RAPPORT D'ACTIVITÉ 2018

Université Fédérale
Toulouse Midi-Pyrénées

INP TOULOUSE

UNIVERSITÉ TOULOUSE III PAUL SABATIER

INSA INSTITUT NATIONAL DES SCIENCES APPLIQUÉES TOULOUSE

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SOMMAIRE

1 Faits marquants

- Projet CADAMIP – CPER 2015-2020
  - Mars 2018 - livraison du nouveau supercalculateur ATOS- Bull Sequana baptisé « Olympe ».
  - Mai-Aout 2018 : Installation et passage des 4 Mésochallenges
  - Septembre 2018 - mise en production d'Olympe.
  - Décembre 2018 - inauguration d'Olympe.

- Comité d'Attribution :
  - Pour la session d'attribution 2018, le comité d'attribution a examiné : 251 demandes de projets et 113 000 000 heures_cpu demandées

- Ouverture aux entreprises et SiMSEO
  - Quatre projets SiMSEO ont été réalisés
  - Deux nouvelles prestations de service avec des entreprises ont été contractualisées pour réaliser des calculs sur le supercalculateur CALMIP

- Mise en plce d'un compte CALMIP sur GITHUP : https://github.com/calmip et partage de deux outils développés à CALMIP : « placement » et « chdb »

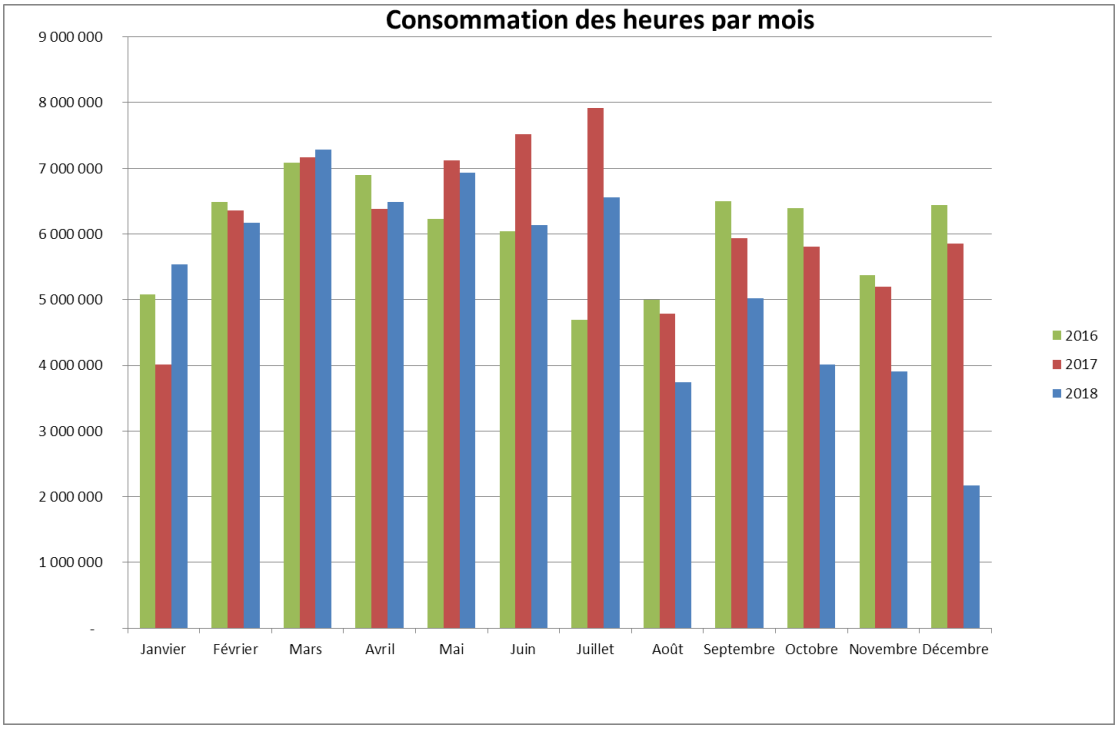
- Décembre 2018 : HACKATHON HPC 2018 organisé par Genci.
  L'équipe HACKALMIP avec le projet « Calcul GPU en mécanique des fluides », IMFT de Toulouse et CALMIP, a été lauréate dans la catégorie "Portage"

- Fin décembre 2018 : Pierrette Barbaresco, Ingénieur de Rechercher de l'Université Paul Sabatier – Toulouse a fait valoir son droit à la retraite

2 Bilan d'exploitation et d'utilisation 2018 pour la recherche académique

***2018**, en quelques chiffres :*

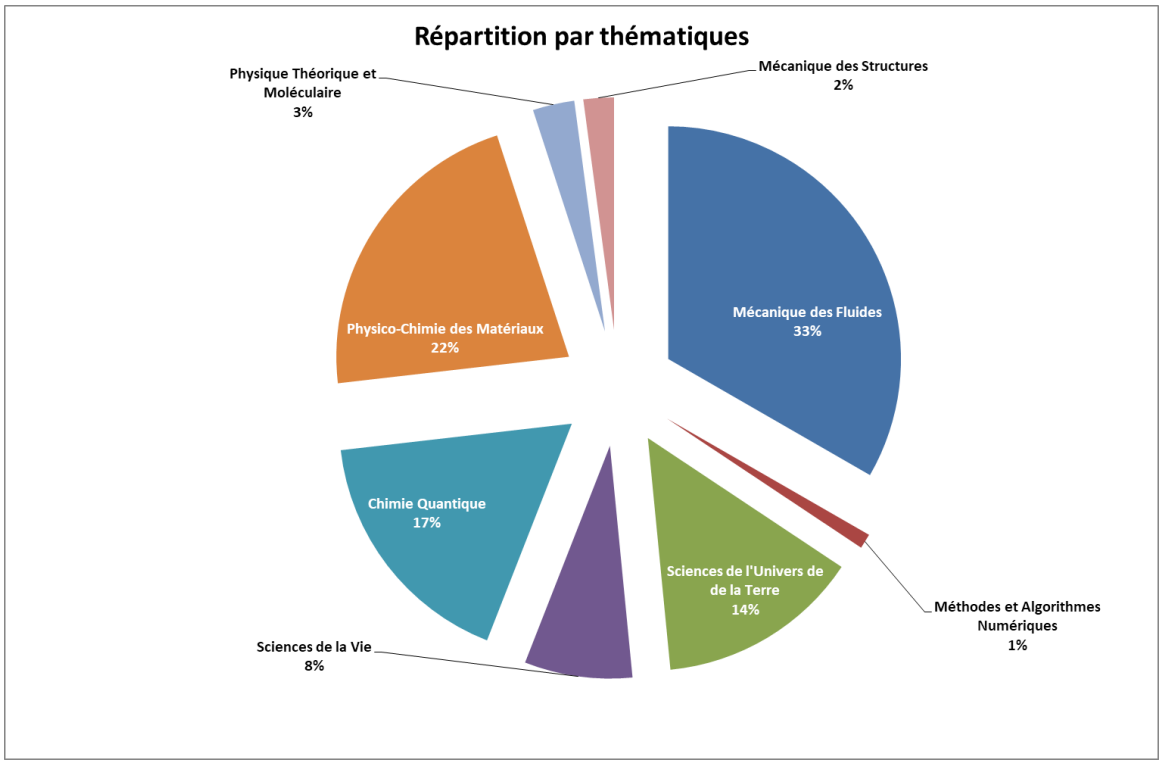
- **251** projets/dossiers soumis au Comité d'Attribution :
  - **62** nouveaux projets,
  - **189** projets renouvelés.
- **35** laboratoires/unités ayant déposés un projet :
- **632** collaborateurs aux projets dont **261** doctorants ou post-doctorants.
- Attribution de ressources :
  - **113 835 089** heures demandées,
  - **85 361 001** heures attribuées,
  - **63 938 634** heures consommées



Le niveau de consommation des heures attribuées sur EOS n'a de sens que jusque septembre 2018, date à laquelle le supercalculateur Olympe a été mis en production. Fin septembre 2018 correspond à la fin de la période de vérification de service régulier d'Olympe. À la fin de cette phase, le supercalculateur Olympe est passé en mode pré-production et ouvert à certains projets. Pour information la consommation sur Olympe (au 12/12/2018) est de 38 766 198 h_cpu normalisées[1].

[1] *Somme des heures CPU et des heures GPU, les heures GPU sont converties en heures CPU via un coefficient de conversion égal à 33.*

2.1 Répartition par thématiques des demandes d'heures de calcul pour la session 2018B



La méta-thématique « Sciences de la Vie » représente 8% des demandes), ce qui est du même ordre de grandeur que la demande de la session B précédente (17B). Cette méta-thématique intègre historiquement la thématique Modélisation Moléculaire qui est pour cette session 2018B la plus grande contributrice de cette méta-thématique « Sciences de la Vie ».

2.2 Ouverture de la plateforme aux entreprises pour des activités d'innovation et de recherche

Dans le cadre du projet Equip@Meso, des entreprises type PME/ETI font du calcul sur CALMIP, jusqu'à 10% des heures CPU de calcul réservées à cette activité.

Leurs objectifs principaux en venant sur CALMIP sont d'avoir l'opportunité de collaborer avec des équipes de recherche, mais aussi de mener des simulations à grande échelle et adapter des méthodes numériques au calcul parallèle.

Sur 2018,

- **7** projets « entreprises » ou projets « test »,
- **5 291 736** heures consommées.

2.3 Formations et animations scientifiques

Formations :

- Introduction aux systèmes de calcul HPC et prise en main du système EOS : deux sessions de deux jours chacune pour 12 inscrits. Encadrants : CALMIP et ATOS
- Formation « HPC pour tous » en collaboration avec l'Observatoir Midi-Pyrénées – 26 Février-1er Mars 2018
- Workshop Applicatif 4-8 Juin « Portage des codes sur Supercalculateur Olympe » – 25 Participants. Encadrants : CALMIP et ATOS
- « Fortran Modernization Workshop » sur les bonnes prtaiques en Fortran moderne, en collaboration avec le Cutis (**C**lub des **U**tilisateurs **T**oulousains de **l'I**nformatique **S**cientifique) et l'éditeur de logiciel NAG – 29 et 30 novembre 2018.

Animations scientifiques :

- Journée JCAD 2018 (ENS Lyon):
    - Présentation du projet CALMIP P09115 " Impact des fines échelles spatiales sur la dynamique océanique en Méditerranée " par *Claude ESTOURNEL* - Laboratoire d'Aérologie, UMR5560, Université de Toulouse - Université Paul Sabatier - CNRS.
    - Présentation du projet CALMIP P1110 " Simulation numérique massivement parallèle de l'hydrodynamique et des transferts d'un réacteur à lit fluidisé gaz-particule réactif polydisperse à l'échelle industrielle (>1 000 000 000 mailles) " par Hervé Neau – Institut de Mécanique des Fluides de Toulosue UMR5502, Université de Toulouse - Université Paul Sabatier - INPT- CNRS.

- Démonstration de l'outil « placement » developpé à CALMIP par Emmanuel Courcelle – UMS3667, Université de Toulouse - Université Paul Sabatier – INPT - CNRS.

- Méso-challenges :

  CALMIP a proposé pendant la phase d'installation de son nouveau système de calcul Olympe, et avant son ouverture massive aux utilisateurs, de permettre la réalisation de "méso-challenges".

  Un méso-challenge poursuit un défi scientifique et technique :
  - Etre capable d'utiliser de manière efficace jusqu'à la totalité d'un grand système de calcul,
  - Permettre de répondre à une problématique scientifique précise grâce à la mise à disposition de ces ressources.

  Les critères de sélection d'un méso-challenge sont principalement : la pertinence scientifique, et la fiabilité technique. CALMIP a reçu 9 propositions et en a retenu 4 (nombre maximal possible) qui sont :

  - ***Spectroscopie in-silico de cyanines***
    Porteur : Michel Caffarel, Laboratoire de Chimie et Physique Quantique

  - ***Impact des fines échelles spatiales sur la dynamique océanique en Méditerranée***
    Porteuse : Claude Estournel Laboratoire d'Aérologie

  - ***Collision oblique de deux sphères dans un fluide visqueux***
    Porteuse : Annaïg Pedrono, Institut de Mécanique des Fluides de Toulouse

  - ***Simulation numérique massivement parallèle de l'hydrodynamique et des transferts d'un réacteur à lit fluidisé gaz-particule réactif polydisperse à l'échelle industrielle (>1 000 000 000 mailles)***
    Porteur : Hervé Neau, Institut de Mécanique des Fluides de Toulouse

3 Mode d'attribution des ressources de calcul

3.1 Attribution des ressources de calcul pour les académiques

- L'accès aux ressources **CALMIP** est ouvert aux projets validés par le **Comité d'Attribution.** Pour cela, les responsables de projets scientifiques doivent faire une demande d'attribution de ressources informatiques sur GRAMC - **G**estion de **R**essources et **A**ttribution pour **M**éso**C**entre**:** **https://attribution-ressources.calmip.univ-toulouse.fr**.
- Deux sessions d'examen de dossiers ont lieu dans l'année :
    - une première session principale "A" a lieu à l'automne, pour distribuer des heures de calcul sur la totalité de l'année suivante (1er Jan. —> 31 Déc.),
    - une seconde session complémentaire "B" a lieu au printemps, pour distribuer des heures de calcul non consommées jusqu'à la fin l'année en cours (1er Juill. —> 31 Déc.).
- Une évaluation scientifique est effectuée par les experts du Comité d'Attribution. Ces experts formulent ensuite des recommandations qui permettent d'effectuer des allocations d'heures sur le supercalculateur CALMIP. Les heures attribuées sont gratuites pour les utilisateurs qui sont dans un laboratoire de la COMUE UT (universités, écoles et EPST), financées par les tutelles des laboratoires. **Un rapport d'activité des travaux réalisés est demandé.**

3.2 Attribution des ressources de calcul pour les entreprises

- Après des échanges entre CALMIP et l'entreprise qui souhaite démarrer un projet de calcul, une première réunion est organisée entre l'équipe HPC de l'entreprise qui porte le projet et l'équipe support utilisateurs de CALMIP. L'idée est de bien appréhender côté entreprise le besoin en calcul, les outils numériques utilisés, la problématique algorithmique … et côté CALMIP, de faire une présentation du service proposé aux entreprises.
- Un premier contrat avec un projet test de 5 000 h de calcul (le nombre d'heures peut être adapté au besoin projet) est conclu avec un ou plusieurs comptes spécifiques ouverts sur le calculateur. Ce projet sert à installer le code de l'entreprise et à faire des premiers tests de fonctionnement et de performance. Deux jours d'ingénieur CALMIP sont dédiés en moyenne à la préparation et mise en œuvre de ce type de projet test.
- Si la PME est satisfaite de ses premiers tests, et si elle souhaite poursuivre son projet, il lui sera alors proposé un contrat de prestation de services adapté à ses besoins de calcul.

4 Bilan scientifique, résumé des projets de l'année 2018

4.1 Mécanique des fluides

Simulations LBM pour les écoulements de suspensions

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Eric Climent**
J'encadre un doctorant (Dominik Schuster <Dominik.Schuster@imft.fr>) qui conduit des simulations avec un code LBM pour la simulation d'écoulements de suspensions. Ce code est opérationnel dans un contexte HPC : http://www.walberla.net/ et nous voudrions déposer un projet CALMIP au prochain appel. Dans l'intervalle, serait-il possible de bénéficier d'un projet test (sur OLYMPE) afin d'installer le code et de faire qqs benchs afin de mieux dimensionner notre demande CPU.

Optimisation et HPC avec le code multi-phasique réactif NEPTUNE_CFD pour la simulation d'écoulements gaz-particules (lit fluidisé) et liquide gaz

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Hervé Neau**
Since 2006, IMFT, LGCT work on the development of mathematical modelling and numerical simulation of hydrodynamic and transfers in reactive gas-particle fluidized beds. The complexity of involved physical phenomena and realistic three-dimensional geometries requires large computer resources. IMFT and LISBP work too on the hydrodynamic behavior of immersed gas cavities. The first step of this work consists in investigating the academic test case of the oscillatory flow appearing during the emptying process of a water bottle also called the glug-glug phenomenon (projet P17034). Simulations are carried out using an Eulerian n-fluid modeling approach for turbulent and polydispersed fluid-particle flows, which is developed and implemented by IMFT in NEPTUNE_CFD. NEPTUNE_CFD is a multiphase flow software developed in the framework of the NEPTUNE project, financially supported by CEA , EDF , IRSN and AREVA. The code solves, for each phase, Eulerian three-dimensional unsteady equations of mass, momentum and enthalpy, coupled through transfer terms between phases, and transport equation of a variable number of scalars. Parallel simulation efficiency of NEPTUNE_CFD has been tested on many platforms. Access to source code programs enable to modify existing models and also to test the build options to improve the performance of the code. Moreover, the excellent parallel performances of the code enable the implementation of multiphysics calculation of flows in actual flow configurations. In 2018, the main objective of this project is to have to an optimized installation of NEPTUNE_CFD on CALMIP supercomputer usable by research project (P0111, P17034, P1132, ...). The main goal is to increase and evaluate NEPTUNE_CFD HPC on EOS and on the new CALMIP super-computer. A fluidised bed reactor with more than 1 billion cells will be used to evaluate NEPTUNE_CFD speed-up and efficiency and to determine the minimum cell number per core to have excellent performances.

Etude de la modulation de la turbulence induite par des rides de sable

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Thomas Bonometti**

When a turbulent flow acts on a deformable or erodible surface (wind blowing along the ocean surface, water flowing over a bed of sediment), the shape surface is modified and ripples arise. The instability mechanism generating these ripples is due to a phase lag between wall shear stress and the shape of the undulated surface. However, the structure of the turbulent flow over sinusoidal boundaries is still not well understood. In particular, some turbulent models, namely using the mixing length theory, are unable to reproduce such flows, unless some ad hoc modifications are done. The aim of this project is to shed some light on the turbulent structures of such flows (turbulent boundary layer over a sinusoidal bottom) using a Large Eddy Simulation numerical approach on orthogonal curvilinear grid (JADIM code). These simulations should help understanding the processes responsible for turbulence modulation in the transitional regime separating laminar from turbulent flows.

PNM

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Marc Prat**

Drying of porous media is central to many environmental and engineering applications. In this context, this project aims at performing a major breakthrough in the modelling of the drying process in capillary porous media from a combination of state of the art pore network modelling (PNM) and pore network simulations. Two- and three-equation continuum models will be developed taking into account the non-local equilibrium condition of the vapour and from the distinction between the percolating and non-percolating liquid clusters. The secondary capillary structures corresponding to the liquid trapped in various geometrical singularities of the pore space will be characterised from numerical simulations and will be taken into account as a distinct and specific phase in the continuum models. The pore network models will be developed so as to perform high performance computing (HPC) simulations, which is necessary to meet the length scale separation constraints allowing the computation of continuum model parameters from pore network simulations. A major objective is thus to develop HPC versions of the PNM drying codes.

Etude des phénomènes instationnaires appliqués aux machines tournantes

Projet démarré en 2018

ISAE/DAEP - Département Aérodynamique, énergétique et propulsion

Porteur de projet: **Yannick Bousquet**

This project aims to analyse the impact of unsteady effects on the performance of axial and radial turbomachinery components. Due to the environmental issues in the aviation domain, engineers have to design more and more efficient components. It is today wheel known that the further rise of efficiency will occur from a good comprehension of unsteady mechanisms and by taking them into consideration during the design procedure. There are many sources of unsteadiness in turbomachinery components. There can be naturally segregated in two categories. The first one considers unsteady effects which are periodic in time and then linked to the blade passing frequency. Interaction mechanisms between rotor and stator fall in this category. The second category concerns unsteady effects which are not linked to the blade passing frequency and includes phenomena such as rotating stall and surge. This project aims to better understand both, the unsteady mechanisms correlated and uncorrelated to the blade passing frequency. It is divided in five sub-project. The first one concerns the analysis of the stall inception process in a high speed centrifugal

compressor. The second one evaluates the impacts of an inlet flow distortion on the stability limit for an axial fan. The third one focuses also on the impacts of an inlet flow distortion but consider an integrated rotor for distributed propulsion application. The fourth one aims to study unsteady mechanisms uncorrelated to the blade passing frequency in an axial fan operating at highly loaded windmilling conditions. Finally, the last project concerns the analysis of unsteady flow field in a variable geometry radial turbine having a rotor with splitter blades.

Study of the response of unsteady heat transfer on cross-flow cylinders to acoustical velocity perturbations

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Benoit Bedat**
The objective of the project concerns the unsteady heat transfer of a single or an array of cross-flow cylinder. Simulations are performed to understand and qualify the influence of periodic incoming flow on unsteady heat transfer. This study is performed in parallel with an experiment on thermo-acoustics at IMFT. It is a electrical Rijke tube. It is known that this set up will conduct to thermo-acoustic instabilities when the unsteady heat release exhibits a delay with the acoustical velocity and overcomes the acoustical power lost at the extremities. Most of the experiments found in the literature lead naturally to an unstable state when enough electrical power is supplied. Depending of the design of the electrical heater, the the IMFT Rijke tube leads to natural transition or not. Design that does not conduct to natural instabilities corresponds to a side by side set-up. In this configuration no wake interactions with another heating elements are possible. Natural triggering happens with a more and less to staggered design. The purpose of the project is to understand and to quatify the response of one or several (side by side) cylinders. The transfer function in term of gain and phase (or delay) will be determined by CFD and used in theoritical study on the stability of this thermo-acoustical set-up.

Simulation numérique d'un panache de bulles en fluides visqueux

Projet démarré en 2018

LISBP - Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (UMR 5504/792)
Porteur de projet: **Alain Line**
The objective of the projet is to simulate the hydrodynamics, mixing and mass transfer induced by a bubble plume. The simulations will be compared to experimental data acquired during the PhD of David Laupsien (LISBP, December 8th 2017). The data bank concerns the frequencies of the bubble plume oscillation, the liquid velocity fields (mean flow, periodic motion and turbulence), bubble characteristics (distributions of sizes and shapes, velocities) and gas fraction distributions. The simulations will be performed with NEPTUNE CFD code. Eulerian model for dispersed bubbly flow will be tested ; the objective is to improve the modelling of the interfacial transfer of momentum and the pseudo-turbulence induced by the bubbles. Then, different large sacles model will be tested (LIM, GLIM and LBM) in the case of spherical caps plumes.

Simulation réservoir géothermique profond (calculs parallèles OpenFoam)

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Rachid ABABOU**

This computational project is being conducted in the framework of an ongoing French R&D project "GEOTREF" (www.geotref.com), funded by ADEME in the context of "Investissements d'Avenir", for developing and modeling the recovery of geothermal energy from deep, high temperature fractured reservoirs. This involves modeling theoretically and numerically water flow and heat transport in fractured porous rocks in the presence of injection and extraction wells. In this context, our work is divided in two parts: (1) upscaling of fractured rock properties (conductivities); and (2) simulation of geothermal exploitation at reservoir scale. The first part in this project is to provide theoretical and numerical upscaling procedures for determining the equivalent continuum hydro-thermal properties of the fractured porous reservoir. This work is well advanced concerning hydraulic properties (Rajeh et al. 2017; Ababou et al. 2017). At this point, we can focus essentially on the computational challenges of the second part of the project: large scale reservoir simulation. It consists in using the previously obtained upscaled properties (equivalent continuum hydro-thermal properties) to simulate scenarios of water injection and heat extraction from the porous fractured reservoir. Typically, this implies large space and time scales: a few cubic km's and tens of years. These scales present a challenge for simulation, and justify the relevance of massively parallel computing. Furthermore, the equivalent hydro-thermal properties of the fractured rock are tensorial & spatially distributed in 3D, e.g. hydraulic conductivity Kij(x,y,z). Also, large discontinuous features like faults & geologic beds have to be represented explicitly on the mesh. Finally, the representation of injection/extraction wells on the numerical mesh (adaptive or not) will be challenging. We have developed the equations for water flow & heat transport, and we have numerically implemented them in the open source software "OpenFoam", written in C++ and massively parallelized based on domain decomposition. The equations for coupled Darcy flow & heat transport are discretized with an unstructured finite volume scheme. A coupled model has been implemented & tested for test cases on mono-processor machine (PC), and on a 24-processor system (short transient simulations in a 3D heterogeneous reservoir with 1 million cells under OpenFoam). Our present aim in this CALMIP project is to apply our OpenFoam simulator for more realistic & larger scale reservoir simulations, with hundreds of finite volume cells, over several months or years of physical time. Our previous experience with OpenFoam indicates that these goals are attainable, given the fully parallelized OpenFoam tool (cf. the RichardsFoam hydrological code developed & published by Orgogozo et al. 2014 on the cluster Hyperion of CALMIP).

Simulation numérique du transfert de matière à travers l'interface d'une goutte

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Eric Climent**

Optimization of separation processes, like liquid-liquid extraction, and improvement of mass transfer rates require most importantly a good understanding of the coupling between internal and external hydrodynamics on mass transfer across the interface. Hence, the study of mass transfer at the scale of a single droplet moving in the surrounding phase is of prime importance. This study represents a major step towards derivation of reliable mass transfer resistance correlations. Many key physical parameters (such as the effects of viscosity ratio, diffusivity ratio, flow configuration, etc.) may impact directly both hydrodynamics of a moving droplet in a continuous phase and extraction efficiency as well. In this study, efforts have been made to investigate the interaction between the internal and the external flows in a single droplet on the one hand, and on the other hand, the influence of the main key parameters on the evolution of the Sherwood number. The temporal evolution and the spatial concentration distribution will be studied, analyzed and then validated on reference test cases. Since under the hydrodynamic conditions

typical of solvent extraction columns, the droplet usually achieves a spherical shape, a fixed (i.e. non deformable) mesh is considered in this study. A numerical investigation has been conducted by DNS to investigate the coupling between the internal and the external flows and their respective effects on mass transfer. JADIM, the CFD code developed at IMFT, was used and adapted in this aim. A specific jump condition has been implemented in order to accurately represent the convection/diffusion and mass transfer coupling at the interface between the droplet and the surrounding liquid. The numerical model will be used to study the sensitivity of the rate of transfer of a non reactive solute to the various hydrodynamical and chemical parameters, accounted thanks to the Reynolds, Peclet, Fourier, Henri numbers. Moreover the respective effect of internal flow circulation and external convection may have drastic changes of the internal and external resistances to mass transfer with increasing values of the Peclet number.

Granular rheology in turbulent bedload transport

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Raphael Maurin**

Considering a granular bed submitted to a surface fluid flow, bedload transport is classically defined by opposition to suspended load as the part of the grains entrained close to the bed. Turbulent bedload transport has been extensively studied with regard to its importance for earth surface processes such as natural riverbed morphological evolution. Despite a century of modern research on the subject, turbulent bedload transport understanding remains limited, and predictions can lead to sediment transport rate up to three orders of magnitude different from what is observed in the field. In this framework, it is important to study the underlying physical mechanisms associated to turbulent bedload transport, in order to strengthen the phenomenon understanding and increase the prediction capabilities for engineering purposes. To do so, we consider simulations of idealised steady uniform configurations of turbulent bedload transport with monodisperse spherical particles. The description of each independent particle with a discrete element method, coupled with a 1D volume-averaged fluid resolution, enable us to analyze precisely the granular behavior and characterize the associated mechanisms. The goal of the present project is to analyze the granular rheology in turbulent bedload transport focusing on the transition from dense to dilute granular behavior. This transition is of importance for the modelling of turbulent bedload transport in the framework of Euler-Euler models, and represents a major challenge in the description of granular media.

Etude thermique dans des canaux millimétriques

Projet démarré en 2018

LGC - Laboratoire de Génie Chimique (UMR 5503)

Porteur de projet: **Nathalie Raimondi**

In the process intensification field, new technologies like compact heat-exchangers reactors have been developed over the past decade to meet the trend of safer, cleaner, more effective and less energy-consuming processes. They integrate two basic concepts of process intensification which are on one hand the miniaturization of the units and on the other hand the multi-functionnality of the apparatuses, exhibiting many advantages, such as good heat transfer performances, better temperature control, reactive volume confinement. However, the reactor size reduction results in laminar flow operating conditions which does not favor transport phenomena. Consequently, complex designs are required in order to enhance mass and heat transfer. Wavy geometries are often used in compact heat-exchanger reactors as

they can interrupt the thermal boundary layer and in return enhance the heat transfer compared with straight tubes. Besides, the resulting complex geometries cause generally higher pressure drop in comparison with straight tubes. The present work consists of the simulation of heat transfer in wavy millimetric channels with square cross-sections of 2 mm length width using the software Ansys CFX 16. The wavy channels consist of periodic zigzag units composed of two straight section lengths and two 90° bends with a curvature radius of 1.5 mm. The straight section length varies from 2 mm to 12 mm. The pressure drop and the evolution of the temperature along the channel are observed in order to determine the friction factor and the Nusselt number. The objective of this study is to investigate the impacts of the fluid velocity and the channel geometry in terms of straight section length between two bends on the thermo-hydraulic performances in wavy channels.

Combustion de particules d'aluminium post-détonation

Projet démarré en 2018

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Laurent Selle**

After the detonation of an oxygen-deficient homogeneous high explosive, a phase of turbulent combustion, called afterburning, takes place at the interface between the rich detonation products and air. Its modelling is instrumental for the accurate prediction of the performance of these explosives. Because of the high temperature of detonation products, the chemical reactions are mixing-driven. Modelling afterburning thus relies on the precise description of the mixing process inside fireballs. There is an additional complexity when the explosive is heterogeneous, i.e. initially seeded with reactive metallic particles. The after burning of these particles greatly impacts the global energy release but the details of their influence on the flow and the post-detonation phase is still unknown. The overall objective of this study is to address these phenomena via unsteady numerical simulation : DNS and LES. This project is at the center of the PhD work of Jimmy Suarez and the continuation of a collaboration between IMFT and CEA (Gramat) over the past 4 years. A previous PhD (Sebastien Courtiaud) paved the way with numerical simulations of homogeneous explosives and we now tackle the influence of aluminium particles. The unsteady simulations aim at understanding the underlying mechanisms of aluminium combustion under such extreme conditions and assessing their influence on the post-detonation processes. On the practical side, the detailed simulations guide the development of low-order models that are routinely used at CEA. The key ingredients of the numerical method are (1) a compressible solver with detailed combustion models and (2) a lagrangian tracking of the particles. The solver is the AVBP code, jointly developed by Cerfacs and IFPEN.

SIMULATION NUMERIQUE DIRECTE DES PROCESSUS D'ATOMISATION

Projet démarré en 2018

ONERA - Office National d'Etudes et de Recherches Aéronautiques

Porteur de projet: **Jean-Luc ESTIVALEZES**

This project focuses on the direct simulation of the atomization of a liquid phase in two different cases. The first concerns the impact of Supercooled Large Droplets on aircraft wings, which can lead to ice formation elsewhere than in protected areas. Since the deposit rate resulting from this type of impact is not well known, for a better understanding of this phenomenon, a direct simulation numerical approach has been chosen. This study will focus on the mechanisms of impact and the emission of secondary drops (splashing). Indeed, this numerical approach allows access to phenomena that are difficult to capture experimentally, such as characteristic times generally lower than the microsecond and the characteristic lengths of the

order of a micrometer. The second concerns the modeling of the assisted primary atomization of fuel. No model is able today to predict the characteristics of the spray atomization air-blast. A fundamental objective of this study is to provide information and data to build and validate models, which would predict the initial characteristics of the spray in a large scale approach. To this end, this project proposes to carry out several direct numerical simulations of assisted atomization on a simplified but relevant configuration, ie a plane liquid layer sheared by a gas flow in a periodic domain.

Lattice Boltzmann Simulation for aerodynamics in rotating geometries (LaBoSAGe)

Projet démarré en 2017

ISAE/DAEP - Département Aérodynamique, énergétique et propulsion

Porteur de projet: **Nicolas Gourdain**

The most popular method to simulate flows in complex geometries (aircraft, car, etc.) is the Reynolds Averaged Navier-Stokes (RANS) approach. Classical RANS models require assumptions about turbulence that are not validated in such geometries. With the increase in computing power, Large Eddy Simulation (LES) emerges as a promising technique to improve both knowledge of complex physics and reliability of flow solver predictions. Unfortunately, the computing cost and the difficulty to represent the real geometry still limit its applicability to engineering applications. In that regard, the use of a Lattice-Boltzmann based flow solver can help to overcome these difficulties. While mesh generation is time consuming for Navier-Stokes flow solvers (due to the "body fitted" approach), this step is usually straightforward with a Lattice-Boltzmann Method. Indeed, the method is based on a Cartesian mesh to avoid building a body-fitted mesh around the provided geometry. Instead, the boundaries are represented through off-lattice boundary schemes, and a match between the Cartesian fluid grid and the curved geometry profile is obtained through adequate interpolation. In 2015 and 2016, the Dpt. of Aerodynamics, Energetics and Propulsion of ISAE-Supaero started to develop [1] and bench LES-LBM for micro-air vehicles [2]. The software considered at DAEP is the open-source flow solver Palabos, mainly developed by the University of Geneva. The code has been tested on EOS, showing a speedup efficiency of 80% with 1600 cores with a 1,000,000 cells grid [2], representing a full contra-rotating shrouded rotor. This project targets the application of LES-LBM to more ambitious configurations: flow control based on aero-elastic capabilities applied to micro-air vehicles and the flow prediction around an hybrid ground vehicle, equipped with a wind-based energy generation device.

Dernières publications:

- N. Gourdain, T. Jardin, R. Serre, S. Prothin and J-M. Moschetta. (2018). Application of Lattice Boltzmann Method to some challenges related to Micro-Air Vehicle, Int. J. of Micro-Air Vehicles, 10(3) - **doi:** pu.doi
- A. Alguacil, T. Jardin and N. Gourdain (2018). Implementation of aero-elastic capabilities in a LBM flow solver: application to a low-Reynolds rotor for micro-air vehicles, European Rotorcraft Forum, paper 148, Delft, Netherlands -

ULTMATE : Ultra Low emission Technology Innovations for Mid-century Aircraft Turbine Engines

Projet démarré en 2017

ISAE/DAEP - Département Aérodynamique, énergétique et propulsion

Porteur de projet: **Xavier Carbonneau**

ULTIMATE or Ultra Low emission Technology Innovations for Mid-century Aircraft Turbine Engines is a research and innovation project in the field of aeronautical engineering. The project has received a funding from the Horizon 2020 research and innovation programme of the European Union and was launched on 1 September 2015. It is set to run for a period of three years (36 months) and is coordinated by Chalmers University of Technology. With the ULTIMATE project, five experienced research groups and four major European engine manufacturers will develop innovative designs for the propulsion and core technologies of aero-engines gas turbines. The ULTIMATE team at the Department for Aerodynamics, Energetics and Propulsion (DAEP) unites strong experience in turbomachinery and gas turbine components performance analysis in severe off-design operation. In ULTIMATE, ISAE leads the Worl Package 3 known as "Advanced Integration and Propulsor Technologies". The ISAE team will target Turbofan configurations, particularly the characterization and optimization of adaptive nacelle concepts, and the Open Rotor configuration, focusing on noise generation.

Dernières publications:

- S.-K. Courty-Audren, G. Napias. Sensitivity Study on Computational Parameters for the Prediction of Tonal Noise Generated by Counter-Rotating Open Rotors in cruise conditions, AIAA Journal (peer-review) -

Simulation Numérique Directe de l'interaction entre la Turbulence et un Changement de phase liquide-vapeur

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Sébastien Tanguy**

The proposed research is a multidisciplinary project at the frontier between Fluid Mechanics, Heat and Mass Transfer at a liquid–gas interface, Applied Mathematics and Scientific Computing. My previous research has contributed to demonstrating the ability and the potential of interface capturing methods, such as Level Set, Ghost Fluid and Volume of Fluid methods, for performing Direct Numerical Simulations in many configurations involving two-phase flows. Many new applications may now be considered, especially in the context of the following two emerging topics: turbulent two-phase flows and liquid-vapor phase change. The proposed research builds upon several current and future collaborations with funding research institutes and industrial partners. We will conclude this short introduction by noting that important progress on this topic may be expected during the next decade due to the previous advances in the field of numerical methods for the simulation of two-phase flows. The new version of the DIVA code may be a leading tool to achieve this result. Especially the recent endeavors devoted to parallel computations with the BlackBox MultiGrid solver will be of great interest to achieve this part of the research project. The important endeavor provided in our recent works on the development and the implementation of numerical methods for two-phase flows is close to reach a sufficient maturity to consider a step forward for my research activities, which will be mainly focused during the next years on more practical applications. All these developments have been integrated in a single and upgraded version of the numerical code DIVA (Dynamics of Interface for Vaporization and Atomization), benefiting of a much more efficient structure (parallel computations for all the solvers, BlackBox MultiGrid, improved WENO scheme for the Level Set method, turbulent inflow generator) than the previous versions in order to push back the current limits of two-phase flows simulations.

Dernières publications:

- A. Dalmon, M. Lepilliez, S. Tanguy, A. Pedrono, B. Busset, H. Bavestrello and J. Mignot. Direct numerical simulation of a bubble motion in a spherical tank under external forces and microgravity conditions. Journal Fluid Mechanics 849, pp 467-497 - **doi:** pu.doi
- A. Urbano, S. Tanguy, G. Huber, C. Colin. Direct numerical simulation of nucleate boiling in micro-layer regime. International Journal of Heat and Mass Transfer 123 (2018) 1128–1137 - **doi:** pu.doi

Hydrodynamique de poches de gaz immergées

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Véronique Roig**

The current research project is part of a new collaboration involving the IMFT, DCNS group and EDF. DCNS group got equipped with the CFD solver NEPTUNE_CFD developed by the CEA, EDF and AREVA-NP and asked the IMFT to assess the performance of the two-phase flow description embedded in the solver on a flow configuration representative of what DCNS want to investigate numerically. To do so we investigate the hydrodynamic behavior of immersed gas cavities. It concerns for example the generic instability of an interface between two non-miscible fluids with different densities when the heavier fluids is at rest above the lighter one (Rayleigh-Taylor instability). This interface evolution problem in a viscous fluid is complex, on one hand because it involves rather fast dynamic with various spatio-temporal scales and on the other hand because it leads to gas-liquid flow regime transitions. The first step of this work consists in investigating numerically the academic test case of the oscillatory flow appearing during the emptying process of a water bottle also called the glug-glug phenomenon (Clanet 2004). This test case is challenging as it implies a broad spectrum of spatio-temporal scales and flow regime transitions. Large gas pockets are created periodically at the bottle neck, then rising in the bottle, the pockets break up to create bubbles of various sizes and shapes. Previous experiments (Heraud 2002 and Clanet 2004) have investigated the different time scales of the flow : the long emptying time scale and the short oscillations time scales depending on the geometry parameters. However the flow regimes has never been characterized so far. The objective here is to compare the performances of NEPTUNE_CFD and JADIM on this test case. An experimental set-up is currently being instrumented at the IMFT in order to assess the accuracy of both numerical solvers. Furthermore an experimental thesis is planed next year, on this apparatus, with the objective to take advantage of the current visualization techniques (PIV and shadowgraphy) to get a new insight in the glug-glug phenomenon. This will also permit to further validate the numerical techniques.

Dernières publications:

- Mer S., Praud O., Neau H., Merigoux N., Magnaudet J., Roig V., The emptying of a bottle as a test case for assessing interfacial momentum exchange models for Euler-Euler simulations of multi-scale gas-liquid flows, International Journal of Multiphase Flow, vol 106, pp. 109–124, 2018 - **doi:** pu.doi

Dynamics of piston-generated vortex rings

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Pierre Brancher**

The project aims at analyzing the production and evolution of vortex rings generated by a moving piston. The study will be based on direct numerical simulations using OpenFOAM, with a dynamic mesh algorithm to mimic the motion of the piston. The project includes the study of vortex ring flows taking into account the influence of confinement, rheology and/or density. The main motivation behind the project is to provide with a crucial complement of on-going experiments, in order to analyze regimes or data which are out of reach experimentally.

Méthodes d'ordre élevé pour la simulation d'écoulements turbulents

Projet démarré en 2017

LAMPS - LAboratoire de Mathématique et de PhySique EA 4217

Porteur de projet: **Stéphane Abide**

The aim of this project is the development of spatially accurate methods to solve incompressible or incompressible-like Navier-Stokes equations, with an emphasis for the simulation of turbulent flows with heat and mass transfer in wall bounded domains. The computational cost of a such simulations is high and can be reduced by combining accurate discretizations and parallel computing. These methods lead to several issues that have to be addressed in order to take advantage of both accurate discretizations and high performance computing. This is even more challenging for variable density flows. In this work, we focus on compact finite differences schemes which have the feature to increase the numerical accuracy (truncature and wavenumber resolution) while having a linear complexity. The core feature of the developed code is based on the common and widely used in the turbulent flow simulations. The incompressible Navier-Stokes equations are discretized with compact finite-difference schemes on a three-dimensional cartesian mesh with avoiding Fourier expansion. The time marching scheme is a third-order Runge-Kutta (RK3), in combination with a Crank-Nicholson scheme for the implicit terms. The incompressibility constraint is ensured up to the accuracy machine with a standard fractional step method which requires to solve a Poisson equation. The pressure and the velocity fields are staggered by half a mesh to avoid spurious oscillations, and to ensure the conservation of the mass and the kinetic energy. The compact scheme derivatives arising in the approximation of the explicit terms are computed with the Parallel Diagonal Dominant algorithm, which achieves good parallel performances. Concerning the Helmholtz/Poisson equations a full diagonalization method has been adapted for a pencil based parallel data distribution. Actually to address variable density flows, iterative methods based on suited preconditioning are investigated.

Control and optimization strategies to improve the aerodynamic performance of complex vehicles

Projet démarré en 2017

ISAE/DAEP - Département Aérodynamique, énergétique et propulsion

Porteur de projet: **Stéphane Jamme**

This project gathers the different numerical studies that are planned to be conducted by our team on the topic of controlling and/or optimizing complex aerodynamic configurations. We mainly focus our work around the following problems: 1. optimizing the mixing between fuel (hydrogen) and oxidizer (air) in the frame of supersonic combustion applications such as the one found in scramjets. This challenge is of fundamental importance both in terms of fuel consumption and pollutant emissions. In that context, we aim at assessing a new idea based on the use of impulsive hydrodynamic instabilities such as Richtmyer-

Meshkov instability (RMI) in order to promote the mixing between the species ; 2. developing innovative active flow control strategies, based on synthetic pulsed jets, also referred as ZNMF for Zero Net Mass Flux, to mitigate the flow separation induced by UHBR (Ultra High Bypass ratio) powerplant installation on the suction side of the wing when the aircraft is operated at high angle of attack and low speed. This topic is led in the framework of the Cleansky 2, European Commission funded research program.

Dernières publications:

- P. Graumer, S. Jamme and Y. Bury. Investigation of the interface stretching within a reshocked mixing zone produced by the Richtmyer Meshkov Instability. 31st International Symposium on Shock Waves, Nagoya, Japan, July 2017. -
- R. Messahel, Y. Bury, J. Bodart, N. Doue. Volumetric Reduced-Order Models of Zero-Net Mass-Flux. AIAA Aviation and Aeronautics Forum and Exposition, Atlanta, USA, June 2018. -

Drag reduction by superimposition of microscopic protrusions on the surface of a sphere

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Jacques Magnaudet**

Janus spherical particles are particles with different physical and chemical properties depending on the zone of the particle considered (cf. Walther & Muller, 2013 for a thorough overview). A particular class of these particles consists of spheres constituted by two hemispheres, one hydrophobic and one hydrophilic. Inspired by these particles, we start our study from fully hydrophobic spheres (ie. bubbles). A review of the literature (cf. Onda et al., 1996; Tricinci et al., 2015; Wenzel, 1936; Cassie & Baxter, 1944) allows us to confidently build hydrophobic surfaces by adding a microscopic roughness to a smooth surface. A particular care is paid to the design of the roughnesses, which can be deterministic or not, regular or irregular, distributed on the whole sphere or only on certain parts (to allow alternation of hydrophilic or hydrophobic materials, a situation whicg has been shown (Swan et al. 2008; Wilmott 2009) to have a significant influence on the overall dynamics of the sphere). In parallel, we develop a macroscopic boundary condition to be imposed at the surface of the "equivalent" smooth sphere. To take into account the different shapes and distributions of the protrusions which constitute the roughness, microscopic problems are solved on a quasi-periodic cell containing a single protrusion to calculate the "slip length" which must be used in the macroscopic condition. A good agreement between the macroscopic model and the full simulations is expected. Using jointly the two approaches, a study of the modifications of the flow is achieved by varying some fundamental parameters, such as the Reynolds and Knudsen numbers (the latter is directly linked to the slip length and, thus, to the shape and distribution of protrusions on the sphere). Several authors (Ramteke & Kishore 2015; Nidhil et al. 2016) recently noticed significant changes in the heat transfer for flow past a cylinder with slip. The present project is based on an extensive use of the open software OpenFOAM. "Ad hoc" solutions and boundary conditions for the present situations of interest will be developed, based on the already implemented solvers.

Dernières publications:

- G. Zampogna, J. Magnaudet & A. Bottaro. Generalized slip condition over rough surfaces. J. Fluid Mech. (submitted) -

Numerical simulation of a vertically stratified flow past a falling sphere

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Jacques Magnaudet**

The present project deals with the study of the dynamics of a sphere moving vertically in a linearly stratified fluid. Such flows, in which the densities are inhomogeneous, are encountered in many natural configurations (oceans, atmosphere, storage basins, etc.), and can influence the aggregation and migration of particles such as plankton for instance (MacIntyre et al. 1995}. Therefore, as a basic model, it is a topic of great interest to study the dynamics of a sphere in such flows, as well as the wake structures behind it in such a stratified environment. The dynamics of this type of flow can be characterized by three non-dimensional parameters, namely the Reynolds number, the Froude number, and the Prandtl number. We consider this problem in the context of the Boussinesq approximation, where the influence of the changes in density on the velocity field is limited to the gravity source in the Navier-Stokes equations; the evolution of the density is governed by an advection-diffusion model. It is now well understood that when a sphere moves vertically in a stably stratified fluid, the wake structure behind it collapses from a near-body structure with attached axisymmetric vortices to a far-wake structure which looks like a jet, in which the velocity can be larger than the speed of the sphere. By means of experiments, it has been observed that the jet structure can be very different depending on the flow parameters (Re, Fr,Pr),; see Hanazaki (2009a). However, the physics of the growth of these different types of three-dimensional wakes/jet structures is not clear. Experimental measurements to access three-dimensional flow structures for both the velocity and the density fields remain a great challenge. Regarding the numerical simulations tackling this problem, because the density boundary layer is very thin (about 5. 10^{-3} the sphere radius for salt stratification with Pr=700), very refined meshes are needed close to the sphere and most of the available numerical works focus on axisymmetric simulations (Torres 2000, Hanazaki 2009b), which cannot cover the situations where wake/jet instability happens. Furthermore, global balances on the sphere, such as the drag/lift force exerted by the flow owing to stratification have not been fully investigated (Yick 2009, Doostmohammadi 2014a} especially in the moderate-Re regimes, and for any values of the Prandtl number. This is a point of great importance in the aim of predicting the sphere dynamics. Therefore, the goal of the present project is to: (i) study the evolution process of the wake/jet structures when the dimensionless parameters are changed, typically 1< Re< 300, 0< Fr< infty and 0.7< Pr< 700; (ii) study the physics of these evolutions when Re, Fr and Pr are varied separately; (iii) establish a correlation between the drag coefficient and the dimensionless parameters, namely C_D=f(Re,Fr,Pr), to determine the variation of the drag force when the stratification of the fluid is changed (no such correlation exists nowadays).

Dernières publications:

- J. Zhang, M. Mercier & J. Magnaudet. Unraveling the mechanims of drag enhancement of bodies settling in a stratified fluid. Phys. Rev. Lett. (submitted) -

Simulation numérique directe d'écoulements turbulents gaz-particules à l'échelle mesoscopique

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Enrica Masi**

Particle-laden flows in dilute or kinetic regime are encountered in several industrial applications as, for example, in combustion chambers using pulverized coal as fuel for combustion or in circulating fluidized bed. In these flows, particle dispersion plays an important role and requires an accurate modeling. In the last years, several experimental and numerical studies have highlighted the important role of the dispersion and of the preferential concentration in particle-laden turbulent flows. It has been shown, for example, that the velocities of neighboring weakly inertial particles are strongly correlated in space, due to the local interaction with the same fluid turbulence. On the other hand, the velocities of close inertial particles are spatially uncorrelated due to the memory they retain of the interactions with the fluid flow at distances comparable to or greater than the spatial integral scale of the turbulence. Taking into account the particle velocity correlation is very important in the statistical modeling of the particle-particle interactions, in particular in order to correctly model the inter particle collision time. As for the dynamics, the effects due to the particulate inertia have a great impact on the thermal statistical properties of a non-isothermal dispersed phase, such as the temperature variance or the heat flux transported by the agitation. The characterization of the temperature of the particles is crucial in the modeling of the dispersed phase reactive flows. It therefore represents one of the goals of this project. The second goal is the characterization of the influence of the collisions on the dispersion of particles in turbulent flow. Indeed, in dispersed-phase turbulent flows, collisions can play an important role on the distribution of particles and on the flow dynamics, even for relatively low volume fractions, typically on the order of 0.1%. This influence results from the fact that, on the one hand, collisions between particles reduce the mean free path of the particles and thus modify the dispersion of clouds of solid particles and, on the other hand, collisions induce a phenomenon of redistribution of particles, which can play a major role in the highly anisotropic regions close the walls. A detailed study of these effects is therefore needed in order to better understand the role of collisions, for example close to the wall, and thus to improve the modeling of dispersed phase flows. The third goal of this project concerns the characterization of the dispersion of particles subjected to electrostatic forces. The modification of the dispersion of the particles due to the long distance interaction forces is in fact a topic of great interest due to its involvement in the field of process engineering. A modeling taking these effects into account is essential to ensure the correct operation of fluidized bed reactors.

Modélisation des vents violents en présence d'effets de relief et de rugusité

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Dominique Astruc**

The project consists of studying the dynamics of the atmospheric boundary layer in the presence of orographic effects (linked to the topography of the environment), roughness effects (linked to land use) and their combined influences. These effects will be studied in the case of violent winds. This configuration allows us to not take into account the effects of thermal stratification, we are in a situation of neutral atmospheric boundary layer.

Dynamique de bulles en présence de surfactants

Projet démarré en 2017

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Dominique Legendre**

The present study aims to explore the complex dynamics of the bubbles motion in liquids containing

surfactants. Two situations will be considered. The first one is an isolated bubble in an infinite stagnant liquid bath. This case has been studied thoroughly by the means of experiments and will allow to make a final validation of our numerical code. The second study is on an isolated bubble in a horizontal cylindrical tube of micrometer lenghtscale (microchannel). In the later, both spherical and elongated bubbles (« Taylor bubbles ») will be considered.

Dernières publications:

- O. Atasi, B. Haut, A. Pedrono, B. Scheid, D. Legendre, (2018). Influence of Soluble Surfactants and Deformation on the Dynamics of Centered Bubbles in Cylindrical Microchannel. Langmuir 34 (34) 10048-10062. - **doi:** pu.doi
- G. Rage, O. Atasi, M. M. Wilhelmus, J. F. Hernández-Sánchez, B. Haut, B. Scheid, D. Legendre, R. Zenit, (2018). Bubbles determine the amount of alcohol in Mezcal. arxiv - **doi:** pu.doi

Développement de CPIV

Projet démarré en 2016

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Pierre Elyakime**
CPIV est un logiciel de vélocimétrie par imagerie de particules (PIV) qui permet à partir des images obtenues lors des expériences de reconstituer le mouvement du fluide filmé. Ce logiciel open source et multiplateforme est développé à l'institut de mécanique des fluides de Toulouse (IMFT) et est utilisé par une dizaine de personnes. Il peut être utilisé de manière séquentiel ou parallèle sur un pc de bureau et a été porté sur le super calculateur de Midi-Pyrénées CALMIP depuis 3 ans. La parallélisation a été faite avec une librairie MPI. Il a été utilisé ses deux dernières années sur le super calculateur EOS par une dizaine de personnes pour environ 200 000h de calcul par an. Ce logiciel utilisé par les expérimentateurs a été originalement porté sur super calculateur pour proposer des temps de calculs extrêmement intéressant : un calcul sur une séquence de 67000 images peut prendre jusqu'à 2 semaines sur une simple machine en séquentiel et ne prend qu'environ 6h sur EOS avec 200 coeurs. CPIV est un code écrit en C/C++ et utilise les librairies opensource OpenCV version 2.4.0 et Qt version 4.8.4.

Dernières publications:

- P. Elyakime, 2017, Présentation d'une technique de parallélisation d'un logiciel de PIV utilisée sur super calculateur, Congrès Francophone de Techniques Laser, CFTL 2018, Dourdan, -
- G. Jodin et al., Electroactive morphing vibrating trailing edge of a cambered wing : PIV, turbulence manipulation and velocity effects, IUTAM Symposium "Critical flow dynamics around moving/deformable structures with design applications" -

RUGOPIV

Projet démarré en 2016

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Frederic Moulin**
Turbulent boundary flows over rough natural beds are studied experimentally at the IMFT using large

flumes that allow access to high values of the Reynolds number. In terms or metrology, PIV (Particle Image Velocimetry) is used in all these experiments. In this context, three research projects are now running, on topics at the core of the HDR of the scientific leader (see [1]). The first research project focuses on the morphodynamics (sediment transport) over a non erodable bed. The second project aims at understanding the turbulent boundary layer structure in very confined (shallow) flows over rough beds formed by prismatic roughness elements (urban-like canopies) or fine glass plates aligned with flow (plant-like canopies), both for submerged and emerged flow regimes. The third project focuses on a combination of shallow flow conditions and bed roughness variation along the transverse direction, involving the development of a scanning PIV measurement technique. In all these research projects, the flow structure is highly three-dimensional and turbulent. To achieve spatial and time convergence, huge amounts of PIV calculations are required.

Dernières publications:

- Chagot L., Moulin F., Eiff O., " Combined effects of relative submergence and roughness aspect ratio on canopy flow", 3 pages, 4th Int. Symposium of Shallow Flows, Eindhoven University Technology, NL, 26-28 June 2017 -
- Chagot L., Moulin F., Eiff O., "Coherent structures in free-surface canopy flows : combined effect of relative submergence and geometrical aspect ratio", 1 page, ETCKTH 2017, 16th 16th European Turbulence Conference, 21-24 August 2017, Stockholm, Suède -

BrainMicroFlow

Projet démarré en 2015

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Sylvie Lorthois**

The morphological, topological and functional study of cerebral microcirculation is a topic of growing interest in the communities of both vascular physiology and neuroimaging. In particular, cerebral blood flow control and diseased-induced modifications at the scale of the vascular network are crucial and unanswered questions. In this context, the development of innovative, cutting edge numerical tools are needed. IMFT is internationally recognized for its work on brain microcirculation modeling (ERC Consolidator Grant BrainMicroFlow #615102 awarded to S.Lorthois). In particular, a new code BrainMicroFlow has been developed, allowing the numerical simulation of blood flow in the cerebro-vascular network. The challenge is now to develop and incorporate mass transfers models (for oxygen, nutrients, tracers). To this end, several tools have been developed with the goal to make a link between the small scale where vessels are individually resolved and larger scales: 1) a 3D-FEM approach solving the advection/diffusion equations has been implemented and is used to check the validity of reduced models 2) a 1D network/boundary element approach, that we recently extended to transient states. The diffusion equation in the brain tissue is solved through integration of Green functions on the boundaries of the capillaries. Then, considering that the capillaries are axisymmetric, the problem is reduced to a pointwize problem along the cylinder axis. 3) a 3D homogenized model of advection/diffusion equation as also been developed, using the volume averaging method. This method allows to take into account the micro-structure of the network to derive effective properties (diffusion coefficients, sources, velocities). These different models will allow us to perform at the same time simulation of blood flow and mass transfers on geometries with total volumes reaching the full human brain scale.

Dernières publications:

- Maxime Berg1, Adlan Merlo1,Yohan Davit1, Michel Quintard1, Sylvie Lorthois. Red blood cells distribution in microvascular networks: a model derived from experiments. Blood flow: current state and future prospects. Paris, Octobre 2017 - **url:** pu.open_url
- M.Peyrounette. Towards brain-scale modelling of the human cerebral blood flow: hybrid approach and high performance computing, PhD Thesis, INPT, Oct 2017. -

Flow within and above a poro-elastic layer

Projet démarré en 2015

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Yohan Davit**
Aerodynamic surfaces in nature are compliant, sometimes porous and most often rough, as opposed to rigid, impermeable and smooth entities that we usually encounter in aeronautics. Understanding the interactions between a fluid and a poro-elastic coating could provide interesting new passive flow control systems for aeronautics with applications to drag reduction, lift enhancement or noise reduction. The scientific project aims at the realistic modelling of natural surfaces and at their simulation, with flow control applications in mind. We will focus on rough surfaces in which the individual roughness elements might be elastic, yielding a collective, compliant behaviour. In the present CALMIP project, we will use OpenFOAM to simulate the flow of a fluid over and within a poro-elastic layer. This will be only a preliminary approach, the goal of which is to gain insight into the physics of the flow and guide us in the process of determining averaged equations for the flow.

Dernières publications:

- Effects of porosity and inertia on the apparent permeability tensor in fibrous media. N. Luminari, C. Airiau, A. Bottaro (2018), International Journal of Multiphase Flow - **doi:** pu.doi
- "A penalization method to treat the interface between a free-fluid region and a fibrous porous medium", Luminari N., Zampogna G.A., Airiau C. & Bottaro A. , J. Porous Media, 2018, in press. -

Modélisation et simulation numérique directe de particules complètement résolues

Projet démarré en 2015

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Enrica Masi**
The goal of the project is to improve the understanding of momentum and heat transfer in poly-disperse flows also in the presence of non-spherical particles, in order to model realistic non-isothermal/reactive dense particle-laden flows on the basis of fully-resolved particle direct numerical simulations. Simulations with thousands particles in several dense configurations will be carried out using a Lagrangian VOF tensorial penalty method implemented in THETIS code developed in collaboration with I2M at Université de Bordeaux (Brandle de Motta, 2013, Vincent et al. 2014).

Dernières publications:

- M.-A. Chadil, S. Vincent, J.-L. Estivalèzes, "Accurate estimate of drag forces using particle-resolved direct numerical simulations", Acta Mechanica (2018) - **doi:** pu.doi

- M.-A. Chadil, S. Vincent, J.-L. Estivalezes, "Novel method to compute drag force and heat transfer for motions around sphere", Thermodynamics of Interfaces and Fluid Mechanics (2018) - **doi:** pu.doi

Dynamique des courants de gravité de configurations complexes

Projet démarré en 2015

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Thomas Bonometti**
The present project deals with fluid mechanics phenomena. The subject of the project is the study of the dynamics of gravity currents of arbitrary density ratio spreading in complex configurations, namely (1) underneath a free-surface or (2) in the upper part of the lithosphere. Such flows are encountered in many natural configurations (submarine currents flowing along the continental shelf slope, diapirs rising in the Earth crust). While gravity currents dynamics is relatively well understood in situation of deep ambient, the case of currents evolving in either a fluid where the top "boundary" is a free-surface, or in highly viscous flows such as those encountered in the upper lithosphere still raises open questions. The goal of the present project is to analyze local phenomena inaccessible to laboratory experiments and in-situ measurements with the use of a numerical approach capable of simulation gravity currents of arbitrary density ratio in configuration where a free-surface is present or in the case of highly viscous fluids. This project is done in collaboration with (1) Marius Ungarish (Technion, Haifa) and (2) Muriel Gerbault, Olivier Vanderhaege, Roland Martin (GET, Toulouse). In the first project, we will focus on the influence of the depth ratio between the gravity current and the free-surface height. In the second project, we will cover a wide range of parameters (density ratio, viscosity ratio, Archimedes number, Buoyancy number) in order to asses the transition between a so-called convection regime from a diapirism regime.

Dernières publications:

- Salinas J., Cantero M., Dari E. & Bonometti T., Turbulent structures in cylindrical density currents in a rotating frame of reference J. Turbul. 19, 463-492 (2018). - **doi:** pu.doi
- Zgheib N., Bonometti T. & Balachandar S., Suspension-driven gravity surges on horizontal surfaces : effect of the initial shape. Comput. Fluids, 158, 84-95 (2017). - **doi:** pu.doi **url:** pu.open_url

Drop motion on solid surface

Projet démarré en 2015

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Dominique Legendre**
The present study aims to explore the complex dynamics of the motion of drop on solid surface. In particular we want to address problems controlled by the dynamic of the contact line. Two situations will be considered: a liquid drop spreading after its contact with a solid surface and a drop sliding on an inclined surface. Liquid drop spreading is a challenging subject that has been studied in countless works and its difficulty to simulate is famous because of the triple line problem and the difficulties rising when trying to simulate its movement. Associated to this phenomena, a new theoretical publication predicts the existence of a series of vortices (Moffat Vortices), induced by the movement of the triple contact line which we pretend to study numerically since they have not yet be seen experimentally. Concerning drop sliding on

inclined plate, we aim to consider the case of pearling drop that have been observed experimentally and reproduced in numerical simulation for the first time using JADIM during the PhD of Marco Maglio.

Dernières publications:

- J-B. Dupont, D. Legendre, A.M. Morgante, Numerical Simulation for Two-Phase Flows in Fuel Cell Minichannels. J. Fuel Cell Sci. Technol 8(4):041008, 2011. -
- M. Febres, D. Legendre. Enhancement of a 2D front-tracking algorithm with a non-uniform distribution of Lagrangian markers Author links open overlay panel. J. of Computational Physics. Volume 358, 2018, p173-200 - **doi:** pu.doi

Ecoulements raréfiés dans les microactionneurs fluidiques

Projet démarré en 2015

ICA - Institut Clément Ader

Porteur de projet: **Lucien Baldas**

Gas flows in microsystems are of great interest for various applications that touch almost every industrial field. This multi-disciplinary nature and diverse range of application is typified through the following examples: • fluidic micro-actuators for active control of gas flows, from vacuum to high pressure level; • vacuum generators and pumps for extraction or insertion of biological samples; • micro heat exchangers for the cooling of electronic components, chemical applications, energy generation, waste heat recovery and efficiency improvement; • microsystems for mixing or separation for local gas analysis (e.g. monitoring of air quality); Recently, many studies have been devoted to the analysis of gas flows through microchannels. Modelling gas microflows necessitates taking several characteristic length scales into account, such as the mean free path of the molecules and the internal dimensions of microsystems. The ratio between these two characteristic scales, called the Knudsen number, is relatively large in microsystems and the flow is, in many cases, consequently rarefied. This causes local thermodynamic disequilibria and statistical fluctuations of the flow parameters, which represent the main difficulties for the flow modelling. This project is organized in two main axis: Development of fluidic micro-actuators for flow control: The active flow control is a research field in broad expansion. Its main objective is the improvement of vehicles aerodynamics by modifying, by means of actuators, the flow in the boundary layer. The objective is here to design efficient fluidic micro-oscillators which will be used for controlling flow separation over a ramp. This will be done through a numerical study of the influence of various geometrical and operation parameters on the oscillator performances (frequency and jet velocity), taking into account 3D and rarefaction effects. Development of Knudsen micro-pumps: In rarefied gases, flows can be generated by a tangential temperature gradient along a wall without any initial pressure gradient. This well-known phenomenon is the so-called thermal creep, or thermal transpiration, effect. It is the basis of the Knudsen pump operation principle, which allows gas pumping without any moving part when the gas is under rarefied conditions. This part of the project will be devoted to the numerical design and optimization of original Knudsen pumps consisting of two facing isothermal ratchet carved surfaces with different temperatures.

Dernières publications:

- S. Wang, L. Baldas, S. Colin, S. Orieux, N. Laurien, A. Kourta, N. Mazellier and S. Loyer. Active flow control of ramp flow by fluidic oscillators. Proceedings of 2nd International MIGRATE Workshop, Sofia, Bulgaria p.MIGRATE-154498 2017 -

- G. Tatsios, D. Valougeorgis, J. Chen, L. Baldas, S. Colin and S. Stefanov. Parametrization study of the thermally driven rarefied flow between saw-tooth like surfaces. Proceedings of 5th Micro and Nano Flows Conference, Milano, Italy 2016 -

Large eddy simulation of complex aerodynamic configurations

Projet démarré en 2014

ISAE/DAEP - Département Aérodynamique, énergétique et propulsion

Porteur de projet: **Julien Bodart**

In our team we mainly focus on turbulent flows applied to external aerodynamics, using Computational Fluid Dynamics and large eddy simulation specifically. We divide this year our demand in three (A-B-C) contributions. We also use eos to run preliminary computations for our current allocation at GENCI (Occigen, Turing) and PRACE (Juqueen) for different kind of problems. Recent developments in the solver include spectral schemes that exhibit optimal accuracy and performance for large scale simulation of turbulent flows. This numerical work will support several of our research topics in which high order schemes are mandatory, together with the legacy finite volume formulation. In this project, we work on the first part (A) which addresses the noise prediction of supersonic jets interaction(collaboration with LMFA). In the second part (B) we study the buffeting phenomenon in the context of reusable launchers (CNES). Finally, the last part of the project (C) aim at studying the flow inside jet actuators within a larger flow control study (Cleansky project XPulse).

Dernières publications:

- Pedro M. Milani; Julia Ling; Gonzalo Saez-Mischlich; Julien Bodart; John Eaton. A Machine Learning Approach for Determining the Turbulent Diffusivity in Film Cooling Flows, Journal of Turbomachinery - **doi:** pu.doi
- Jack Weatheritt; Richard D. Sandberg; Julia Ling; Gonzalo Saez; Julien Bodart, "A Comparative Study of Contrasting Machine Learning Frameworks Applied to RANS Modeling of Jets in Crossflow", Proc. ASME. 50794; Volume 2B: Turbomachinery, V02BT41A012.June 26, 2017 GT2017-63403 - **doi:** pu.doi

Ecoulement autour d'obstacles immergés

Projet démarré en 2013

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Ludovic Cassan**

The project about macroroughness fishways, linked to the Agence Française pour la Biodiversité (AFB) ex ONEMA, aims to determine the diphasic flow structure in these kinds of channels. They are constituted by blocks rows in a staggered arrangement on the bottom of a slopped channel. The blocks can have different shapes but they are taken as circular sections cylinders in this study. In order to determine if the flow structure is adapted to fish aptitude and due to difficulties to perform measurement in such flows, numerical simulations are necessary. The aim of these studies is to define a well adapted model for the problem. Turbulence and free surface flow models will be existing ones, the focus will be on their validity range and computation convergence criteria as mesh structure and density, Froude number, initial and boundary conditions. In order to validate the model, experiments were performed on a laboratory flume firstly on an unique plot (T. Ducrocq thesis) and on full plots ramps (Tien Trang thesis). During the year

2017, a new meshing methodology was applied to build a computational grid permitting to apply cyclic boundaries conditions. The numerical results were compared to measurements and confirm the applicability of VOF method associated with URANS turbulence modelling or better with LES method. Complementary runs are necessary in order to obtain detailed mean and unstationary flow characteristics and so help to fish passes conception. The new tilted glassed flume at IMFT (on spring 2018) will permit to make fine flow experiments and to test real fishes behavior in these flows.

Dernières publications:

- Ducrocq, T. (2016). "Etude de l'écoulement à forte pente autour d'un cylindre émergent," Thèse de Docteur Ingénieur, Institut National Polytechnique de Toulouse, Toulouse, France - **url:** pu.open_url
- Ducrocq, T. and al. (2017) Flow and drag force around a piercing cylinder for environmental applications. Environmental Fluid Mechanics, 17(4) - **doi:** pu.doi

Détermination de propriétés physiques de milieux poreux

Projet démarré en 2013

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Gérald Debenest**

This project aims to study the numerical determination of transport properties of real porous media. This is a complex subject related to fluid mechanics in tortuous geometries at a small scale and very demanding in terms of computations. Thanks to the developments of advanced visualization techniques (microtomography, microscopy), we are now able to obtain at a small scale a real image of the porous medium. The following step is now to use these data to determine the real properties of porous media in terms of permeability, conductivity and effective diffusion. To do so, we need to calculate flow and concentration field at the local scale and then, solve closure problems in periodic cells. This will give us the estimates of larger scale coefficients we could use to represent the transport phenomena. For real media, the challenge consists to find a way to determine effective properties without any influence of boundary values. This year is really devoted to multiphase flow and then to the development of new solvers able to treat the physics at all scale, i.e. microscopic or macroscopic.

Dernières publications:

- Guibert R., Nazarova M., Horgue P., Hamon G., Creux P., Debenest G., (2015) Computational permeability determination from pore-scale imaging: sample size, mesh and method sensitivities, TiPM -
- Horgue, P., Soulaine, C., Franc, J., Guibert, R., & Debenest, G. (2015). An open-source toolbox for multiphase flow in porous media. Computer Physics Communications, 187, 217-226. -

Traversée d'une interface de densité par un obstacle

Projet démarré en 2013

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Jacques Magnaudet**

La situation générique dans laquelle un corps rigide en mouvement rectiligne traverse de manière normale une interface séparant soit deux fuides immiscibles, soit deux régions du même fluide entre lesquelles

existe une discontinuité de densité, se rencontre dans de nombreuses applications allant de la métallurgie (remontée de bulles et de particules dans le métal liquide) à l'hydrodynamique sous-marine (mouvement d'engins auto-propulsés ou de capteurs passifs, bulles de culot), en passant par la pollution atmosphérique et océanique (dispersion de particules) et les processus d'encapsulation (pharmacie notamment). Cette situation a été beaucoup moins étudiée que celle où l'obstacle se déplace parallèlement aux surfaces iso-densité (sillages stratifiés en particulier). Il existe un réel besoin d'obtenir des données et un modèle général pour ces phénomènes, l'objectif étant de prédire la forme de la colonne entraînée et la vitesse de l'obstacle en fonction de sa forme, du rapport des densités et des viscosités des deux fluides, voire des tensions interfaciales impliquées, pour des conditions où l'inertie et les effets visqueux sont tous deux présents. La démarche proposée pour cette thèse consiste à utiliser intensivement la simulation numérique directe afin de cartographier ces écoulements en couvrant une large gamme de paramètres (nombres de Reynolds, de Froude et de Weber, rapports de densités et de viscosités) et de situations physiques (obstacles bi- et tridimensionnels indéformables, bulles et gouttes déformables). En parallèle il s'agira de développer un modèle théorique aussi général que possible en utilisant des techniques asymptotiques (un petit paramètre clé étant la différence relative de densité entre les deux fluides), d'une part dans la limite des écoulements non-visqueux, d'autre part dans celle des écoulements de Stokes.

Dernières publications:

- J.L. Pierson & J. Magnaudet 2015 Settling of a sphere through a fluid-fluid interface: influence of the Reynolds number. 68th APS DFD Annual Meeting, Boston, USA. -
- J. MAGNAUDET & J.-L. PIERSON 2017 Pinch-off dynamics of a liquid column pulled by a sphere settling through an interface. 70th APS DFD Annual Meeting, Denver, USA. -

Interaction fluide-structure d'un cylindre en rotation.

Projet démarré en 2012

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **David Lo Jacono**

Vortex-induced vibration (VIV) are of fundamental and practical importance. Indeed, the interactions between a structure within a flow are encountered in many engineering problems. The coupling between the solid and the fluid becomes of prime importance when the former has a natural frequency comparable to the typical frequency of the detached eddies that could occur behind those structures. One can imagine the disastrous impact if both those frequencies become similar (lock-in). On a fundamental viewpoint the strong coupling between the solid and the fluid is a canonical problem where one can study the interaction phenomena between the body and the fluid, including the mechanisms of energy transfer. Here, in this study we are interested in the particular response of the coupled fluid-structure system when one force a steady rotation on a solid (drill pipe in offshore stations) within a uniform flow. The symmetry breaking that the rotation imposes on the equations might lead to a new class of solutions that will be of interest within the VIV and more generally within the bluff body flow community.

Dernières publications:

- Three-dimensional mode selection of the flow past a rotating and inline oscillating cylinder, D. Lo Jacono, R. Bourguet, M. Thompson & J. Leontini, Journal of Fluid Mechanics, 855, 2018 -

- Flow-induced vibrations of a rotating cylinder in an arbitrary plane, R. Bourguet, Journal of Fluid Mechanics, sous presse, 2018 -

Simulation et assimilation de données d'écoulements à surface libre en géophysique

Projet démarré en 2012

IMT - Institut de Mathématiques de Toulouse (UMR 5219)

Porteur de projet: **Frédéric Couderc**

This project is mainly focus on parallel numerical simulations of free surface geophysical flows considering unstructured grids. The numerical environment is fully developed at the Toulouse Mathematics Institute in Fortran 2008. At the top level, a library named FUnMesh has been developed with advanced structures to consider unstructured meshes with particular attention to sequential performance and in context of distributed parallel computing (using only the MPI library for the moment). If main activity is to design new models and numerical schemes, it is crucial to test these models and numerical schemes in "real" context with large computations for geophysical flows (time scales implying very large number of time steps). The numerical environment includes several software's applications: - Omanu: resolving the multilayer shallow water equations using original explicit and semi-implicit Finite Volume schemes with low Froude asymptotic consistency property on collocated or staggered unstructured grids. Main application is (coastal) oceanography in collaboration with the SHOM under a research contract. - Mingus: resolving original shallow water type models considering surface tension developed in the laboratory under hyperbolic time step restriction, and so avoiding the surface tension one. Applications are industrial film flows with eventually wet/dry fronts in collaboration with ONERA and LIMSI. - Monk: resolving the multifluid compressible Navier-Stokes equations using an original Finite Volume scheme with low Mach asymptotic consistency property as an original implicit surface tension treatment adding a new transported variable. Main application for the moment is again film flow in collaboration with LIMSI with possibility to test with in future wave breaking for our SHOM activities.

Dernières publications:

- Semi-implicit staggered mesh scheme for the multi-layer shallow water system. - **doi:** pu.doi
- Centered-Potential Regularization for the Advection Upstream Splitting Method. - **doi:** pu.doi

Simulation numérique de lits fluidisés réactifs gaz-solides

Projet démarré en 2011

LGC - Laboratoire de Génie Chimique (UMR 5503)

Porteur de projet: **Renaud Ansart**

LGC and IMFT, in the frame of the Fermat Research Federation and in collaboration with PROMES laboratory, Institut Français du Pétrole,... are working on the development of mathematical modelisation and numerical simulation of hydrodynamic and transfers in reactive gas-particle fluidized beds. The complexity of involved physical phenomena (interparticle collisions, aggregate formation, evaporation, heat transfer, chemical reaction, ...) and realistic three-dimensional geometries (biomass gasification plants, concentrating solar power plants) lead to use powerful computer resources such as SGI Altix ICE 8200. Simulations are carried out using an Eulerian n-fluid modeling approach for turbulent and polydispersed fluid-particle flows, which is developped and implemented by IMFT (Institut de Mécanique des Fluides de

Toulouse) in a specific version of the NEPTUNE_CFD software, known as NEPTUNE_CFD V1.08@Tlse. NEPTUNE_CFD is a multiphase flow software developed in the framework of the NEPTUNE project, financially supported by CEA (Commissariat à l'Énergie Atomique), EDF (Électricité de France), IRSN (Institut de Radioprotection et de Sûreté Nucléaire) and AREVA-NP. The code solves, for each phase, Eulerian three-dimensional unsteady equations of mass, momentum and enthalpy, coupled through the terms of transfer between phases and transport equation of a variable number of scalars. Parallel simulation efficiency of NEPTUNE_CFD has been tested on many platforms Linux PC, supercomputer (SGI ALTIX ICE, NEC, clusters based on AMD Shangaï and Barcelona). Access to source code programs enables the possibility to modify existing models and also to test the build options to improve the performance of the code. Moreover, excellent parallel performances of the code enable the implementation of multiphysics calculation of flows in real flow configurations. One first objective of the projet is the comparison between experimental measurements realised in the LGC and numerical results from the code NEPTUNE_CFD. The aim of the research is the modeling of the coupling between hydrodynamic, and heat and mass transfer to account for additional mechanism such as radiative transfer and chemical reaction in gaz-solid flow.

Dernières publications:

- R. Ansart, P. Garcia Triñanes, B. Boissière, H. Benoit, J.P.K. Seville, O. Simonin. Dense gas-particle suspension upward flow used as heat transfer fluid in solar receiver : PEPT experiments and 3D numerical simulations. Powder Technology, Volume 307, Pages 25-36, 2017. - **doi:** pu.doi **url:** pu.open_url
- H. Benoit, R. Ansart, H. Neau, P. Garcia Triñanes, G. Flamant, O. Simonin, 3D numerical simulation of upflow bubbling fluidized bed in opaque tube under high flux solar heating. AIChE Journal. - **doi:** pu.doi **url:** pu.open_url

Intégration de données topographiques LIDAR dans des codes hydrodynamiques pour la simulation de la propagation de champ d'inondations

Projet démarré en 2011

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Jacques Chorda**

The aim of the project is to make an efficient usage of the topographic airborne LIDAR data in order to improve modeling of flood areas delimitations that are of particular interest to flood planners and risk assessors. Modeling floods areas in lowland is challenging. In such zones flood distribution is significantly influenced by small changes in surface elevation and manmade structures. So, we worked successively on flood dynamics for different lowlands locations : the Lèze and Touch rivers with geographs and sociologists, the Garonne river downstream Toulouse. For the last one, in the SWOT project (CNES-NASA) context, various simulations permitted to test data assimilation algorithms giving a discharge value from periodical satellital observations. Moreover, collaboration with BRGM (MARTHE code), must provide a better understanding of water exchanges between alluvial aquifers and river particularly during low water periods. A hard point is that airborne LIDAR data does not penetrate through water surfaces and so, the bathymetric data are not available, which imposes a limitation particularly for large rivers as Garonne. In order to explore and extend the LIDAR data usage application to environmental hydrodynamics modeling, we joined this year the CRUESIM project which associates physicians of atmosphere, hydrologists and oceanographs in order to model and study the Mediterranean flash floods including bedload and suspension conjugated with intense rainfalls on watershed. Atmosphere/Ocean coupling effect will provide the retroactive effect of sea level on flood extension. These modeling will be based at different scales on the cascade of : SWAT (Soil and Water Assessment Tool) low resolution model, then medium resolution MARINE (IMFT), the

hydrologic spatially distributed, physical basement model. River hydrodynamics will be treated with 2D high resolution TELEMAC2D model.

Dernières publications:

- Yoon, Y., P.-A. Garambois, R. C. D. Paiva, M. Durand, H. Roux, and E. Beighley (2016), Improved error estimates of a discharge algorithm for remotely sensed river measurements: Test cases on Sacramento and Garonne Rivers - **doi:** pu.doi
- Brisset, P., Garambois, P-A, Monnier, Roux, H. (2016), Identifiability and Assimilation Of Sparse Altimetric Data In 1D Saint-Venant River Models - **url:** pu.open_url

Modélisation du transport sédimentaire par une approche de simulation numérique locale

Projet démarré en 2010

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Laurent Lacaze**
Physical mechanisms involving solid particles and fluid flow are still poorly described due to the lack of knowledge in the local characterization and thus modelling of solid-liquid and solid-solid interactions. However, these local processes play a fundamental role at larger scales such as sediment transport encountered in many natural flows for which environmental impacts become of major societal concern. Erosion and accretion are two important processes involved in these natural issues. The impacts of granular transport can, in fact, be encountered at different scales and applications, ranging from the process industries to landslides and avalanches. In this proposal, we will focus our attention on the environmental context of river, coastal flows, as well as natural hazard such as subaerial or submarine landslides. The objective of this proposal is to provide a better understanding of the physical processes involved in the transport of solid particles, induced by gravity or flow entrainment, at the scale of the grains, via the development of adapted numerical tools. The aim of these numerical methods is the modelling and quantification of such physical processes. The key objective of the numerical strategy proposed here is the ability to resolve interactions between the solid and liquid phases at the scale of the grains, which are critical in coastal and river flows. To this end, we plan to develop two different numerical tools which can be viewed as complementary by virtue of the type of interaction each method can accurately capture (solid-solid vs. fluid-solid).

Dernières publications:

- Izard E., Bonometti T. and Lacaze L. 2014 Modelling the dynamics of a sphere approaching and bouncing on a wall in a viscous fluid. J. Fluid Mech., 747, p. 422—446 - **doi:** pu.doi **url:** pu.open_url
- Izard E., Lacaze L., Bonometti T. & Pedrono A. Numerical modeling of a granular collapse immersed in a viscous fluid. Advances in Hydroinformatics, Springer, Singapore, 1099-1116 (2018). - **doi:** pu.doi

Propriétés de transport des écoulements inertiels de suspension en canal

Projet démarré en 2010

LGC - Laboratoire de Génie Chimique (UMR 5503)
Porteur de projet: **Micheline Abbas**

La plupart des procédés industriels impliquent un écoulement de milieux divisés. Il est important d'en comprendre les propriétés de transport, dans plusieurs domaines d'ingénierie (génie pétrolier, génie de la réaction chimique ou génie agro-alimentaire). En fonction de l'inertie de l'écoulement, de la fraction volumique de la phase solide, de la taille des particules par rapport à la taille de la conduite et aux structures de l'écoulement, du rapport de densité particule/fluide, la présence des particules peut altérer le transfert de quantité de mouvement. Ce projet vise, par l'intermédiaire de la simulation locale, à étudier la dépendance de la dynamique de la suspension sur tous les paramètres déjà énumérés. Par dynamique je sous-entends la modification des propriétés de l'écoulement par la phase dispersée et/ou structuration (ou organisation) de la phase dispersée due à l'écoulement.

Dernières publications:

- Gupta, A., Magaud, P., Lafforgue, C., & Abbas, M. (2018). Conditional stability of particle alignment in finite-Reynolds-number channel flow. Physical Review Fluids, 3(11), 114302. - **doi:** pu.doi
- Wang, G., Abbas, M., & Climent, E. (2018). Modulation of the regeneration cycle by neutrally buoyant finite-size particles. arXiv preprint arXiv:1806.02862. - **doi:** pu.doi **url:** pu.open_url

Modèles de la dynamique des bulles pour la simulation des grandes échelles des écoulements turbulents

Projet démarré en 2009

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Rémi Zamansky**

Bubbly flows (consisting of a continuous liquid phase and a dispersed gas phase) are of great importance for many industrial applications, which include chemical reactors, water treatment (flotation, oxidation, ..), steam generators, drag reduction system or some CO2 capture devices. In these situations, the Reynolds number is usually large and the complexity of such a flow lies in the coupling between the various physical phenomena involved. When the Reynolds number of the flow is very large, the liquid present turbulent fluctuations on the scale of the bubble. Moreover, the large number of bubbles in the flow may induce hydrodynamic interactions between bubbles and can also cause a significant alteration of the carrier phase. Our goal is to propose an approach to perform Large Eddy Simulation (LES) for this kind of two-phase flows. The realistic description of the bubbles dispersion as well as their influence on the continuous phase requires to compute the hydrodynamic forces on the bubbles. These depend on the relative speed of the bubble and the local fluid acceleration. And since these two quantities are mainly set by the small (unresolved) scales of the flow, the LES approach remains challenging. The question is therefore to estimate correctly the turbulent liquid fluctuations at subgrid scales and particular those "seen" by the bubble. This is our motivation for introducing a stochastic modeling of the flow at unresolved scales. The advantage of the approach of coupling LES with stochastic models at subgridscale is to give access to the unresolved intermittent structures of the flow, while taking into account the large scale organization of the flow. The project aims to devise stochastic models representing the bubble/liquid and the bubbles/bubbles interactions at subgrid scales. These models should be based on theoretical and experimental knowledge of the Lagrangian acceleration properties of high Reynolds number turbulent flows. Contributions from the coupling of the LES with a subgrid stochastic modeling for bubbly flows will be studied by comparison with Direct Numerical Simulations (DNS), experimental results and with standard LES.

Dernières publications:

- Shear-induced self-diffusion of inertial particles in a viscous fluid (2009) Abbas M., Climent E., Simonin O., Phys. Rev. E 79, 036313 -
- Etude numérique de la réduction de traînée par injection de bulles en écoulement de Taylor-Couette, thèse soutenue par Agathe Chouippe le 12 juillet 2012, INP-Toulouse -

Sensibilité et contrôle des écoulements par simulations numériques h-p

Projet démarré en 2008

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Christophe Airiau**
The present work is associated to the new RTRA STAE project 3C2T (2018-2021) about the control of the turbulent and transitional compressible boundary layer. The three partners (IMFT, CERFACS, ONERA) will build together a new numerical common suite (plateforme) in which high order h-p simulations, based on DNS, LES and Euler equations will be coupled with their discrete adjoint counter part to solve sensitivities, control and optimisation of flows around complex geometry in a large range of Mach number and Reynolds number regimes. At the beginning, and more especifically, the work will concern the control of the instabilities in the transitional flow or of the small scale structures in the turbulent boundary layer flow, in the subsonic and hypersonic regime. The main numerical simulation tool is the recent JAGUAR code developped at CERFACS, in which Discontinuous Galerkin scheme with Spectral Difference are implemented, optimized and validated for HPC purpose. The Adjoint version of each approach will be developped and implemented at IMFT, in collaboration with the partners using the discrete adjoint formulation, but in respect with the scheme consistancy and the numerical discretization. The first year, 2018, will be dedicated to the first implementation of the adjoint DNS, its validation by comparing with existing solution (for instance ASIA and adjoind ASIA, a 2D compressible code ever developped inside this CALMIP project in the periode 2008-2014). The discrete adjoint will be carefully implemented, without a code of automatical differentiation in order to supervise and qualify each step of the process. Possibly, in a short period, a continuous then discretized adjoint DNS JAGUAR will be designed to validate some sensitivity results on the 2D boundary layer flow. The details about the test cases (Mach, Reynolds, pressure gradients, geometry, ...) will be decided in january, at the beginning of the project.

Dernières publications:

- Rona, A. ; Monti, M ; Airiau, C. On the generation of the mean velocity profile for turbulent boundary layers with pressure gradients under equilibrium conditions, The Aeronautical Journal, (16), N° 1180, 569 -597, - **doi:** pu.doi
- Spagnoli, B ; Airiau, C. Adjoint analysis for noise control in a two-dimensional compressible mixing layer. COMPUTERS & FLUIDS, 37(4), 475-486, - **doi:** pu.doi

Simulation numérique de l'hydrodynamique et des transferts dans les réacteurs gaz-particules à lit fluidisé

Projet démarré en 2001

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Pascal Fede**
Since 2006, IMFT work on the development of mathematical modelling and numerical simulation of

hydrodynamic and transfers in reactive gas-particle fluidized beds. The complexity of involved physical phenomena (inter-particle collisions, aggregate formation, evaporation, heat transfer, chemical reaction, ...) and realistic three-dimensional geometries (catalyst injection zone in polymerization reactor, cyclone separator) requires large computer resources. Simulations are carried out using an Eulerian n-fluid modeling approach for turbulent and polydispersed fluid-particle flows, which is developed and implemented by IMFT (Institut de Mécanique des Fluides de Toulouse) in NEPTUNE_CFD. NEPTUNE_CFD is a multiphase flow software developed in the framework of the NEPTUNE project, financially supported by CEA (Commissariat à l'Énergie Atomique), EDF (Électricité de France), IRSN (Institut de Radioprotection et de Sûreté Nucléaire) and AREVA-NP. The code solves, for each phase, Eulerian three-dimensional unsteady equations of mass, momentum and enthalpy, coupled through transfer terms between phases, and transport equation of a variable number of scalars. Parallel simulation efficiency of NEPTUNE_CFD has been tested on many platforms. Access to source code programs enable to modify existing models and also to test the build options to improve the performance of the code. Moreover, the excellent parallel performances of the code enable the implementation of multiphysics calculation of flows in actual flow configurations. In 2018, the main objective of the project is to continue the development a original n-Eulerian LES modeling approach which accounts for the subgrid particle segregation effect on the momentum transfer between the gas and the particles. Also, time will be dedicated to the development and validation of the modeling of heat and mass transfers, coupled with chemical reactions as to the numerical simulation of bioreactors.

Dernières publications:

- Hamidouche, Z.; Masi, E.; Fede, P.; Ansart, R.; Neau, H.; Hemati, M. & Simonin, O. Numerical Simulation of Multiphase Reactive Flows Academic Press, 2018 - **doi:** pu.doi
- Neau H., Fede P., Ansart R., Simonin O., Renon N., Barbaresco P., Baudry C., Merigoux N., Massively Parallel Numerical Simulation of Hydrodynamics and Transfers in a Polydispersed Reactive Gas-Particle Fluidized Bed at Industrial Scale, Journées Calcul et Données JCAD'2018, 2018 -

SIMULATION DIRECTE ET MODELISATION DES ECOULEMENTS TRIDIMENSIONNELS TURBULENTS DE TYPE SILLAGE

Projet démarré en 2000

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)

Porteur de projet: **Marianna Braza**

This project focuses on development of new simulation methods for the Direct Numerical Simulation as well as new strategies for turbulence modelling for unsteady flows around aerodynamic bodies, including deformable wing structures under the effect of electroactive morphing in order to increase the aerodynamic perfrmances. A new direction of this project focuses on the Fluid-Structure Interaction Modelling and Simulation. The project uses and develops advanced simulation tools for solving the Navier-Stokes equations in incompressible and compressible regimes, taking into account phenomena related to transition and turbulence. This project aims at investigating the successive stages of the flow transition towards turbulence around bodies. Concerning the high-Reynolds number regimes, this project aims at developing advanced turbulence modelling methodologies and Reduced Order Modelling (ROM) to accurately predict the aerodynamic coefficients in unsteady regimes, especially in the context of Fluid-Structure Interaction. Furthermore, the Electroactive Morphing concept of new generation of airvehicles is a major concern of the present project that aims at associating a very efficient Aeroelasticity integrated model, coupling the most advanced CFD to novel electroactive materials CSM (Computational Structural

Mechanics), to achieve Morphing of aileron's structure. The CFD-CSM kernel is coupled with optimum shape design MDO, especially based to surrogate order modelling, to give the appropriate shape to the control surfaces in order to avoid nuisance phenomena (aileron flutter and vibration sources) and to improve manoeuvrability. This is achieved by acting on the Electroactive materials to enable deformation of the solid surface according to optimum shape design.

Dernières publications:

- V. Shinde, E. Longatte, F. Baj, M. Braza, "A theoretical model of fluidelastic instability in tube arrays", Nuclear Engineering and Design, 337, pp. 406-418, 2018 -
- M. BRAZA, K. HOURIGAN, M. TRIANTAFYLLOU Sci. Eds., (2018)-(2019) "Critical flow dynamics involving moving/deformable structures with design applications", Notes on Numerical Fluid Mechanics and Multidisciplinary Design, à paraître, Publisher Springer -

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4.2 Sciences de la Vie

Interaction de porphirines métallées avec un ARN quadruplex

Projet démarré en 2018

LCC - Laboratoire de Chimie de Coordination (UPR 8241)
Porteur de projet: **Jean-Luc Stigliani**
Les acides nucléiques G-quadruplex sont des structures particulières d'ADN ou d'ARN se formant par l'assemblage de 4 brins riches en guanines. Leur rôle en biologie devient de jour en jour plus évident. Ils sont impliqués dans la régulation des processus fondamentaux du vivant comme la réplication, la transcription, la traduction, ... La présence de G-quadruplex dans le génome de certains virus comme HIV-1, a été mise en évidence récemment. ils sont situés dans des zones cruciales pour le cycle viral. L'équipe a montré que des ligands de G-quadruplex de type métallo-porphyrines inactivent le virus HIV-1. Certains de ces dérivés ont une activité comparable à celle de l'antiviral de référence, l'AZT. Cette dernière est par ailleurs conditionnée par la présence et la qualité du métal central : la suppression du métal entraine une forte baisse de l'activité inhibitrice. Des étude préalables de modélisation moléculaire basées sur des méthodes de mécanique moléculaire n'ont pas permis de mettre en évidence l'effet du métal sur l'interaction entre la porphyrine et le quadruplex, les effets électroniques n'étant pas vraiment pris en compte par ces méthodes. Afin de décrire ces effets, les méthodes de mécanique quantique sont plus adaptées. Dans ce travail préliminaire, l'interaction entre la porphyrine métallée (avec de l'or) ou bien non métallée et un ARN quadruplex sera étudiée à l'aide de la méthode mixte QM/MM implémentée dans le logiciel Gaussian 09 (méthode ONIOM). Le but est de déterminer l'énergie d'interaction entre le quadruplex et la porphyrine (métallée ou non métallée) afin de mettre en évidence l'effet du métal sur l'interaction.

Concours IGEM : Cerberus

Projet démarré en 2018

LISBP - Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (UMR 5504/792)
Porteur de projet: **Sophie Barbe**

Ce projet s'inscrit dans le cadre du concours international de biologie synthétique iGEM (International Genetically Engineered Machine), lancé en 2004 par le MIT (Massachusetts Institute of Technology) localisé à Boston. Pendant plusieurs mois, des groupes d'étudiants mettent en commun leurs compétences pour développer un système biologique doté d'une fonction nouvelle et innovante. Cette fonction doit répondre à un besoin particulier, que cela soit une meilleure connaissance de la biologie ou une application concrète dans un domaine défini. Parmi les domaines proposés se trouvent l'environnement, la santé, mais aussi l'énergie, le traitement de l'information, et même l'art. L'aspect humain et éthique fait partie intégrante du projet, et sa bonne conduite conditionne les récompenses obtenues. Ainsi, les participants sont invités à vulgariser leur projet pour le rendre accessible au grand public ainsi qu'à informer sur les possibilités offertes par la biologie synthétique. Notre projet iGEM 2018 "Cerberus" s'inscrit dans le contexte du développement de matériaux innovants. Dans ce domaine, la fonctionnalisation de la cellulose laisse entrevoir d'intéressantes perspectives. Étant utilisée dans les domaines du médical, du textile et de la papeterie, ce matériau aux propriétés déjà largement exploitées peut encore se voir implémenter de certaines fonctionnalités novatrices. La simplification de la conjugaison de molécules bio-actives à la cellulose permettrait d'en élargir le champ des possibilités. Du papier conducteur d'électricité aux dispositifs hygiéniques prévenant l'infection de souches pathogènes, notre design d'une protéine « linker » tricéphale nommée Cerberus (en référence au chien de la mythologie grecque) permettra la fixation de composés chimiquement variés. Ce design repose sur la fusion de trois structures protéiques fixatrices représentant les trois têtes du système. La première tête est un domaine protéique de la famille des Carbohydrates Binding Module de type 3 (CBM3), se liant à la cellulose. La deuxième est un des plus forts systèmes de liaison du vivant : la streptavidine, fortement affine pour la biotine. La dernière tête est constituée d'un acide aminé non-naturel, l'Azoture de Phénylalanine (AzF), catalysant des liaisons covalentes par un système de click chimique. Ce système Cerberus designé permettra de conjuguer de manière versatile une grande diversité de molécules biologiques, organiques et inorganiques. Ces travaux impliquent la construction d'un modèle 3D du système Cerberus d'intérêt afin de comprendre l'arrangement 3D des différents composants moléculaires. Il s'agit également d'étudier la stabilité, et les réarrangements conformationnels de ce système dans différents environnements (solvant, T°, ...). En particulier, ces travaux nécessitent de réaliser des simulations de dynamique moléculaire et des calculs d'énergie libre avec le logiciel de simulation de biomolécules AMBER. De longues simulations extrêmement coûteuses en temps de calcul sont nécessaires afin d'accéder à un large échantillonnage de la dynamique du système étudié dans différentes conditions. De plus, chaque simulation sera réitérée avec des vitesses initiales différentes afin de vérifier la reproductibilité des résultats. L'analyse de l'ensemble de ces trajectoires de dynamiques moléculaires permettra de guider la sélection des molécules pouvant être greffées sur notre système Cerberus afin de fonctionnaliser la cellulose. Les études envisagées nécessitant d'avoir recours à des simulations numériques très coûteuses en temps CPU, nous déposons comme convenu une demande de 50.000 heures de calcul.

High-resolution 3D structure determination of Pks13, the condensase of mycolic acids, by single-particle cryo-electron microscopy

Projet démarré en 2018

IPBS - Institut de Pharmacologie et de Biologie Structurale (UMR 5089)

Porteur de projet: **Cecile BON**

Type I polyketide synthases (PKS) are large multifunctional enzymes responsible for the biosynthesis of a structurally diverse range of natural products with a comparably broad spectrum of biological activities. The structure elucidation of PKS is of both fundamental and applied interest, with considerable potential for structure-based engineering and drug design. Most of the current knowledge about structure-function

relationships of PKS has been deduced from structures of the related type I fatty acid synthase (FAS) enzymes and on combining high-resolution structural data for individual domains or didomains derived from PKS. Although there are not yet any atomic resolution structures of intact PKS, low-resolution models have been more recently derived from single-particle electron cryo-microscopy (SP cryo-EM) or by hybrid approach combining X-ray crystallography and small angle X-ray scattering (SAXS). Pks13 is a type I PKS involved in the final step of the biosynthesis pathway of mycolic acids, and is essential for the viability of mycobacteria. It has been the focus of intensive research aiming at characterizing its mechanism of action and druggability. In parallel with these studies, we have embarked on the structural characterization of such a complex megasynthase (186 kDa, 1733 residues comprising five catalytic domains interconnected by linker regions). Our strategy was to work on the full-length enzyme and on domains or fragments, and to use a combination of SAXS and crystallography to provide low- and high-resolution information, respectively. For instance, the crystal structure of a 52-kDa fragment containing the acyltransferase domain has been determined in different states. Our goal now is to make use of SP cryo-EM, which is nowadays "becoming a dominant technology", to determine the atomic structure of the full-length enzyme. Preliminary results, in collaboration with Célia Plisson-Chastaing (LBME, CBI) led to images of such quality that structure determination can now easily be foreseen. The objective of this application is to carry out single particle reconstruction from data already available and hopefully from data obtained at higher resolution on an even more powerful electron microscope. We would like to use RELION and Ctffind4, already installed on the CalMIP facilities, to be able to investigate the structure of Pks13 at the highest possible resolution, with the most time-efficient manner.

Développement de modulateurs de l'interaction entre la protéine oncogénique virale HBZ et les facteurs de transcription à domaine bZIP

Projet démarré en 2018

IRIM - Institut de Recherche en Infectiologie de Montpellier

Porteur de projet: **Laurent Chaloin**

HTLV-1 (Human T-cell Leukemia Virus type 1) infection promotes the Adult-T-leukemia (ATL) several years post-infection. As viral genes do not integrate into the host genome within a proto-oncogenic region or in a tumor suppressor gene, this cellular transformation has been attributed to the only viral protein present in all leukemic cases, HBZ for HTLV-1 basic zipper factor. This protein, which is expressed all along the infection, was suspected to induce the leukemic transformation. Indeed, HBZ has a leucine-rich basic domain (bZIP) which is found in many transcription factors of the ATF/CREB and AP-1 families, allowing it to interact with numerous partners already identified like Jun-D. Recent published data have shown that its interaction with a truncated isoform of JunD was sufficient to promote cell transformation. Our project aims to better understand the mechanisms governing this transition resulting in a malignant clone, by studying at the molecular and cellular level, the interactions of HBZ with its various partners of the ATF / CREB family and those of the AP- 1family. To reach our objectives, we will first design a family of chemical compounds able to modulate or block the interactions involving the basic zipper domain of this viral protein. By using the tridimensional molecular models obtained for HBZ alone or in complex with Jun-D as a heterodimer, a large virtual screening campaign will be carried out using a chemical library of 2 million of drug-like compounds by targeting the leucine-rich region of this basic zipper domain. All the hit compounds predicted as good binders will be evaluated for their ability to bind and/or to dissociate the HBZ/Jun-D heterodimer. In addition, several cellular models harboring a luciferase reporter gene under the control of the AP-1 promoter sequence will be used in order to evaluate the potency / efficiency of identified hit compounds to inhibit the transcriptional activity mediated by HBZ/Jun-D.

Modélisation de nanoparticules d'or et d'argent

Projet démarré en 2018

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)
Porteur de projet: **Mathias Rapacioli**
Modeling Silver and Gold nanoparticles In the present project, we investigate gold and silver clusters and nanoparticules. This topic is relevant from a fundamental side (understanding noble metal nanoclusters properties) but also in several contexts such as catalysis, health or sensors design. We are using the Density Functional based Tight Binding (DFTB) method, an approximated DFT scheme with a much lower computational cost than DFT, while conserving an explicite quantum description. We have developed a set of DFTB parameters and showed that they provide a good description of Ag/Au properties from clusters to bulk, opening the route to the modeling of large nanoparticules. The combination of this potential with global exploration schemes of the complexe Au/Ag potential energy surfaces allows for the determination of structural and thermodynamical properties for systems containing from a few tens to hundreds of atoms. More precisely, our current and future works consist in characterizing the structural nature of large gold clusters (regular or amorphous, presence of cavities, cages) and to establish the size and charge effects on the heat capacity curves of Ag/Au clusters.

Dernières publications:

- M. Rapacioli, N. Tarrat, and F. Spiegelman. Melting of the au20 gold cluster: Does charge matter? J. Phys. Chem. A, 122, 16, 4092 (2018) - **doi:** pu.doi **url:** pu.open_url
- N. Tarrat, M. Rapacioli, and F. Spiegelman. Au147 nanoparticles: Ordered or amorphous? The Journal of Chemical Physics, 148, 20, 204308 (2018) - **doi:** pu.doi **url:** pu.open_url

Investigating Structure-Function Relationships of Carbohydrate-Active Enzymes to guide development of novel biocatalysts: A focus on Glycoside-Phospho

Projet démarré en 2018

LISBP - Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (UMR 5504/792)
Porteur de projet: **Jeremy Esque**
Oligosaccharides represent a class of very diverse biomolecules consisting in linear or ramified chains of sugar moieties or sugar derivatives that are linked together by different types of α or β osidic linkages. The wide structural diversity of oligosaccharides comes from both the combination of sugar moieties and the types of covalent linkages. These molecules are involved in a multitude of cellular processes, including cell signaling/differentiation, modulation of immune response, inflammation, and mediation of microbial and host-microbe interactions. Because of their highly versatile structures and biological functions, oligosaccharides are used for a broad range of applications in food (functional foods, prebiotics or as additives) and health (as drugs, drug carriers or vaccine intermediates) industries. Development of novel synthetic routes to access more easily to these complex carbohydrates is thus of utmost interest. Within this context, the current study will be integrated into a more ambitious project funded by the ANR, the project OLIGOMET (2016-2020), which aims at developing new bio-based synthetic routes for the efficient production of added-value oligosaccharides. Within this project, we will focus mostly on a particular family of Carbohydrate-Active enzymes (CAZymes), i.e. Glycoside Phosphorylases (GPs), among which several members have been recently discovered in our laboratory, the LISBP, using functional metagenomics (Tasse

et al., Genome Res., 2010 ; Ladevèze et al., J. Biol. Chem. 2013 ; Cuskin et al., J. Biol. Chem. 2015). These enzymes, produced by gut bacteria, could play a role in polysaccharide phosphorolysis of plant cell wall and phosphorolysis of glycans from host intestinal epithelium. Nowadays, few studies have been dedicated to GPs. Therefore, better understanding their mechanism and their structure-function relationships seems to be crucial for developing their biotechnological applications. Our objective in fine is to use this fundamental knowledge to guide rational engineering of GPs toward novel catalytic reactions and substrates. These enzymes will be integrated in E. coli metabolic chassis to produce oligosaccharides of high-added value, mostly eukaryotic glycan cores and prebiotics.

Modélisation multi-échelle des molécules constitutives de la membrane des mycobactéries et leurs interactions avec la membrane de la cellule hôte

Projet démarré en 2017

IPBS - Institut de Pharmacologie et de Biologie Structurale (UMR 5089)
Porteur de projet: **Matthieu Chavent**
Mycobacterial infections, and in particular human tuberculosis (TB), remain major public health problems throughout the world, especially in developing countries. About two billion individuals worldwide are estimated to be carriers of Mycobacterium tuberculosis (Mtb), the etiological agent of human TB. This enormous reservoir of latently infected people, who may develop the disease decades after their infection and transmit the bacillus to other people, fuels the ongoing TB pandemic. We want to use molecular modeling to develop new strategies to understand the biological mechanisms of molecules involved in Mtb virulence and protection. Some of these molecules contribute to modulate the protective host immune responses. Using multi scale molecular dynamics simulations, we will study different types of molecules from complex lipids to proteins in order to shed lights on the biophysical mechanisms involving this molecules and also to develop a global understanding of the biological mechanisms taking place in the Mtb enveloppe.

Dernières publications:

- Interactions of the EphA2 Kinase Domain with PIPs in Membranes: Implications for Receptor Function - **doi:** pu.doi **url:** pu.open_url

Etudes par dynamique moléculaire d'hydrocarbures aromatiques polycycliques interstellaires et d'asphaltènes environnés

Projet démarré en 2017

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)
Porteur de projet: **Aude Simon**
This project aims at characterizing polycyclic aromatic hydrocarbon (PAH) monomers and clusters in an environement using molecular dynamics simulations (MD). In these simulations, the electronic structure is computed on-the-fly using the self-consistent charge density functional based tight-binding approach. This project can be divided into two parts. We aim at characterizing: -(i)- PAH(H2O)n clusters. This is an ongoing research project in our team, and it follows an ANR project which is ending (PARCS 2014-2017). Our goal is to characterize the structures, binding energies and vibrational and electronic spectra of PAH(H2O)n clusters in which the PAH is either planar or curved (typically pyrene and coranulene). This is done in

collaboration with Nadia Ben Amor (LCPQ) and with experimentalists in Bordeaux (V. Blanchet and J. Mascetti). It is funded by the PCMI (physicochimie du milieu intertellaire) national program. -(ii)- asphaltenes in solution at the interface with liquid water. Asphaltenes are PAH derivatives that include heteroatoms and aliphatic chains. There exists varieties of asphaltenes that are present in fuel, coals, nanoparticles resulting from biomass combustion. Asphaltenes are regarded as the most enigmatic component in petroleum because of their negative influence on stabilizing the water-in-crude oil emulsion, that should be closely related to their self-aggregation. This has motivated experimental and theoretical studies (MD with force-fields) that sometimes lead to contradictory conclusions. In this context, we propose to characterize structural, energetic and dynamic properties of asphaltene molecules and clusters in solution at the interface with water, at the molecular level. We aim at determining asphaltenes' propensity to aggregate at the water interface, and with which orientation. The influence of the monomer size and chemical nature (presence of alkyle side chains, heteroatoms) on these properties will be studied. This new project in our group is done in collaboration with V. Pauchard (experimentalist, Engineering Department, City College of New York). It is funded by the NSF for 5 years.

Dernières publications:

- V. Deguin, J. Mascetti, A. Simon, N. Ben Amor, C. Aupetit, S. Latournerie, J. Noble* 'Photochemistry of Fe :H2O Adducts in Argon Matrices : A Combined Experimental and Theoretical Study in the mid-IR and UV-Visible Regions" J. Phys. Chem. A 2018, 122, 529-542 - **doi:** pu.doi
- E. Michoulier, N. Ben Amor, Mathias Rapacioli, J. A. Noble, J. Mascetti, C. Toubin, A. Simon*, 'Theoretical determination of adsorption and ionisation energies of polycyclic aromatic hydrocarbons on water ice ', Phys. Chem. Chem. Phys. 2018, 20, 11941-11953 - **doi:** pu.doi

Design computationnel et conception « à façon » d'enzymes pour la synthèse chimio-enzymatique programmée d'oligosaccharides antigéniques

Projet démarré en 2016

LISBP - Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (UMR 5504/792)
Porteur de projet: **Isabelle Andre**
Ce projet vise à concevoir "sur mesure" des enzymes déployant de nouvelles spécificités vis-à-vis de substrats non naturels pouvant être utilisées en couplage avec la chimie pour synthétiser de façon efficace et contrôlée des molécules glucidiques complexes. Ce travail s'inscrit dans le cadre d'une longue collaboration avec l'Institut Pasteur et vise in fine à développer des procédés chimio-enzymatiques originaux de synthèse d'oligosides antigéniques représentatifs des sérotypes prévalents de S. flexneri pour le développement de vaccins contre la shigellose, une forme de dysenterie bacillaire. La conception " à façon" des enzymes ayant les activités requises s'appuiera fortement sur des techniques de modélisation moléculaire et du design computationnel de protéines qui a récemment fait ses preuves pour accélérer le développement d'enzymes capables de catalyser des réactions nouvelles, n'existant pas dans la nature. L'objectif sera ainsi d'adapter des glucane-saccharases de la famille 70 des Glycoside-Hydrolases, des enzymes de haut poids moléculaire (entre 120 et 180 kDa) utilisant des agro-ressources (saccharose) comme substrat donneur, à la glucosylation spécifique d'intermédiaires tétrasaccharidiques intervenant dans la synthèse des oligosaccharides antigéniques. La réaction de glucosylation est fortement dépendante de la reconnaissance enzyme/substrat et de tous les déterminants structuraux et dynamiques impliqués dans l'ensemble du processus conduisant à la réaction enzymatique. Dans le cadre de ce projet, il s'agira dans un premier temps d'approfondir nos connaissances sur les relations structure-dynamique-fonction des enzymes retenues de la famille GH70, jamais étudiées à ce jour par modélisation moléculaire. En particulier,

nous chercherons à décrire en détails les sites de liaison et le mode de reconnaissance des substrats donneur et accepteurs (naturels et non-naturels). Aussi, nous étudierons les réarrangements conformationnels, notamment la dynamique des boucles participant à la topologie du site actif, pouvant se produire au cours de la catalyse. Prenant appui sur ces résultats, nous explorerons ensuite le remodelage du site actif et des régions clés des enzymes d'intérêt afin de les adapter à la reconnaissance des intermédiaires tétrasaccharidiques cibles. Ceci sera réalisé à l'aide de méthodes computationnelles automatisées de design de protéines permettant d'optimiser la combinatoire de séquences et de conformations afin de proposer les séquences les plus prometteuses qui seront ensuite étudiées en détail par modélisation et dynamique moléculaire avant de les soumettre à l'évaluation expérimentale.

Dernières publications:

- Vergés A., Cambon E., Barbe S., Moulis C, Remaud-Siméon M., André I. 2017. Novel product specificity toward erlose and panose exhibited by multi-site engineered mutants of amylosucrase. Protein Sci. 26,566-77 -
- Vergés A., Cambon E., Barbe S., Moulis C., Remaud-Siméon M., André I. 2017. Isolation and characterization of an efficient mutant of Neisseria polysaccharea amylosucrase for the synthesis of controlled size maltooligosaccharides. Carbohydrate polymers 173, 403-411 -

MoMA: Molecular motion algorithms for highly-flexible biomolecules

Projet démarré en 2016

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)
Porteur de projet: **Juan Cortes**
Algorithms originating from robotics research have recently appeared as a complement or an alternative to classical methods to explore the conformational space of flexible bio-molecules. LAAS-CNRS is one of the pioneering labs in developing these novel approaches. These algorithms can be applied to small and middle-sized molecules (e.g. small peptides) using a single personal computer. However, analyzing large systems in reasonable computing time, while considering accurate models and full flexibility, requires parallelized implementations running on computer clusters. A few years ago we developed a distributed-memory implementation that we could successfully test on the MareNostrum supercomputer in Barcelona. We are now developing a more sophisticated parallelization strategy, combining shared memory and distributed memory operations, aiming at optimizing its performance using multi-core processors in current computer clusters. Preliminary tests in CALMIP (thanks to a "Test Project") have shown an excellent performance of this new implementation for proteins of different sizes. Our objective is to continue the development of these algorithms that will be applied to the study of intrinsically disordered proteins (IDPs) in the context of the PhD thesis of Alejandro Estaña, co-advised by Pau Bernadó (Centre de Biochimie Structurale, Montpellier).

Dernières publications:

- Alejandro Estaña, Kevin Molloy, Marc Vaisset, Nathalie Sibille, Thierry Siméon, Pau Bernadó, Juan Cortés. Hybrid parallelization of a multi-tree path search algorithm: Application to highly-flexible biomolecules. Parallel Computing, 77, pp.84-100. - **doi:** pu.doi **url:** pu.open_url

- Alejandro Estaña, Nathalie Sibille, Elise Delaforge, Marc Vaisset, Juan Cortés, Pau Bernadó. Realistic ensemble models of intrinsically disordered proteins using a structure-encoding coil database. Structure. In press. -

Molecular mechanism of glycoside-phosphorylases inferred by QM/MM metadynamics simulations

Projet démarré en 2016

LISBP - Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (UMR 5504/792)
Porteur de projet: **Isabelle Andre**
Ce projet, à l'interface entre les sciences du vivant et la chimie théorique, vise à développer et à mettre en œuvre des méthodes computationnelles hybrides, reposant sur l'utilisation conjointe de mécanique quantique et de métadynamique associées à de la dynamique moléculaire, pour appréhender à différents niveaux de détails la cascade d'évènements, y compris dynamiques, conduisant à la catalyse enzymatique. Il s'agira plus particulièrement de de mieux comprendre le mécanisme réactionnel de glycoside-hydrolases d'intérêt biotechnologique.

modélisation des alliages léger à base d'aluminium: couplage chimie/mécanique

Projet démarré en 2015

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)
Porteur de projet: **Alain Esteve**
In this project, our goal is to investigate, at the atomic scale, the coupling of chemistry with the mechanical properties of model-nanostructures. Two viewpoints will be considered in this study: (i) evaluation of the impact that a chemical modification can print on the mechanical properties of a system, and conversely, (ii) what could be the impact of mechanical strain on a chemical process. Our long-lasting experience on the basic mechanisms of oxidation of semiconductors as well as metallic surfaces will help us providing new insights into these chemical processes under mechanical strain. In particular, we will work on the hydrogenation of light alloy nanostructures to explore the relation of hydrogen chemistry with mechanical properties in terms of embrittlement, in relation with aeronautic applications. We will investigate in detail the interaction of hydrogen with light alloys, i.e. aluminum and its alloy derivatives including Cu, Zn or Mg-based aluminum alloys. More specifically, we will focus on the interaction of Hydrogen with defects such as vacancies, impurities, dislocations, and up to grain boundaries. Note that, in aeronautic applications, aluminum-based alloys are deemed cured in their mechanical strength, but at the expense of some of the fundamental and intrinsic properties of pure aluminum: resistance to corrosion and ductile behavior. The proposed fundamental study at the crossing of chemistry and mechanics will also have potential large societal impact, for instance in corrosion science as well as in pure metallurgy, well beyond aeronautics.

Solvants issus de la biomasse expansés par le CO2 : Étude des propriétés physicochimiques par dynamique moléculaire.

Projet démarré en 2015

LGC - Laboratoire de Génie Chimique (UMR 5503)
Porteur de projet: **Yaocihuatl Medina-Gonzalez**
CO2-expanded liquids (CXLs) are mixtures of a room-temperature organic liquid and a gas at high-pressure

or supercritical fluid. CXL's are a very promising group of innovative solvents since they present advantages such as: 1) a solvent power that is higher than their supercritical fluids counterpart, which is advantageous to dissolve catalysts and reactants; 2) CO2 can be used to tune the mixture's solvation power across a large polarity range, and 3) CXLs present a more convenient combination between chemical reaction and product separation. This project proposes to use molecular dynamics to study the physicochemical behavior of some members of different families of bio sourced solvents when expanded by CO2. In particular the renovation of the access to the super calculator will allow continuing the work started during 2016 by performing calculations on new CXL's in order to continue with the construction of the library of behaviors started last year; this project is part of Emanuel Granero PhD thesis. For that, we will perform molecular dynamics calculations on boxes containing between 1000 and 2000 molecules; the size of the boxes is chosen as to pertinently model a continuous phase and to be sure that the results will be representative of the entire phase. These calculations will be performed by using the open source code LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator). This method will allow calculating properties such as density, molecular packing fraction and other physicochemical and transport properties such as viscosity. It is expected that polarity and proticity of these mixtures decrease with pressure. Results obtained from molecular dynamics calculations will be compared with experimental results obtained by using a high-pressure view cell coupled to an UV-Vis spectrophotometer. Simulations performed during last year and by using this methodology are encouraging and allowed results with very good agreement with literature data.

Dernières publications:

- Molecular Dynamics Simulations of Gas-Expanded Liquids - **doi:** pu.doi

Atlas Anatomique de Primates

Projet démarré en 2014

AMIS - Anthropologie moléculaire et Imagerie de Synthèse

Porteur de projet: **Jean Dumoncel**

The « Imagery » research team of the AMIS laboratory uses anatomical data essentially obtained by CT, micro-CT, or by synchrotron imaging. Through innovative technologies as well as academic and industrial collaborations (notably in the areas of image processing and the acquisition of high resolution data), we can better characterize the variability of phenotypic traits in teeth and bones amongst past and present populations of primates. Indeed, variability studies represent a prerequisite for future developments investigating evolutionary processes. Even if geometric morphometric studies (based on landmarks only) have proved to be useful, there is a need for automated tools and reproducibility anatomical comparison. Methods based on deformable models are increasingly used in medicine and should be better implemented in biological investigations as ours. We use a program developed by Stanley Durrleman (INRIA Researcher, ICM, Brain and Spine Institute). It computes anatomical atlases based on deformation maps without landmarks. These statistical atlases are based on average templates and local deformations, and then used to classify anatomical data.

Dernières publications:

- C. Zanolli, L. Pan, J. Dumoncel, O. Kullmer, M. Kundrát, W. Liu, R. Macchiarelli, L. Mancini, F. Schrenk, C. Tuniz. Inner tooth morphology of Homo erectus from Zhoukoudian. New evidence from an old collection

housed at Uppsala University. Sweden, Journal of Human Evolution, Volume 116, March 2018, Pages 1-13, ISSN 0047-2484 - **doi:** pu.doi

- J. Dumoncel, G. Subsol, S. Durrleman, A. Oettlé, Z. Lockhat, F. E. Suleman, E. De Jager, A. Beaudet, 2018. A quantitative comparison of the brain and the inner surface of the cranium. 10th Symposium national de Morphométrie et Evolution des Formes, Bordeaux, France. -

Cartographie et étude des duplications segmentaires intra- et interchromosomiques

Projet démarré en 2014

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)

Porteur de projet: **Sylvain Cussat-blanc**

Segmental duplications (SDs) are DNA sequences of minimum 1kb and 95% identity between copies. They represent a key substrate for gene conversion, and an underestimated source of genomic diversity. However, few algorithm have been designed to extract efficiently SDs from complex genomes. In 2016, we have developed ASAGRT, a powerful algorithm searching for SDs in any genome properly assembled. We have compared ASGART performances in regard to the most similar algorithm existing in literature. Comparative performances performed on 5 model organisms showed that ASGART is systematically better than Last and than Mummer (in CPY time and memory used). However, if SD mapping is easy and fast at the intra-chromosomic level, it appears more complicated at inter-chromosomic level (ull genome). We now, need to go futher on SD's full genome acquisition, probably by modify ASGART and the alignment procedure. Once solved we will be able to address 2 fundamental biological questions: 1) the role played by SD on sex chromosomes as an alternative substrate for gene conversion and 2) the real duplicative scenario that affected the vertebrate genomes (exploring fish genomes).

Etude structurale de particules pré-ribosomiques eucaryotes par cryo-MET et analyse d'images

Projet démarré en 2014

LBME - Laboratoire de Biologie Moléculaire eucaryote (UMR 5099)

Porteur de projet: **Célia Plisson-Chastang**

Ribosomes are ubiquitous macromolecular machines ensuring the translation of mRNA into proteins. The synthesis of ribosomes is one of the major cellular activities, both from a quantitative and a qualitative point of view. Ribosomes are composed of a small and a large subunits, respectively termed 40S and 60S in eukaryotes. Assembly of those huge ribonucleoprotein complexes is a very complex and dynamic process, that requires more than 200 maturation factors interacting transiently with the forming particles. Ribosome biogenesis defects have recently been associated to an increasing list of human genetic diseases and cancers; understanding those diseases calls for a better knowledge of ribosome maturation pathways in human cells. Our group focuses on studying the mechanisms enabling the assembly of eukaryotic ribosomes, using both yeast and mammal cells as models. To do so, we notably use cryo-electron microscopy coupled to image analysis techniques to determine the 3D structures of pre-40S particles. Cryo-electron microscopy (cryo-EM) is a very powerful method that allows determination of the 3D structure of very large complexes. We have already made use of cryo-EM and image analysis on the computing facilities of CalMIP to solve the first 3D structure of a pre-40S particle purified from human cells, to 19 Å resolution. This work has given rise to a first scientific article, published in the journal Nucleic Acids Research. We have more recently acquired cryo-EM datasets of other pre-40S particles purified at various maturation steps, either from baker's yeast or human cells, that we are processing using CalMIP's computational facilities. The various 3D reconstructions that we have obtained, at 6-7 Å resolution allow us to propose the first

morphogenesis depiction of the assembly of the eukaryotic small ribosomal subunit. We now would like to process more images, and reach an atomic resolutions for the structures of these pre-ribosomal particles.

Dernières publications:

- Structure of a human pre-40S particle points to a role for RACK1 in the final steps of 18S rRNA processing Natacha Larburu; Christian Montellese; Marie-Francoise O'Donohue; Ulrike Kutay; Pierre-Emmanuel Gleizes; Celia Plisson-Chastang Nucleic Acids Research 2016 - **doi:** pu.doi **url:** pu.open_url

Développement de méthodes pour la conception assistée par ordinateur de protéines

Projet démarré en 2013

LISBP - Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (UMR 5504/792)
Porteur de projet: **Sophie Barbe**
Ce projet porte sur le développement et la validation de nouvelles méthodes algorithmiques afin de proposer de nouveaux outils de design computationnel de protéines (Computational Protein Design, CPD). Plus particulièrement, les travaux envisagés au cours de l'année 2018 visent à étendre nos méthodologies vers la résolution de problèmes de design multi-états et multi-objectifs ainsi qu'à combiner et intégrer dans le processus de design de la connaissance dérivée de l'apprentissage sur la masse de données sans cesse croissante de séquences et structures de protéines. Fondées sur une association de techniques algorithmiques développées en intelligence artificielle et en biologie structurale computationnelle, ces nouvelles méthodes devraient permettre de fournir des solutions uniques ou de petites librairies de mutants qui puissent être plus facilement et rapidement criblées au niveau expérimental tout en augmentant les chances de construire les protéines dotées des propriétés ciblées. Les méthodes développées seront validées sur un large nombre de systèmes protéiques représentatifs de différents problèmes de design des protéines. Exposer le problème scientifique, la situation de l'équipe par rapport au problème (résultats ou expérience déjà acquis dans le domaine, ou projet nouveau).

Dernières publications:

- Simoncini D, Zhang KYJ, Schiex T, Barbe S. (2018) A Structural Homology Approach for Computational Protein Design with Flexible Backbone. Bioinformatics. In press -
- Charpentier, A., Mignon, D., , S., Cortés, J., Schiex, T., Simonson, T., Allouche, D. (2018) Variable Neighborhood Search with CostFunction Networks to Solve Large Computational Protein Design Problems. Journal of Chemical Information and Modeling. In press -

Relations Structure-Dynamique-Fonction et Design de protéines d'intérêt biotechnologique

Projet démarré en 2012

LISBP - Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (UMR 5504/792)
Porteur de projet: **Sophie Barbe**
Pendant de nombreuses années, les relations entre la structure et l'activité des protéines ont été étudiées en négligeant complètement les aspects dynamiques du comportement moléculaire. Or, de plus en plus nombreux sont les travaux qui montrent que la flexibilité et les mouvements collectifs des (macro)molécules sont des composantes absolument essentielles des mécanismes d'interaction

moléculaire et de l'activité catalytique des enzymes. Il en résulte que la vision statique de la catalyse enzymatique est insuffisante pour rendre compte du comportement cinétique de nombreuses enzymes. Ce projet a donc pour objectif d'améliorer notre compréhension de l'impact de la dynamique sur la catalyse de systèmes enzymatiques très variés dont l'activité catalytique est susceptible d'être reliée à des réarrangements conformationnels importants : des enzymes actives sur des sucres (glycoside-hydrolases, hémicellulases), sur des lipides (lipases, fatty acyl synthases), des enzymes d'oxydo-reduction (aldehyde deshydrogenases), des enzymes de dépolymérisation (PLA-dépolymérases) Nous étudierons également l'impact de la dynamique sur les interactions protéine-protéine (JO/IN). L'étude de ces liens nécessite l'exploration de différents types de mouvements (macro)moléculaires pouvant couvrir de larges échelles temporelles et spatiales. Nous faisons appel à différentes techniques de dynamique moléculaire (classiques et dérivés) pour explorer cette hiérarchie de mouvements. Les résultats de ces simulations sont confrontés à des données expérimentales acquises au sein de l'équipe (ou à travers des collaborations) et visent ainsi à caractériser les facteurs structuraux et dynamiques impliqués dans l'activité, la spécificité et la sélectivité des protéines d'intérêt pour mieux comprendre différents processus biologiques. Sur la base de cette meilleure compréhension des relations structure-dynamique-activité des systèmes protéiques étudiés, nous proposons des régions ad hoc à remodeler pour adapter et optimiser les protéines vis à vis de propriétés recherchées.

Dernières publications:

- Allouche D., André I., Barbe S., Davies J., de Givry S., Katsirelos G ., O'Sullivan B., Prestwitch S., Schiex T. and Traoré S.. 2014. Computational Protein Design as an optimization Problem. Artificial Intelligence 212:59-79 (JCR = 2.566) -
- Faten Arab-Jaziri, Bastien Bissaro, Sophie Barbe, Olivier Saurel, Hélène Débat, Claire Dumon, Virginie Gervais, Alain Milon, Isabelle André, Régis Fauré and Michael J. O'Donohue. The functional roles of H98 and W99 and b2a2 loop dynamics in the a-L-arabinofuranosidase from Thermobacillus xylanilyticus. 2012. FEBS Journal, 279(19):3598-3611. -

Simulation à l'échelle atomique pour l'oncologie structurale:Criblage des mutations de l'oncoprotéine Ras

Projet démarré en 2012

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Marie Brut**

This request supports a long term collaboration with CRCT-INSERM which aims at proposing new strategies to target Ras oncoproteins, mutated in ~30% of all human tumors. Our team has a strong background in the treatment of biological issues, notably with enzymes as therapeutic targets. Our collaboration with CRCT to investigate some mechanisms involved in the regulation activity of Ras family proteins lead us to identify new mutations allowing to modulate NRas activity, mutations that we need to characterize on both structural and chemical sides. To this end, weuse both traditional tools from molecular simulation (DFT and Molecular Mechanics) and "lab-made" tools that allow original in silico experiments on biomolecules. We complement this strategy thanks to steered QM/MM calculations to understand the local chemistry induced by the mutations we have predicted. Our ultimate goal if to propose a new therapeutic strategy able to mimic the effect of such mutations.

Dernières publications:

- Water distribution within wild type N-ras protein and its oncogenic mutations at position 61 during unrestrained QM/MM molecular dynamics, Biophysical Journal Volume 115, Issue 8: 1417-1430 - **doi:** pu.doi **url:** pu.open_url
- Hybrid QM/MM vs pure MM molecular dynamics for evaluating water distribution within p21Nras and the resulting GTP electronic density - **doi:** pu.doi

Modélisation de complexes de métaux de transition. Optimisation de géométrie et structure électronique.

Projet démarré en 2012

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Jacques Bonvoisin**
The project concerns the modelization of a specific ruthenium complex. It is a mononuclear ruthenium complex with more than one hundred surrounding atoms which constitute the so-called ligands. In this project we would like to follow the electronic properties of this complex when we vary the oxidation state of the ruthenium atom. Modelization means geometry optimization as well as prediction of electronic properties. We would like to predict the IR and UV-Vis spectrum. The oxidation state of the ruthenium atom may vary from 2 to 4. We would like to study all the three oxidation states and follow on the UV-Vis spectrum in order to compare them with the experiments. The different forms of this complex will be studied by DFT in order to have a good understanding of the electronic and magnetic properties by using the resident GAUSSIAN program on CALMIP. We may also vary the ligands around the ruthenium atom in order to see the impact on the electronic properties and the UV-Vis spectrum. This system described here is a part of a bigger nuclearity complex which would have a potential interest in nanosystem device. I would like to use the CALMIP platform because the system under study cannot be modelized with our resource; the computed time would be too long. In Ru(III) form, the system has to be studied in UHF mode and it is very time consuming relative to the size of the system.

Dernières publications:

- "Spectral signature of a Ru(II, III, IV) complex: a combined experimental and theoretical investigation" J. Bonvoisin & I. Ciofini. Dalton Transactions (2013) 42, 7943-7951. - **doi:** pu.doi
- "Two-Dimensional Halogen-Bonded Self-Assembly of copper beta-diketonato Complexes" Fabien Silly, Christine Viala & Jacques Bonvoisin. J. Phys. Chem. C (2018) 122, 17143-17148 - **doi:** pu.doi

Spectroscopie in silico de systèmes biologiques et de phases liquides. Apport de la dynamique moléculaire classique et ab-initio.

Projet démarré en 2007

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)
Porteur de projet: **Franck Jolibois**
Understanding the structural, dynamic and spectroscopic properties of chemical systems in the liquid phase at different temperatures and / or at different pressures is a matter of fundamental importance both in biological, physical or chemical sciences. As part of the theoretical simulation of such systems , the accurate modeling of the interactions and a correct sampling of the configuration space is a prerequisite for calculating spectroscopic parameter . We propose to conduct ab initio molecular dynamics studies on three

liquid systems with a priori different properties: water (H2O) , ammonia (NH3) and nitromethane (CH3NO2). A DFT approach within periodic boundary conditions and using plane wave basis sets will be used for calculating the energy and gradients . The validation of our results will be performed by comparing two types of parameters to existing experimental data: the structure of the liquid obtained by calculating the radial distribution function and a spectroscopic signature with the theoretical determination of NMR chemical shielding. We intend, through this project, to establish a comprehensive and effective strategy for the precise modeling of liquid systems. For this, different parameters will be analyzed on the three aforesaid chemical systems : the inclusion of dispersion forces and exact exchange in DFT functional, the necessity to introduce nuclear quantum effects , the number of molecules explicitly used in the primitive box for the calculation of the energy, gradients and NMR parameters, the influence of isotope effects on the hydrogen atom and the influence of temperature. In parallel with this study, we also propose to exploite the capability of classical molecular dynamics to explore configurations space of large systems in order to investigate the structural properties of "bio-inspired" molecules (peptoids). These studies coupled with the calculations of specific spectrocopic properties (mainly NMR and Circular Dichroïsm) and their comparison to experimental spectra will allow the elucidation of their 3D structures.

Dernières publications:

- Exploring the Conformation of Mixed Cis–Trans α,β-Oligopeptoids: A Joint Experimental and Computational Study. G.Dumonteil, N.Bhattacharjee, G.Angelici, O.Roy, S.Faure, L.Jouffret, F.Jolibois, L Perrin, and C.Taillefumier, J.Org.Chem. (2018) 83, 6382–6396. -
- Evaluation of Gas to Liquid 17O and 1H Shift of Water: a Test Case for Molecular and Periodic Approaches. J.Cuny, F.Jolibois and I.C.Gerber J.Chem.Theo.Comp. (2018) 14, 4041–4051 -

Etude des propriétés structurales, spectroscopiques et dynamiques de Molécules et Agrégats

Projet démarré en 2000

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Fernand Spiegelman**

This project is a long-term project on the structural, spectroscopic, dynamical and thermodynamical properties of various complexes and clusters (molecular complexes, homogeneous clusters, atoms and molecules adsorbed or embedded on/in clusters). The methodology is based on the development of the Density Functional Tight Binding methods for a quantum description of the electronic structure and the combination with various simulation codes for on-the-fly classical or quantum molecular dynamics to derive structural and spectroscopic properties. The advantages of DFTB are: (i) DFTB efficiency evolution towards very large systems, (ii) combination with dynamics and global exploration methods to derive finite temperature properties, (iii) combination with Path-Integral Molecular dynamics. The current applications are: (i) structure, reactivity and thermodynamics of water clusters containing impurities for atmospheric chemistry, (ii) structure, spectroscopy (IR and electronic) and fragmentation dynamics of carbonaceaous complexes and PAH clusters (poly-aromatic hydrocarbons) displaying astrochemical interest.

Dernières publications:

- I. Braud, S. Zamith, J. Cuny, Z. Linjie, J.-M. L'Hermite, Size-Dependent Proton Localization in Hydrated Uracil Clusters : A Joint Experimental and Theoretical Study, J. Phys. Chem, 2018, soumise -

- A DFTB approach to ruthenium clusters and nanoparticles, C. Marti, F. Spiegelman, M. Rapacioli and J. Cuny, J. Chem. Phys, soumise -

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4.3 Sciences de l'Univers et de la Terre

Darwin

Projet démarré en 2018

EcoExMoulis - Station d'Ecologie Expérimentale (USR 2936)

Porteur de projet: **Jose Maria Montoya Teran**

Climate change is a global phenomenon whose effects pervade all biomes, from the tropics to the poles. Different biomes, however, are affected at different rates of change, and the characteristics of the local ecosystems, in particular species interactions, can ameliorate or exacerbate the ecological consequences of climate change. Thus, one of the greatest challenges of this project is to investigate how local differences in both the environmental stressors and biotic interactions modulate the effects of climate change. Marine phytoplankton play a critical role in marine food web, global biogeochemical cycles and climate processes, making them important indicators for ecosystem state under climate change. Thus, we use a global ecosystem model combined with ocean circulation model to gain mechanistic insights into how changes in species interactions modify global distribution patterns of plankton species across spatial scales and how future climate change affects the marine ecosystems worldwide.

Modélisation des jets zonaux dans les océans équatoriaux

Projet démarré en 2018

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)

Porteur de projet: **Yves Morel**

The request for opening a project at CALMIP for our study is motivated by the need to implement high resolution ocean basin scale simulations using the CROCO (Coastal and Regional Ocean Com munity Model) numercial model. This model solves the primitive equations from small scale fluid mechanics to geophysical flows. It is developed by a consortium of French laboratories, including LEGOS and LA in Toulouse. This model is capable of modeling all scales of fluid mechanics (from turbulence to global circulation of the ocean). It is parallelized and optimized for multiprocessor computing. Our project is a process study related to equatorial ocean circulation. The aim is to identify the mechanisms involved in the creation of deep jets recently observed in the ocean circulation of the tropical / equatorial band. Our goal is to test various configurations, forcings and parameters of a simplified ocean model to understand the origin of these jets, which are currently not properly described in realistic models of the ocean.

Le silure glane (Silurus glanis L.) : connaissances et estimation des stocks dans le bassin de la Garonne-Dordogne

Projet démarré en 2018

ECOLAB - Laboratoire d'écologie fonctionnelle (UMR 5245)

Porteur de projet: **Ivan Paz Vinas**

Cette étude concerne le Silure glane (Silurus glanis) une espèce de poisson introduite dans le bassin de la Garonne-Dordogne il y a environ 35 ans, et qui y a proliféré depuis. L'objectif de ce projet est d'évaluer le stock de silures dans ce bassin, afin d'obtenir des informations concernant le fonctionnement de ses populations. Pour cela, nous avons déterminé au préalable les niveaux de diversité et structuration génétiques de ces populations à l'aide de marqueurs microsatellites. Nous avons ensuite analysé ces données avec des méthodes classiques d'estimation de tailles efficaces des populations. Bien que ces premiers résultats soient encourageants, ils reposent sur des hypothèses initiales très restrictives (populations considérées à l'équilibre, absence de flux de gènes provenant d'autres populations...), et sont potentiellement biaisées par la structure particulière de l'écosystème (réseau dendritique). Afin d'obtenir des estimations précises, nous envisageons une approche basée sur la comparaison de (i) données génétiques simulées sous des modèles de génétique des populations qui "mimeraient" la structure spatiale du bassin Garonne-Dordogne, et (ii) les données génétiques observées. Cette comparaison ce fera au travers des procédures de type "calcul Bayésien approché" couplées à des méthodes d'apprentissage automatique (forêts aléatoires). Ce projet test nous permettra d'adapter à cette problématique un "pipeline" de programmes qui permet à la fois de simuler des jeux de données génétiques et de calculer des statistiques descriptives pour chaque simulation. Ce pipeline est composé de plusieurs programmes académiques non parallèles, et a déjà été utilisé sur Eos dans le cadre du projet p1003 (2010-2015, voir rapports d'activité passés et Paz-Vinas et al 2015 Mol Ecol 24:4586-4604 pour plus de détails sur le pipeline). En fonction des résultats obtenus, nous effectuerons une demande plus conséquente lors du prochain appel d'offres. Cordialement,

General ecosystem models under climate change scenarios and their consequences for species interactions, ecosystem productivity and stability

Projet démarré en 2018

EcoExMoulis - Station d'Ecologie Expérimentale (USR 2936)

Porteur de projet: **Jose Maria Montoya Teran**

Description Environmental change affects ecosystems across spatial scales. Ongoing climate change, in particular, is a global phenomenon whose effects pervade all biomes, from the tropics to the poles. Different biomes, however, are affected at different rates of change, and the characteristics of the local ecosystems, in particular species interactions, can ameliorate or exacerbate the ecological consequences of climate change. Thus, one of the greatest challenges of biodiversity and climate change research is to develop global models of biodiversity change that allow for local differences in both the stressors (e.g., mean temperature, temperature variability) and local processes (e.g., biotic interactions) that modulate the effects of environmental change. The general objective of this project is twofold: (1) to gain mechanistic insights into how changes in species interactions (e.g., via changes in specialization) modify species distribution patterns across spatial scales, and ultimately how they affect diversity-productivity and diversity-stability relationships; (2) to forecast climate change effects on ecosystems worldwide using a suite of warming scenarios. For this project, we use the DARWIN model that simulates the physical conditions of the global ocean coupled with the ecological traits of species from different trophic levels. Climate change scenario 1) "control" run : the pre-industrial fields for 240 years --- this is so we can keep track of the drift. 2) "all" run : The temperature, circulation, mixing, and sea ice fields change as projected by the Earth system model from 1860 to 2100. 3) "direct" run : The temperature fields that affect biological rates change from 1860 to 2100, but the circulation, mixing, and sea-ice fields remain as for pre-industrial conditions. 4) "indirect" run : Temperature fields remain as for pre-industrial conditions, but the circulation,

mixing, and sea-ice fields change from 1860 to 2100 conditions. Model setup for climate change scenario deltaT :3 min longitude : 2 degree latitude : 2.5 degree depth : 23 levels offlineForccingPeriod: 1 month deltaToffline : 4 min language: Fortran and C compiler: gfortran and gcc application: MPI, python(to combine them into one slice), netcdf

Infrarouge Thermique

Projet démarré en 2018

CESBIO - Centre d'Etudes Spatiales de la BIOsphère (UMR 5126)

Porteur de projet: **Ahmad Al Bitar**

Dans le cadre du Projet ESA_ITT_TIR pour l'agence spatiale Européenne (ESA) Nous effectuons des calcules intensifs pour simuler la reflectance et la radiance des surfaces terrestres en 3D. L'objectif étant de mettre à disposition de la communauté scientifique des bases de données simulant les différentes configurations d'une futur mission en Infra-rouge thermique. Ainsi nous considérons des objets 3D dans une scènes simulant du Mais, du Blés, des citronnier et des environnements urbains avec des détails centimétriques et une multitude de configuration: stage de développement des plantes, direction du soleil, direction de vue, températures de la végétation et du sol, type du sols...Ainsi une centaines de millier de simulation sont à prévoir. --Logiciel: DART (Discrete Anisotropic Radiative Transfer Model) http://www.cesbio.ups-tlse.fr/dart/#/ (Licence distribuée par l'Université Paul Sabatier) --Bibliothèques: ---------- - libc 2.15+ (ainsi que libm, libpthread, librt et libdl à la même version) - zlibc -> bibliothèque C de compression, base du "zip". - OpenGL 1.2+ -> Pour l'importation des objets 3D au format .obj. - bash - xvfb et nohup (ou équivalent, pour le lancement à distance sans interface graphique) --logiciel académique (développé au CESBIO) --logiciel multi-thread

Modélisation de la dynamique et de la chimie atmosphérique à mésoéchelle : chimie en phases gazeuse, aqueuse et aérosols

Projet démarré en 2018

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Céline Mari**

This project aims at understanding the dynamical and chemical processes which control the atmospheric composition and air quality over the southern West Africa (FP7 DACCIWA) and south east Asia (ANR TTL-Xing). The DACCIWA airborne field campaign took place in June-July 2016, the aircraft campaign was deployed with three aircrafts covering Benin, Togo, Ghana and south-east of Ivory Coast. Scientific flights were dedicated to the quantification of city emissions from Lome, Accra, Abidjan, Cotonou and Kumasi, characterization of power plant emissions, oil and gas flaring, shipping emissions. The campaign produced an unique dataset to quantify the current pollution sources and dispersion over the coastal belt of southern West Africa. The Meso-NH model will be run in its LES configuration (around 100 m resolution) which explicitly resolves the convective boundary layer. The simulations will be performed including the gas and aerosol species with sensitivity tests to assess the impact of anthropogenic and natural sources on the pollution levels sampled on board the aircraft platforms. The french ANR TTL-Xing project is devoted to the study of the impact of monsoon convection on the composition of the UTLS and on the formation of the Asian Tropopause Aerosol Layer (ATAL). High resolution simulations with the Meso-NH cloud resolving model in the Asian monsoon region will be performed to explicitly represent convective clouds and associated processes (scavenging of particles, aerosol-cloud interactions and in-cloud chemistry). Simulations with passive tracers mimicking emissions from the different Asian regions will provide

information about the transport processes (fast convective uplift versus slow diabatic heating) and about the origin of the pollutants.The high resolution Meso-NH simulations will be performed for case studies observed during the StratoClim 2017 monsoon campaign.

Dernières publications:

- Brosse, F ; Leriche, M ; Mari, C ; Couvreux, F., LES study of the impact of moist thermals on the oxidative capacity of the atmosphere in southern West Africa, ACP, doi :10.5194/acp-18-6601-2018, 2018 - **doi:** pu.doi

Non-hydrostatic modelling investigations over the strait of Gibraltar

Projet démarré en 2018

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Laurent Roblou**

The Mediterranean Sea is a semi-enclosed basin featuring an active thermohaline circulation that is maintained by the atmospheric forcing and regulated by the Strait of Gibraltar. Briefly, over the Mediterranean Sea, the ocean-atmosphere fluxes are balanced by the exchange flow that takes place within the strait of Gibraltar. Within the strait, the ocean circulation features a two-way exchange, directly influenced by the interaction between the intense tidal forcing and the complex geometry of the strait, through the mixing mechanism due to internal tides and a hydraulic control. Some aspects of the strait hydrodynamics could not be well reproduced by standard numerical model. This especially concerns the evolution of the internal tidal bore generated in the main sill area. After its generation, the bore progresses toward the Mediterranean, evolving into a series of short internal solitary waves of large amplitude. These waves are strongly nonlinear and nonhydrostatic, thus their modeling requires fully nonhydrostatic codes such as the new-generation ocean modelling system CROCO (https://www.croco-ocean.org/) from the Coastal and Regional Ocean Community (CROCO). Thus, the main goal of this proposal is the investigation of several open questions on the hydraulic behavior of the strait of Gibraltar applying the nonhydrostatic assumption, AGRIF grid refinement and new monotonic implicit large eddy simulations (MILES) parameterizations. Specifically, the evaluation of the impact of these novel features on the internal solitary waves forced by the tides in the strait of Gibraltar is one of the scopes of this proposal. In this framework, the project team is applying for 130 000 hours of computing time and associated data storage on the CALMIP platform.

Gravity field and tidal deformations of small bodies of the solar system

Projet démarré en 2018

ISAE/DEOS - Département Electronique, optronique et signal

Porteur de projet: **Raphael Garcia**

As elementary bricks of planets, asteroids are a special target of interest for scientists in order to grasp a better understanding of the early Solar system formation and therefore determining the internal structure of planets and small bodies. Several space missions with asteroids as their main goal have already been launched and more are planned to follow suit. Therefore there is a real need to improve our models of asteroids for the smooth progress and planning of these missions. For this project, we choose to focus on the gravity field and seismic measurements among the available observables for asteroids: the gravity field

having already been measured and being essential for missions getting closer to asteroids, and seismic measurements as it is one of the most efficient ways to determine the internal structure of celestial bodies. The aim of this project is to determine the global gravity field of any asteroid, their tidal deformations and potential sources of seismic waves. Especially, we study the tidal forces exerted upon an asteroid so that tidal displacements, and thus tidal stress, can be calculated. This gives us information about the stress state of the asteroid and if material failure is likely to happen, which would mean tidal quakes happening and thus allowing passive seismology at the surface of these bodies. Because of the highly diverse shapes and internal structure of asteroids, standard methods used on almost spherical bodies cannot be applied here, and specific numerical methods are required. This project will use and expand the library FreeFEM++ for solving gravity field and tidal deformations of small objects of the solar system.

SenSAgri

Projet démarré en 2018

CESBIO - Centre d'Etudes Spatiales de la BIOsphère (UMR 5126)

Porteur de projet: **Eric Ceschia**

Our team is part of the Sentinels Synergy for Agriculture (SenSAgri) project that is financed by the European Commission. The goal of this project is to develop an innovative portfolio of prototypes agricultural monitoring services. In this project, our team focuses on the construction of dynamic crop maps of the land usage updated regularly over the agricultural season. Those maps are created from the Sentinel satellite image series and in-situ field data by using supervised classification algorithms. One of our main goals is to be able to construct those maps as soon as possible during the agricultural season [1]. The new satellite images acquired by Sentinel mission initiate a new area in Earth Observation. As main novelty, Sentinel mission provides systematic global acquisitions of high-resolution multi-spectral and radar imagery with a high revisit frequency, [2]. The use of both radar and optical data in synergy is the main motivation of the SensAgri project. The complementarity of both sources of information allows accurate land cover discrimination. Therefore, the generation of accurate maps is possible thanks to this huge amount of information. However, the processing of these large data volumes requires an important number of computational resources. The first classification experiments of Sentinel images times series have been performed by using a processing chain prototype, which has been developed at CESBIO. The main programs are developed in C++ and they are interfaced with Python. Thus far, this chain has been successfully tested for three satellite tiles (110km x 110km each) on the CESBIO server named s2calc. The first results have been very promising and our goal is now to evaluate the proposed methodology on a large scale. Specifically, in the framework of SenSAgri project, we would like to test the algorithms on a surface of 35 satellite tiles covering the diversity of the European landscapes . To make this deployment we would like to use CALMIP's services.

Orogen

Projet démarré en 2018

GET - Géosciences Environnement Toulouse (UMR 5563)

Porteur de projet: **Frederic Mouthereau**

One of the most important question regarding the evolution of the continental lithosphere is why and how shear zones and faults localizes ? Although, conceptual models try to explain relationships between inheritance (pre-orogenic structure, lithology and rheology) and mountain belt structures it is still widely unknown from a physical point of view. With this project we want to investigate how rifted margins

influence the orogens structure ? Or more precisely, how along strike variations in the maturity of passive margins control the thermal regime in the collision from initial stage of the inversion as well as the final structure of orogens? The study will be performed using pTatin2d, a parallel implementation of the finite element method, which employs an Arbitrary Lagrangian Eulerian discretization, together with the material point method in order to resolve the Stokes equation for incrompressible fluids with non-linear viscosity. The conservation of momentum and mass are coupled with the heat conservation equation. We also use simple diffusive erosion sedimentation law which captures the age of sedimentation and account for the rheology and the heat production of sediments.

Modélisation numérique directe du mélange de traceurs océaniques

Projet démarré en 2017

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)
Porteur de projet: **Yves Morel**
The general context of the project is the TEASAO IDEX project which aims at the preparation of the next generation of prediction systems for both the atmosphere and the ocean. A major scientific challenge to do so is to improve understanding and modelling of the effect of small-scale turbulence and vertical mixing on the evolution of chemical or biological species in both the ocean and the atmosphere and its integrated effect at larger scales. This has strong relevance for societal problems such as fresh water resources, air or water quality, pollution development and spreading, primary ocean production (plankton) and fisheries. Many of the outstanding scientific questions in this area are common to both ocean and atmosphere and the rationale for the TEASAO project is that there is much to be gained by the atmosphere and ocean scientific communities in Toulouse from exploiting this commonality. The project is based on the long-term visit of Professor Peter Haynes, from University of Cambridge (UK), who is an international expert on the dynamics of atmosphere and ocean and on the transport and mixing of trace species, including reacting chemical and biological species. The project is built with an original combination of theoretical to applied studies. One scientific goal of the TEASAO project is thus to build a common framework to address the theoretical aspects of the evolution of active tracers in turbulent stratified flows, in particular the evolution of their distribution along density classes. Data and more realistic applications will be provided by specific studies for the ocean (plankton growth in along an upwelling front) and for the atmosphere (the interaction between turbulence, mixing and microphysics on different scales in the tropical tropopause layer). The global expected fallouts for Toulouse are cohesion and visibility, on a subject at the frontier of the present scientific concerns, and the preparation of the next generation operational systems for both the atmosphere and the ocean. The TEASAO project will also benefit the local higher education programs and several actions are planned with this perspective.

Characterizing stellar parameters from high resolution spectra of cold stars/ young

Projet démarré en 2017

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)
Porteur de projet: **Jean-François Donati**
Having well constrained stellar parameters is essential for deducing the properties of planets and magnetic field from radial velocity and polarimetric data. Stellar parameters for F-G-K stars can be directly estimated by comparing observations to a stellar spectral library with a reliable estimation tool. But for M dwarfs, existing stellar spectral libraries struggle to account for observed molecular lines accurately. We propose to create a high resolution spectral library in the optical and infrared range with PHOENIX model atmospheres

code (Allard et al. 2011ASPC-448-91A) that can precisely compute molecular lines. The chosen grid of stellar parameters will be as follow: dTeff =25K, dlog g = 0.05, d[M/H] =0.05, ranging between: Teff =[2500-4000]K, log g=[4.0-5.5], [M/H]= [-1 – 1] and will be made available to the community. This spectral library used along with Bayesian estimation tools will accurately characterize stellar parameters of the main sequence (MS) low-mass stars of masses 0.1-0.5 solar mass and later on the parameters of the pre-main sequence (PMS) stars of masses 0.3-1 solar mass. This work is an essential step in the preparation of the scientific exploitation of the new high-resolution near-IR velocimeter and polarimeter SPIRou which will be installed on the Canada-France-Hawaii-Telescope (CFHT) in 2017.

Dernières publications:

- SF2A-2017: Proceedings of the Annual meeting of the French Society of Astronomy and Astrophysics - **url:** pu.open_url

Eddy fluxes in the Atlantic Ocean: role of air-sea interactions

Projet démarré en 2017

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)
Porteur de projet: **Serena Illig**
Project 17016 is a high-resolution regional modeling project for the study of turbulent flows in the Atlantic Ocean and their roles on the atmospheric boundary layer on the one hand and on the oceanic biogeochemical properties on the other hand. Model experimentation will be carried out, both in idealized conditions and in more realistic conditions. Four areas in the Atlantic sector in which large meso-and submeso- scale activities are reported have been identified, namely, the Benguela upwelling system, the Agulhas current area, the Iberian Peninsula and the Gulf of Mexico. An inter-comparative approach should not only transpose tools and study methods into different ecosystems but also better understand the specificities of each system in relation to the fine scale processes that control the ocean mean state and ecosystem conditions. This project takes advantage of developments in coupled modeling (hydrodynamic, biogeochemical and atmospheric) carried out by the SYSCO2 team (LEGOS) within CALMIP P1044 (PI. B. Dewitte) and P1134 (PI. I. Dadou) projects. It is based on the use of three community models: the ROMS-CROCO hydrodynamic model, the WRF atmospheric model and the BioEBUS biogeochemical model. The coupling between oceanic and atmospheric codes is carried out thanks to the OASIS3-MCT coupler developed at CERFACS. Our need for the first semester of 2017 are estimated to 200 000h, and will concern the development of two complementary sub-projects dedicated to the study of turbulent flows in the Iberian Peninsula and in the Gulf of Mexico.

TROLL

Projet démarré en 2017

EDB - Évolution et Diversité Biologique (UMR 5174)
Porteur de projet: **Jerome Chave**
We have developed an individual-based forest growth simulator to model the dynamics of carbon in a tropical forest ecosystem but also to jointly monitor its biodiversity. This model TROLL, offers unique potentialities to constrain global dynamic vegetation models, that are now commonly coupled with climate models in Earth System Models. We have assembled a long-term knowledge of tropical forests of French

Guiana and aim to implement this strategy as part of the activities of Labex CEBA. Specifically, we propose to (1) improve TROLL by including the carbon, water, and nutrient balances, and including a species-level parameterization of the main plant-level processes for the tropical forest of French Guiana; (2) mobilize high-resolution remote-sensing data (aerial LiDAR scanning) to inform plant allometry and canopy structural properties, as well as topographical features; (3) mobilize forest dynamic data to validate the model, implement a forest management module and a forest fire module; (4) as a exercise of the model's scaling properties, scale-up the simulations to the entire area of French Guiana (c.a. 84,000 km2) making use of recent progress in our understanding of tree species distribution and ecological processes at this scale; (5) provide scenarios to assess the impacts of land use change, forest management and climatic change on selected forest types of French Guiana. The findings of this project should have an impact beyond French Guiana, in other Neotropical forests. It should also provide to the scientific community of Labex CEBA a modeling tool to assimilate information from several research lines (forest ecology, remote sensing, climate science, socio-economics), and suggest optimal development paths for the coastal forests for regional policy and local managers of natural areas, who are faced with practical challenge of maintaining wood production while protecting biodiversity and carbon stocks.

Dernières publications:

- Maréchaux, I., & Chave, J. (2017). An individual-based forest model to jointly simulate carbon and tree diversity in Amazonia: description and applications. Ecological Monographs. -

Signatures observationnelles de la migration planétaire dans les poussières des disques protoplanétaires

Projet démarré en 2016

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Clément Baruteau**

Planets form in a protoplanetary disc of gas and dust surrounding young stars. The gravitational interaction between planets and the gas component of their protoplanetary disc can decrease or increase the distance between planets and their star, at a pace that depends on the planet mass and the physical properties of the disc (density, temperature etc.). This is known as planetary migration. It plays a prominent role in our understanding of the orbital properties of extrasolar planets, and of the observations of protoplanetary discs, for which the extremely diverse gas and dust distributions (spirals, rings, lopsided asymmetries etc.) are often interpreted as signatures of planets buried in the discs. However, contrary to the gas component of protoplanetary discs, planet-disc interactions in the dust remain largely unknown. In particular, the implications of planetary migration on the spatial distribution of the dust in protoplanetary discs have never been investigated. This is the scope of this application for CalMip computing time. In this project, I will carry out hydrodynamical simulations modelling both the gas and dust components of a protoplanetary disc where a planet forms. Numerical simulations will make use of the public hydrodynamical code Fargo to which I have recently implemented a dust particle integrator (tested, validated and published). The planet's mass and the disc's physical properties will be varied to explore various regimes of planetary migration. Their impact on the distribution of dust grains of various sizes will be examined. Inclusion of several planets is also anticipated in this project. The results of simulations will be used to produce synthetic images of the dust continuum emission as it would be observed via interferometric imaging (like with the ALMA telescope).

Dernières publications:

- Fuente, Baruteau, Neri, Carmona, Agúndez, Goicoechea, Bachiller, Cernicharo & Berné, "Probing the cold dust emission in the AB Aur disk: A dust trap in a decaying vortex?", 2017, ApJ Letters, 846, L3-8 -
- Ataiee, Baruteau, Alibert & Benz 2018, "How much does turbulence change the pebble isolation mass for planet formation?", 2018, A&A, 615, 110-120 -

Modèles 3D de transport de flux magnétique solaire et assimilation de données

Projet démarré en 2016

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)
Porteur de projet: **Laurène Jouve**
This project aims at building a 3D numerical model of the generation and evolution of the magnetic field in the solar interior and then assimilating observational data into this model. The first part of the project was dedicated to solving the mean-field induction equation in a 3D model of the solar convection zone in spherical geometry. In these types of mean-field and kinematic models, the velocity field (differential rotation, meridional circulation and convective flows) is prescribed. We thus also need to provide an algorithm which will enable the magnetic flux produced in the interior to be buoyantly transported towards the surface to produce spots. To do so, the open source MAGIC code was modified by the postdoc fellow R. Kumar and myself and a link to solar wind models developed in IRAP was established. A paper was submitted in October 2017 to « Frontiers in Space Sciences » on this topic. Thanks to session 2017B, a thorough parametric study was started but we need to investigate more the role of the meridional circulation in such models since it turns out to have a crucial role in the cycle period for example. The second part of the project consists in incorporating observational data into models via modern techniques of data assimilation. We started a first step which consists in regularly introducing into the model the magnetic field observed at solar minimum. The next step is to perform real data assimilation. These methods have been used in meteorology on Earth for decades now and allow one to combine physical models and observational data in order to obtain predictive models and thus forecasts of future states of the system. First attempts have been made to apply similar techniques to solar physics (Jouve et al. 2011, Dikpati et al. 2014, Chung et al. 2015, 2017). Observations coming from the Hinode or SDO satellites of photospheric motions, of sunspots characteristics and of the behaviour of the global magnetic field will be assimilated (via a sequential assimilation technique) in the kinematic 3D model developed in the first part of the project. The goal is to characterize the predictive skills of such models and produce forecasts of the future solar activity.

Dernières publications:

- Kumar, Jouve, Pinto & Rouillard, Frontiers in Space Sciences, submitted -

Magnetisme des amas (MAMAS)

Projet démarré en 2016

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)
Porteur de projet: **Francois Rincon**
This project aims at investigating the effects of convective fluid instabilities such as the magnetothermal (MTI) and heat flux buoyancy driven (HBI) instabilities in galaxy clusters. These instabilities are thought to contribute to the magnetisation of the intracluster medium (ICM) and extragalactic plasmas, and may also

provide a significant non-thermal pressure support to the ICM, with potentially important implications for cosmological studies relying on clusters. As a first step, in 2016 we developed new functionalities in the MHD code SNOOPY, in order to be able to perform high-resolution simulations including the effects of anisotropic heat conduction and Braginskii viscosity on the stability of stratified magnetised plasmas. We also performed a preliminary scan of parameter space for 3D simulations. We now plan to extend these simulations to higher resolution in order to assess the effects of dissipative processes on the MTI and HBI, to characterise carefully how they may affect heat transport and induce magnetic field in clusters, and to quantify the pressure support associated with the subsequent turbulence, with the goal of improving phenomenological dynamical and thermodynamical models of galaxy clusters.

Portage du modèle hydrologique MGB et apport combiné précipitation/altimétrie satellitaires pour la modélisation fluviale

Projet démarré en 2015

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)
Porteur de projet: **Sylvain Biancamaria**
Tropical river basins are among the biggest ones. However, their hydrological cycle and especially the precipitation and their runoff are not well known because of lack of in-situ measurements. Satellite measurements have therefore an important role to play to have a more accurate estimate of the basin hydrological state and variability. The Global Precipitation Measurement (GPM) constellation of satellites (and especially the CNES/ISRO Megha-Tropiques satellite) brings a valuable forcing to hydrological model which is used to compute distributed river discharge and surface water elevation and extent. Future NASA/CNES/CSA/UKSA wide swath altimeter Surface Water and Ocean Topography (SWOT) will provide 2D maps of continental water bodies surface elevations which could be used to correct hydrological model parameters and outputs. The purpose of this project is therefore to combine GPM and SWOT data to get a better estimate of river discharge variability, through a focus on the Amazon and Niger Rivers. The first step will be to study and quantify satellite rainfall uncertainty propagation into hydrological modeling. Then, the second step will be to assimilate virtual SWOT data to decrease error on discharge resulting from satellite rainfall estimate errors. Two hydrological models will be used: ISBA-TRIP (developed at CNRM, Toulouse) and MGB (developed in Brazil). The project is led by GET and LEGOS, with some contributions from IPH (Brazil), CNRM (Toulouse), CERFACS (Toulouse), ABN (Niger). The purpose of this project is to port hydrological models to CALMIP supercomputer, generate precipitation ensembles, model output ensembles and finally assimilate virtual SWOT data through ensemble method (Ensemble Kalman Filter).

Modélisation des environnements ionisés

Projet démarré en 2015

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)
Porteur de projet: **Pierre-louis Blelly**
The Magnetosphere / Ionosphere / Thermosphere (MIT) system plays a critical role in the Sun-Earth connections and it is a key element in Space Weather. The couplings between the three different subsystems are a complex mix of fluid / kinetic transport, chemistry and electrodynamics with charged particles trapped in the background magnetic field and the three regions are so deeply intricated that deconvoluting the various interactions is a tough challenge in view of developping any service dedicated to Space weather. The project aims to focus on some aspects of these couplings. Especially, we wish to study the interactions within the plasmasphere, which is the inner part of the magnetosphere. For that, we have

developped a time dependent numerical model which is able to solve the interhemispheric dynamics of the ionospheric plasma along convecting magnetic field lines inside the plasmasphere. This code has been parallelized so that we can follow a large number of flux tubes at different locations (~2000) and thus we can reconstruct the 3D motion of the ionospheric plasma. Such an approach is rather innovative in the sense that this model has a high resolution along the magnetic field line and accounts for a large number of processes controlling the lower part of the ionosphere. We are interested in the steady state equilibrium of the plasmasphere that could arises from such a convecting model because it provides background conditions for the inner magnetosphere stability. For that, we want to model the plasmasphere for different solar illumination cases : solstice, equinox, high solar activity, low solar activity, ... and follow the dynamics of the plasma between the two hemispheres with a focus on the magnetic equatorial plane.

Dernières publications:

- D. Sarria, F. Lebrun, P.-L. Blelly, R. Chipaux, P. Laurent, J.-A. Sauvaud, L. Prech, P. Devoto, D. Pailot, J.-P. Baronick et M. Lindsey-Clark, Taranis XGRE and IDEE detection capability of terrestrial gamma-ray flashes and associated electron beams. Geoscientific Instrumentation, Methods and Data Systems, 6(2):239–256, 2017 - **doi:** pu.doi
- Marchaudon, A., P.-L., Blelly, M., Grandin, A., Aikio, A., Kozlovsky, and I. Virtanen, IPIM Modeling of the Ionospheric F2 Layer Depletion at High Latitudes During a High-Speed Stream Event, J. Geophys. Res., 123, doi:10.1029/2018JA025744, 2018. - **doi:** pu.doi

Assombrissement gravitationnel des étoiles à enveloppe convective

Projet démarré en 2015

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)
Porteur de projet: **Michel Rieutord**
This project focuses on the problem of gravitational darkening of rapidly rotating stars with an outer convective envelope. For this, we shall examine the dependence of the convective flux on latitude for a set of simplified models made of a rotating spherical layer heated from below. We use direct numerical simulations of this set-up with the code MAGIC that solves the hydrodynamic equations with a pseudo-spectral method based on Chebyshev polynomials and spherical harmonics. The point is to explore the range of parameters reachable with a DNS and then devise models that can be applied to the extreme (in terms of numbers) case of stars.

Dernières publications:

- Raynaud R., Rieutord M., Petitdemange L., Gastine T. and Putigny B. (2017), "Gravity darkening in late-type stars. I Coriolis effect", in Astron. & Astrophys. vol. 609, A124 - **doi:** pu.doi

Structure et dynamique du vent solaire lent

Projet démarré en 2015

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)
Porteur de projet: **Alexis Rouillard**
This project addresses the outstanding problem of the origin of strongly twisted magnetic flux-tubes

detected by spacecraft in the slow solar wind streams. These are coherent structures extend, in principle, from the lower layers of the solar atmosphere up the the interplanetary space. Their origin remains illusive, at present date, even though a few competing hypothesis have been proposed. These rely on magneto-hydrodynamical processes whose effects have not yet been properly quantified and confronted with observations. Beyond the problem of their origin, the actual dynamics of these magnetic structures are still misunderstood (e.g, are these transient Alfven-like wavefronts or large-scale quasi-stationnary structures?). This is a key issue for the Space Weather activities, as the dynamics of these magnetic structures affects the way solar surface perturbations are propagated up to the Earth environment. This proposal relies on a well-tested 3D MHD numerical setup tailored for the purpose and based on the PLUTO code (with excellent MPI scaling and perfectly adapted to massively parallel computing environments) and on PIC simulations using the code SMILEI.

Dernières publications:

- Pinto, Bemporad, Arge, Solar wind structure in the corona : new insights from models and coronography, [Astrophysical Journal], soumis -
- Pinto, Rouillard, Tao, Real-time computation and forecast of solar wind from Sun to Earth, [Journal of Space Weather], soumis -

Analyse des impacts hydro-sédimentaires et morphologiques afférents à l\'installation de dispositifs houlomoteurs sur des ouvrages portuaires et litto

Projet démarré en 2014

IMFT - Institut de Mécanique des Fluides de Toulouse (UMR 5502)
Porteur de projet: **Dominique Astruc**
Improving research in renewables energies is crucial to face current climate evolutions and cater for the increasing needs in energy. Coastal and harbour structures are suitable sites for wave energy converters installation: first, they are ideally situated to collect wave energy and second, wave energy devices could possibly help to provide protection of the inlands from overtopping. Since the first attempts to represent OWC hydrodynamics, much progress has been made to calculate the hydrodynamic efficiency of the device, both in analytical and numerical ways. Until very recently, potential wave theory was favoured. Accounting for rotational and viscous effects, combined Direct Numerical Simulation with level-set and immersed boundary methods showed better agreement with experimental results. The aim of the present projetc is to assess the effects of OWC systems on sediment transport and bed morphology in the vicinity of the device and the possible feedback on hydrodynamic effciency The work consists in modelling numerically the flow in an OWC. Navier-Stokes equations are solved by the code JADIM (IMFT). Wave train generation is simulated to propagate on a complex bathymetry towards an OWC. Free surface, air and water velocity and pressure fields, turbulence and hydrodynamic efficiency of the OWC are investigated. Bottom shear stress are calculated before evaluating sediment transport and bed morphology. The situations with and without wave energy device are then compared.

Dernières publications:

- V. Rameliarison, D.Astruc, G. Chapalain. Assessment of Navier-Stokes modelling of an oscillating water column wave energy converter. In Proceedings of the 11th European Wave and Tidal Energy Conference, Nantes 2015. -

Assimilation SWOT SURFEX

Projet démarré en 2014

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)
Porteur de projet: **Sylvain Biancamaria**
The future SWOT (Surface Water and Ocean Topography) satellite mission, jointly developed by NASA and CNES for a proposed launch around 2020, will provide 2D maps of ocean and continental water bodies surface elevations. This mission will therefore provide unprecedented information on the seasonal and spatial variability of the continental water cycle at global scale. Currently, hydrological models (like ISBA-TRIP which is part of the SURFEX platform developed at CNRM) are commonly used to study the global continental water cycle. However, it is extremely difficult to gather global datasets to estimate all of the parameters needed for such hydrological models (such as river depth/width, friction coefficientï¿½) and are currently approximated using empirically-based parametrizations. Yet, this is the kind of information which can be derived from SWOT. Thus the goal of our overall project, mainly based at LEGOS, is to investigate the potential of SWOT measurements to improve parameter specification and their spatial distribution for a coupled hydrological-routing model, using data assimilation techniques. An Extended Kalman Filter has already been developed at CNRM to assimilate virtual SWOT observations into ISBA-TRIP to correct friction coefficient. The purpose of the CALMIP project is to do some sensitivity analysis of ISBA-TRIP, run this assimilation platform and assess the needed improvement (on the code, but also if the assimilation scheme needs to be upgraded to an Ensemble Kalman Filter and the issue of correcting other model parameter as the bankful depth). This project will be done at LEGOS in collaboration with CNRM and CERFACS.

Dernières publications:

- Emery C., S. Biancamaria, A. Boone, P.-A. Garambois, S. Ricci, M. Rochoux and B. Decharme. "Temporal Variance-based Sensitivity Analysis of the River Routing Component of the large scale hydrological model ISBA-TRIP: Application on the Amazon Basin". Journal of Hydrometeorology, 17(12), 3007-3027 - **doi:** pu.doi
- Emery C., A. Paris, S. Biancamaria, A. Boone, S. Calmant, P.-A. Garambois, J. da Silva. "Large scale hydrological model river storage and discharge correction using satellite altimetry-based discharge product". Hydrology and Earth System Sciences, 22, 2135-2162 - **doi:** pu.doi **url:** pu.open_url

Modelling Infrasounds from Solid/Atmosphere Coupling and Applications

Projet démarré en 2014

ISAE/DEOS - Département Electronique, optronique et signal
Porteur de projet: **Raphael Garcia**
Low-frequency events such as tsunamis generate acoustic and gravity waves which quickly propagate in the atmosphere. Since the atmospheric density decreases exponentially as the altitude increases and from the conservation of the kinetic energy, those waves see their amplitude raise (to the order of 10^5 at 200km of altitude), allowing their detection in the upper atmosphere. Various tools have been developed through years to model this propagation, such as normal modes modeling or to a greater extent time-reversal techniques, but none offer a low-frequency multi-dimensional atmospheric wave modelling. A modeling tool is worthy interest since there are many different phenomena, from quakes to atmospheric explosions, able to propagate acoustic and gravity waves. In order to provide a fine modeling of the precise

observations of these waves by GOCE satellite data, we developed a new numerical modeling tool. Starting from the SPECFEM program that already propagate waves in solid, porous or fluid media using a spectral element method, this work offers a tool with the ability to model acoustic and gravity waves propagation in a stratified attenuating atmosphere with a bottom forcing or an atmospheric source. Atmospheric attenuation is required in a proper modeling framework since it has a crucial impact on acoustic wave propagation. Indeed, it plays the role of a frequency filter that damps high-frequency signals. The bottom forcing feature has been implemented due to its ability to easily model the coupling with the Earth's or ocean's surface (that vibrates when a surface wave go through it) but also huge atmospheric events. Applications span from tsunami and/or atmospheric explosions detection on Earth to remote seismology when studying other solar system planets. Indeed, understanding these kind of events would eventually give the opportunity to avoid using ground seismometers when atmospheric conditions are too rough to properly settled down ground stations.

Dernières publications:

- A. Spiga et al., "Atmospheric Science with InSight," Space Sci. Rev., vol. 214, no. 7, p. 109, Oct. 2018. - **doi:** pu.doi
- L. Martire et al., "Numerical Simulation of the Atmospheric Signature of Artificial and Natural Seismic Events," Geophys. Res. Lett., Nov. 2018. - **doi:** pu.doi

Modélisation des écosystèmes planctoniques en Méditerranée

Projet démarré en 2013

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Caroline Ulses**

The objective of the project is to study the coupling of hydrodynamic and biogeochemical processes in the Mediterranean basin. The project is linked with another project about the study of the variability of physical processes in the Med Sea. Here we intend to do simulations of the impact of physical processes on the planktonic development. More precisely, the project is dedicated to establish budgets of biogenic elements and to study how the planctonic ecosystem is shaped by hydrodynamics. It aims particularly at: (i) Characterizing the history of the thermodynamic and biogeochemical properties of the water masses in a wide range of scales (from the event to the annual cycle and interannual variations and from the submesoscale to the scale of the basin) (ii) Understanding how the ecosystem is shaped by hydrodynamics in the temporal dimension and in the spatial dimension (iii) Calculating budgets of biogenic elements in relation with dense water formation (iv) Evaluating the impact of atmospheric deposition on primary production and global budget of nutrients (v) Evaluating the flux of CO2 and O2 at the ocean-atmosphere interface (vi) Studying the impact of environmental changes on the variability of biogeochemical cycles

Dernières publications:

- Kessouri, F., C. Ulses, C. Estournel, P. Marsaleix, T. Severin, M. Pujo-Pay, J. Caparros, P. Raimbault, O. Pasqueron de Fommervault, F. D'Ortenzio, V. Taillandier, P. Testor, and P. Conan (2017). Nitrogen and phosphorus seasonal budgets in the Northwestern Mediterranean deep convection region. J. Geophys.l Res. Accepted. - **doi:** pu.doi

• Kessouri, F., Ulses, C., Estournel, C., Marsaleix, P., D'Ortenzio, F., Severin, T., et al. (2018). Vertical mixing effects on phytoplankton dynamics and organic carbon export in the western Mediterranean Sea. Journal of Geophysical Research: Oceans, 123 - **doi:** pu.doi

Modélisation océanique à haute résolution en Mer Méditerranée

Projet démarré en 2013

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Patrick Marsaleix**

The present request is mainly based on the LEFE "NUMEROFIX" program. The main objective of the NUMEROFIX project is to improve the representation of not explicitely resolved turbulence in circulation ocean models. The frame of the project is the mediterranean sea. Model outputs are compared to in situ measurements of turbulence (Gulf of Lion, Med. Sea) performed by the Marseille university. I am in charge of the numerical simulation of the 3D high resolution model of the NorthWestern Mediterranean sea. Here is a summary of our team's recent work on NUMEROFIX: Using the comparison with in situ data of kinetic energy dissipation rate ε and eddy viscosity KZ , measured in the Gulf of Lion (NW Mediterranean Sea), a 3-D ocean circulation numerical model is used to assess the different performance of k − ε and k − closure schemes in predicting microscale turbulence. Two different surface boundary conditions are considered in order to clarify their influence on these closure schemes performance. The effect of two types of stability functions on the k − ε is also explored. Overall, the 3-D model predictions are much closer to the in situ data in the surface mixed layer as opposed to below it. Furthermore, the results show that the k − scheme's predictions of ε are closer to the observations than the k − ε scheme's ones, especially below the mixed layer depth. Above the mixed layer depth, the to schemes' predictions are comparable when k − employs a boundary condition supposing the equilibrium between the production and dissipation terms in the dynamic equation for the kinetic energy. The two closure schemes perform similarly in estimating KZ with no strong influence of the boundary conditions. Nevertheless, the KZ predictions of the k − ε scheme improves when the Canuto A stability functions are employed.

Dernières publications:

• Damien, P., Bosse, A., Testor, P., Marsaleix, P. and Estournel, C. (2017), Modeling postconvective submesoscale coherent vortices in the northwestern Mediterranean Sea. J. Geophys. Res. Oceans. doi:10.1002/2016JC012114. http://dx.doi.org/10.1002/2016JC012114 - **doi:** pu.doi **url:** pu.open_url

• Kessouri, F., Ulses, C., Estournel, C., Marsaleix, P., D'Ortenzio, F., Severin, T., et al. (2018). Vertical mixing effects on phytoplankton dynamics and organic carbon export in the western Mediterranean Sea. Journal of Geophysical Research: Oceans, 123 - **doi:** pu.doi

Regional Climate and Atmospheric Chemistry Interactions in the Mediterranean Basin

Projet démarré en 2013

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Fabien Solmon**

The evolution of anthropogenic and natural particles and gases emissions is expected to generate in fine outstanding climate and health changes (climate warming, precipitation regime changes, degradation of public health and ecosystems …). It is now necessary to address more in detail the issue of the

characterization of spatial and temporal scales of particles and gases emissions, their transport in the atmosphere and their impacts. The project team has both knowledge and long-time expertise to study these various aspects through a regional modelling of the physical and chemical variability of the atmosphere using the regional climate model RegCM (Giorgi et al., 2012). Building this regional climate modelling needs long term (10+ years) and high resolution (15km) numerical simulations of the emission and the transport of gases and particles in the atmosphere. At the regional scale, the Mediterranean basin is located at the crossroads of air masses carrying gas phase species such as ozone and precursors, as well as natural (desert dust, sea-salt, SOA) and anthropogenic (black carbon, sulphate, etc.) particles. These species contributes to regional pollution and can have strong effects on the regional radiative budget with ensuing impact on regional climate fluctuations from daily to multi-decadal scales, as well as on ecosystems and air quality over the Mediterranean basin. Based on IPCC climate change and anthropogenic emission projections, the scientific objective of the MedCORDEX and ChARMEx WP7 international programs are to better quantify the possible evolution of regional aerosol and ozone budget, associated particulate matter concentrations, and aerosol radiative forcing over the Mediterranean basin. Three temporal windows are targeted for present, middle and end of the century. As part of these projects, we plan is to use the ICTP RegCM4 regional climate model including an interactive aerosol and chemistry module to perform climate-chemistry simulations over an extended Mediterranean domain. These simulations involve intense parallel supercomputing and CALMIP resources offer an ideal environment for this project. For all these reasons, the project team is applying for computing time and data storage on the CALMIP platform.

Dernières publications:

- Somot, S., Ruti, P., Ahrens, B., Coppola, E., Jordà, G., Sannino, G. and Solmon, F., 2018. Editorial for the Med-CORDEX special issue. Climate Dynamics. -

Modélisation physique et biogeochimique des estuaires en Afrique Centrale et en Asie : Application aux estuaires du Cameroun, du Gabon et du Golfe du

Projet démarré en 2013

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Thomas Duhaut**

One of the main objectives of the modelisation of hydrodynamic and biogeochemical modelisation in central Africa and Asian estuaries is to develop and test new numerical methods for coastal circulation with SYMPHONIE model which take into account mangrove forest, siltation, Sea level rise change and climate changes. This project will also help to describe the ocean circulation in east of Gulf of Guinea and Gabon who are very poor in physicals oceanography studies. This project intends to enforce the exchanges between the different teams (POC ,ECOLA) and different laboratory (LA, LEGOS). More recently we are extending our work to other estuaries in Africa (in Gabon, Benin) but also in Asia (Gulf of Tonkin, South China Sea) and we also propose to go further into biogeochemical point of view of those highly anthropologically constrainted systems. A first step is to simulate the circulation with different forcing : ocean circulation (MERCATOR,COPERNICUS), atmospheric forcing (GLORYS and ECMWF) , Tidal Forcing (FES2014) and River discharges and sediment transport in area. Circulation models on various test cases, including fully realistic cases requiring strong computing resources motivating the present request made to CALMIP.

Prévisibilté des épisodes de précipitations intenses dans la région méditerranéenne (Code Méso-NH)

Projet démarré en 2012

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Evelyne Richard**

This proposal aims at improving the predictability of heavy precipitation events that frequently hit the Mediterranean coastal regions. It is closely linked to the recent international field experiment HyMeX (http://www.hymex.org/). Our goal is to develop ensemble forecasting methologies suited for the convective scale. The work will be based upon the Meso-NH atmospheric model (http://www.hymex.org). Both initial state uncertainties and model errors will be accounted for.

Dernières publications:

- Lac, C., Chaboureau, J.-P., Masson, V., Pinty, J.-P., Tulet, P., Escobar, J., Leriche, M., Barthe, C., Aouizerats, B., Augros, C., Aumond, P., Auguste, F., Bechtold, P., Berthet, S., Bielli, S., Bosseur, F., Caumont, O., Cohard, J.-M., Colin, J., Couvreux, F., Cuxart, J., Delautier, G., Dauhut, T., Ducrocq, V., Filippi, J.-B., Gazen, D., Geoffroy, O., Gheusi, F., Honnert, R., Lafore, J.-P., Lebeaupin Brossier, C., Libois, Q., Lunet, T., Mari, C., Maric, T., Mascart, P., Mogé, M., Molinié, G., Nuissier, O., Pantillon, F., Peyrillé, P., Pergaud, J., Perraud, E., Pianezze, J., Redelsperger, J.-L., Ricard, D., Richard, E., Riette, S., Rodier, Q., Schoetter, R., Seyfried, L., Stein, J., Suhre, K., Taufour, M., Thouron, O., Turner, S., Verrelle, A., Vié, B., Visentin, F., Vionnet, V., and Wautelet, P.: Overview of the Meso-NH model version 5.4 and its applications, Geosci. Model Dev., 11, 1929-1969. - **doi:** pu.doi
- Seyfried, L., P. Marsaleix, E. Richard, C. Estournel. Dynamics of North Balearic Front during an autumn Tramontane and Mistral storm : air-sea coupling processes and stratification budget diagnostic. Ocean Sci. Discuss., https://doi.org/10.5194/os-2018-14, 2018 Revised manuscript under review for OS - **doi:** pu.doi

Application d'OpenFOAM aux Transferts dans les sols

Projet démarré en 2012

GET - Géosciences Environnement Toulouse (UMR 5563)

Porteur de projet: **Laurent Orgogozo**

On continental surfaces, a part of rain waters infiltrates in soils. These direct infiltrations are among the main recharges of the groundwaters, which are the most commonly used drinkable water reservoirs. Consequently the study of water transfers through soils is an important stake for water engineering. Moreover, many other applications involve the transfer of water into soils (geotechnics, agronomics, environmental engineering, …). In basic research in geosciences, these phenomena are also of great interest. For example the infiltration of water into soils and parent rocks is the cause of the weathering processes, which are key processes of the carbon cycle. Infiltration of water into soils is classicaly modelled by the so-called Richards equation. A solver for Richards equation have been implemented in the framework of OpenFOAM, a CFD tool box which allows massively parallel computing. 2 publications in Computer Physics Communications present this solver (RichardsFoam2) and its parallel performances (Orgogozo et al., 2014, Orgogozo 2015). The ongoing applications of this solver are various (experimental watersheds modelling in India and Laos, wineyards hydrology, studies of transfers in complex porous media). In the case of boreal continental surfaces, one need to be able to take into account of permafrosts. In order to do so, a multiphysic solver, permaFoam, which solves the thermal transfers with phase changes and the water flow into soils has been developed in the framework of OpenFOAM. This solver has been presented at the EGU 2015, at the ICOP 2016 and at the InterPore conference 2017. The application to field

data sets acquired in experimental watersheds in Central Siberia (collaboration with the Sukachev Institute of Forest de Krasnoiarsk) is the subject of a manuscript in revision for publication. For these purposes we need dedicated allocation of about 300 000 hours of CPU time on CALMIP for the year 2018.

Dernières publications:

- Accepted. L. Orgogozo, A.S. Prokushkin, O.S. Pokrovsky, C. Grenier, M. Quintard, J. Viers, S. Audry. Water and energy transfer modelling in a permafrost-dominated, forested catchment of Central Siberia: the key role of rooting depth. Permafrost and Periglacial Processes. - **doi:** pu.doi
- 2018 L. Orgogozo, A.S. Prokushkin, O.S. Pokrovsky, C. Grenier, M. Quintard, J. Viers, S. Audry. Numerical investigation of evapotranspiration processes in a forested watershed of Central Siberia. Oral presentation at the 5th European Conference On Permafrost, Chamonix, juin 2018. - **doi:** pu.doi **url:** pu.open_url

Dynamique dans l'upwelling du Benguela et dans l'océan Atlantique Tropical

Projet démarré en 2011

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)
Porteur de projet: **Isabelle Dadou**
A serious consequence of global warming that is increasingly gaining importance is the decrease of the dissolved oxygen content of the world ocean. Deoxygenation and extension of the oxygen minimum zones, in particular in the Eastern Boundary Upwelling systems, are predicted because oxygen is less soluble in warmer waters and also because the changing oceanic stratification and circulation are expected to reduce the supply of O2 to the ocean interior. However, the biogeochemical contribution due to the O2 consumed by the aerobic processes (e.g. remineralisation/respiration, nitrification) remains to be quantified. This deoxygenation of subsurface waters will have widespread consequences due to the role O2 and organic matter degradation plays in the biogeochemical cycling of carbon, nitrogen and other important elements such as P, Fe, Mn, S. Oxygen is essential to all aerobic life and sublethal and lethal O2 thresholds vary greatly between marine organisms. The oxygen minimum zones and associated upwelling regions are key areas where climatically relevant gases such as CO2, N2O, are released from the ocean to the atmosphere. In this area, the coupled physical/biogeochemical processes are very active, especially at (sub)mesoscale. In order to develop innovative predictive management tools and strategies to resolve the dynamic interactions of climate change drivers, i.e. changes in ocean circulation, climate, ocean acidification, etc. on the structure and functioning of marine ecosystems in these vulnerable oceanic areas, we propose to employ a combination of data synthesis and numerical simulations (coupled physical(ROMS)/biogeochemical(BioEBUS) model). We focus our efforts on two eastern boundary upwelling systems with oxygen minimum zones of the upwelling off Peru in the Eastern South Pacific ocean and in the Benguela upwelling systems in the Eastern South Atlantic ocean. During the year 2018, we will carry out different coupled physical/biogeochemical (ROMS/BioEBUS) simulations in the Benguela including the Eastern Tropical Atlantic ocean for the Alti-ETAO project (OSTST-CNES) (2017-2020).

Dernières publications:

- Bachèlery, M.–L., S. Illig, and I. Dadou, 2015, Interannual variability in the South–East Atlantic Ocean, focusing on the Benguela Upwelling System: Remote versus local forcing, J. Geophys. Res. Oceans, 121(1), 284–310. doi:10.1002/2015JC011168 - **doi:** pu.doi

• Bachèlery, M.–L., S. Illig, and I. Dadou, 2016, Forcings of nutrient, oxygen, and primary production interannual variability in the southeast Atlantic Ocean, Geophys. Res. Lett., 43, doi:10.1002/2016GL070288 - **doi:** pu.doi

Dynamique spatio-temporelle des populations de truite commune (Salmo trutta) de la province de Navarre

Projet démarré en 2011

ECOLAB - Laboratoire d'écologie fonctionnelle (UMR 5245)
Porteur de projet: **Christophe Laplanche**
Brown trout (Salmo trutta) has colonized alpine freshwaters at a global scale. Stream-dwelling brown trout requires high quality water and can therefore be used as a global bio-indicator of the ecological status of rivers. Brown trout population density is highly variable, both temporally and spatially, which makes trout populations at the edge of its spatial distribution vulnerable to environmental changes. This is the case for brown trout populations which are located in the Spanish Pyrénées. Fish density is driven by internal factors (e.g., density of mature females) as well as external factors (e.g., stream discharge). The complex inter-relationships between internal and external variables make ecological models the only sensible approach that can be used to predict the future of brown trout populations. We work on a dataset that has been collected in the southern Pyrénées by the GAN (Gestion Ambiental de Navarra) since 1993 (> 20 years) over 48 localities distributed over a 6420 km² area. We are creating a hierarchical Bayesian model that simulates brown trout population dynamics that fits these long-term, large scale data. At the current stage, the model successfully simulates the spatio-temporal dynamics of trout growth over the study area for the last 20 years. The model has been extended with a mortality component that also provides very satisfactory results. The model is currently being supplemented with a recruitment (birth) component. The aim is first to simulate population dynamics (growth, mortality, recruitment) over the region of interest for the last 20 years. In a final step, the model will be used to predict future values of brown trout density and test for different scenarios of management and environmental change.

Dernières publications:

• Lecomte, Jean-Baptiste and Laplanche, Christophe A length-based hierarchical model of brown trout (Salmo trutta fario) growth and production. (2012) BiometricalJournal, vol. 54 (n°1). pp. 108-126. ISSN 0323-3847 -
• Laplanche, Christophe and Leunda, Pedro and Ardaiz, José and Francis Juanes. Hierarchical Bayesian modelling of stream-dwelling salmonid growth over a large spatio-temporal scale (en cours d'évaluation) -

Mesure des vitesses horizontales de la surface solaire via la CST

Projet démarré en 2011

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)
Porteur de projet: **Thierry Roudier**
Based on observations of the Sun, it seems clear that the medium which transfers the disturbances in the solar corona through the filament is the magnetic field. It is natural to study the evolution of the movement of material below the filament and the coronal magnetic field when specific motions can be imposed at the feet of the filaments. The goal of our program is to detect twisting or shearing of the filaments around the

feet. Our first results show that the horizontal surface flows crossing the reversal polarity line where the filament is located, allow parasites polarities crossing the line inversion. Our studies also highlight the likely role of differential rotation for the destabilization of the filament, through the stretching of magnetic field lines, leading the filament to a sudden disappearance. The goal of our application to CALMIP is to measure the surface motions all over the Sun surface by using satellite images and Coherent Structure Tracking. The study of such large-scale photospheric motions is also a search on the precursors of solar flares and therefore contributes to the understanding of space weather.

Dernières publications:

- Horizontal photospheric flows trigger a filament eruption Roudier, T. , Schmieder , B. , Filippov , B., Chandra, R. , and Malherbe, J.M. 2018 A&A 618, 43 - **url:** pu.open_url
- Dynamics of Trees of Fragmenting Granules in the Quiet Sun: Hinode/SOT Observations Compared to Numerical Simulation Malherbe, J.M., Roudier, T. , Stein, R.; Frank, Z. 2018 Solar Physics 293, 4 - **url:** pu.open_url

Instabilités magnétiques dans les intérieurs stellaires

Projet démarré en 2011

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Laurène Jouve**

This proposal aims at understanding the interaction between differential rotation and magnetic fields in a stellar radiative zone. One possible application is the magnetism of main-sequence A-type stars, which possess a radiative envelope. Observations have revealed a lower bound in the strong magnetic field observed in a small fraction (5%) of those stars and a two orders of magnitude magnetic desert among those stars between this lower bound and a new type of sub-Gauss magnetism, first discovered in Vega. A bifurcation between stable and unstable large scale magnetic configurations in differentially rotating stars has been advanced to explain this apparent magnetic dichotomy. To test this scenario, we perform global 3D spherical simulations of a magnetic field subject to the differential rotation of a radiative stellar envelope, with the open-source MAGIC code. The first part of this project was devoted to the evolution of an incompressible magnetized fluid (Jouve et al, 2015). We then moved the project to a more realistic situation where stable stratification is taken into account. The calculations of CALMIP session 2015 showed that other instabilities may set in in this stable situation, results were presented in the thesis defence of M. Gaurat in November 2016 but need to be continued with a thorough parametric study. Session 2016A was dedicated mostly to the study of cases with a forced differential rotation, such that a steady state could be reached for the magnetic configurations. D. Meduri, working as a postdoc in our group, performed a large parameteric study for these axisymmetric calculations. Thanks to the calculations of session 2016B and 2017, he showed that when magnetic field is added, the flow is prone to MHD instabilities again. An article is in preparation on these subjects (Meduri et al., in prep.). Hydrodynamical simulations performed by a Master student during the 1st semester of 2017 also enabled us to properly characterize the influence of stable stratification and thermal diffusion on the calculated steady states, for values of the parameters realistic for stellar radiative zones. We now wish to continue this project by characterizing the hydrodynamical stability of those solutions. We then want to perform similar simulations with a different kind of forcing for the differential rotation (a volumetric forcing) which could mimic the contraction or expansion of different regions in the star. We also wish to extend this study to the non-linear phases of possible MHD instabilities developing in such systems, in particular to investigate the possibility of dynamo action in stellar radiative zones.

Dernières publications:

- Pasek, M., Lignières, F., Georgeot, B., & Reese, D. R., A&A 546, A11, 2012 -
- Ballot, J., Lignières, F., Reese, D., Lecture Notes in Physics 865, Springer, 91, 2013 -

Caractérisation de milieux poreux par modélisation numérique multi-échelle de la propagation d'onde et d'écoulements (in)compressibles

Projet démarré en 2011

GET - Géosciences Environnement Toulouse (UMR 5563)

Porteur de projet: **Roland Martin**

In order to realise this project, we need 550 000 computation hours on EOS. With this project we want to develop a numerical code that allows us to image complex media with different rheologies like in granular and/or porous media in presence or not of fluids or attenuation. At different scales (micro to macroscale), interactions between fluids and solids must be taken into account in the wave propagation modelling. And for each phase intrinsic attenuation due to viscous or interphase friction effects must be taken into account. We model two different problems, one at the laboratory scale in granular or porous media and another one at the atmospheric scale (Earth/Atmosphere coupling). These models introduce similar mechanical behaviors : fluid-solid coupling, attenuation due to presence of fluids, etc... Different numerical techniques (high order finite differences, finite volumes or spectral elements) are used to model wave propagation in complex media at different scales. At the laboratory scale, porous media properties like permeabilities can be we evaluated at the Darcy or Biot scale to constrain our porous media models. We intend to develop here numerical tools suitable to perform upscaling on real experimental or field data sets by the use of massive parallel implementation of the solvers of flow transport and closure problems associated to the chosen upscaling technique, namely volume averaging. Finally, an example of upscaling from pore scale to darcy scale of a realistic 3D porous medium will be studied. We aim at modelling attenuation, poroelasticity and non-linear rheologies for non-consolidated media at the scale of the near subsurface. This project is a multidisciplinary project. AT GET laboratory, expertise is brought for wave propagation modelling using finite differences, finite spectral element methods and inversion tools are provided. At METIS laboratory, the data sets at the laboratory scale and the signal processing tools are provided. And at LAUM laboratory of Le Mans, V. Tournat provides physical expertise in granular and complex solid media in presence of water or not. The scientific results obtained will be valorised by scientific publications.

Dernières publications:

- Quentin Brissaud, Roland Martin, Raphaël F. Garcia and Dimitri Komatitsch, Hybrid Galerkin numerical modeling of elastodynamics and compressible Navier-Stokes coupling: applications to seismo-gravito acoustic waves, Geophysical Journal International, vol. 210(2), p. 1047-1069, doi: 10.1093/gji/ggx185 (2017) -
- R. Martin , L . Bodet, V. Tournat, F. Rejiba. 3D numerical modelling of non-linear viscoelastic wave propagation using auxiliary differential equations. Geophysical Journal International, Volume 216, Issue 1, 1 January 2019, Pages 453–469, https://doi.org/10.1093/gji/ggy441(soumis en Avril 2018, accepté en Octobre 2018, on-line Janvier 2019). - **doi:**pu.doi

Modélisation et assimilation de données pour l'étude de la circulation océanique dans le Golfe de Gascogne et autres régions côtières

Projet démarré en 2011

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)
Porteur de projet: **Nadia Ayoub**
We aim to constrain a coastal OGCM with sea surface height and temperature satellite data. The objective is to provide a more realistic ocean state estimation at monthly time scales, with a specific focus on the surface layers. Modeling and assimilation in coastal areas present specific challenges because of the numerous physical processes that need to be taken into account and the wide range of their associated spatial and temporal scales. In such a context, data assimilation can effectively constrain the model if the method is able to take into account the complexity of the model error space due to the richness of the processes at work and the specificity of the studied region. For this reason, we are working on an Ensemble Kalman Filter (EnKF) method where the full multivariate forecast error covariances are used. Our OGCM is SYMPHONIE in realistic configurations of the Bay of Biscay and Gulf of Lion. We also plan to use it in the Gulf of Tonkin (South China Sea). The ensembles are generated by randomly perturbing the wind forcing. We use the S-DAP (SEQUOIA data assimilation Platform) software that includes a code for the EnKF (http://sourceforge.net/projects/sequoia-dap/). Our objective for requesting computing resources at CALMIP is 1/ perform ensemble simulations and assimilation runs; these tests based on synthetic data allow us to evaluate the impact of both sea surface height and high-resolution sea surface temperature data on the estimation of the ocean surface circulation and stratification and calculate several types of ensemble statistics 2/ run the ocean model in a high resolution configuration (without assimilation) to study interactions between the river plume, tides and shelf circulation and to simulate altimetric observations of the future satellite mission SWOT, 3/ test the feasibility and performance of a downscaling method based on data assimilation in a high-resolution coastal model.

Dernières publications:

- Toublanc F., N. Ayoub, F. Lyard, P. Marsaleix, D. Allain, 2018. Tidal downscaling from the open ocean to the coast: a new approach applied to the Bay of Biscay. Ocean Modelling, 124, 16-32, doi: 10.1016/j.ocemod.201802001 - **doi:** pu.doi

CASSANDRE « Calcul Haute performance pour la modélisation de la propagation d'ondes et les méthodes potentielles »

Projet démarré en 2011

GET - Géosciences Environnement Toulouse (UMR 5563)
Porteur de projet: **Roland Martin**
In the mean term the goal will be to solve joint inversion problems on High performance clusters. For this purpose we identified four problems requiring high performance computing : three-dimensional efficient and fast wave propagation modelling at the laboratory or regional scale, the Pyrennes chain or Tibetan plate using joint seismic and gravity inversion and the electrical capacitance tomography which should be correlated in the future with (electro)magnetic imaging. In 2017 we have been able to perform a gravity inversion of one profile through the Pyrenees chain but we would like to perform the same kind of inversion for three other transects through the Pyrenees. In order to extend these techniques to other

zones of the Earth, we aim at applying joint gravity/seismic inversions using teleseismic waves and the whole seismic and density models of the Earth to constrain the regional inversions. An application of this technique to dense gravity and seismic data arrays will allow us to illuminate structures of the lithosphere form below and obtain better images of the first 200kms depth heological structures. We aim at applying our adjoint theory-based inversion techniques on huge data sets collected during the PYROPE and TOPOIBERIA campaigns at the scale of the Pyrenees chain. In collaboration with BRGM and TOTAL companies through the "OROGEN" project we will perform full waveform inversion constrained by gravity data provided by BGI and BRGM to obtain both seismic velocities and densities. Pyrennees are a nice pilot site to validate our tools before applying them to other parts of the world like Tibet and South Europe including the Mediterranean sea for which we already have the data too. We have also performed some joint gravity and seismic data recently in the Mauleon basin thriugh pyrenees by introducing petrophysical and geological constraints in the same way it is done for Mansfield and Yerrida region in Western Australia. The main goals of this joint inversion project are : (i) performing joint inversions on synthetic models in presence of Moho jump inversions (ii)performing joint gravity and seismic inversions on PYROPE+BGI+TOTAL/OROGEN data sets using the adjoint method for the full sesismic waveform inversion and introduce bith petrophysical and geological constraints from the BRGM database. (iii) comparing with the models obtained by joint inversion of time delays and gravity data. (iv) performing joint inversion on three south-North transects (v) applying the methodology to other sites in the world : Western Australia (Mansfield and Yerrida regions), Tibetan plate, Mexico (MASE experiment), Mediteranean sea imaging When comparing the tomographic images to nowadays geological knowledge, we wish thus identify and establish the origin and nature of deep structures under the Pyrenees in order to better constrain the geodynamic evolution of the chain.

Dernières publications:

- Jérémie Giraud, Evren Pakyuz-Charrier, Mark Jessell, Mark Lindsay, Roland Martin, and Vitaliy Ogarko (2017). "Uncertainty reduction through geologically conditioned petrophysical constraints in joint inversion." GEOPHYSICS, 82(6), ID19-ID34. https://doi.org/10.1190/geo2016-0615.1 -
- J. Giraud, E. Pakyuz-Charrier, Vitaliy Ogarko, M. Jessell, M. Lindsay and R. Martin, [2018, submitted], Impact of uncertain geology in constrained geophysical inversion, Expanded Abstract AEGC Sidney 2018. -

Simulation explicite des propriétés microphysiques et électriques des orages avec le modèle MésoNH

Projet démarré en 2011

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Jean-Pierre Pinty**

We are using our "MésoNH" tool, a highly parallelized and vectorized code of an atmospheric multipurpose non-hydrostatic research model. Our project is first concerned by the cloud scheme LIMA that includes explicitly the effects of a population of aerosols of different origin. These are used here to compute the number concentrations of the cloud droplets (CCN activation process) and those of the pristine ice crystals (IFN heterogeneous nucleation) to initiate the ice phase. An issue is to illustrate the initialization of the 3D aerosol fields with the MACC analyzes available at ECMWF, Reading, UK. In addition, our purpose is to enrich LIMA by predicting the shape of the pristine ice crystals which is deemed to be important for accurate cloud physics and radiative transfer modeling. The other point under investigation in LIMA is the on going evaluation of new ice multiplication processes (ice break-up and raindrop shattering) which may play a role in building huge ice contents found in tropical storms. The second part of the project focuses on

the modeling of cloud electricity through the CELLS scheme that we developped in MesoNH. Here the purpose is to improve the treatment of the cloud-to-ground flashes and the lightning optical detector simulator through simulations performed over: 1- HyMeX domain (Gulf of Lion area) to simulate the many electrical events observed by a LMA "Lightning Mapping Array", 2- central Africa (Congo bassin and Victoria lake) where an intense electrical storm activity was currently observed by the LIS optical detector onboard TRMM, 3- New Mexico, which was overflown by LIS of TRMM with coincident LMA data, 4- Corsica and surroundings where Lab. Aérologie owns and operates the SAETTA network of 12 LMA stations and where the ANR "EXAEDRE" field experiment is scheduled in 2018. Typically the 24h simulation domain is 500x500 gridpoints with 60 levels. A 2-model simulation lasts 20 hours without (~40 hours with) electricity for 250 core run.

Dernières publications:

- * Barthe, C., M. Chong, J.-P. Pinty, C. Bovalo, and J. Escobar, CELLS v1.0: updated and parallelized version of an electrical scheme to simulate multiple electrified clouds and flashes over large domains, Geosci. Model Dev., 4, 2849-2892, 2011. -
- Hoarau T., Pinty J.-P., and C. Barthe, A representation of the collisional ice break-up process in the two-moment microphysics scheme LIMA of Meso-NH, submitted to Geosci. Model Dev. - **url:** pu.open_url

Modélisation océanique et atmosphèrique dans le Pacifique Sud-Est

Projet démarré en 2010

LEGOS - Laboratoire d'Etudes en Géophysique et Océanographie Spatiale (UMR 5566)
Porteur de projet: **Boris DEWITTE**
This project is the continuation of activities carried out within the project n°1044 focusing on modeling activities dedicated to the study of the Peru/Chile current system dynamics and the equatorial Pacific dynamics associated to extreme El Niño event. We plan to update our simulation based on updated oceanic Reanalyses that serve as boundary conditions of our configurations, updated version of the code (in particular CROCO will replace our ROMS version) and taking into account new developments on air-sea coupling parametrizations. We also plan to start coupling a biogeochemical component to the existing platforms, which shall require tuning experiments and development. This project benefits from international collaborations and is in line with international projects within which the team is active (eg. TPOS2020, SCOR WG EBUS). Two new students have been incorporated who will start using the models' configurations for their PhD works. Our needs for the first semester of 2018 are estimated to 250000h, which is an amount comparable to the previous demand.

Dernières publications:

- Meerhoff E., B. Yannicelli, B. Dewitte, E. Díaz-Cabrera, C. Vega-Retter, M. Ramos, L. Bravo, F. Hernández-Vaca and D. Véliz, 2018: Asymmetric connectivity of the lobster Panulirus pascuensis in remote islands of the Southern Pacific: importance for its management and conservation. Bulletin of Marine Science, https://doi.org/10.5343/bms.2017.1114. - **doi:** pu.doi
- Tapiador F. J., R. Roca, A. Del Genio, B. Dewitte, W. Petersen and F. Zhang, 2018: Is Precipitation a Good Metric of Model Performance? Bull. Amer. Meteor. Soc., doi:10.1175/BAMS-D-17-0218.1. - **doi:** pu.doi

Calcul ab initio des propriétés de partage isotopique (silicium, lithium) de minéraux et de solutions.

Projet démarré en 2010

GET - Géosciences Environnement Toulouse (UMR 5563)

Porteur de projet: **Méheut Merlin**

Measurement of the isotopic composition of minerals and rocks is a tool of primary importance to interpret geological processes. The last decade of geochemistry research has led to stable isotope measurements of unprecedented accuracy for many elements. In order to fully realize the full potential of these new measurements, it is important to understand the basic mechanisms causing isotopic fractionation through careful theoretical studies and laboratory experiments. Among the new elements that can be measured, silicon is of particular interest, both due to its ubiquity and high abundance in planetary environment (planetology and deep earth studies), and as an important nutrient for biosphere (environmental studies). Here we propose a systematic theoretical investigation of the equilibrium stable isotope geochemistry of silicon, supported by laboratory experiments and empirical studies of selected natural assemblages. Mineral-solution fractionation of Si will also be a focus of this investigation. While less abundant in Nature, Li isotopes show large isotopic fractionations between minerals and solutions, that have been recently investigated in details by experiments. They therefore represent a good case study of mineral-solution fractionation.

Dernières publications:

- Blanchard, M. , Méheut, M. Deon, L., Poirier, M., Micoud, P., Le Roux, C. , Martin, F., Infrared spectroscopic study of the synthetic Mg-Ni Talc series. Physics and Chemistry of Minerals 45, 843 - **doi:** pu.doi
- Oxygen isotope fractionation during smithsonite formation from aqueous solutions - **doi:** pu.doi

Variabilité interannuelle de la circulation en Méditerranée occidentale

Projet démarré en 2009

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Claude Estournel**

The project aims at modelling the oceanic circulation in the western Mediterranean at interannual scales. We intend to better understand the variability of the extent of convection events and dense water cascading in response to the variability of the atmospheric forcing and of the large scale oceanic forcing. Beyond this thematic, we want to understand the important trends that appeared in the characteristics of the Mediterranean deep water mass since 2005. Are they the result of climate change or do they reflect a decadal oscillation of the Mediterranean circulation and of the dense water formation? A new observation program of the Levantine basin should take place over one year between summer 2018 and summer 2019. We are a partner of this project and our objective is to participate with our simulations from the preparation of the cruises to the scientific analysis of the results. All the studies listed above are associated to national and international projects (HYMEX and MERMEX) whose aim is to understand the modifications of the oceanic circulation and the consequences on marine ecosystems. The second part of the project are dedicated to the study of extreme events in the coastal zone (AMORAD ANR project- PhD of GuillaumeMikolajczak). A coupling of the circulation model with a sea state model and a sediment transport

model is used. This complex model will be used to study the fate of water and matter brought by rivers to the coastal zone and possibly the export to the deep sea.

Dernières publications:

- Damien P., Bosse A., Testor P., Marsalei P., Estournel C. Modeling post convective submesoscale coherent vortices in the Mediterranean Sea. Journal of Geophysical Research - **doi:** pu.doi
- Estournel C., Testor P., Damien P., D'Ortenzio F., Marsaleix P., Conan P., Kessouri F., Durrieu de Madron X., Coppola L., Lellouche J.M., Belamari S., Mortier L., Ulses C. and Prieur L. High resolution modelling of dense water formation in the north-western Mediterranean: benefits from an improved initial state in summer. Journal of Geophysical Research - **doi:** pu.doi

Peanuts

Projet démarré en 2009

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)
Porteur de projet: **Francois Rincon**
Le processus d'accrétion de matière dans les environnements stellaires jeunes constitue une étape fondamentale de la formation des planètes. Il est désormais largement admis que la turbulence joue un rôle critique dans le processus d'accrétion, cependant la question de son origine au sein des disques reste encore en grande partie ouverte. Ce projet a donc pour objectif principal d'identifier et de mieux comprendre des mécanismes de transitions possibles vers la turbulence dans des écoulements en rotation différentielle Keplerienne représentatifs des systèmes accrétants. Nous utilisons pour cela des approches numériques originales dans le contexte astrophysiques mais utilisées dans d'autres communautés scientifiques. Il s'agit notamment de calculer des solutions non-linéaires 3D des équations pertinentes, dont on pense qu'elles représentent les briques fondamentales de la transition vers le chaos et la turbulence, et d'analyser de manière détaillée l'anisotropie des transferts spectraux non-linéaires dans le system Keplerien.

Dernières publications:

- "Periodic magnetorotational dynamo action as a prototype of nonlinear magnetic field generation in shear flows", J. Herault, F. Rincon, C. Cossu, G. Lesur, G. I. Ogilvie, P.Y. Longaretti, Phys. Rev. E 84, 036321 (2011) - **doi:** pu.doi **url:** pu.open_url
- "Magnetorotational dynamo chimeras. The missing link to turbulent accretion disk dynamo models ?", A. Riols, F. Rincon, C. Cossu, G. Lesur, G. I. Ogilvie, P.-Y. Longaretti, Astron. Astrophys. in press (2016) - **doi:** pu.doi **url:** pu.open_url

Astérosismologie des étoiles variables pulsantes

Projet démarré en 2002

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)
Porteur de projet: **Stéphane Charpinet**
Evolved compact stars populating the extreme horizontal branch (also called sdB stars) and the white dwarf cooling sequence represent respectively an intermediate stage and the ultimate product of the evolution of

intermediate to low-mass stars forming up to 98% of all stars in the Universe. The discovery of several classes of nonradial pulsators among these objects over the past decades has open huge opportunities to probe their interior with asteroseismology. These stars show rapid multiperiodic oscillations of low amplitude that are usually captured through high precision high speed photometry carried out from ground based mono- or multi-site campaigns, or from space instruments such as COROT, KEPLER, and KEPLER2. These stars often show sufficient number of independent oscillation modes to allow in-depth probing of their internal structure and dynamic through asteroseismology. We have developed in our team powerful and unique numerical tools to exploit the asteroseismic potential of these stars. These include a massively parallel real-coded-hybrid-genetic-algorithm named LUCY that can perform high dimension multimodal optimization to "invert" the internal structure of these stars from the observed pulsation periods. This code, with appropriate stellar modeling and pulsation codes, is exploited and continuously improved with the goal to analyze objects among a still growing sample containing to date more than 110 known pulsating sdB stars and up to 200 pulsating white dwarfs, many of them having ultra high precision seismic data available from space instruments. This fantastic pool of seismic information about the interior of evolved stars requires important computational power to be fully exploited. Running our codes on EOS/CALMIP has been the most efficient solution found so far to pursue this project.

Dernières publications:

- Van Grootel, Valérie; Péters, Marie-Julie; Green, Elizabeth M.; Charpinet, Stéphane; Brassard, Pierre; Fontaine, Gilles, OAst, 27, 44 - **doi:** pu.doi
- Charpinet, Stephane; Giammichele, Noemi; Zong, Weikai; Van Grootel, Valérie; Brassard, Pierre; Fontaine, Gilles, OAst, 27, 112 - **doi:** pu.doi

Dans le cadre de la tache de service MESONH labélisé INSU Portage/Développement de modèle MésoNH sur architecture HPC

Projet démarré en 2001

LA - Laboratoire d'Aérologie (UMR 5560)

Porteur de projet: **Juan Escobar**

MESO-NH Modélisation à moyenne échelle de l'atmosphère En 1993, des équipes de modélisation atmosphérique de méso-échelle du CNRM (Météo-France) et du Laboratoire d'Aérologie (UMR 5560) se sont regroupées au sein du projet MESO-NH visant à développer un nouveau code de modélisation météorologique intégrant les avancées scientifiques et techniques les plus récentes dans le domaine. Dès 1998, le projet a atteint ses objectifs initiaux et a débouché sur un outil de recherche performant du niveau des meilleurs codes de la communauté internationale. Il est aujourd'hui utilisé par une large communauté (atmosphériciens, hydrologues,...) de plus d'une centaine de chercheurs rattachés à 37 équipes dans 8 pays. Ce code : * intègre un système d'équations non-hydrostatique, permettant de traiter avec le même outil une vaste gamme de phénomènes atmosphériques allant de la méso-échelle alpha (quelques milliers de km) jusqu'à l'échelle des tourbillons (quelques m) * est doté d'un jeu complet de paramétrisations physiques, de divers niveaux de complexité et adaptées aux différentes échelles considérées * dispose de capacités d'auto-imbrication lui permettant de relever de nouveaux défis (prévisibilité des systèmes orageux par exemple) * est couplé avec des modules de chimie gazeuse, aqueuse et des aérosols qui offrent un cadre dynamique privilégié pour toute étude numérique de physico-chimie atmosphérique * est doté d'opérateurs d'observation qui permettent de comparer directement les sorties du modèle avec des observations satellite ou radar. Les utilisations scientifiques de MESO-NH sont extrêmement variées. Le modèle est largement utilisé sur les thématiques des grands projets nationaux et internationaux

(TOGACOARE, FASTEX, ACE II, TRACAS, PICO3, ESCOMPTE, ESQUIF, TRACE P, PEM, MAP, TROCCINOX, AMMA, MEDEX,...). L'INSU a labellisé les missions de Service (maintenance du code, assistance aux utilisateurs, veille scientifique)

Modes propres des étoiles

Projet démarré en 2001

IRAP - Institut de Recherche en Astrophysique et Planétologie (UMR 5277)

Porteur de projet: **Michel Rieutord**

This project is devoted to various studies of stellar oscillations in order to give theoretical background to the interpretation of data coming from the space missions CoRoT (CNES) and KEPLER (NASA). The project is divided into three parts: the first part is focused on the oscillations of rapidly rotating stars and aims at deciphering the dynamics of both acoustic and gravity modes. The second part is devoted to the influence of magnetic fields and aims at modeling the oscillation spectrum of the so-called roAp stars. The third and last part focuses on the case of tidally forced oscillations, which are important for the understanding of the dynamics of binary stars. All these parts require in a more or less important way, 2D models of rotating stars and thus part of the computing time is dedicated to run and test such models (computed with the ESTER code).

Dernières publications:

- Rieutord M. and Valdettaro L. (2018), "Axisymmetric inertial modes in a spherical shell at low Ekman numbers" in J. Fluid Mech. vol. 844, 597-634 - **doi:** pu.doi
- Evano B., Lignières F. and Georgeot B. (2018), "Correlations in the chaotic spectrum of pressure modes in rapidly rotating stars", submitted to Europhysics Letters -

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4.4 Physique théorique et moléculaire

KPZ fluctuations in finite volume

Projet démarré en 2018

LPT - Laboratoire de Physique Théorique (UMR 5152)

Porteur de projet: **Sylvain Prolhac**

KPZ universality describes the dynamics of large scale fluctuations in a variety of one-dimensional systems such as growing interfaces, directed polymers in random media, strongly interacting driven particles, or fluids with few conservation laws. It has become in the past few years a prominent topic at the interface between non-equilibrium statistical physics (theory, numerics and experiments) and probability theory (Markov processes, stochastic differential equations, random matrices). At the KPZ fixed point, the fundamental object of interest is a very singular random function depending on space and time. Many exact results have been obtained in the past twenty years for KPZ fluctuations, mainly in two limiting cases: the infinite system, and the finite system in its stationary state. In these two cases, universality is well established from numerics, exact results for various integrable models, mathematical proofs for other types of models, and even experiments. This project focuses on the crossover between the two regimes, which

describes finite volume relaxation from a state where fluctuations are connected to random matrix theory to a non-equilibrium steady state where KPZ fluctuations describe rare events in terms of large deviation functions. Analytical results have been obtained recently for the exact time evolution of fluctuations in a specific exactly solvable model of hopping particles called TASEP (for totally asymmetric simple exclusion process) with specific initial conditions (flat, stationary and domain wall). The main goal of the project will be to provide numerical evidence of the universality of these exact results in the crossover regime by comparing with numerical simulations of another model, the Kardar-Parisi-Zhang equation, a stochastic partial differential equation describing the evolution in time of a growing interface between stable and metastable thermodynamic phases, and which gives its name to the universality class.

Physique des solitons dans les plasmas magnétisés

Projet démarré en 2018

LAPLACE - Laboratoire Plasma et Conversion d'Energie (UMR 5213)
Porteur de projet: **Renaud Gueroult**
Solitons are non-linear waves which feature unique properties. For example, solitons maintain their form while propagating in a dispersive media and also preserve their shape and speed after colliding with another soliton. Further to these unique physical properties, the concept of solitons has played a central role on theoretical developments in nonlinear wave physics and applied mathematics. We have recently shown through particle-in-cell simulations that shocks in magnetized plasmas can lead to the formation of magnetosonic solitons, both in perpendicular astrophysical shocks [1] and in fast magnetic compression experiments [2]. One of the long standing questions in astrophysics is what acceleration mechanism can explain the observation of cosmic energetic particles. Here, the new result that solitons can under some conditions mediate the reformation process [1] by which astrophysical shocks propagate offers new avenues to study particle shock acceleration and its role on energetic particles. Furthermore, improving our basic understanding of the physics of solitons in magnetized plasmas could also help designing control techniques to mitigate the effects of electron dephasing which typically limit the performances of plasma-based particle accelerators [2]. We propose here to build on our earlier results from Refs [1,2] and to explore and study the rich physics uncovered by these past studies using electromagnetic particle-in-cell (PIC) simulations. [1] Gueroult R., Ohsawa Y. and Fisch N.J, Physical Review Letters, 118, 125101 (2017) [2] Gueroult R., Fisch N. J., Physics of Plasmas, 23, 032113 (2016)

Non-adiabatic dynamics and dissipation in the reactivity of PAH-related complexes and of molecule-surface systems

Projet démarré en 2018

LCAR - Laboratoire Collisions Agrégats Réactivité (UMR 5589)
Porteur de projet: **Didier Lemoine**
The present project seeks HPC support for two selected scientific projects, one from a European ITN consortium, http://www.europah.eu, and the other from the LABEX NEXT, http://www.next-toulouse.fr. I. The ITN EUROPAH LCAR PhD project aims at developing and applying new, efficient approaches to non-adiabatic dynamics and dissipation in the reactivity of PAH-related complexes and of hydrogen atoms or small molecules interacting with PAHs or graphene. Namely, these approaches are built upon the Density Functional-based Tight Binding "DFTB" theory and upon its so-called Time-Dependent DFTB "TD-DFTB" version. Implementation in the Toulouse open source DeMonNano package (http://demon-nano.ups-tlse.fr) will enable simulations with full dimensional classical molecular dynamics. The code development

and production steps are a) TD-DFTB calculation of excited states, of their gradients and of the non-adiabatic (dynamical) couplings; b) Interfacing with a multiple-state mixed quantum-classical molecular dynamics scheme such as Trajectory Surface Hopping "TSH"; c) Testing and benchmarking; d) Application to the relaxation of an electronically-excited PAH molecule; Analysis of direct versus indirect fragmentation and of the role of electronic-to-electronic and electronic-to-vibration energy conversions. II. The NEXT EXSTAS project addresses two key topics of EXcited STate dynamics At Surfaces 1. Adsorbate coupling to electron-hole pairs (EHPs) in reacting systems: Surface and subsurface chemistry of atomic and molecular hydrogen with Ag and Au; 2. Pathways by which EHPs localize electronic excitation on adsorbate molecules: Electronic quenching of excited states NO(A&B) or of CO on Ag or Au. The model systems are chosen to provide insights about how the elementary degrees of freedom of atoms or molecules (electronic, translational, vibrational and rotational) interact with EHPs. New theoretical methods (similar and/or complementary to those for EUROPAH) will be applied to compare with experimental observations. As an alternative to the TD-DFTB/TSH interface, the development of a friction version of molecular dynamics within DFTB-DeMonNano, will extend computational feasibility to (much) larger systems. In the future, both strategies will be applied to either EUROPAH and EXSTAS targeted applications.

Foudre et composite

Projet démarré en 2018

ISAE/DMSM - Département Mécanique des structures et matériaux
Porteur de projet: **AUDREY BIGAND**
L'objectif est de pouvoir simuler les effets multiphysique de la foudre sur les structures composites. Pour cela, on va utiliser le module electro-thermo-mécanique d'abaqus afin de prédire la vaporisation de la protection foudre, la redistribution du courant dans le composite et les effets d'explosions associées. Abaqus est un logiciel commercial et parallèle.

vortex optiques dans les cristaux liquides

Projet démarré en 2018

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **gonzague agez**
Bonjour, L'objectif est de simuler la propagation de la lumière dans des cristaux liquides cholestériques afin de générer des vortex optiques. J'utilise le logiciel Meep (bibliothèques BLAS, LAPACK, GUILE, libctl, HDF5) Logiciel sous licence GNU GPL Je l'utilise sur mon poste en monoprocesseur mais j'aimerais l'utiliser en parallèle (MPI) sur Calmip

Modélisation de Radiothérapie par Méthode Monte-Carlo

Projet démarré en 2018

CRCT - CRCT UMR 1037 - Centre de Recherches en Cancérologie de Toulouse
Porteur de projet: **Luc SIMON**
Notre Laboratoire réalise des modélisations par la méthode Monte-Carlo de Radiothérapie interne et externe. Il s'agit de calculer la distribution de dose absorbée au sein des patients traités pour différents cancers (en particulier les cancers bronchiques). Ces modélisations ont un intérêt quand les algorithmes de

routine clinique atteignent leur limites (par exemple les petits champs). La plateforme GATE/Geant4 contient l'ensemble des données physiques nécessaires à la simulation ainsi que des outils de construction de géométrie et des outils permettant de définir des régions "sensibles" (régions dans lesquelles il est possible de récupérer des données de sortie). Notre cluster actuel a montré ses limites et nous souhaitons trouver une autre solution pour certaines de nos applications. Nous sommes venus sur le site de CALMIP pour un premier contact et cette entrevue a motivé une demande de "projet test".

Molecular network of coordination complexes

Projet démarré en 2016

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Veronique Langlais**
CALMIP support is needed for the success of the project MoNet. Time consuming quantum chemistry calculations and simulations are necessary in order to understand and to interpret experimental results as well as to determine the chemical effects at play in the on-surface-synthesis reactions. On-surface-synthesis on ultrathin oxide insulating films to build 2D Covalent Molecular Network (CMN) will be explored in the project Monet. The strategy proposed here is based on designing molecular precursors to control the synthesis directly on the surfaces of oxide ultrathin films. The properties of these unique systems will be experimentally explored by scanning probe microscopy and advanced synchrotron techniques to get a clear understanding of their properties at local and collective level. Calculations will be performed to predict and to understand the mechanisms which govern the intermolecular bonding, molecule-substrate interaction, electronic transfer and magnetic coupling.

Dynamique microscopique d'agrégats ou de molécules sous irradiation intense

Projet démarré en 2012

LPT - Laboratoire de Physique Théorique (UMR 5152)
Porteur de projet: **Phuong Mai Dinh**
The structure and the dynamics of a collection of atoms (molecules, clusters, nanostructures, materials, etc.) come from a subtle balance between electronic effects (by essentially valence electrons) and ionic ones (an ion being the remaining system composed by the atomic nucleus and the core electrons). The analysis of the dynamics of such objects relies on a simultaneous description of the electronic and ionic degrees of freedom. The difference between the femtosecond time scale of (quantum) electrons and that of the (classical) ions, of the order of the picosecond, makes this task difficult. To simulate realistic processes with many electrons/ions, a goal that represents a real theoretical and numerical challenge, we have developed tools to cope this multiscale dynamics, from the femtosecond to the picosecond. Relying on our expertise of more twenty years on the ionization of free clusters by intense electromagnetic excitations, this project aims at studying dynamical scenarios when a molecule or a cluster is irradiated by a laser. In particular, the advent of new sophisticated light sources, as train of attosecond pulses in the XUV, opens the road for new types of excitation and ionization in multielectronic systems. At the same time, the use of higher and higher laser intensities calls for a better description of dissipation in such systems, and therefore calls for "beyond mean-field" approaches. Finally, we would like to extend our approach to the case of irradiation of small systems by a positron, this project being motivated by a brand-new collaboration with experimentalists in Lyon. Indeed, the understanding of the damage dynamics induced by the interaction with a positron is scarce or even inexistent.

Dernières publications:

- C.-Z. Gao, P. M. Dinh, P.-G. Reinhard, E. Suraud, and C. Meier, Phys. Rev. A 95, 033427 - **doi:** pu.doi
- L. Lacombe, P. M. Dinh, P.-G. Reinhard, and E. Suraud, J. Phys. B 49, 245101 - **doi:** pu.doi

Plasmonique hybride

Projet démarré en 2011

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)

Porteur de projet: **Christian Girard**

This project aims to get a better understanding of optical properties of plasmonic structures composed of colloidal and lithographied metal nanoparticles deposited on dielectric substrates and their coupling with fluorescent nanoparticles. The team has already a solid experience in that field, theoretically as well as experimentally (see references for more information). A program based on Green's dyadic method has been developed. This algorithm reproduces with a good agreement experimental results, but it needs an efficient supercomputer such as EOS, to be run in reasonable times. In that perspective, we intend to parallelize our program, which would allow us to study more complex structures with a better precision.

Dernières publications:

- J. Opt. 20 075004 (2018) -
- Phys. Rev. B 97 (8), 085411 (2018) -

Agrégats quantiques

Projet démarré en 2010

LCAR - Laboratoire Collisions Agrégats Réactivité (UMR 5589)

Porteur de projet: **Nadine Halberstadt**

In this project we study dynamics processes in or on quantum clusters. We focus on helium droplets, which exhibit outstanding superfluid properties. The challenge consists in describing the N-body dynamics as a function of time and using quantum techniques. We have developped a simulation method based on MCTDH (Multi-Channel Time-Dependent Hartree) in Gaussian wave packets, to take into account both correlation and boson exchange symmetry. We are also making extensive use of the simulation program of Barranco and Pi, from the Barcelona University, which is based on helium density functional (He-DFT) and its time-dependent version. We take advantage of the IDEX Chaire d'Excellence of Manuel Barranco to start developping a mixed approach with the MCTDH techniques for the dopant and their nearest neighbor helium atoms, and He-DFT for the rest of the droplet.

Dernières publications:

- Desorption dynamics of RbHe exciplexes off He nanodroplets induced by spin-relaxation, F. Coppens, J. von Vangerow, M. Barranco, N. Halberstadt, F. Stienkemeier, M. Pi and M. Mudrich, Phys. Chem. Chem. Phys. 20, 9309-9320 (2018); - **doi:** pu.doi
- - Impulsive alignment of 4He-CH3I: A theoretical study, P. Vindel Zandbergen, J. Jiang, M. Lewerenz, Ch. Meier, M. Barranco, M. Pi and N. Halberstadt, J. Chem. Phys. 149, 124301 (2018) - **doi:** pu.doi

Simulation numérique des propriétés optiques de nanostructures plasmoniques

Projet démarré en 2008

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Arnaud Arbouet**
This project aims at predicting the optical properties of metallic nanoparticles. It is well-known that gold and silver nanostructures support optical resonances termed surface plasmon resonances, the properties of which strongly depend on the particle morphology, its size and environment. The ability of Surface Plasmons to enhance the electric field and shrink it into regions of subwavelength dimensions open exciting perspectives in nano-optics. The investigation of the peculiar properties of Surface Plasmons has motivated several important experimental breakthroughs such as near-field optical probes, electron spectroscopies and nonlinear microscopies. The modelization of these complex experiments is the main motivation of the present project. The interpretation of nano-optics experiments requires the resolution of Maxwell's equations taking into account the morphology and material properties of a given nanosystem. In our case, we use the Green Dyadic Method and use a discretization of the volume of the investigated nanosystems. This has clear advantages as virtually particles of any shape can be described but it also has important constraints as the size of the linear systems to be manipulated in our algorithms can be quite large. The numerical implementation of our resolution algorithm is based on an hybrid OpenMP/MPI parallelization which fully exploits the ressources of EOS.

Dernières publications:

- Decay rate of magnetic dipoles near nonmagnetic nanostructures Peter R. Wiecha, Arnaud Arbouet, Aurélien Cuche, Vincent Paillard, and Christian Girard Phys. Rev. B 97, 085411, 2018 - **doi:** pu.doi
- Development of a high brightness ultrafast Transmission Electron Microscope based on a laser-driven cold field emission source F. Houdellier, Giuseppe Mario Caruso, Sébastien Weber, Mathieu Kociak and Arnaud Arbouet Ultramicroscopy, 186, 128-138, 2018 - **doi:** pu.doi

Molécules et/ou nanofilms métalliques sur surface

Projet démarré en 2008

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Xavier Bouju**
Our studies on the adsorption of molecules on metal surfaces will continue in 2018. We plan to address relatively large molecules in terms of size which will require significant calculations. Right now, we plan to use semi-empirical methods, although the use of DFT can also be considered. The metal surfaces we expect to use are surfaces conventionally used as Au (111). We are considering the possibility to tackle the adsorption of molecules near surface defects, such as kinks or step edges.

Dernières publications:

- Giant (12×12) and (4×8) reconstructions of the 6H-SiC(0001) surface obtained by progressive enrichment in Si atoms - **doi:** pu.doi
- Three-dimensional hydrogen bonding between Landers and planar molecules facilitated by electrostatic interactions with Ni adatoms - **doi:** pu.doi

Simulations quantiques des processus ultrarapides dans des systèmes complexes

Projet démarré en 2002

LCAR - Laboratoire Collisions Agrégats Réactivité (UMR 5589)

Porteur de projet: **Christoph Meier**

The aim of the project «Simulations quantiques des processus ultrarapides dans des systèmes complexes» is the theoretical study and numerical simulation of atomic and molecular processes at the femtosecond timescale. In particular, the quantum aspects of the time evolution, and the possibility to actively control its dynamics by shaped laser pulses are at the hart of the project. In many areas, quantum effects are extremely important for the detailed understanding of the dynamical processes at the atomistic level, like chemical reactivity, catalysis or biological functioning. Additionally, quantum dynamics in general, its coupling to an environment and the possibility to control its time evolution are keystones for possible future implementations of quantum information processing. As far as the possibility to control quantum processes are concerned, several experimental advances have substantially increased the general interest , like pulse shaping techniques, developed in the optical regime,that have been transposed to : -- the UV/XUV regime, with a possibility to control the optical phase withing the intensity of the envelope (carrier / envelope phase), opening new possibilities for attosecond control of atomic processes. -- the IR regime, with the possibilty to control nuclear dynamics directly on the electronic ground state From the theoretical point of view, the dynamic quantum mechanical modelling of atomic processes are still restricted to a few degrees of freedom, very often insufficient for complex systems, like proteins, or embedded or deposited molecules and clusters. In this context, the complexity not only stems form the number of atoms involved, but also from the from the different types of interactions, the effects of a coupling to an environment, and the non-linear response to strong, external pulses of high complexity. As a consequence, the development of novel quantum or mixed quantum/classical methods is an important part of the project, alongside with simulations of realistic systems with well established methods.

Dernières publications:

- "Quantum dynamics modeled by interacting trajectories" L. Cruz-Rodriguez, L. Uranga-Pina, A. Martinez-Mesa, and C. Meier, Chem. Phys. 503, 39 (2018) -
- Quantum trajectory study of laser-driven atomic ionization, L. Cruz-Rodriguez, L. Uranga-Pina, A. Martinez-Mesa, and C. Meier, Chem. Phys. 715, 211 (2019) -

APPLICATIONS DES METHODES DU CHAOS QUANTIQUE: INFORMATION QUANTIQUE, PHYSIQUE DU SOLIDE, PHYSIQUE ATOMIQUE, ETUDE DES RESEAUX

Projet démarré en 2001

LPT - Laboratoire de Physique Théorique (UMR 5152)

Porteur de projet: **Bertrand Georgeot**

The project is devoted to the application of methods from quantum chaos to solid state physics, quantum computation, atomic physics and networks. A first part of the project studies studies the effects of interaction on many-body systems, in particular the transition towards a quantum chaos regime characterised by delocalized wavefunctions. This theme was originally developped in the context of the Anderson localization of electrons in solids, which is still studied in the group in particular in the understanding of the multifractal properties of the wave functions at the transition. A second aspect of the

project concerns the simulation of chaotic systems by a quantum computer. Algorithms developped in the group, enabling to simulate efficiently quantum and classical physical systems in a regime of dynamical chaos, are implemented and tested in presence of realistic imperfections. These developments towards the study of quantum computers led us to more fundamental studies on decoherence in quantum systems, the creation of entanglement and interference in quantum processes, and their link with the efficiency of quantum algorithms. A recent development concerns the study of molecular computation in link with experimentalists at CEMES. These studies and the recent experimental progress in the control of cold atoms led us to new developments towards the application of these different methods to the physics of cold atoms and Bose-Einstein condensates. A new direction recently initiated corresponds to the application of these methods to networks like the World Wide Web, in particular in the context of the Google PageRank algorithm.

Dernières publications:

- Gabriel Lemarié, "Glassy properties of Anderson localization: pinning, avalanches and chaos ", submitted (2018)(arXiv:1809.02329 preprint) -
- Gabriel Lemarié, Ilaria Maccari, Claudio Castellani, "Kane-Fisher weak link physics in the clean scratched-XY model ", submitted (2018)(arXiv:1811.09203). -

4.5 Chimie quantique

Développement d'un modèle mixte de chimie quantique et d'apprentissage automatique pour prédire les paramètres RMN de structures de carbone amorphe de

Projet démarré en 2018

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)
Porteur de projet: **Céline Merlet**
Ce projet test correspond à l'arrivée d'un post-doctorant. L'objectif du projet post-doctoral est de développer un modèle mixte de chimie quantique et d'apprentissage automatique pour prédire les paramètres RMN de structures de carbone amorphe de grandes dimensions et de l'utiliser pour améliorer notre compréhension des carbones poreux désordonnés. Ces carbones consituent une classe de matériaux utilisés dans de nombreuses applications incluant le stockage d'énergie, le stockage de gaz, le traitement de l'eau et la catalyse. Dans tous les cas, la caractérisation des matériaux poreux, qui reste un défi du point de vue expérimental, est une étape essentielle si l'on veut comprendre et optimiser les performances de ces matériaux. L'approche utilisée sera basée sur un couplage entre un modèle de type « tight-binding » et la détermination de polarisabilités magnétiques atomiques afin de calculer des paramètres RMN. Le modèle sera d'abord appliqué et testé sur des molécules aromatiques relativement petites avant d'être étendu à des solides périodiques. Ce modèle devrait alors nous permettre d'explorer l'influence de la présence de défauts sur les propriétés électroniques et magnétiques des carbones poreux. Nous serons aussi en mesure de discriminer les différentes structures atomiques proposées dans la littérature. Pour pouvoir faire l'apprentissage du modèle puis sa vérification, nous allons calculer, via des méthodes de chimie quantique, des paramètres RMN pour un certain nombre de structures de carbone. Ce projet test, avec l'utilisation de Gaussian, correspond à des tests préliminaires pour des molécules aromatiques de petites et moyennes dimensions afin d'estimer les coûts associés pour la suite du projet. Nous allons aussi profiter des ces

heures de calcul pour essayer d'identifier le programme que nous utiliserons pour les calculs sur des solides périodiques.

Morphologie de nanoparticules de ruthénium

Projet démarré en 2018

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)
Porteur de projet: **Romuald Poteau**
Jusqu'à très récemment, les nanoparticules de ruthénium (RuNP) de petite dimension, produites par voie colloïdale, avaient été observées le plus fréquemment sous forme de sphéroïdes cristallins hcp, ou dans de plus rares cas fcc. L'équipe Nanostructures et Chimie Organométallique du LPCNO vient ces dernières semaines d'observer des RuNP de forme icosaédrique! Des calculs DFT menés en amont il y a environ 5 ans montraient la possible existence d'une phase icosaédrique. Sans support expérimental, ces travaux n'ont jamais été publiés. Le présent projet consiste à reprendre ces anciens travaux et à vérifier si on peut justifier que cette morphologie soit observée dans les conditions expérimentales de la synthèse de ces RuNPs, c'est-à-dire à température modérée (< 400K) et avec des molécules d'acides laurique en tant que ligands stabilisants. Les 700000h demandées devraient permettre de comparer la stabilité relative de différents modèles de RuNPs nus et saturés avec des taux variables d'acides à leur surface.

Modélisation de l'activation de liaisons chimiques inertes par des complexes organométalliques via un nouveau mode de coopération métal-ligand

Projet démarré en 2018

LCC - Laboratoire de Chimie de Coordination (UPR 8241)
Porteur de projet: **Dmitry Valyaev**
The proposal is focused on the theoretical study of the activation of inert E-H bonds (E = H, B, C, Si) by transition metal complexes using a new mode of metal-ligand cooperation. The project is based on the experimental results recently obtained in the team "Molecular design of transition metal pre-catalysts" of Laboratory of Coordination Chemistry (LCC), namely facile dihydrogen activation by a series of manganese complexes bearing bidentate ligands incorporating phosphine and N-heterocyclic carbene moieties and their high activity in hydrogenation of carbonyl compounds. The first part of the project will be devoted to the study of the electronic structure and bonding mode of the reactive manganese intermediates and the mechanism of E-H bond activation (concerted or stepwise). Then the modeling of entire catalytic cycle for selected manganese catalysts and relevant model organic substrates (ketones, imines, esters, alkynes) as well as the expansion of this concept to other first row transition metals (Fe, Co, Ni) will be performed.

Systematic study of the structure and bonding of halogens on low index Pt surfaces

Projet démarré en 2018

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)
Porteur de projet: **Chiara Dinoi**
Heterogeneous catalysis is one of the most important chemical processes of various industries performed on catalyst nanoparticles with different sizes or/and shapes. In the past two decades, thanks to the spectacular advances in syntheses of metal nanomaterials, the catalytic performances of different catalytic

reactions on metal nanoparticles with well controlled sizes or shapes have been extensively studied. It has been shown, in particular, that the structure and morphology (size and shape) of metal nanoparticles may have a substantial influence on their catalytic activity. One of the current goal of nanoscience and nanotechnology is therefore to provide the ability to create controlled structures and geometries to investigate and optimize a broad range of catalytic processes. The team of B. Chaudret and K. Soulantica recently discovered that the presence of different halides on the surface of Pt nanoparticles influences the growth mode of these particles, leading to different catalytic activities and selectivities during the catalytic hydrogenation process of several compounds. The synthesis of Pt nanoparticles, obtained by reaction of Pt halides with octadecylamine under exogenous H2 pressure, indeed, has shown that the use of PtCl2 at a 99.9% of purity affords Pt nanoparticles with a multipode crystallographic orientation, whereas the use of PtCl2 at a 98% of purity (containing therefore other halides as impurity) affords Pt nanoparticles with a concave cube crystallographic orientation in the 110 surface. Interestingly these two crystallographic orientations, either multipodes or concave cubes, display different catalytic activities and selectivities in the catalytic hydrogenation reaction of several substrates. To understand the reason for this behavior, we recently started, in collaboration with this experimental group, a theoretical work aimed at studying the structure and bonding of halogens on Pt low index surfaces (100, 110 and 111) by means of density functional theory (DFT) calculations using periodic slabs to model the surface. By computing the halogen absorption energies, in particular, we plan to determine which halogens (or mixtures of halogens) are preferentially absorbed by a fixed surface and which surface has the lower absorption energy for a fixed halogen (or mixture of halogen). Once we have determined and explained the correlation between the halogen composition and the structure of the Pt nanoparticules, our second goal is to establish the correlation between the shape of the Pt nanoparticule surfaces and the corresponding catalytic performances.

Etude des propriétés photophysiques de complexes d'Iridium(III)

Projet démarré en 2018

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Fabienne Alary**

Cyclometalated iridium(III) complexes typically display intense and highly tunable luminescent emission and can be used as phosphors incorporated into light-emitting electrochemical cell devices for artificial lighting applications, as molecular sensors and as phosphorescent cellular imaging agents for confocal microscopy. Key to their exploitation in these applications is the engineering of the organic ligand supporting the metal centre to enable efficient tuning of the electronic and electrochemical properties. These ligand tuning effects can also determine the localisation and character of the emissive excited state which can have a profound influence on the photophysical properties. In the current project a series of cationic biscyclometalated iridium(III) complex incorporating a pyridyl- (pytz) , pyrimidinyl- (pmtz) or pyrazinyltriazole-based (pztz) ancillary ligand have been experimentally prepared and their photophysical properties investigated. The data show that the ancillary ligand has a significant affect on the photophysical properties leading to a general trend of increasing wavelength of emission in the order pytz < pmtz < pztz. Further, the change in the nature of the ancillary ligand leads wo a switching in the nature of the emissive state from 3MLCT/3ILCT character (MLCT = metal-to-ligand charge transfer, ILCT = intraligand charge transfer) favoured for pytz to 3MLCT/3LLCT for pztz based complexes (LLCT = ligand-to-ligand charge transfer). In addition, for some of the complexes the excited state is observed to switch between these states on warming from 77 K (3MLCT/3ILCT) to room temperature (3MLCT/3LLCT). Indeed, it is significant that for the complex [Ir(ppy)2(pmtz)]+ dual emission from both excited states persists to above room temperatures. The aim of this study, with experimental data directly comes from our collaborator Paul

Elliott (U. Huddersfield, UK),is therefore to provide crucial computational data in in order to understand that photophysical properties of these complexes and offer insights into the emissive excited state dynamics involved. This will entail the optimisation of the ground state and lowest triplet excited states of each complexes, the calculations of their optical absorption spectra and characterisation of the transition involved, determination of the electronic structure through examination of their molecular orbitals and determination of the localisation of the emissive states.

Photoréactivité de complexes de ruthénium(II) et d'osmium(II)

Projet démarré en 2018

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Isabelle Dixon**

Ruthenium complexes are inescapable in solar energy conversion, photocatalysis or photodynamic therapy. They lie at the heart of novel anticancer therapeutic strategies involving the photorelease of biologically active moieties. Microscopic photoreactivity mechanisms have remained elusive during 40 years because they involve excited states that bear no distinct spectroscopic signature (so-called 'dark states'). In 2016, for the first time, our theoretical calculations [a] have allowed us to identify and rationalize the key role of such excited states in photorelease mechanisms, opening the way to a better understanding of photoinstability issues in this family of complexes. This project aims at extending these studies to a large family of complexes (Ru/Os) that display rich and original photoreactivities. Experimental data directly comes from two of our collaborators (Paul Elliott, U. Huddersfield, UK [b] and Sylvestre Bonnet, U. Leiden, NL [c]), following interactive approaches combining experiment and theory in close synergy. [a] Göttle, A.J.; Alary, F.; Boggio-Pasqua, M.; Dixon, I.M.; Heully, J.-L.; Bahreman, A.; Askes, S.H.C.; Bonnet, S. Inorg. Chem. 2016, 55, 4448. [b] Welby, C. E.; Rice, C. R.; Elliott, P. I. P. Angew. Chem. Int. Ed. 2013, 52, 10826; Scattergood, P. A.; Ross, D. A. W.; Rice, C. R.; Elliott, P. I. P. Angew. Chem. Int. Ed. 2016, 55, 10697; Scattergood, P. A.; Khushnood, U.; Tariq, A.; Cooke, D. J.; Rice, C. R.; Elliott, P. I. P. Inorg. Chem. 2016, 55, 7787. [c] Cuello-Garibo, J.-A., Pérez-Gallent, E., van der Boon, L., Siegler, M. A., Bonnet, S., Inorg. Chem. 2017, 56, 4818.

Dernières publications:

- Theoretical Chemistry Accounts (2018) 137:37 - **doi:** pu.doi
- Inorg. Chem. 2018, 57, 3192−3196 - **doi:** pu.doi

Stochastic Quantum Chemistry

Projet démarré en 2018

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Pierre-François Loos**

In the last decade, supercomputers and their ever-growing capabilities have transformed the way one must think and implement quantum chemistry algorithms. In the footsteps of this technological shift, this project aims at revisiting the traditional quantum chemistry methods to make them stochastic by nature. Contrary to their conventional, deterministic parents, these methods are well suited to massively parallel architectures and have proven to be scalable up to hundreds of thousands of cores. A key aspect of this proposal is validate a number of strategies to make the stochastic implementation of these methods both general and practical for large systems. In particular, we propose to take advantage of the zero-variance

principle in order to significantly reduce the statistical uncertainty and weds deterministic and stochastic algorithms to produce an hybrid semi-stochastic massively-parallel method, thereby achieving the best of the two worlds.

Dernières publications:

- Selected configuration interaction dressed by perturbation, Y. Garniron, A. Scemama, E. Giner, M. Caffarel, and P. F. Loos. J. Chem. Phys. 149, 064103 (2018). - **doi:** pu.doi **url:** pu.open_url
- Perturbatively selected configuration-interaction wave functions for efficient geometry optimization in quantum Monte Carlo Monika Dash , Saverio Moroni , Anthony Scemama and Claudia Filippi (2018), in: Journal of Chemical Theory and Computation - **doi:** pu.doi **url:** pu.open_url

Design d'acides nucléiques contraints

Projet démarré en 2018

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Nathalie Tarrat**
Depuis une dizaine d'année nous développons une famille de nucléotides contraints (CNAs) dédiés au contrôle de la conformation des acides nucléiques en particulier dans leurs structures atypiques de la double hélice et biologiquement impliquées dans les processus fondamentaux tels que les interactions protéines /acides nucléiques, les repliements des ARN, l'activité catalytique de certains acides nucléiques.... Nous avons synthétisé des dinucléotides reliés par un cycle dioxaphosphorinane (cycle à six chaînons incluant le phosphore et les deux oxygènes reliés par un pont propylène) qui permet le contrôle des angles de torsion du squelette sucre/phosphate de la chaine polynucléotidique. Des calculs DFT ainsi que des simulations de dynamique moléculaire classique [Angewandte 2006, OBC 2008, Eur. JOC 2011, NJC 2011, Eur. JOC 2012, JNA 2012] nous ont permis de déterminer les conformations et les énergies associées à ces acides nucléiques contraints et se sont avérés en parfait accord avec les structures établies par l'analyse de diffraction de rayons X. Très récemment, la tentative d'introduction d'un atome de sélénium sur le phosphore du cycle, afin de faciliter la cristallisation et le phasage au cours des analyses de diffractions a mis en évidence une migration de ce dernier et une inactivation de la synthèse automatisée des oligonucléotides. Afin de résoudre ce problème, notre piste principale consiste à rendre le phosphore le plus affin possible pour le sélénium. Nous allons pour cela générer deux nouvelles familles : les séléno-aza-dioxa-phosphorinanes et les séléno-diaza-phosphorinanes. Afin de guider les synthèses vers les composés les plus prometteurs, nous souhaitons en amont déterminer à l'aide d'une étude DFT les structures d'énergies minimales des différents candidats (substitutions possible des atomes d'azote du cycle) ainsi que les nouvelles charges partielles portées par le phosphore. Ce travail est réalisé dans le cadre d'une collaboration entre deux laboratoires toulousains : le LSPCMIB (J-M. Escudier - Synthèse organique des acides nucléiques contraints) et le CEMES (N. Tarrat – Modélisation des acides nucléiques contraints).

Mechanism of a Ru catalysed concomitant dihydrogen/B-H activation process: a computational study

Projet démarré en 2017

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)
Porteur de projet: **Chiara Dinoi**

The use of transition metal catalysts may allow the challenging activation of unsaturated bonds such as the inert E-H σ-bonds (E= H, B, Si, C, N). Contrarily to the C=C bond engineering, the synthetic strategies relying on the formation and post-functionalization of embedded-Bsp2-Nsp2 bonds remain challenging and still under-explored. As pioneered by Dewar, they are mostly obtained by Friedel-Crafts cyclization reactions leading to conjugatively stabilized Bsp2-Nsp2 bonds such as azaborines and related compounds.Other approaches such as intramolecular hydroboration or dehydrogenative cylization have also been reported to a lesser extent for the synthesis of different BN-embedded molecular scaffolds. We investigate here the formation of Bsp2-Nsp2-embedded cyclic systems via a recently discovered Ru catalysed concomitant dihydrogen/B-H activation process. As attested by NMR and X-ray diffraction studies this catalytic reaction affords uncommon benzazaborolidines species in good yields. We plan here to study from a theoretical point of view the nature of this catalytic transformation by using DFT calculations. The thermodynamic aspects as well as the mechanistic profile of the reaction will be rationalized and the main parameters enabling the activation processes involved in this selective and efficient transformation will be investigated.

Dernières publications:

- Beguerie, M.; Dinoi, C.; del Rosal, I.; Faradji, C.; Alcaraz, J.; Vendier, L.; Sabo-Etienne, S., ACS Catal., 2018, 8, 939-948. -

DNA polypep

Projet démarré en 2017

LCC - Laboratoire de Chimie de Coordination (UPR 8241)

Porteur de projet: **Colin Bonduelle**

Biologically-inspired nanotechnologies are technologies developed to mimic biological systems and to take advantage of nature's evolution that have resulted in highly efficient and sophisticated systems. To design these innovative nanotechnologies, biology, at the "nano" level, serves as inspiration: the building blocks in the biological world are nanometer-sized natural molecules such as proteins that, when assembled into intermediate length-scaled objects determine and control biological functions. By using bio-inspired chemistry, nanometer-sized biomimetic molecules can now be prepared and organized in nano objects able to interact with the biological world. In this context, the project entitled DNApolypep is a pluridisciplinary project, which associates experimental science and molecular modeling to prepare a new class of polymers fully constituted of amino acids. These polymers are polypeptides obtained by N-carboxyanhydride polymerization in which a nucleic acid moiety will be introduced through the use of post-polymerization click chemistry. This strategy will result in multifunctional pre-structured macromolecules from which interesting self-assembly properties are expected. These macromolecules will be at the origin of innovative drug delivery systems or new classes of therapeutics. Molecular modeling is aimed to be performed by using CALMIP facilities (EOS supercomputer) and includes DFT minimizations of molecular models that perfectly mimic our polymeric structures. These calculations will intend to reveal the structuring properties of the material in aqueous solutions. Non-covalent interactions will be modeled by using appropriate methods within Gaussian software and the solvent effect will be achieved by implicit solvation (energetic continuum).

Dernières publications:

- Biomacromolecules, 2018, 19, 4068−4074 - **doi:** pu.doi

Etudes théoriques des espèces moléculaires impliquées dans les premiers instants de synthèse de nanoparticules métalliques

Projet démarré en 2016

LCC - Laboratoire de Chimie de Coordination (UPR 8241)
Porteur de projet: **Christine Lepetit**
The morphology and the size of the metallic nanoparticles (NPs) prepared in the team Nanochemistry Organisation and Sensors (NOS) in LCC, are strongly dependent of the organometallic precursor and synthesis route, which are determinant for the control of the microelectronic, plasmonic or biological applications of these nano-objects. In order to help in understanding and controlling the nano-objects nucleation and growth processes, the organization of the metallic centers and the chemical reactivity of the molecular species formed during the very first steps of the organometallic synthesis, will be studied using various theoretical tools that will be calibrated from the available experimental spectroscopic data (X-Ray Diffraction, Nuclear Magnetic Resonance (NMR), Infrared (IR) and Raman spectroscopy). On the one hand, using a computational molecular approach, a series of mono- or polymetallic, homo- ou hetero-metallic precursors built with various metallic centers (M or M' = Ni, Cu, Zn, Ag) in various oxidation states and with various amidinate ligands substitution patterns, will be studied using ELF (Electron Localization Function) topological analysis, QTAIM (Quantum Theory of Atoms In Molecules) and NCI (Non-Covalent Interactions) analysis, in order to characterize metal-ligand bonding and metal-metal interactions. On the other hand, the interactions between the stabilizing ligand and the surface metal atoms of the metallic nanoparticle will be investigated using periodic DFT calculations and QTAIM and ELF topological analyses, and carried out for crystalline metallic surfaces used as models of the facets of the nanoparticles.

Dernières publications:

- M. Boukallaba, B. Kerkeni, C. Lepetit, D. Berthomieu Coordination complexes of 4-Methylimidazole with ZnII and CuII in gas phase and in water: A DFT Study J. Mol. Model. 2016, 22, 301/1-10. -
- C. Lepetit, P. Fau, K. Fajerwerg, M. L. Kahn, B. Silvi, Topological analysis of the metal-metal bond: a tutorial review, Coord. Chem. Rev. 2017, 345, 150-181. -

Dianions géminés: des complexes carbéniques aux complexes dimétalliques

Projet démarré en 2016

LHFA - Laboratoire d'Hétérochimie Fondamentale et Appliquées (UMR 5069)
Porteur de projet: **Marie Boutignon**
Due to the increasing number of examples of stable geminal dianions, this kind of species received a growing interest in the 2000's (ACIEE 1999, 38, 1483-1484). The double negative charge carried by a single carbon atom proved to be easily stabilized by a various set of electron-withdrawing substituents, from silyl groups to hypervalent phosphorus. This interest was also supported by the fact that such geminal dianions can be used as precursor for the synthesis of carbene complexes of various metals, especially d0 metals and rare earths metals (Chem. Soc. Rev. 2011, 40, 2164). In some case they also proved to act as non-innocent ligands for CH activation (Organometallics 2005, 24, 4838-4841 ; Chem. Eur. J. 2012, 18, 16136-16344) or hydrogen transfer (Chem. Eur. J. 2015, 21, 1-11). They can also be used as carbenoids precursors (ACIEE 2007, 46, 5947-50)), that can further activate borane (J. Am. Chem. Soc. 2013, 135, 8774-8777). In any of these outbreaks, the use of DFT calculation brought some crucial insight on reaction mechanisms, or fine

understanding of the charge stabilization mechanism. Our project is built on two axes. Firstly, the development of the chemistry of geminal dianions as ligands for transition metal needs some reinforcement. A palladium (II) complex bearing the bis(thiophosphinoyl)methanediide ligand coordinated as a pseudo-carbene has been used in cooperative catalysis for the cycloisomerization of alkynoic acids. A mechanism for this transformation has been proposed. Meanwhile, a variety of analogous platinum (II) complexes have been synthesized in our group; we whish to extend the study to these species, in order to rationnalize and optimize the experimental conditions. Secondly, we will deepen our work on a set of first-row transition metal complexes that were isolated recently but are not properly described yet on an electronic point of view. Amongst those, a homodimetallic complex of iron II features a short iron-iron distance that rise a doubt about the existence of an iron-iron bond. Furthermore, its structure is close to this of the MoFe cofactor, which is the active site of nitrogenase enzymes. Theoretical modelling has already proved to be a helpful tool in the understanding of activation of molecular nitrogen by model complexes (Nature 2015, 526, 96-99). In many aspects, a detailed study of the electronic structure of this homodimetallic complexe – and any related one – is necessary for a proper development of its chemistry.

Dernières publications:

- A. Pujol, M. Lafage, F. Rekhroukh, N Saffon-Merceron, A. Amgoune, D. Bourissou, N. Nebra, M. Fustier-Boutignon, N. Mézailles; Angew. Chem. Int. Ed. 2017, 56, 12264 –12267 - **doi:** pu.doi

Structuration de mélanges de semi-conducteurs organiques pour la photo détection. Etude sur les propriétés photophysiques et photochimiques.

Projet démarré en 2016

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)
Porteur de projet: **Fabienne Alary**
This demand is a cooperative project between four public laboratories in Toulouse (LAAS, Laplace, LCC, LCPQ). Our main objective is to reach a detailed understanding of the electronic structure and of electronic transfers occurring at interfaces present in organic photovoltaic (OPV). Achieving this goal will able us to design and to synthetize original and efficient organic devices for photoconversion. The description of the nano-morphology created upon blending of the two organic semi-conductors (OSCs) will be the subject of extensive theoretical and experimental studies in order to achieve a rationalization and a full description of the electronic phenomena such as the efficiency of excitons diffusion as well as the efficiency of dissociation into free charges from which originates the current. The interfacial morphology and its electronic interactions will be studied by using a set of advanced characterization methods.

Dernières publications:

- JOURNAL OF PHYSICAL CHEMISTRY A. 122, 6532-6545. - **doi:** pu.doi

Modélisation du phénomène de double-échange

Projet démarré en 2015

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)
Porteur de projet: **Nicolas Suaud**

This project concerns the modeling of doped linear transition metal complexes like nickelates (Y2-xCaxBaNiO5) and manganites (La1-xCaxMnO3.) Since the discovery of compounds showing colossal magneto resistance (CMR) in the 1950's, followed by the discovery of high Tc superconductivity in layered cuprates 27 years ago, there has been renewed interest in the study of doped transition metal complexes. Although one can hardly exaggerate the importance of the study of such novel materials, the renewed interest can be attributed to the surprising observation that an anti-ferromagnetic insulator can be transformed into a a superconducting material simply by doping with charged impurities. Taking nickelates for example, such complexes can be represented as a spin-1/2 two-leg ladder of finite length with variable number of holes. The system is modeled using a modified Double Exchange hamiltonian and full/Krylov-Schur diagonalization is used to obtain the low energy spectra. The parallel computational software library SLEPc is employed to get the eigenvalues of the matrices which can grow to very large sizes of the order of 10^9x10^9 elements. Such methods being massively parallel render large calculations feasible. Taking a number(N = 3, 4, 5, 6, 7) of sites and one or two holes the entire parameter (J=t,K=t) phase space is explored to pin-point the phase transitions and critical points of the hamiltonian. Then, detailed calculations are done using physical values of the exchange/coulomb integrals. It is known that there is a ferromagnetic cloud surrounding the impurities, this qualitative result is verified in our calculations. A novel method, in the form of a truncated spin density operator, is used to ascertain the extent of this ferromagnetic cloud. The interaction between two such ferromagnetic regions, due to two holes, is then quantified. Effect of the magnetic field on the transport properties is calculated using the Localization Tensor. We have performed pilot calculations with a set of canonical hamiltonian matrices on the EOS super-cluster and have developed a driver subroutine to couple our code with the SLEPc library. These calculations have successfully shown that SLEPc would be adequate for our matrix diagonalization needs.

Dernières publications:

- Chem. Euro. J , 23, 4380- 4396 (2017). - **doi:** pu.doi
- Mol. Phys. , 115, 2684-2695 (2017). - **doi:** pu.doi

Étude de la réactivité et de la caractérisation des propriétés catalytiques de systèmes allant du cluster à la Nanoparticule

Projet démarré en 2014

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Iker Del Rosal**

Nanoparticles (Nps) exhibit physical and chemical properties intermediate between those properties exhibit of small molecular compounds and the bulk material, resulting from surface or quantum size effects. Special sites are also known to play a role in heterogeneous catalysis and in synthesis over nanoparticles.More efficient nanocatalysts need to be developed, yet the task of discovering novel alternatives has proven to be extremely challenging. Non-magnetic ruthenium (NPs)constitute an important class of catalysts, involved in hydrogenolysis reactions, olefin metathesis, hydrogenation of aromatic compounds, and the FischerTropsch reaction. It is a catalyst of utmost importance which deserves a deeper understanding of its surface properties under the NP state, a range of sizes with possible quantum size effects. In the same way, magnetic nanoparticles are of interest because of their outstanding magnetic properties are expected to lead to a specific catalytic behavior due to their enhanced magnetic moment, and because of their wide range of possible applications, such as data storage, spintronics etc. In this context, we plan to realise in 2014 an extended study of different magnetic and non-magnetic nanomaterials and their use in catalysis.

Dernières publications:

- An Unprecedented Reaction Mode of phosphorus in phosphinidene rare-earth complex: a joint experimental-theoretical study, H. Tian, J. Hong, K. Wang, I. del Rosal, L. Maron, X. Zhou, and L. Zhang, J. Am. Chem. Soc., 140 : 102 – 105, 2018. -
- Surprising Differences of Alkane C-H Activation catalyzed by Ruthenium Nanoparticles: Complex Surface-Substrate Recognition? N. Rothermela, D. Bouzouitab, T. Röthera, I. del Rosal, Simon Tricard, R. Poteau, T. Gutmanna, B. Chaudret, H.-H. Limbachc and G. Buntkowsky, ChemCatChem, doi.org/10.1002/cctc.201801022, 2018. -

Modélisation quantique et classique de systèmes en phase condensée par les méthodes SCC-DFTB et DFT

Projet démarré en 2013

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Jérôme Cuny**

Since a long time, the «Modelling, Aggregates and Dynamics» group (MAD), which is part of the Laboratoire de Chimie et Physique Quantiques (LCPQ), has been interested in combining quantum chemical approaches with molecular dynamics to study and characterise various chemical systems. In particular, a number of studies have been devoted to the characterisation of aggregates such as water and polycyclic aromatic hydrocarbons (PAHs) clusters. The P1320 project intends to extend the expertise of the MAD group to the field of condensed matter science through two main subjects: - Study the influence of nuclear quantum effects (NQE) on the structural and spectroscopic properties of condensed matter systems, in particular aqueous systems. This subject was initiated in 2013 and we are now at the point where we can simulate liquid water including NQE in combination with the self-consistent-charge density-functional based thigh-binding (SCC-DFTB) description of the electronic structure. Our aim is to extend this study to other phases of water. - Study the impact of thermal fluctuations on a range of physico-chemical problems in the liquid and solid phases. In particular, we are interested on the luminescence, fluorescence and reactive properties of various molecular species in solution. We are now also looking at the proton-conduction properties of solid-state compounds. Our goal is to rationalise the influence of the solvent and/or thermal fluctuations on these properties at the atomistic scale level. This work is performed in full collaboration with various members of the MAD group, in particular M. Rapacioli and A. Simon as permanent members.

Dernières publications:

- G. Daigre, J. Cuny, P. Lemoine, M. Amela-Cortes, S. Paofai, N. Audebrand, A. Le Gal La Salle, E. Quarez, O. Joubert, N. G. Naumov, S. Cordier, Metal Atom Clusters as Building Blocks for Multifunctional Proton-Conducting Materials: Theoretical and Experimental Characterization, Inorg. Chem., 2018, 57, 9814–9825 - **doi:** pu.doi
- J. Cuny, F. Jolibois, I. C. Gerber, Evaluation of Gas-to-Liquid 17O Chemical Shift of Water: A Test Case for Molecular and Periodic Approaches, J. Chem. Theory Comput. 2018, 14, 4041−4051 - **doi:** pu.doi

Propriétés moléculaires relativistes

Projet démarré en 2013

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Trond Saue**

The overall theme of the proposed project concerns the calculations of molecular properties in a relativistic framework. In the present period we will proceed along three lines of research: i) We will continue our simulations of X-ray absorption spectroscopy for molecules containing heavy atoms. We would like to add electron correlation through DFT to the method STEX (static exchange approximation), which otherwise shows good performance in that it take into account the significant relaxation effects. We also want to benchmark our methods against experiments for selected molecules. This project will involve a Master student (Timothé Melin). ii) We would like to study the contribution of nuclear volume effects to the isotope fractionation of tungsten (4 stable isotopes). This will be a collaboration with a geochemist (Merlin MEHEUT, assistant professor in the GET lab in Toulouse). iii) We would like to further explore the power of 4-component relativistic coupled-cluster calculations. We plan in particular to study performance and convergence of the calculation of core ionization energies. Another project concerns the calculation of the electric field gradient at the bismuth nucleus in the diatomic molecules BiN and BiP. Combined with experiment, this allows the extraction of the electric quadrupole moment of the bismuth nucleus.

Dernières publications:

- Christopher South, Avijit Shee, Debashis Mukherjee, Angela Wilson and Trond Saue, 4-component relativistic calculations of L_{3} ionization and excitations for the isoelectronic species UO_{2}^{2+} , OUN^{+} and UN_{2} , PCCP 18 (2016) 21010 - **doi:** pu.doi
- Adel Almoukhalalati, Stefan Knecht, Hans Jørgen Aagaard Jensen, Kenneth G. Dyall and Trond Saue, Electron correlation within the relativistic no-pair approximation, J. Chem. Phys. 145 (2016) 074104 - **doi:** pu.doi

Dianions géminés et carbénoides / trimérisation vs oligomérisation de l'éthylène/ réduction de N2

Projet démarré en 2013

LHFA - Laboratoire d'Hétérochimie Fondamentale et Appliquées (UMR 5069)

Porteur de projet: **Nicolas Mézailles**

Over the past years, we have been developing the use of dianions, where the two charges are located on the same carbon atom. These highly sensitive molecules are then used to transfer electron density to metal fragments (transition metals, lanthanides, actinides) in order to form metal carbene complexes. We are interested in probing the nature of the interaction between the M and C by experimental and theoretical methods as well as rationalizing the reactivity of the complexes. We have shown in particular that these dianions can allow the stabilization of the first gold carbene complex. Calculations have guided reactivity tests. In parallel, we study the reduction/functionalization of N2 using designed Mo/Fe fragments. The reactivity is studied in a dual experimental/theoretical approach. Finally, we are interested in finding the experimental parameters that allow the selective trimerisation of ethylene catalysed by Ti complexes. In order to do so, modelisation of the various pathways of oligomerisation/polymerisation have to be done and compared.

Dernières publications:

- Angew. Chem., Int. Ed, 2018, 57, 1874 - **doi:** pu.doi
- Chem. Commun. 2018, 54, 11953 - **doi:** pu.doi

Interaction de pesticides avec les fractions minérale et organique du sol.

Projet démarré en 2012

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Fabienne Bessac**

The first molecule under study was atrazine molecule, 2-chloro-N4-ethyl-N6-isopropyl-1,3,5-triazine-4,6-diamine. It is the active substance of a pesticide which has an herbicide effect. This molecule is one member of the triazine family characterized by an s-triazine cycle. Forbidden within the European Union since 2004, it has still been used in about 80 countries all over the world and is one of the most employed pesticides. The use of atrazine is highly controversial because of its negative impact on the environment. Thus, understanding fate and transport of this compound in soils and water is of great interest. Since 2014, our work has also been dealing with metamitron (herbicide) and fenhexamid (fungicide). To start, the soil has been modeled by only the mineral part. A Ca-montmorillonite clay has been chosen. Our project uses a multiscale approach organized in four levels starting from gas phase molecular systems to condensed phase: • Isolated pesticide ; • Complexes with one or two atomic cations ; • Pesticide on dry montmorillonite ; • Pesticide on hydrated montmorillonite. In order to obtain information on the adsorption of the pesticide on a clay surface, we use the CPMD program with periodic DFT (PBE functional with a D2 dispersion correction). Static calculations and Car-Parrinello Molecular dynamics allow to access physical and chemical properties of the adsorption and desorption of pesticides in soils. Modeling such large systems of about 600 atoms (pesticide + clay surface + water solvent) demands important computing resources.

Dernières publications:

- "Pesticide interaction with environmentally important cations: A molecular dynamics and DFT study of metamitron and fenhexamid." Bastien Belzunces, Sophie Hoyau, Jérôme Cuny, Fabienne Bessac, Computational and Theoretical Chemistry 1117 (2017) 220–234. - **doi:** pu.doi
- Metamitron and fenhexamid interaction with Ca2+-Montmorillonite clay surfaces: a DFT molecular dynamics study. Bastien Belzunces, Sophie Hoyau, Fabienne Bessac, Journal of Computational Chemistry, submitted for publication. -

Etudes mécanistiques de propriétés photochimiques de chromophores organiques

Projet démarré en 2012

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Martial Boggio-Pasqua**

In this project, we propose to study the photochemical mechanisms of various organic chromophores with different applications in view. Two classes of organic chromophores are currently under investigation: 1) photoisomerizable chromophores found in various proteins (PYP, GFP, etc.) 2) photochromic compounds (DHP/CPD, dithienylethenes, DHA/VHF, etc.) used as photoswitches The study of photoisomerizable chromophores will help us to get a better understanding of the initial photochemical events taking place in proteins. We need first to characterize the excited states involved in the competing photochemical processes and to determine the potential energy surfaces associated with these electronic states. We can then explore the various routes leading to the photoizomerization process, including non-adiabatic routes taking place through conical intersections. Such studies require first performing accurate ab initio

calculations on the isolated chromophores. Then, environment effects can be included via a hybrid QM/MM approach and dynamics simulations can be performed. The second type of photoisomerizable chromophores are highly interesting because of their photochromic properties. Photochromic molecular systems have entered the new generation of innovative functional materials with high added value. Applications are already widespread in nanosciences, biology, and photonic or optoelectronic devices as light-activated switches. However, the underlying mechanisms by which these molecular switches operate are often not fully understood. Computational photochemistry provides a very efficient tool to bring detailed insights into these mechanisms. The purpose of this part of the project is to use our expertise in computational photochemistry to rationalize original photochromic behaviors in realistic conditions and to design new systems with improved photoswitchable properties.

Dernières publications:

- Efficient photoswitch system combining a dimethyldihydropyrene pyridinium core and ruthenium(II) bis-terpyridine entities - **doi:** pu.doi **url:** pu.open_url
- Electrochemical control of the switching process of photochromic dimethyldihydropyrene derivatives - **doi:** pu.doi **url:** pu.open_url

Hydrogénation catalytique de nitriles sur une surface de palladium

Projet démarré en 2012

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)
Porteur de projet: **Iker Del Rosal**
Nitriles are important materials in the chemical and pharmaceutical industries. These materials are widely used on the manufacture, via a hydrogenation process, to their corresponding primary amines which have found widespread applications as solvents, fibers for textiles.... However, in contrast to other hydrogenation processes, which usually proceed relatively simply, in the hydrogenation of nitriles a mixture of primary, secondary and tertiary amines are formed. The generally accepted hydrogenation mechanism, proposed by J. von Braun et al. in 1923, suggests that the hydrogenation reaction involves the formation of an imine intermediate. This imine can, in addition to hydrogenation reaction which leads to the primary amine, react with the initially formed primary amines in order to, trough a reductive amination process, give the secondary and tertiary amines. However, although the formation of an imine intermediate as well as the reductive animation process involved in the hydrogenation mechanism of nitriles are generally accepted, several questions remain unanswered. The most important controversy concerns the reactive intermediates for which no experimental evidence allows to clearly determine their nature. The present project is realized in order to shed light on this controversy, by the determination of the synthesis process of the different amines as well as the elucidation of the nature and geometry of the different surface intermediates.

Transition magnétique induite par application d'un champ électrique dans des ions Polyoxométallates

Projet démarré en 2011

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)
Porteur de projet: **Nicolas Suaud**

Magnetic properties of Polyoxometalate (POMs) are particularly attractive for experimentalists and theoreticians. In a series of paper, we clearly identified the microscopic origin of the magnetic properties of 2-electron-reduced POM. This was based on a 2-step approach: i) evaluation of the interactions between metal centers; ii) use of these parameters in a well-suited model Hamiltonian. From this approach, we expect a para- to dia-magnetic transition induced by an external electric field. This result is strenghtened by some DFT calculations. Now, these calculations have to be performed on the POM structure optimized under the influence of an electric field. Moreover, other POMs seem to be good candidates to exhibit such a property but for a much smaller intensity of the electric field. The purpose of the request of computer time is to confirm this assumption.

Dernières publications:

- J. Phys. Chem. Letters, 8, 1695-1700 (2017) - **doi:** pu.doi
- Euro. J. Inorg. Chem. - **doi:** pu.doi

Etude ab-initio des propriétés électroniques dans des systèmes de basses dimensionalités

Projet démarré en 2010

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Thierry Leininger**

The main objective of our project concerns carbon nanotubes as energy storage devices. A few year ago, we showed that ionic nitrogen clusters could be used as high energy density materials. We recently start calculations on the inclusion of N3- and N5+ in zig-zag carbon nanotubes of different sizes. As the nanotubes present some open-shell edge orbitals, it is necessary here to use CASSCF and NEVPT2 calculations. We already determined the carbon nanotube minimum size to fit each cluster. The next step will be to study the inclusion of both salts into the nanotube. We will also repeat the calculations with arm-chair nanotubes which present the advantage to be closed-shell systems and thus allow to use DFT approaches which are less time consuming. Ultimately, these results will serve as starting point to dynamical calculations done by our colleagues in Perugia. Finally, as a background task, we should work on the implementation of the Total Position Spread Tensor (and its counterpart, the Total Momentum Tensor) at the MRCI level in Molpro.

Dernières publications:

- A. Segalina, A. Francé-Monerris, M. Pastore, T. Leininger, S. Evangelisti et A. Monari, Theoret. Chem. Acc. 137, 163 (2018). Conical intersection properties unraveled by the position spread tensor. -
- A. Diaz-Marquez, S. Battaglia, G. L. Bendazzoli, S. Evangelisti, T. Leininger et J.A. Berger, J. Chem. Phys. 148(12), 124103 (2018). Signatures of Wigner localization in one-dimensional systems. -

Structure et Activité Catalytique en Chimie Organométallique

Projet démarré en 2009

LCC - Laboratoire de Chimie de Coordination (UPR 8241)

Porteur de projet: **Mary Grellier**

Our research focuses on the transition metal complex development with non- conventional coordination

modes and specially the understanding of the metal-ligand interaction. One of the main research concerns the chemistry of complex M (sigma- HE) (E = H, C, Si, Ge) including one or more sigma -HE Bonds. Applications in catalysis are at the heart of our studies. The importance of DFT calculations using the Gaussian 09 software is essential for the characterization, the interpretation of the stability and reactivity of our complexes. These calculations are important to confirm our experimental observations and to model the reactivity of these compounds. Our study is divided in two parts: a) Understanding of the stability of various complexes of iron and ruthenium in association with the experimental characterization of these compounds (such as NMR predictions). b) Reactivity studies of these species from a catalytic point of view. We will calculate the energies of the different possible transitions and intermediate states in catalytic hydrofunctionnalization reactions by Iron and ruthenium complexes. We would like to develop increasingly predictive approach of calculations for selecting ligands function of the desired properties in the complexes.

Dernières publications:

- Angew. Chem. Int. Ed. 2017, 56, 16191-16196 - **doi:** pu.doi **url:** pu.open_url
- Dalton Transactions, 2018, 47, 10139-10146 - **doi:** pu.doi **url:** pu.open_url

Etude théorique de propriétés photophysiques et photochimiques de complexes polypyridine de ruthénium

Projet démarré en 2008

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)

Porteur de projet: **Martial Boggio-Pasqua**

Ruthenium nitrosyl complexes have found utility in a variety of applications, such as optical switches and data storage [1], or medicine [2]. Depending on the ancillary ligands, environment, and irradiation wavelength, these complexes can undergo either intramolecular N→O linkage photoisomerization [3] or NO photorelease [4]. However, the mechanism behind these two competing processes is lacking. Preliminary results obtained by our group on the [RuClNO(py)4]2+ complex using density functional theory (DFT) points toward a complex two-photon mechanism on the lowest triplet potential energy surface [5]. A dynamical study using TD-DFT performed by the group of L. González in Vienna provides some information on the initial steps of the photorelease mechanism for a different ruthenium nitrosyl complex [6]. To unravel the photoisomerization and photorelease mechanisms and the factors governing their competition, we propose to study the photodynamics of different ruthenium nitrosyl complexes using ab initio or TD-DFT molecular dynamics (MD), including the description of the intersystem crossings (ISC) between initially populated singlet states to the lower triplet states. In 2016 and 2017, we have performed a theoretical study of the [RuClNO(py)4]2+ complex using highly-accurate ab initio multireference calculations.[7] In particular, we have described the most probable ISC pathways accounting for triplet state population. We have also computed the relevant potential energy surfaces along the N→O linkage photoisomerization pathways and interesting information has been obtained on the photoswitching mechanism of this complex, which confirms and completes our previous DFT study. TD-DFT calculations have also been performed to establish a computational protocol that will be viable for the photodynamics study.[8] In 2018, we wish to continue our study of this complex by computing the NO photorelease pathways. The results are expected to provide some important insight into the competition between the photorelease and the photoisomerization processes. Finally, the photodynamics of this system will be studied by "on-the-fly" nonadiabatic dynamics.

[1] M. Imlau et al., in Nanoelectronics and Information Technology, Ed. R. Waser, Wiley-VCH, 2003, p. 659.
[2] (a) E. Culotta et al., Science 1992, 258, 1862–1865. (b) J. S. Stamler et al., Science 1992, 258, 1898–1902.
[3] (a) P. Coppens et al., Chem. Rev. 2002, 102, 861–883 and 1803. (b) T. A. Bitterwolf, Coord. Chem. Rev.

2006, 250, 1196–1207. [4] N. L. Fry et al., Acc. Chem. Res. 2011, 44, 289–298. [5] J. Sanz Garcia et al., Inorg. Chem. 2015, 54, 8310–8318. [6] L. Freitag et al., Phys. Chem. Chem. Phys. 2015, 17, 14383–14392. [7] F. Talotta et al., J. Chem. Theory Comput. 2017, DOI: 10.1021/acs.jctc.7b00982. [8] A. J. Atkins et al., J. Chem. Theory Comput. 2017, 13, 4123–4145.

Dernières publications:

- Adiabatic versus nonadiabatic photoisomerization in photochromic ruthenium sulfoxide complexes: a mechanistic picture from density functional theory calculations, A. J. Göttle, I. M. Dixon, F. Alary, J.-L. Heully, M. Boggio-Pasqua, J. Am. Chem. Soc. 133, 2011, 9172–9174. - **doi:** pu.doi **url:** pu.open_url
- Linkage photoisomerization mechanism in a photochromic ruthenium nitrosyl complex: new insights from a MS-CASPT2 study - **doi:** pu.doi **url:** pu.open_url

Étude théorique de la structure et réactivité d'un catalyseur greffé sur une surface de silice.

Projet démarré en 2008

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)
Porteur de projet: **Laurent Maron**
The major disadvantage of homogeneous catalysis as well as heterogeneous is the need to remove the catalyst and the ligands (after polymerization) by tedious and expensive treatment (liquid / liquid extraction, adsorption resin, etc.). An attractive alternative is to graft the catalyst systems on insoluble solid supports such as silica or polystyrene reticulated. This technique is at the interface between homogeneous and heterogeneous catalysis, and it avoids the steps of purification of synthesized polymers and to encourage the reuse of the catalyst system. However, by supporting the catalyst on a support coordination entails a loss of control of the intermediate steps of polymerization. The study we want to do is focus on catalysis by d and/or f metal grafted complexes on silica support. So far, we have created different models of an amorphous silica surface treated at different temperatures. We showed that to the five created models, two are in agreement with experimental data obtained for a silica surface treated at 700 ° C, while five models are in agreement with the data obtained for a silica surface treated at 300 ° C. The data used for the theoretical/experimental comparisons is both structural (distance) and spectroscopic (IR and NMR). This work, conducted in collaboration with the experimental team of R. Gauvin (Université des Sciences et Technologies, Lille) and M. Taoufik (Chemistry, Catalysis, Polymers and Processes, Lyon), it is made in the context of the theory of density functional. Our studies has shown that (i) grafting plays an important role on the catalytic activity of grafted complexes compared to their homogeneous counterpart; (ii) the grafting mode it is also important and can strongly modify the catalytic activity; (iii) the NMR is a tool of choice for the characterization of possible grafting modes but also to establish a fruitful exp/théo dialogue.

Dernières publications:

- DFT study of the ring opening polymerization of epsilon--caprolactone by grafted lanthanide complexes : 2-Effect of the initiator ligand. I. del Rosal, R. Poteau, and L. Maron. Dalton Trans., 40 : 11228–11240 (2011). - **doi:** pu.doi
- Reductive CO2 homocoupling: de novo synthesis of a borylated C3 carbohydrate, A. Béthegnies, Y. Escudié, N. Nuñez-Dallos, L. Vendier, J. Hurtado, I. del Rosal, L. Maron, S. Bontemps, ChemCatChem,, accepted, 2018 - **doi:** pu.doi

Clusters et nanoparticules métalliques : structure, propriétés électroniques, spectroscopie et état de surface

Projet démarré en 2006

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)
Porteur de projet: **Romuald Poteau**
Metal particles at the nanoscale are currently an area of intense scientific interest, due to a broad variety of potential applications and from a fundamental point of view as well. These NPs are not so easy to stabilize, owing in particular to their mutual interaction which increases their possible coalescence. A valuable strategy to synthesize colloidal NPs is use an organometallic route. Our 2018 project consists in two main parts and two projects currently in standby: (i) nanocatalyzed water splitting (Year 2) (i_a) coadsorption properties of THF and carboxylate ligands on RuNPs. See progress report, part II (i_b) adsorption properties of photosensitizers grafted on RuNPs (preliminary calculations only at the end of 2017, see progress report) (i_c) redox properties of RuNPs (will be evaluated in 2018) (ii) modification of the catalytic properties of RuNPs by dilution of iron atoms (new topic started in autumn 2017, see progress report, part I) (iii) the dissociation of CO and H2 co-adsorbed on and ReNPs, followed by their recombination (continuation of 2016, no calculations performed in 2017 on this topic) (iv) platinum NPs stabilized by thiol ligands and their influence on the self-organization of the PtNPs (not finished in 2016, no calculations performed in 2017 on this topic, in standby)

Dernières publications:

- J. Creus, S. Drouet, S. Suriñach, P. Lecante, V. Colliere, R. Poteau, K. Philippot, J. García-Antón & X. Sala Ligand-capped Ru Nanoparticles as Efficient Electrocatalyst for the Hydrogen Evolution Reaction ACS Catal., 2018 , 8 , 11094-11102 - **doi:** pu.doi
- J. A. Vargas, V. Petkov, E. S. Nouh, R. Ramaamorthy, L.-M. Lacroix, R. Poteau, G. V. and* Pierre Lecante & R. Arenal Ultrathin Gold Nanowires with the Polytetrahedral Structure of Bulk Manganese ACS Nano, 2018 , 12 , 9521-9531 - **doi:** pu.doi

METHODES MONTE CARLO QUANTIQUE POUR LES MOLECULES

Projet démarré en 2005

LCPQ - Laboratoire de Chimie et de Physique Quantiques (UMR 5626)
Porteur de projet: **Michel Caffarel**
The proposal presented here is part of our long-term project to develop and apply quantum Monte Carlo (QMC) techniques to the electronic structure problem as it is expressed in quantum chemistry (see, the web site of our project "QMC for chemistry at Toulouse", http://qmcchem.ups-tlse.fr). Let us emphasize that from the computational point of view QMC is particularly well-suited to high-performance computing and, more specifically, to massively parallel calculations. For the year to come, we propose to study the following points: i) Application of QMC to the calculation of the vertical excitation energy of several cyanines of increasing size. Comparison with state-of-art methods (CASPT2, GW/BSE, and TDDFT). ii) Detailed QMC study of the singlet and triplet electronic manifolds of formaldehyde including the calculation of many excited-states. iii.) Development of a massively parallel implementation of selected CI approaches (and variants). Such studies being very CPU-intensive we ask for a large amount of computing time on Eos, namely 1 500 000 CPU hours. Such a demand is motivated by the fact that Eos turned out to be an

extremely efficient and useful computational platform for our studies. A Ph.D. student, Yann Garniron will work full-time on this project.

Dernières publications:

- Alternative definition of excitation amplitudes in Multi-Reference state-specific Coupled Cluster - **doi:** pu.doi **url:** pu.open_url
- Hybrid stochastic-deterministic calculation of the second-order perturbative contribution of multireference perturbation theory - **doi:** pu.doi **url:** pu.open_url

Modélisation de composés de coordination et organométalliquespour la catalyse homogène et la polymérisation radicalaire contrôlée

Projet démarré en 2004

LCC - Laboratoire de Chimie de Coordination (UPR 8241)
Porteur de projet: **Rinaldo Poli**
Our computational work is directly connected with the experimental studies going on in our research group, which are centered on homogeneous catalysis and on controlled radical polymerization. It involves the optimization of molecular geometries (global and local minima, transition states when dealing with the study of reaction pathways or catalytic mechanisms, "minimum energy crossing points" when dealing with reaction with a change of spin states), with computation of the energy and of the normal modes of vibration for compounds containing in most cases only one heavy atom (transition metal) plus a certain number of lighter atoms. The calculations may need hybrid QM/MM methods, but in certain cases a full QM treatment is necessary. The group research activity is organized along two distinct topics: (i) controlled radical polymerization; (ii) homogeneous catalysis.

Dernières publications:

- Inorg. Chim. Acta 2018, 470, 365-372 - **doi:** pu.doi
- Eur. J. Inorg. Chem. 2018, 2285-2299 - **doi:** pu.doi

4.6 Mécanique des structures

Foudre Composite

Projet démarré en 2018

ICA - Institut Clément Ader
Porteur de projet: **Christine ESPINOSA**
The lightning damage mechanism for carbon laminate aeronautical structure is a complex multi-physical phenomenon. The lightning current entering into the surface metallic protection, called LSP (Lightning Strike Protection) and the carbon plies generates Joule's effects and magnetic forces which both induce mechanical forces and surface explosion that has a significant mechanical impact. The aim of the project is to compute the damage generated by a high current injection on a CFRP structure using estimations of

explosive load induced by the metallic protection vaporization during a typical lightning strike current injection.

Optimisation topologique de la structure d'attache moteur voilure

Projet démarré en 2018

ICA - Institut Clément Ader

Porteur de projet: **Christian Gogu**

Engine deformations during operation of an aircraft have a sensible impact on the engine's fuel consumption and are thus are an increasing concern for both engine and aircraft manufacturers. The tip-clearance, defined as the radial gap between the blade tip and the engine casing, can show small variations induced by aircraft maneuvers both on the ground and in flight. These variations can produce increased tip leakage flow, secondary flows and vortex losses that can sensibly increase the engine trust specific fuel consumption (TSFC). The topology of the structure connecting the engine to the rest of the aircraft through the wing pylon will directly impact the tip clearances and thus the thrust specific fuel consumption. The project aims at carrying out high fidelity topology optimization of the engine-pylon structure in order to minimize the TSFC. A specific topology optimization framework was developed by the team for this purpose, involving static condensation of the aircraft engine model, mesh coupling of the design zone and condensed engine model, adjoint sensitivities for solving the optimization problem. A main challenge in obtaining high fidelity designs resides in increasing the number of the degrees of freedom (DOF) considered in the design zone (tens or even hundreds of millions of DOFs). To achieve this, the project builds upon recent developments in highly parallel topology optimization frameworks that were recently able to achieve up to a billion DOFs in a HPC environment on simpler minimum compliance topology optimization problems. Upon completion the project is expected to provide innovative high fidelity structural designs for the engine wing assembly that will help reduce the lifetime fuel consumption of future aircraft.

Identification de paramètres pour le modèle thermodynamique du système Cu-Fe-H2SO4-H2O

Projet démarré en 2018

LGC - Laboratoire de Génie Chimique (UMR 5503)

Porteur de projet: **Laurent Cassayre**

Our research project focuses on the process of dissolving a copper ore in sulfuric acid, which is part of the process of producing metallic copper from ore, in order to find the optimal conditions (improve the extraction yields and minimize the acid consumption). The approach consists in establishing a thermodynamic model for the description of the complex system Cu-Fe-H2SO4-H2O. The free PhreeqC geochemical computation software allows the calculation of thermodynamic equilibria involving electrolytic aqueous phases. We have selected the SIT model (Specific ion Interaction Theory), which describes the activity coefficients of aqueous ions notably by taking into account the short range interactions between ion pairs i and k thanks to a parameter εi,k (T). The work in progress consists of identifying the values of the parameters εi,k over the temperature range 25-90 ° C. We estimated at approximately 10 the number of interactions to be considered in describing the full system. The principle adopted for the determination of the parameters is, for each temperature step, to vary the values of each εi,k in a fixed range, to calculate the thermodynamic equilibrium, and to minimize the difference between all calculated values and an experimental data set. The determination of the interaction parameters has been initiated on the H2SO4-H2O subsystem, with two interaction parameters. To do this, we have developed a procedure based on the use of a Fortran code that calls the Phreeqc software. This approach made it possible to determine the two

interaction parameters as a function of temperature, with calculation times of a few hours. Further work on the Fe-H2SO4-H2O subsystem, however, comes up against the length of the calculations. Thus, in the current configuration (4 pair interactions), a calculation takes about ten days, which is very penalizing to test our approach. The present request to Calmip therefore aims to allow us to progress in our modeling work, by reducing the computation time. We estimated it at 50,000 hours, which corresponds to about 200 computational configurations.

Traitement numérique de la localisation et de la rupture dans les matériaux structuraux sous sollicitations sévères

Projet démarré en 2016

ICA - Institut Clément Ader
Porteur de projet: **Patrice Longère**
Under severe loading, including shock and impact, structural materials are subjected to large strain, high strain rate and temperature rise, at least locally. The resulting thermal- and/or damage induced-softening may lead to strain localisation in narrow bands and further fracture. The standard finite element method is known to suffer from pathological mesh dependence in the softening regime. There exist different technique aiming at attenuating this mesh dependence. The one adopted herein consists in embedding the band of localised deformation in the representative volume element and developing enriched constitutive models and/or finite element kinematics in user subroutines for solving complex initial-bounadry value problems. Those developments are currently in progress in the framework of Johannes Wolf and Dorothy Hannah-Lois PhD studies.

Dernières publications:

- H.L. Dorothy and P. Longère. Modelling of high strain rate Adiabatic Shear Banding induced failure: a comparison of two approaches. International Journal of Impact Engineering. 110, 219-227. 2017 - **doi:** pu.doi

Amélioration des méthodes de prédiction du glissement dans les assemblages vissés dû à des chargements thermoélastiques et vibratoires

Projet démarré en 2015

ICA - Institut Clément Ader
Porteur de projet: **Alain Daidié**
The thesis entitled "Improving prediction methods of the slip in screw connections due to thermo- elastic and vibratory loads" is a continuation of a work initiated at Icam Toulouse. It is followed by CNES and Thales Alenia Space and started in September 2014 at the Icam Toulouse Mechanics Department. The main objective of the thesis is a better prediction of the slip in screw connections (conventional screws , screw / nut) for several types of space applications. First, we aim to reduce the size of connections to gain mass to improve mission costs and / or increase the payload. On the other hand , the actual stiffness of the screw connections have to be determined according to their application , in order to improve the finite element model representing the behavior of the complete structure . Slip can have several more or less important consequences. For example , in the case of an observation telescope, the performance of the equipment may be affected by a single micro-slip . In the case of a structural screw, sliding can induce a change in the

modal behavior of the equipment involved and lead to critical eigenmodes couplings between the equipment and the satellite. Ultimately, this thesis aims to provide comprehensive and optimized methods for calculating slip . In practice, this involves the construction of detailed finite element models to correctly model the mechanisms of sliding, the realization of a substantial number of tests to compare modelizations to practice and programming of advanced slip prediction tools.

Dernières publications:

- R. Thanwerdas, E. Rodriguez and A. Daidié. Stiffness and slip laws for threaded fasteners subjected to a transversal load. Proceedings of International Joint Conference on Mechanical Design Engineering & Advanced Manufacturing (JCM2016) p.517-526, 2016 - **doi:** pu.doi
- R. Thanwerdas, E. Rodriguez, A. Daidié, M. Heim and C. Fabries. Industrial Equivalent Modelling of a Screw Assembly Subjected to a Thermal Load. Proceedings of 14e European Conference on Spacecraft Structures, Materials and Environmental Testing (ECSSMET) p.1-15, 2016 -

Étude des pièces composites de formes complexes /// Développement d'un essai Arcan dynamique

Projet démarré en 2012

ICA - Institut Clément Ader
Porteur de projet: **Steven Marguet**
This thesis work deals with the characterization and the modeling of the mechanical behaviour up to failure of laminated composite structures involving complex shapes. One of the major failure modes of laminated composite parts is the demalination. A way to prevent this issue is to design the parts in such a way that avoids the occurence of these phenomenon. Double curved parts present these suited characteristics in terms of prevention of delamination. The study is going to follow three steps: - parametric experimental study on elementary coupons to identify and understand the phenomena - characterization and modeling of the local orientation of the fibers of the composite - modeling of the whole part with suited mechanical behaviours

Dernières publications:

- B. Vales, S. Marguet, R. Créac'hcadec, L. Sohier, J.-F. Ferrero and P. Navarro. Numerical study of the local behaviour of adhesive bonds under dynamic loading. Journal of Adhesion Science and Technology. 30(12)1319-1339. 2016 under Dynamic Loading - **doi:** pu.doi
- B. Vales, S. Marguet, R. Créachcadec, L. Sohier, J.-F. Ferrero and P. Navarro. Experimental & numerical study of the Tensile/Compression-Shear Arcan test under dynamic loading. International Journal of Adhesion and Adhesives. 78, 135-147. 2017 - **doi:** pu.doi

MOdélisation CInétique de Plasmas sur Supercalculateur dans le contexte de sources d'ions - MOCIPS

Projet démarré en 2011

LAPLACE - Laboratoire Plasma et Conversion d'Energie (UMR 5213)
Porteur de projet: **Laurent Garrigues**
Most of the time low temperature plasmas (LTP) can be simulated using fluid approaches because the

distance between two collisions is orders of magnitude lower than the characteristic length of the system. At low pressure, when the number of collisions becomes rare, fluid approaches fails. One way to simulate LTPs at low pressure is to solve the Boltzmann equation using kinetic-particle approaches, where the unknown is the distribution function of the particles that constitute the plasma in phase space. In particle methods used in LTPs, the computational domain is divided in cells. The plasma (electrons and ions) is simulated with a larger number of particles. From a given distribution of electromagnetic fields, particle trajectories are integrated. The charged densities are calculated on grid nodes from the positions of all the particles. From charged particle distributions, the electromagnetic fields are obtained solving Maxwell equations. Collisions between charged particles and background gas are treated with statistical methods. This technique is referred as Particle-In-Cell Monte Carlo Collisions (PIC-MCC) in the literature. PIC-MCC methods are well suitable for parallel computing. PIC-MCC methods are developed and used in the LAPLACE laboratory in the GREPHE research group in the context of projects with CNES and SNECMA for plasma propulsion for satellites, EUROfusion for ion sources of the ITER neutral beam injector. PIC-MCC methods are used to better understand the electron transport across magnetic field barriers in these ion sources. This technique has been already successfully used on the Eos cluster through the study of electron transport in a Hall Thruster for plasma propulsion, extraction of negative ions in the ITER context (a new type of source will be also studied). A new topic concerns the study of magnetron whose geometry and plasma conditions are relatively closed to the Hall thruster but whose application is related to coating for industrial applications. The goal of this project is to use a previously parallel hybrid OpenMP/MPI PIC-MCC model in a 2D, 2.5D and few 3D versions.

Dernières publications:

- G. Fubiani, L. Garrigues, and J. P. Boeuf, "Modeling of negative ion extraction from a magnetized plasma source: Derivation of scaling laws and description of the origins of aberrations in the ion beam", Physics of Plasmas 25, 023510 (2018) - **doi:** pu.doi
- J. P. Boeuf and L. Garrigues, "ExB Electron Drift Instability in Hall Thrusters: Particle-In-Cell Simulations and Theory", Physics of Plasmas 25, 061204 (2018) - **doi:** pu.doi

Modélisation au crash de structures composites élémentaires

Projet démarré en 2010

ICA - Institut Clément Ader

Porteur de projet: **Samuel Rivallant**

Thanks to their high strength-to-weight ratio, composite materials are widely used in the field of transport and especially in aerospace applications, where weight savings are important. But specificity and complexity of composite fractures modes make difficult the prediction of the mechanical behaviour of composite structures subjected to crush loading. Numerous studies have been done in the last decades and the interest in crashworthiness is still present as show the recent works on the subject. But there is still a lake in numerical simulation. Most of the models developed in the last few years are based on global tests characterisation that make the model depend on global parameters, which do not permit to have predictive models. Some models are based on material characteristics, but often need an a priori knowledge of the crush damage mode developed in the crush front. The challenge today in crashworthiness simulation is then to be able, from elementary material characterisation data, to predict both crush damage modes and energy absorption in any structures. This study propose a finite element model for simulation of crushing of composite plates and sandwich structures under impact.

Dernières publications:

- ISRAR H.A.. : Etude expérimentale et numérique de l'écrasement de stratifiés composites à base de fibres de carbone. Thèse de doctorat de l'Université de Toulouse, soutenue le 21/02/2014. -
- - Wilhelm A. Rivallant S. Ferrero JF. : Study of the deformation of a sandwich shield subjected to bird impact: A behaviour analysis tool using vector decomposition, Journal of Sandwich Structures and Materials, 2018 online -

Modélisation d'endommagement sur plaque stratifiée composite

Projet démarré en 2010

ICA - Institut Clément Ader
Porteur de projet: **Christophe Bouvet**
The project presented here is focused on the numerical modeling of composite laminates made of unidirectional plies. The objective is to develop predictive models of impact and post-impact residual strength. At the same time, experimental studies are conducted to investigate the damage scenario during impact and compression after impact (CAI), and provide experimental data to validate the simulations. A finite element modeling with a Discrete Ply Model (DPM) approach is performed based on previous work done at the laboratory. This approach allowed us to simulate damage development in composite structures for aeronautical applications. This approach was applied during the phds of Benjamin Ostré and Hakim Abdulhamid for impact solicitations and is currently used during the phds of Nicolas Dubary, Pablo Garcia Perez and Fadhel Chatti.

Dernières publications:

- Dubary N., Bouvet C., Rivallant S., Ratsifandrihana (2018) Damage tolerance of an impacted composite laminate, Composite Structures, Vol. 206, pp. 261-271 - **doi:** pu.doi
- Chatti F. ., Bouvet C., Poquillon D, Michon G. (2018) Numerical modelling of shear hysteresis of entangled cross-linked carbon fibres intended for core material, Computational Materials Science, Vol. 155, pp. 350-363 - **doi:** pu.doi

Flux réactif activé par décharges couronne

Projet démarré en 2010

LAPLACE - Laboratoire Plasma et Conversion d'Energie (UMR 5213)
Porteur de projet: **Olivier Eichwald**
Le projet concerne l'optimisation des réacteurs plasmas utilisant des décharges électriques de type couronne pour la décontamination biologique et/ou chimique de l'air ou de l'eau. Ces réacteurs sont très efficaces lorsque la concentration des polluants est très faible (quelques centaines de ppm) dans le mélange gazeux. Quelques soient leurs configurations, on distingue deux phases dans les procédés corona qui se suivent et se répètent en permanence. Ces deux phases sont caractérisées par des échelles de temps et d'espace très différentes : - Dans la première phase, dite phase de décharge et qui dure quelques centaines de nanosecondes, des ramifications de décharges filamentaires (de diamètres de quelques dizaines de microns) génèrent par collisions entre électrons énergétiques et molécules du gaz des radicaux chimiquement actifs dans des proportions similaires à celles des polluants. - Dans la seconde phase, dites

phase de post-décharge et qui dure quelques millisecondes, les radicaux sont transportés par le gaz réactif en écoulement, diffusent et réagissent avec les polluants pour les transformer en espèces inoffensives. L'optimisation des procédés plasmas de type corona passe par l'estimation de la production et de la répartition des radicaux formés durant les phases de décharge et par une meilleure compréhension des mécanismes physico-chimiques de transformation des polluants lors des phases de post-décharge. L'étude par la simulation de la première phase fait l'objet de demandes régulières dans le cadre du projet CALMIP (Projet « Plasma Removal »). Ce nouveau projet concerne l'utilisation du logiciel FLUENT pour la simulation instationnaire d'un écoulement gazeux réactif activé régulièrement par des décharges filamentaires de type couronne.

Dernières publications:

- M. Meziane, O. Eichwald , J.P. Sarrette , O. Ducasse and M. Yousfi, "Multi dimensional simulation of a polluted gas flow stressed by a DC positive multi-pins corona discharge reactor", International Symposium on Non-Thermal Plasma Pollution Control Technology & Sustainable energy, ISNTP 8, 25-28 june 2012, Camaret, France (Invited Conference) -
- J.P. Sarrette, O. Eichwald, O. Ducasse, "Electro-hydrodynamics simulation of ozone production in a multi pins to plane corona discharge reactor", 22nd International Conference on Gas Discharges and Their Applications (GD 2018), Novi Sad Serbia, September 2-7, 2018 -

Impact sur structure composite (pales d'hélicoptère)

Projet démarré en 2009

ICA - Institut Clément Ader

Porteur de projet: **Pablo Navarro**

This project aims to study the degradation of helicopter blades in composite material subjected to high velocity impact loadings. The final objective is to develop a strategy for modeling the physical phenomena involved in order to be able to predict the residual state of a blade after impact. The numerical model must be validated by performing impact tests. The phenomena are strongly non-linear, and many variable are required to characterize the state of the components of the composite blade. A significant computing power is indispensable to progress at this stage.

Dernières publications:

- F. Pascal, O. Dorival, P. Navarro, S. Marguet and J.-F. Ferrero. Impact damage prediction in thin woven composite laminates – Part I: Modeling strategy and validation. Composite Structures. 190, 32-42. 2018 - **doi:** pu.doi
- F. Pascal, A. Rogani, B. Mahmoud, P. Navarro, S. Marguet and J.-F. Ferrero. Impact damage prediction in thin woven composite laminates – Part II: Application to normal and oblique impacts on sandwich structure. Composite Structures. 190, 43-51. 2018 - **doi:** pu.doi

Plasma ReMoval

Projet démarré en 2006

LAPLACE - Laboratoire Plasma et Conversion d'Energie (UMR 5213)

Porteur de projet: **Olivier Eichwald**

The 3D-Streamer project aim is to optimize plasma reactors (corona discharges) in the framework of biological and/or chemical decontamination of air or water (acting in surface). To optimise the plasma reactor, we have to estimate the production of radical species (O, OH, N, HO2) within the discharges channels produced during the discharge period by electronic impacts on the gas molecules (N2, O2, CO2, H2O). The radical production is important to quantify, since radicals participate to the transformation of oxides and bacteria, during the post-discharge. But, experimentally it is very difficult to obtain the radical concentration and their nature within the channels, due to their thickness (about 10µm), formation velocity (about 10ns on 1cm), and due to its unpredictable localisation. Thus, the objective is to estimate the radical production within the plasma channels, during the discharge period by means of modelling. Then, indirectly, the numerical results (species concentration, but also nature and chemical scheme) are experimentally validated with an electric diagnostic and an optical one.

Dernières publications:

- O. Ducasse, J-M. Plewa, O. Eichwald, P. Dessante, C. Jacobs, N. Renon and M. Yousfi, "Simulation of 3D Streamer branching using High Performance Computing", Conference SFE, Grenoble -
- O. Ducasse, J-M. Plewa, O. Eichwald, "3D Streamer Simulation in a point to plane configuration", Conference GD2018, Novi Sad -

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4.7 Physico-chimie des matériaux

Approche multi-méthodes pour l'exploration du paysage énergétique dans les systèmes complexes

Projet démarré en 2018

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Marie Brut**

Ce projet accompagne une nouvelle thèse dont le but est d'exploiter et de coupler l'algorithme des Modes Statiques (MS) avec des calculs DFT pour guider ces derniers et ainsi diminuer l'intervention de l'utilisateur nécessaire pour fournir la liste exhaustive des événements utilisés pour alimenter d'autres codes, tels que le Monte Carlo Cinétique. La méthode des MS a été initialement développée pour traiter les mouvements de biomolécules et la complexité des paysages énergétiques associés. Nous visons maintenant à rendre cette méthodologie transférable à tous les types de matériaux d'intérêt (biohybride et inorganique). Cette nouvelle approche doit donc permettre de gagner du temps dans l'exploration du paysage énergétique en guidant la DFT et en optimisant le choix des évènements significatifs pour l'évolution du système, et donc de participer à la conception d'une méthodologie multi-échelle innovante, prédictive, adaptée aux systèmes complexes tout en conservant un temps de calcul réduit.

erosion dynamics of wet granular materials

Projet démarré en 2018

LMGC - Laboratoire de Mécanique et Génie Civil (UMR 5508)
Porteur de projet: **Thanh-Trung Vo**

Fracture of silicate glasses : Insight from atomistic simulations

Projet démarré en 2018

L2C - Laboratoire Charles Coulomb (UMR 5221)
Porteur de projet: **Simona Ispas**
Silicate glasses are traditionally considered as brittle materials, since they break without appreciable deformation and by rapid crack propagation. However the fracture mechanisms of silicate glasses are far from well understood, and noticeable structural rearrangement and plasticity are expected at the microscopic scale (nm). We aim to use computer simulations in order to obtain a deeper understanding of the fracture behaviour of glasses at the atomic scale. Atomistic simulations have the advantages that they provide detailed information of the atom arrangements that are hardly accessible by current experimental techniques. With these atomic scale structural and mechanical information, we thus can make comparison and connections to the macroscopic mechanical behaviours. Our preliminary simulation results have suggested that reliable insight can be obtained only if one generates big simulation samples. We thus need to carry out simulations with relatively large system sizes, i.e. ~400,000 atoms, and thus minimize the finite size effect. These simulations require computer time that is outside the capacity of our current computer resources, and thus we apply to use the resources of CALMIP center. We use LAMMPS, a classical molecular dynamics code, to carry out such simulations. Lammps is used mainly for academic purpose, and it is distributed as an open source code under the terms of the GPL. Openmpi and fortran libraries are prerequisites in order to compile and run LAMMPS properly. LAMMPS runs on single processors or in parallel on multiple CPUs using message-passing techniques and a spatial-decomposition of the simulation domain.

Manipulation de la Charge de nanoparticules métalliques sur des surfaces isolantes

Projet démarré en 2018

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **David MARTROU**
Electron or hole transfer processes in semiconductor or insulating interfaces, which are sandwiched between metallic electrodes, are important elementary processes in any kind of micro- or nano-electronic component. To reach a level of information at the atomic level it is necessary to work on model systems composed of metallic 3D nanoparticles or 2D islands (indistinctly labelled NP in the following) which are supported on an insulating layer, and with non-contact AFM (nc-AFM) and related techniques like EFM and Kelvin probe force microscopy (KPFM) which allow explicitly charging metal NPs and quantifying their charge via measuring the electrostatic interaction between the tip and the surface. The objective of this project is to study CT processes (1) between a metallic NP and a conducting support through an insulating thin film of thickness t (1 nm< t <100 nm) and (2) between two NPs under the influence of the insulating film. Such CT processes will be studied in dependence on the film thickness and structure (monocrystalline, polycrystalline, amorphous), and on the NP morphology (e.g., size). In an ideal, defect-free film, CT mechanisms involve tunnelling or internal field emission. They depend on the electronic structure of the insulating film but also on the metal-insulator interfaces where, even in the absence of extrinsic defects, specific states (e. g., metal induced gap states (MIGS) or insulator surface states) can play a role. Modelisation and theoretical calculations will be used to assist experiments describing and predicting

charge/discharge phenomena of NPs. In particular the calculations will consider two systems: 2D Au islands on AlN(0001) and Au or Pd NPs on MgO(001) for which preliminary experiments suggest that charge can be injected from the AFM tip in a controlled way. The understanding gained in the study of these systems will be used to interpret same experiments for metal NPs grown on amorphous hafnium oxide (hafnia, HfO2) films.

Dernières publications:

- Giant (12×12) and (4×8) reconstructions of the 6H-SiC(0001) surface obtained by progressive enrichment in Si atoms David Martrou, Thomas Leoni, Florian Chaumeton, Fabien Castanié, Sébastien Gauthier, and Xavier Bouju Phys. Rev. B 97, 081302(R) (2018) - **doi:** pu.doi
- Stabilization of Au Monatomic-High Islands on the (2×2)−Nad Reconstructed Surface of Wurtzite AlN(0001) Benoit Eydoux, Bulent Baris, Hassan Khoussa, Olivier Guillermet, Sébastien Gauthier, Xavier Bouju, and David Martrou Phys. Rev. Applied 8, 044002 (2017) - **doi:** pu.doi

Structure atomique et conductivité électrique de matériaux pour mémoires à changement de phase

Projet démarré en 2017

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Alain Claverie**
Ce projet va probablement faire intervenir un stagiaire de 5ème année INSA ou un stagiaire M2 de l'UPS (un sujet de stage vient d'être proposé aux étudiants sur ce thème). L'étudiant recruté commencera son stage en 2017. Nous allons nous concentrer sur l'étude du lien entre la structure atomique et chimique locale de composés à changement de phase dont la composition est proche de celle de Ge2Sb2Te5, et les propriétés électriques de ces composés, en particulier leur conductivité électrique. Il s'agira de comprendre si la conductivité peut être ajustée via le désordre d'alliage (lorsque les conditions de synthèse ou les traitements termiques sont telles qu'une proportion non négligeable d'atomes sont sur des anti-sites), via la composition chimique globale (écarts à la stoïchiométrie de Ge2Sb2Te5) ou lorsque la successions des plans cristallins compacts (ainsi que leur composition chimique) est intermédiaire entre celle correspondant à la phase cubique et celle correspondant à la phase hexagonale. La structure cristalline des ces phases cristallines et de leur écart à l'ordre parfait sera étudiée soit dans des supercellules (avec les codes Wien2k et Vasp, ce qui donnera accès aux longueurs de liaison chimique précises qui peuvent changer d'un site atomique à l'autre, en fonction de la nature précise des premiers voisins qui peut être modifiée par le désordre) soit par la méthode CPA qui permet d'étudier le cas de systèmes dans lequel le désordre atomique est parfait. La conductivité électrique sera calculée à l'aide du code SPR-KKR.

Modélisation des processus physico-chimiques liés au water-splitting pour la production d'hydrogène

Projet démarré en 2017

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)
Porteur de projet: **Alain Esteve**
The photo-induced splitting of water molecules using sunlight to produce hydrogen is currently attracting interest as a long term technological route, with the potential for low to zero greenhouse gas emission. Our goal is to support this technological development, and particularly LAAS-experiments on this subject, by

addressing fundamental issues at the core of the design of optimized devices. During the year 2017, we will first focus on the basic understanding of the chemistry of water dissociation on neutral ZnO model-surfaces (polar Zn or oxygen terminated surfaces, orientation, hydroxylated surfaces, surface defects) to draw scenario for H2 or/and O2 production. In a second step, we will concentrate on the comparison of these gas/surface mechanisms with results obtained when treating explicitly a liquid phase (water environment). The setting up of phenomenological kinetic Monte Carlo or continuum models and electronic transport issues are planned in the mid term (2018).

Dernières publications:

- Water dissociation and partial hydroxylation of perfect and defective polar ZnO model-surfaces, Mathilde Iachella, Jeremy Cure, Mehdi Djafari Rouhani, Yves Chabal, Carole Rossi, Alain Estève ACS J. Phys. Chem. C 122 (38), 21861 -

Étude des couches minces nanocomposites à base de nanoparticules d'Ag enrobées dans la silice pour des propriétés antimicrobiennes contrôlées

Projet démarré en 2017

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Magali Benoit**
This project aims to study nanocomposite thin films based on Ag nanoparticles coated in silica for controlled antimicrobial properties. Metallic nanoparticles, in particular Ag nanoparticles (AgNPs), are known for their chemical activity but also for their plasmonic properties. In order to control their interaction with the environment and to protect them from rapid oxidation, one strategy is to coat them. Coatings containing an antibacterial agent such as AgNPs have the potential to simultaneously exhibit a high antibacterial efficiency and a high exaltation of the vibrationnal and luminescent signals originating from molecules located in their vicinity. It is precisely this potential that we wish to exploit in this project by means of specific dielectric layers containing AgNPs. In this context, small AgNPS (<20 nm) coated in silica matrices were manufactured at CEMES. By studying their eco-toxicity (by measuring the inhibition of photosynthesis of green algae), it has been shown that the release of silver atoms is controlled by the depth at which the AgNPs are embedded in the silica host matrix. However, mechanisms for the release of Ag ions and their diffusion through the thin layer of silica are not well understood. The objective of this project is therefore to provide some answers to these questions by performing simulations at the atomic scale. In particular, we intend to model the SiO2/Ag interface for more or less hydrated silicas in order to study the influence of the water content on the diffusion mechanisms of the Ag ions. The SiO2/Ag interfaces will be prepared using classical molecular dynamics simulations, then they will be annealed by ab initio molecular dynamics in order to obtain more reliable structural characteristics of the interface as well as its electronic properties. The calculation of the spectral signatures of the different chemical species present at the interface can also be envisaged for the purpose of a direct comparison with experimental results. Finally, once the interfaces are characterized, we intend to study the diffusion mechanisms of the different chemical species involved in the release of Ag ions through the silica matrix.

Etude de la ségrégation aux joints de grains cfc et cc

Projet démarré en 2017

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)
Porteur de projet: **Damien Connétable**
The aim of this project is to use a multi-scale approach coupling electronic structure calculations (DFT) and statistical approach to predict the amount of hydrogen and phosphorus (or sulfur) that can simultaneously segregate on grain boundaries (Fe cc and Ni fcc) and to understand whether the co-segregation of these two species induces further embrittlement of the materials. To do this, a multi-physics approach is developed: the results of the first-principles calculations (segregation energies) will be used in a statistical physics model to compute segregation rates, specific segregation isotherms... These informations can not be obtained experimentally because of the low concentrations of impurities involved and the difficulty of quantifying the chemistry of the material around grain boundaries. DFT calculations have already shown that they provide valuable information for understanding impurity segregation embrittlement phenomena, but the effect of an interaction of different impurities remains unexplored.

Mechanical properties of structured polymer gels

Projet démarré en 2017

SPO - Sciences pour l'œnologie
Porteur de projet: **Virginie Hugouvieux**
Certain biopolymers transform into a gel because of a catalytic reaction in which freely moving catalysts, called enzymes, convert repulsive monomers of the polymers into attractive ones. These attractive monomers stick to each other and make that the polymer solution slowly transforms into a gel. Important examples for such systems occur in plant cell walls where some polysaccharides (pectins) undergo gelation due to the presence of an enzyme (pectin methylesterase). We have developed a simple model consisting of bead-spring polymers (~pectins) and soft particles (~enzymes) that can serve to describe such systems. Using large scale computer simulations we have studied how the homogeneous polymer solution becomes unstable due to the increasing fraction of attractive monomers making that at low temperatures the system transforms indeed into a gel. We have found that before the system reaches at long times one of these two phases, it forms at intermediate times a surprisingly regular cluster phase. The goal of the present project is to determine the mechanical properties of this novel gel phase. In particular we want to determine the elastic moduli as well as the Poisson ratio and correlate these quantities with the internal structure of these materials. Very few numerical investigations on this topic can be found in the literature and none of them address the connection between the internal structure of the gel with its mechanical properties. Comparison with standard polymer gels will give insight into the advantages of such structured gels for applications. Since gels show disorder on large length scales, one needs to consider samples that are relatively large (200,000 particles) and simulate them for long times (O(10^8) time steps). This is the reason why we will need a supercomputer to carry out this investigation.

Simulations de l'adsorption des ions dans des carbones poreux modèles pour étudier les relations structure – performance dans les supercondensateurs

Projet démarré en 2017

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)
Porteur de projet: **Céline Merlet**
Supercapacitors are of great interest as energy storage systems because they exhibit very high rates of charge/discharge, long cycle lifes, and they are made of cheap and light materials. These attractive properties arise from the electrostatic nature of the charge storage which results from ion adsorption in the

electrode pores. Recently, it was demonstrated that ions can enter pores of sub-nanometer sizes leading to a huge increase of capacitance. This was an important breakthrough as the energy density of supercapacitors, relatively low compared to batteries, is what currently limits their application. The progress towards more powerful supercapacitors is limited by our incomplete understanding of the relation between their performance, in particular their capacitance and charging rate, and the complex structure of the porous carbon electrodes. To make progress we need a better fundamental understanding of the ion transport and electrolyte structure in the pores. In this project we are planning to use classical molecular dynamics simulations to calculate the capacitive and transport properties of a range of systems. We will focus on model ordered three-dimensional porous carbons which are currently the missing link between oversimplified geometries, such as planar graphitic structures and carbon nanotubes, and disordered realistic structures. This will allow us to vary geometric descriptors, e.g. pore size and ion size, in a systematic way and obtain relevant microscopic information. This classical molecular dynamics study will be coupled with the development of original mesoscopic models in order to allow for a systematic screening of porous carbons for energy storage application.

Méthodes stochastiques pour l'exploration du paysage énergétique de systèmes moléculaires : Application aux biomolécules sur surfaces

Projet démarré en 2016

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Nathalie Tarrat**
Comprendre la structure et le comportement des biomolécules sur des surfaces est d'un grand intérêt pour la recherche fondamentale et les applications technologiques. Ces dernières années, des algorithmes issus de la recherche en robotique sont apparus comme une nouvelle approche pour l'exploration du paysage énergétique de systèmes moléculaires. En collaboration avec le Prof. Dr. Christian Schön du Max Planck Institute for Solid State Research (Stuttgart, Allemagne) et l'université de Koskalin (Pologne), nous appliquons ces méthodes à l'étude de petites molécules organiques (disaccharides) sur des surfaces métalliques. Notre projet consiste à identifier un ensemble de conformations correspondant aux états les plus probables du système. Etant donné que les états les plus probables sont ceux qui minimisent l'énergie du système, il s'agit donc de résoudre un problème d'optimisation globale, dans lequel il ne s'agit pas de calculer seulement le minimum global, mais un ensemble de minima suffisamment représentatif. Pour traiter ce problème en très haute dimension, nous travaillons au couplage de méthodes stochastiques d'exploration et d'échantillonnage inspirées d'algorithmes utilisés en robotique avec des méthodes d'optimisation locale et des méthodes de clustering. Afin de valider cette approche, il a été nécessaire de comparer les minima localisés avec ceux issus de calculs à haut niveau de théorie. Pour cela nous avons confronté nos résultats à ceux issus d'une étude DFT-D, i.e. en tenant compte explicitement des électrons et des forces de Van der Waals. Le système modèle étudié était constitué d'une molécule de tréhalose déposée sur du Cu(100). Nous avons également mis au point un protocole nous permettant d'aller de l'étude de la molécule unique validée sur le trehalose à la simulation de sucres auto-organisés. Nous souhaitons maintenant nous assurer que notre approche nous permet de prévoir les différences de réactivité des différentes facettes cristallographiques du cuivre Cu(XXX) mais également de deux autres métaux de type d9 très utilisés pour des applications in vivo ou en tant qu'antibactériens, l'or et l'argent. Pour cela nous allons dans un premier temps réaliser des décompositions énergétiques pour les différents couples M(XXX) / molécule, puis dans un second temps, confirmer par DFT les résultats obtenus par robotique en terme de structure et de stabilité. Des expériences sont également réalisées au sein du MPI auxquelles seront confrontés nos résultats.

Interprétation atomistique du fonctionnement d'un capteur de gaz

Projet démarré en 2016

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)

Porteur de projet: **Anne Hemeryck**

Water vapour is the omnipresent interfering component for gas sensing in ambient conditions. Even more than four decades after the first SMOX-based gas sensor came on the market, the cross sensitivity to water vapour is still one of big issues for gas sensing in ambient conditions. Most of the current models describing the interaction of water vapour with SMOX surface were empirically developed more than one or two decades ago and fail to satisfactory explain the recent experimental findings. A critical revision based on modern theoretical calculations seems to be inevitable. DFT calculations approach is considered to be a powerful approach to understand the surface reactions on an atomistic level, determining involved surface species and their influence on the electronic structure of the solid. This project is developed in the frame of a collaboration between the LAAS from Toulouse and the University of Tuebingen in Germany. Several metal oxides materials are under study, namely SnO2, WO3 and In2O3. The goal of this project is to get a detailed picture of the reaction of gas molecule (CO, CO2, H2, N2, NO2...) on clean and defective surfaces of the metal oxides, and also to understand how humidity can affect the detection process. The study of water effect is thus performed on SnO2, WO3 and In2O3 surfaces. The concentration and type of defects such as bulk/surface oxygen vacancies or surface hydroxyl groups will be considered.

Dernières publications:

- Ambient humidity influence of CO detection with SnO2 gas sensing materials - a DRIFTS/DFT investigation - Susanne Wicker, Mathilde Guiltat, Udo Weimar, Anne Hemeryck, Nicolae Barsan, Journal of Physical Chemistry C 121 (2017) 25064–25073 - **doi:** pu.doi **url:** pu.open_url

Simulations micromagnétiques de réseaux ultradenses de nanofils magnétiques

Projet démarré en 2016

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)

Porteur de projet: **Thomas Blon**

This project aims at simulate the magnetic hysteresis loops of assemblies of nanomagnets. These assemblies consist in Co nanowire arrays which are experimentally synthesized and measured in the LPCNO. A major problem in nanomagnet assemblies concerns the dipolar interactions between neighboring magnets which hide the intrinsic magnetic properties. Some analytical models in the mean field approximation can give valuable information but numerous consequences of interactions can only be modeled using numerical simulations. The effect of interactions has to be taken into account in order to suppress its influence in the measured hysteresis loops and then to determine the intrinsic parameters of the nanowire array, more specifically the switching field distribution of the nanowires which is the fundamental figure of merit of the system. The project focuses on simulations of Co nanowire arrays with variable interwire distances in order to tune the interactions. Preliminary results have shown that the interactions scale with the packing fraction of nanowires, and that the coercivity is modified whereas it is not expected in the mean field approximation. The numerical approach needs now to simulate larger nanowire arrays, with fine meshing, in order to introduce a predefined and significant distribution of nanowire switching fields and test the procedure of decorrelation of the interactions to be able to

determine the expected distribution. The aim is here to develop and validate a method that will be applied experimentally to determine the switching field distribution of a measured nanowire array which is unknown by definition. Moreover the global coercivity of the nanowire arrays will also be investigated to define its dependence with interactions.

Effets de déplacement atomique dans le silicium pour le durcissement des capteurs CMOS

Projet démarré en 2015

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)
Porteur de projet: **Anne Hemeryck**
Today, the development of new experimental facilities surrounded by a nuclear environment is accompanied by a need for resistant systems to radiation, so-called "hardened" for diagnostics and security. The improvement and adaptation of the holding of these systems to these extreme environments can be achieved through the adaptation of their architecture. However, it appears essential to help the hardening of the component thanks to a better knowledge of the physical phenomena of degradation under irradiation taking place in the material layers constituting component. This is particularly the case for the new generation of imagers based on CMOS sensors (for "Complementary Metal Oxide Semiconductor"). These are planned to replace CCDs (for "Charge-Coupled Device") in nuclear installations. Therefore, a multi-levels study dedicated to the understanding of the formation of defects and the effects of these atomic displacements due to radiation in silicon constituting CMOS sensors is set up using Dynamic Molecular technique, kinetic Activation Relaxation Technique and ab initio calculations. The current step of calculations concerns ab initio characterizations of the permanent formed defects using LDA methodology and GW methodology, then those data will be used to establish the link with the experimental DC-Random-Telegraph-Signals in macroscopic models. Now the modeling approach is validated, we expect to draw a complete, detailed and well-characterized list of all kind of defects that can exist in Silicon-based devices.

Dernières publications:

- Simulation of Single Particle Displacement Damage in Silicon – Part II: Generation and Long-Time Relaxation of Damage Structure - Antoine Jay, Mélanie Raine, Nicolas Richard, Normand Mousseau, Vincent Goiffon, Anne Hémeryck, Pierre Magnan - IEEE Transactions on Nuclear Science 64 (2017) 141-148 - **doi:** pu.doi
- Simulation of Single Particle Displacement Damage in Silicon – Part III: Generation and Long-Time Relaxation of Damage Structure - Antoine Jay, Anne Hémeryck, Nicolas Richard, Layla Martin Samos, Mélanie Raine, Alexandre Le Roch, Normand Mousseau, Vincent Goiffon, Philippe Paillet, Marc Gaillardin, Pierre Magnan - IEEE Transactions on Nuclear Science 65 (2018) 724-731 - **doi:** pu.doi

Heudyn

Projet démarré en 2015

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Nicolas Biziere**
The Heudyn project aims at calculating the spin waves frequencies in magnonic crystals made of Co2MnSi alloys. To achieve this goal, we perform micromagnetic simulations in time domain from a quasistatic equilibrium position of the magnetization. The calculation is performed in cubic cells and the results of the

time varying magnetization position is recorded for FFT post-treatment revealing the spin waves amplitudes and frequencies in the magnonic crystal. The results of this calculation are compared to experimental measurements realized at the CEMES lab. The spin wave measurement are performed on millimeters samples in microstrip configurations up to 30 GHz. The size of the simulated samples must avoid artefacts in the determination of the stationary modes such as reflection of spin waves on the edge of the sample. Then we want to simulate the dynamic magnetic states of big samples composed of few millions of nanometric cells.

Dernières publications:

- Magnetic Configurations in Co/Cu Multilayered Nanowires: Evidence of Structural and Magnetic Interplay - **doi:** pu.doi

Representative models of polymer surfaces using MD and DFT studies: poly-epoxy and organosilicates surfaces

Projet démarré en 2015

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)
Porteur de projet: **Corinne Dufaure**
The aim of our project is to construct models of polymer surfaces and to simulate XPS spectra of the surfaces to validate our computational approach by comparison with experimental XPS spectra. We work on two materials : (i) Poly-epoxy polymers and (ii) Organosilicates hybrids. Poly-epoxy polymers major applications lie in the aeronautical/aerospace industry where a need for substituting metallic or ceramic parts with polymers has emerged. We have already develop a model of a bulk poly-epoxy polymer using a cross-linking procedure and classical MD simulations. The thermal and volumetric properties of the model poly-epoxy were also obtained (density, coefficient of volumetric thermal expansion, and glass transition temperature, Tg) with good agreement with available experimental data. Our aim at the moment is to develop a model representing the poly-epoxy surface using the same computational approach (cross-linking code/MD simulations) and to study the adsorption of Cu metallic atoms on the polymer model surface by DFT. Organosilicate membranes are promising materials for the detection, purification or separation of liquids and gases where sorption of species at the surface of the membranes is one key-step. Therefore, we want to design models for the surface of organosilicate membranes and for the adsorption of the different interacting species. We will choose first a polymer composition corresponding to conventional PDMS to get a bulk model and in a second step a surface model (cross-linking code + MD simulations). Moreover, we will perform the simulation of XPS spectra for the pristine polymer using first a molecular model (deMon2k code and uGTS level of theory) and next using the developed model of the surface.

Dernières publications:

- T. Duguet, C. Bessaguet, M. Aufray, J. Esvan, C. Charvillat, C. Vahlas, C. Lacaze-Dufaure, Toward a computational and experimental model of a poly-epoxy surface. (2015) Applied Surface Science, 324, 605. -
- Gavrielides A., Duguet T., Esvan J., Lacaze-Dufaure C., Bagus P.S., A poly-epoxy surface explored by Hartree-Fock ΔSCF simulations of C1s XPS spectra, The Journal of Chemical Physics, 145, 074703 (2016) -

Calcul ab initio de spectres XANES et EELS pour l'interprétation de spectres expérimentaux.

Projet démarré en 2015

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Benedicte Warot-Fonrose**
In this project, we propose to use DFT-based first principles methods to calculate the electron energy loss spectra (EELS) and/or the X-ray absorption near-edge structures spectra (XANES) of different kinds of oxides potentially very important for technological applications. These calculations will be very helpful for experimentalists (in particular those working at the CEMES) to interpret experimental spectra in terms of the local electronic structure. Used as finger prints, the calculated spectra will also help experimentalists identifying crystal phases in complex samples, when nanocrystals are too small for being studied individually with conventional diffraction techniques and when experimental spectra recorded on reference crystals are not available. Displaying calculated spectra is moreover a task in which we are actively involved within the framework of the european network ESTEEM2 (Enabling Science and Technology through European Electron Microscopy). We will in particular calculate oxygen K-edge EELS spectra in complex oxides potentially strongly interesting for electronic and spintronic applications (half-metals, ferroelectrics or multiferroics). A comparison of the spectra obtained with different DFT-based codes and with different methods will be performed.

Dernières publications:

- M. Lee, R. Arras, B. Warot-Fonrose, T. Hungria, M. Lippmaa, H. Daimon and M. J. Casanove, Phys. Chem. Chem. Phys. 19, 28676 (2017). - **doi:** pu.doi
- M. Lee, R. Arras, R. Takahashi, B. Warot-Fonrose, H. Daimon, M.-J. Casanove, M. Lippmaa, ACS Omega 3, 2169 (2018). - **doi:** pu.doi

STRUCTURE ELECTRONIQUE ET INJECTION DE SPINDANS LES JONCTIONS METAL FERROMAGNETIQUE/ISOLANT/SEMICONDUCTEUR

Projet démarré en 2014

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Lionel Calmels**
CE PROJET A ETE SOUMIS CETTE ANNEE A UN APPEL D'OFFRE EN VUE D'OBTENIR LE COFINANCEMENT D'UNE THESE PAR LA REGION MIDI-PYRENEES ET LE PRES. NOUS VENONS D'APPRENDRE QUE NOTRE PROJET A ETE SELECTIONNE. UN DOCTORANT DEVRAIT DONC ARRIVER A L'AUTOMNE POUR TRAVAILLER SUR CE PROJET. Cette thèse sera centrée sur l'étude théorique des états électroniques de multicouches permettant l'injection de spin dans des semiconducteurs. Les fonctions d'onde décrivant le comportement des électrons seront calculées au CEMES par des méthodes ab-initio, avec des codes déjà existants basés sur la théorie de la fonctionnelle de la densité (DFT), tels que les codes Wien2k et VASP. Ces codes permettent de décrire le raccordement des fonctions d'onde aux interfaces de la multicouche, en fonction de leur structure atomique. Les multicouches qui seront étudiées sont les jonctions CoFeB (ou Fe)/MgO/GaAs(001), ainsi que des multicouches à base de semiconducteurs bidimensionnels (domaine de recherche en plein essor à l'heure actuelle) tels que MoS2, WS2, WSe2. Ces calculs devraient être très lourds (plusieurs interfaces dans le même système, un grand nombre d'atomes à prendre en compte). C'est pourquoi nous avons besoin de 250000 heures pour le lancer (automne/hiver 2014).

Dernières publications:

- Spin-Polarized Electron Tunneling in bcc FeCo/MgO/FeCo(001) Magnetic Tunnel Junctions -
- Half-metallicity, magnetic moments, and gap states in oxygen-deficient magnetite for spintronic applications -

Compréhension des mécanismes de croissance des matériaux et de formation des interfaces

Projet démarré en 2014

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)
Porteur de projet: **Anne Hemeryck**
The overall aim of this project is help technological development toward the integration of ultra-thin and nanoscale mastered oxide layers in the context of Microelectronics. These integrated materials must be now characterized by tailored structural and electronic properties, achievable thanks to the control of the atomic arrangement. The main objective of this project is to push forward these developments through a fundamental understanding of the local mechanisms involved during the growth of integrated materials. We want to provide models required by technologists in order to master the steps of deposition process of metal oxides layers as a function of the applied technological process. In fine, our challenge is to be able to provide a macroscopic model as TCAD tool dedicated to the deposition process simulation (based on kinetic Monte Carlo methodology where DFT data are used as input parameters). In order to provide a multi-processes, multi-materials simulation platform, this project is developed on four main materials: - Simulationg the growth of Si/SiO2 interface as a thermal oxidation process thanks to the ARTn/VASP coupling developed by A. Hemeryck and coworkers - Setting up of a Si/SiO2 interface model systems. - Growth of Bi nanowires on Silicium substrates

Dernières publications:

- Strain-driven diffusion process during silicon oxidation investigated by coupling Density Functional Theory and Activation Relaxation Technique - Nicolas Salles, Nicolas Richard, Normand Mousseau and Anne Hemeryck, Journal of Chemical Physics 147 (2017) 054701 - **doi:** pu.doi
- Modeling Of The Interface Formation During CuO Deposition On Al(111) Substrate: Linking Material Design and Elaboration Process Parameters Through Multi-Levels Approach - Mathilde Guiltat, Nicolas Salles, Marie Brut, Georges Landa,Nicolas Richard, Sébastien Vizzini, Anne Hémeryck - Modelling and Simulation in Materials Science and Engineering 25 (2017) 064005 - **doi:** pu.doi

Simulation de cycles d'hysteresis et calcul du torque de nanoparticules magnétiques en interaction.

Projet démarré en 2014

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)
Porteur de projet: **Julian Carrey**
We have successfully developed an algorythm simple and fast enough to be able to simulate the high-frequency hysteresis loop of thousands of magnetic nanoparticles in interaction. The simulations describe accurately the superparamagnetic regime as well as the ferromagnetic regime. This constitutes ou "first program" Using as a basis our initial code, we have also modified it so as we could calculate the torque undergone by an assembly of nanoparticles in a rotating magnetic field; this is our "second program". We have finished to develop this code, and performed a full theoretical study of the torque undergone by an assembly of nanoparticles under a rotating magnetic field. This problem had never been adressed

theoretically, and we have published these results. We have unfortunately discovered recently a bug (the same one) in the two programms that we have used so far. Our priority for this year is to evaluate the consequences of this bug on the results we have obtained and published so far. If necessary, errata will be published in order to present the exact results. After this step of verification, further research will be performed using our "second programm" : the torque properties of magnetic nanoparticles in interaction is a complex topic which requires additionnal theoretical work from our part. Moreover, we will use our "first programm" in order to simulate experimental results. Our objectives require calculation time on EOS.

Dernières publications:

- J. Carrey and N. Hallali, Phys. Rev. B 94, 184420 (2016) - **doi:** pu.doi
- J. Carrey and N. Hallali, Phys. Rev. B 98, 139902(E) (2018) - **doi:** pu.doi

Effets de la contrainte épitaxiale et des défauts de structure sur la structure électronique d'oxydes complexes

Projet démarré en 2013

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Rémi Arras**
This project consists in using first principles methods to calculate the modifications of the electronic structure induced by structural defects (vacancies or interstitial adatoms...) and strain or surface effects in complex oxides for technological applications. We will focus on magnetic oxides for spintronics. The problem of cation distribution inside the lattice will be also addressed.

Dernières publications:

- J. Phys.: Condens. Matter 25, 256002 (2013) -
- M. Lee, R. Arras, B. Warot-Fonrose, T. Hungria, M. Lippmaa, H. Daimon & M.-J. Casanove, Phys. Chem. Chem. Phys. 19, 28676 (2017). - **doi:** pu.doi

Modélisation et optimisation de nanoparticules métalliques bactéricides

Projet démarré en 2013

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Nathalie Tarrat**
L'objectif de ce projet est d'étudier les liens entre la morphologie d'une nanoparticule d'or et sa capacité d'adsorption de molécules antibactériennes en surface. Afin d'étudier ces systèmes, nous travaillons à l'adaptation d'une méthode approximée, la SCC-DFTB. En effet, cette dernière nous permettra d'étudier des systèmes très étendus comprenant la nanoparticule et son environnement organique avec une précision proche de celle des calculs DFT mais avec un coût calculatoire bien moindre. En parallèle, afin d'acquérir une compréhension précise de l'interface nanoparticule d'or / (bio)-molécule et de générer un jeu de données permettant de tester la validité de cette méthode quasi quantique, nous réalisons une étude DFT sur des surfaces d'or fonctionnalisées par des antibiotiques ou par des fonctions modèles.

Dernières publications:

- J. Phys. : Condensed Matter 2018, 30, 303001 - **doi:** pu.doi
- Materialia - In press - **doi:** pu.doi

Linear and nonlinear optical properties of high refractive index dielectric nanostructuress: A numerical study

Projet démarré en 2012

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Vincent Paillard**
High refractive index dielectric nanostructures exhibit enhanced absorption and scattering efficiencies as compared to their bulk counterparts. These properties can be predicted theoretically by the analytical Lorenz-Mie theory for an infinitely long single nanowire with circular cross-section embedded in a non-absorbing, homogeneous medium. To determine deviations from this ideal case (finite length, presence of a substrate, non-circular shape …), approximative numerical methods must be used such as the Green Dyadic method (GDM). Recently we focused on nonlinear effects in Silicon nanowires, in particular the experimental observation of an intense polarization-dependent Second Harmonic Generation (SHG), normally forbidden in bulk silicon. As in other centrosymmetric nanostructures such as gold nanorods and nanoparticles, there are different electric dipolar (surface) and higher order (volume) contributions for SHG. We developed code to calculate the possible contributions to SHG from centrosymmetric media. Comparison with experimental results showed that several sources meet in SHG from SiNWs. Thanks to extensive numerical simulations we found that these sources can be individually addressed by simply changing the polarization state of the illuminating fundamental light, or by varying the nanowire diameter. The latter is leading to a transition between a field-gradient induced bulk- and a local surface contribution to SHG. In a second project, we coupled the GDM to an evolutionary optimization algorithm, capable to target multiple optimization objectives simultaneously. Thanks to this, we are able to automatically design double-resonant nanostructures, having polarization dependent, individually addressable resonances at arbitrary, user-specific wavelengths.

Dernières publications:

- Wiecha, P. R. et al. Multi-resonant silicon nanoantennas by evolutionary multi-objective optimization. in Computational Optics II 10694, 1069402, SPIE Proceedings, invited talk at SPIE Frankfurt (May 2018). - **url:** pu.open_url
- Fano-resonances in High Index Dielectric Nanowires for Directional Scattering, P. R. Wiecha, V. Paillard, et al., in Fano Resonances in Optics and Microwaves, Springer Series in Optical Sciences 219, Springer Nature Switzerland AG 2018 1, E. Kamenetskii et al. (eds.). -

DFT STUDIES OF THE INHIBITION OF THE CORROSION OF ALUMINUM AND OXIDES

Projet démarré en 2012

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)
Porteur de projet: **Corinne Dufaure**
Recently, the high toxicity of chromates has imposed restrictions on their use in industrial applications. It is mandatory to find new environmentally friendly compounds as corrosion inhibitors of aluminum and aluminum alloys. This project aims to investigate, at the atomic scale, the corrosion inhibition mechanisms affecting

aluminum. We propose to determine the mode of action of an efficient corrosion inhibitor by using ab initio calculation. In the past years, we studied the interaction of the 8-hydroxyquinoline (8HQ) and derivatives with aluminum surfaces with a periodic/DFT-D approach. We also investigated the reactivity towards molecular oxygen of the organic layers adsorbed on Al(111). O2 dissociation was not observed on the most compact layers. In addition, we studied the adsorption of the 8HQ molecule on hydroxylated aluminum oxide. The chemisorption of the organic molecules led to an electronic redistribution in the systems that could change the surface reactivity. In order to demonstrate it, we want now to investigate the interaction of molecular oxygen with the oxide covered by the organic layer. Moreover, we began to study a set of organics inhibitors analogues to 8-HQ but showing no corrosion inhibition efficiency. We perform DFT computations on the isolated molecules but also on Al complexes in order to determine energetic, structural, electronic, topological… descriptors in relation with corrosion inhibition. We expect that all these ab initio calculations will give insights in the relation between the chemical nature of the surface, the chemical structure of the inhibitor, the inhibitors/surface interactions and the inhibition efficiency of a molecule. It will help us to rationalize the search of alternative inhibiting species against the corrosion of aluminum and its alloys.

Dernières publications:

- Surface Science 2011, 605, 341 -
- F. Chiter, M-L. Bonnet, C. Lacaze-Dufaure, H. Tang and N. Pébère, Phys. Chem. Chem. Phys., 20 (2018) 21474. -

Mobilités des joints de grain sous contrainte

Projet démarré en 2012

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Nicolas Combe**
Structural materials with nanoscritalline grains (<100nm) are very promising due to their very good mechanical properties. These mechanical properties are noticeably related to the mobility of grain boundaries (GB). The present project proposes to study homogeneous nucleation of disconnection in Aluminum grain boundaries and the inhomogenous nucleation of disconnections resulting from the absorption of bulk dislocations in copper. The structural and energetic study of the GB migration will be studied using the Nudge Elastic band method between two states corresponding to the positions of the GB before and after the migration. In addition, the calculation of the free energy of the migration as a function of a collective variables will be performed using the Adaptive Biasing Forces and the metadynamic method.

Dernières publications:

- Unidimensional model of the adatom diffusion on a substrate submitted to a standing acoustic wave II. Solutions of the ad-atom motion equation. -
- Phys. Rev. Mat., 1, 033605 (2017) - **doi:** pu.doi

Structure électronique de multicouches extrinsèquement multiferroïques et gaz d'électrons bidimensionnel aux interfaces tout-oxydes

Projet démarré en 2012

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Rémi Arras**
The first part of this project aims using first principles calculations for studying a very particular class of materials: extrinsic multiferroic materials. These systems consist in transition metal oxide ferroelectric (or piezoelectric)thin layers associated with magnetic thin layers. Among all the possible extrinsic multiferroic materials, we will focus on multilayers containing magnetic oxides with the spinel structure (Fe3O4, CoFe204, NiFe2O4), or ferromagnetic metal thin films (Co, Fe...) and ferroelectric oxides with the perovskite structure (BaTiO3, PbTiO3, Pb(Zr,Ti)O3). The theoretical work which we plan to do on these materials will be based on ab-initio calculation of the electronic structure. The results which will be obtained will be useful for understanding spintronic materials of which the magnetic configuration could be controçled by an external electric field, or four-logic-states devices for high density memories. The second part of the project will be focused on the study of oxide-based heterostructures, at the interfaces of which an intrinsic and (fully-spin polarized) electron gas can be stabilized. Such system is also of great interests for spintronic applications, like (spin-)FET.

Dernières publications:

- M. Studniarek, S. Cherifi-Hertel, E. Urbain, U. Halisdemir, R. Arras, B. Taudul, F. Schleicher, M. Hervé, C.-H. Lambert, A. Hamadeh, L. Joly, F. Scheurer, G. Schmerber, V. Da Costa, B. Warot-Fonrose, C. Marcelot, O. Mauguin, L. Largeau, F. Leduc, F. Choueikani, E. Otero, W. Wulfhekel, J. Arabski, P. Ohresser, W. Weber, E. Beaurepaire, S. Boukari, and M. Bowen, Adv. Funct. Mater. 1700259 (2017). - **doi:** pu.doi
- M. J. Veit, R. Arras, B. J. Ramshaw, R. Pentcheva, and Y. Suzuki, Nat. Commun. 9, 1458 (2018). - **doi:** pu.doi

ETUDES NUMERIQUES DE SYSTÈMES FORTEMENT CORRELES EN MATIERE CONDENSEE OU DANS LES SYSTEMES D'ATOMES ULTRA-FROIDS SUR RESEAUX

Projet démarré en 2012

LPT - Laboratoire de Physique Théorique (UMR 5152)
Porteur de projet: **Didier Poilblanc**
The scientific activity briefly described here is directly connected to the most active domains of research in the fi

eld of correlated systems such as unconventional and high-Tc superconductors, quantum phase transitions, low-dimensional conductors, novel fractional quantum Hall states and emerging non-Abelian excitations, ultra-cold atoms loaded on optical traps, entanglement & quantum information, etc. Our activity is two-fold: (i) using well optimized numerical methods (such as home-made Lanczos exact diagonalisation, Density Matrix Renormalization Group algorithm or variational quantum Monte Carlo algorithm) to tackle models of correlated systems and achieve the best refined comparison with many of the related experimental systems and (ii) develop new numerical methods like tensor network techniques borrowing novel concepts from quantum information to be able to address larger systems, still with a very good accuracy.

Dernières publications:

- Discrete lattice symmetry breaking in a two-dimensional frustrated spin-1 Heisenberg model, Ji-Yao Chen, Sylvain Capponi, Didier Poilblanc - **doi:** pu.doi
- Non-Abelian chiral spin liquid in a quantum antiferromagnet revealed by an iPEPS study, Ji-Yao Chen, Laurens Vanderstraeten, Sylvain Capponi, Didier Poilblanc - **doi:** pu.doi

Anisotropie magnétique des couches minces et multicouches pour l'électronique de spin

Projet démarré en 2012

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Etienne Snoeck**
This project consists in calculating the magnetic anisotropy energy of several kinds of magnetic multilayers which are interesting for their potential application in spintronic devices. We will calculate the anisotropy energy of crystals in which the magnetic anisotropy is strongly enhanced by interfaces between magnetic and non-magnetic materials. The magnetic materials which will be sudied here are: - thin Fe layers grown on the top of a non magnetic bcc substrate - thin layers of full Heusler alloys such as Co2MnSi, Co2FeSi, Co2FeAl, Co2Fe(Al,Si)which will be sandwiched between non magnetic metals such as Pt and Pd. We will calculate which thicknesses and which interfaces must be chosen to reach a magnetic anisotropy perpendicular to the interfaces. The magnetic anisotropy of these multilayers will be interpreted in terms of the electronic structure, starting from the perturbation theory which describes the modification of the ground state energy induced by spin-orbit coupling: the electron states responsible for the perpendicular anisotropy will be either degenerated states near the Fermi level (they contribute at the first order perturbation theory), or occupied and unoccupied non degenerated states (they contribute at the second order perturbation theory).

Dernières publications:

- PHYSICAL REVIEW B 90, 45411 (2014) -
- JOURNAL OF PHYSICS-CONDENSED MATTER 25, 256002 (2013) -

Étude de nanoparticules cœur-coquille Fe@Au

Projet démarré en 2011

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Magali Benoit**
Bimetallic nanoparticles are of great interest due the effect of the reduced size on their properties but also due

to the effect of the chemistry of the system. The chemical composition inside the particle is a very important parameter with respect to the properties. Au-Fe nanoparticles have potential applications in catalysis and bio-medicine. It is therefore fundamental to know their morphology, which can be controlled by the growth parameters. Experimentalists at CEMES have elaborated Au-Fe nanoparticles with a Fe core and an Au shell. The epitaxial relationships have been studied by transmission electronic microscopy. In order to understand the formation mechanism of these particles, in 2012 and 2014, we have studied the Au(001)/Fe(001) interface, using spin-polarized DFT calculations in the GGA approximation, and have extracted the interface energy from these calculations. In 2016, we have shown that Fe@Au nanoparticles may have different surface reactivity depending on the number of gold layers in the Au shell. Finally, in 2017, we have developed a new Fe-Au EAM potential that we have started to use for large-scale molecular dynamics and Monte Carlo simulations. In 2018, we will continue the study of the morphology of these nanoparticles with particular emphasis on the growth mechanisms during gold deposition.

Dernières publications:

- P. Benzo, M. Benoit, N. Tarrat, C. Langlois, R. Arenal, B. P\'ecassou, A. Le Priol, N. Combe, A. Ponchet and M.-J. Casanove, IEEE Nanotechnology Materials and Devices Conference (NMDC) (2017) -
- C. Langlois, M. Benoit, J. Nicolai, N. Combe, R. Arenal, A. Ponchet, and M.-J. Casanove, Nano Letters 15, 5075 (2015) -

Modelisation du depot et de l'initiation de materiaux energetiques nano-structures de type thermite

Projet démarré en 2010

LAAS - Laboratoire d'Analyse et d'Architecture des Systèmes (UPR 8001)
Porteur de projet: **Alain Esteve**
Energetic materials have attracted a growing interest these last years due to their capability to provide on-board energy. Within this context LAAS experimentalists are developing new techniques for integrating Al/CuO thermite in pyrotechnic microsystems. However, the properties of thermites are not well understood neither from the synthesis nor their thermal characteristics. Therefore, we use multi-scale calculations in order to gain a better understanding involved during the deposition and initiation processes in order to build a meso- or macroscopic model for guiding experimentalists in the design of ad-hoc materials.

Dernières publications:

- Al Interaction with ZnO Surfaces Yuzhi Gao, Mathilde Iachella, Eric Mattson, Antonio T. Lucero, Jiyoung Kim, Mehdi Djafari Rouhani, Yves Chabal, Carole Rossi, Alain Estève ACS J. Phys. Chem. C 122 (31), 17856, -
- Al Interaction with ZnO Surfaces Yuzhi Gao, Mathilde Iachella, Eric Mattson, Antonio T. Lucero, Jiyoung Kim, Mehdi Djafari Rouhani, Yves Chabal, Carole Rossi, Alain Estève ACS J. Phys. Chem. C 122 (31), 17856, -

Simulation des propriétés optiques de nano-objets et nanostructures métalliques.

Projet démarré en 2009

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Adnen Mlayah**
Les nano-objets et nanostructures métalliques absorbent, diffusent, transmettent et guident la lumière dans une gamme de longueur d'onde qui s'étale du proche UV (0.3 nm) jusqu'à l'infrarouge lointain (3 µm) grâce à l'excitation optique d'oscillations collectives de leurs électrons libres, les plasmons de surface. De plus, leur taille nanométrique et le grand rapport surface/volume leur confèrent la capacité de localiser spatialement l'énergie électromagnétique. De ces propriétés découlent des applications dans des domaines aussi variés que ceux des télécommunications, de la production d'énergie, des capteurs chimiques et biologiques, du diagnostic et de la thérapie en cancérologie. La simulation/modélisation des propriétés optiques de nano-objets métalliques est un outil non seulement d'interprétation des expériences de spectroscopies optiques (absorption,luminescence, Rayleigh-Mie, Raman-Brillouiun, Luminescence à deux photons) mais aussi de "design" de la nature, de la taille, de la forme des nano-objets visant une propriété optique particulière (exaltation de l'émission, guidage optique, hyperthermie). Le projet présenté ici s'inscrit dans cette thématique de recherche "plasmonique". Il vise l'utilisation d'un programme de modélisation des spectres d'extinction et d'absorption optique et de simulation du champ proche électromagnetique au voisinage des surfaces de nano-objets métalliques. Le projet s'inscrit dans le cadre des activités "plasmonique" du CEMES, axe transversal au sein du laboratoire. Ce projet a fait l'objet de collaborations internationales (Institute for Material Research and Engeneering/ Singapore, Donostia International Physics Center de San Sebastian; Rice University, Houston) qui se poursuivent et de thèses N. Large UPS/Donostia, A. Mezni UPS/Bizerte, I. Abid UPS. D'autres collaborations internationales se mettent en place notamment avec la Chine (Laser Fusion Center, Mian-Yang, Sishuan) et les états unis (RICE university, Houston).

Dernières publications:

- Temperature dependent plasmon-exciton interation in hybrid MoSe2/Au nanostructures Inès Abid, Weibing Chen, Jiangtan Yuan, Arash Bohloul, Sina Najmaei, Carolina Avendano, Renaud Péchou, Adnen Mlayah and Jun Lou ACS Photonics 2017, 4, 1653−1660 - **doi:** pu.doi
- Resonant Surface Enhanced Raman Scattering in Hybrid MoSe2/Au Nanostructures Inès Abid, Weibing Chen, Jiangtan Yuan, Arash Bohloul, Sina Najmaei, Carolina Avendano, Renaud Péchou, Adnen Mlayah and Jun Lou Optics Express, Vol. 26, Issue 22, pp. 29411-29423 - **doi:** pu.doi

Calculs DFT des nanoparticules FeRh : effet de taille et de la morphologie

Projet démarré en 2009

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Hao Tang**
Close to the equiatomic composition, the chemically ordered FeRh alloy with B2 cubic structure (B2-FeRh), presents a remarkable magnetic phase transition from an antiferromagnetic (AFM) state at low temperature to a ferromagnetic (FM) state above 370K. In recent years, there has been a strong interest for this alloy for applications in microelectronics, heat-assisted magnetic recording or magnetic random access memories. While the FM-AFM transition is sharp in the bulk alloy, the persistence of a FM component at low temperature in FeRh thin films raised important questions about the effect of size reduction, interfaces and surface termination on their magnetic properties. Incomplete transitions upon cooling were also reported in FeRh nanoparticles. However, whereas pure size effects were studied in nanoparticles (NPs), the role of surface termination remains to be addressed. In this project, we will perform DFT calculations in order to understand the effect of size reduction, interfaces and surface termination on the magnetic properties in the particular case of equiatomic composition B2-FeRh NPs.

Dernières publications:

- "Magnetism and morphology in facetedB2-ordered FeRh nanoparticles", M. Liu, P. Benzo, H. Tang, M. Castiella, B. Warot-Fonrose, N. Tarrat, C. Gatel, M. Respaud, J. Morillo and M. J. Casanove, Eur. Phys. Lett., 116, 27006 (2016). - **url:** pu.open_url
- "Prediction of Co nanopareticle morphologies stabilized by ligands : towards a kinetic model", Van Bac Hguyen, M. Benoit, N. Come and H. Tang , Phys. Chem. Chem. Phys., 19, 4636-4647 (2017). - **url:** pu.open_url

Étude de la solubilité et de la diffusion de l'oxygène dans les superalliages à base de nickel

Projet démarré en 2009

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)
Porteur de projet: **Damien Connétable**
In the context of lifetime prediction of numerous industrial devices working at high temperature and oxidizing atmospheres (heat converter in nuclear power plants, solar hoven, gaz turbines, …). we propose to study the mechanisms involved in high temperature oxidation of nickel-based superalloys which result in the formation of cavities in the substrate. The project will involve both, numerical studies by the mean of atomistic simulations together with a mesoscopic model and experimental studies on model materials. The project is focused on the formation of cavities in the substrate, that are observed during high temperature oxidation of nickel-based superalloys, and the diffusion of the O atoms in the substrat and its interactions with others defects.

Dernières publications:

- B. Amin-Ahmadi, D. Connétable, M. Fivel, D. Tanguy, R. Delmelle, S. Turner, T. Pardoen, J. Proost, D. Schryvers and H. Idrissi, Acta Materialia 111 (2016) 253-261. - **doi:** pu.doi
- D. Connétable, M. David, A. Prillieux, D. Young and D. Monceau, Journal of Alloys and Compounds 708 (2017) 1063-1072 - **doi:** pu.doi

Structure électronique des matériaux d'électrodes pour jonctions tunnel magnétiques Métal/MgO/Métal

Projet démarré en 2008

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Lionel Calmels**
Les calculs que nous souhaitons mener au cours des prochaines années permettront de comprendre la structure électronique des jonctions tunnel magnétiques dont les électrodes sont constituées de métaux 3d (essentiellement le fer et le cobalt). Il s\'agira également de calculer les spectres EELS permettant de faire des mesures locales de cette structure électronique afin de comprendre et interpréter les résultats des mesures expérimentales menées sur ces systèmes. •Calcul de la structure électronique des jonctions « Métal 3d/MgO/Métal 3d »: Le but de notre projet est de comprendre les mécanismes de transport dans les jonctions tunnel ainsi que la connection entre les propriétés de magnétotransport et le couplage magnétique entre les deux électrodes. En l'absence de polarisation et pour des jonctions peu épaisses avec des interfaces parfaitement planes, le couplage n'est pas dû aux interactions dipolaires de type "peau d'orange" mais aux électrons qui traversent la jonction par effet tunnel, dans les deux sens et avec un courant résultant nul. Les calculs de structure électronique permettront de comprendre comment les fonctions d'onde se comportent aux

interfaces de la barrière et au travers de celle-ci lorsqu'on modifie la nature des électrodes magnétiques et des interfaces. Une première série de calculs portera sur la jonction Co(hcp)/MgO/Co(hcp). La structure atomique de cette jonction est telle que l'axe c du cobalt est couché dans le plan de croissance et la fine barrière de MgO est contrainte sur le cobalt. La structure atomique (hcp) des électrodes magnétiques et des interfaces de cette jonction est différente de celle des jonctions à électrodes bcc qui ont jusqu'à présent été abondamment étudiées. Ces calculs vont permettre de comprendre comment des états électroniques ayant une symétrie autre que celles des électrodes bcc peuvent être mis en jeu dans des expériences de magnétotransport. Une seconde série de calculs portera sur les jonctions de type Fe(100)/Co(bcc)/MgO/Fe(100) ou Fe(100)/Co(bcc)/MgO/Co(bcc)/Fe(100). L'intercalation d'une couche ultra mince de Co épitaxiée permet d'envisager l'existence d'états de puits quantiques dans la couche mince de cobalt, le nombre et l'énergie de ces états dépendant de la largeur de la couche de cobalt. Ces états localisés entre l'électrode de fer et la barrière isolante devraient modifier les propriétés de transport d'une façon que l'on pourra ajuster en modifiant l'épaisseur de la couche de cobalt (et donc le nombre d'états de puits quantique occupés et inoccupés des électrons de spin majoritaire et minoritaire). •Structure fine au seuil L23 des métaux de transition dans les jonctions « Métal 3d/MgO/Métal 3d »: L'étude de la structure fine des spectres EELS au seuil L23 des métaux de transition concernera les jonctions tunnel Fe/MgO/Fe et FeCo/MgO/FeCo. Il s'agira par exemple de calculer le moment magnétique des atomes au voisinage des interfaces (en tenant éventuellement compte de la présence d'une couche d'oxyde) et de relier la valeur de ce moment magnétique au rapport d'intensité I(L3)/I(L2) mesuré près de l'interface par spectroscopie de pertes d'énergie d'électrons. Remarque: un chercheur post-doc financé par l\'ANR viendra compléter cette équipe en cours d\'année.

Dernières publications:

- PHYSICAL REVIEW B 90, 45411 (2014) -
- JOURNAL OF PHYSICS-CONDENSED MATTER 25, 256002 (2013) -

Propriétés physico-chimiques de nanostructures à base de carbone et autres matériaux 2D: fonctionnalisation, dopage, effets du substrat

Projet démarré en 2008

LPCNO - Laboratoire de Physique et Chimie des Nano-Objets (UMR 5215)
Porteur de projet: **Iann Gerber**
The design of innovative materials based on nano materials requires a thorough understanding of the physics and chemistry at the atomic scale. The study by DFT calculations of the physico-chemical properties of carbon-based nanostructures has become almost an inescapable fact in many case studies. Indeed it is a major issue to understand complex phenomena related to the functionalization, the doping, the effects of external stress which can be mechanical, electrical or even imposed by a substrate. All this, with future applications in nanocatalysis, or to improve electronic transport properties, or even for a more fundamental understanding of the nature of metal-carbon interactions. Besides, lamellar dichalcogenide based materials have unique physical properties that offer a new field of investigations in optoelectronic mainly. Electronic band structure calculations beyond standard DFT are essential in this study in order to understand photoluminescence experiments.

Dernières publications:

- Theor. Chem. Acc. 137, 156 (2018) - **doi:** pu.doi
- ACS Appl. Nano Mater. 1, 5885 (2018) - **doi:** pu.doi

interstitial-solute interactions in Al and Ni studied by numerical simulations, implications on materials' properties (diffusion, cohesion and plastic

Projet démarré en 2007

CIRIMAT - Centre Inter-universitaire de Recherche et d'Ingénierie des Matériaux (UMR 5085)
Porteur de projet: **Damien Connétable**
The context of the project is the damaging of metallic alloys in their environment. We want to predict, on the long term, the loss of mechanical properties of structural materials (nickel based alloys, steels and aluminum alloys) due to Stress Corrosion Cracking (SCC), hydrogen embrittlement, metal dusting or internal oxidations. The goal of this project is to enhance applications' safety (air plane, civilian nuclear plants, pipelines...) and to reduce maintenance costs. The project consist in the development of a multi-scale simulation (coupling first-principles calculations –DFT- and classical modeling of diffusion processes via Molecular Dynamics, Monte Carlo and explicit equations) of some key mechanisms involved in metallic embrittlement. We will focus on the interactions between interstitials and crystalline defects in aluminum and nickel: point defects, dislocations and solutes.

Dernières publications:

- "Stress-controlled carbon diffusion channeling in bct- iron : a mean-field theory.",P. Maugis, S. Chentouf and D. Connétable , J. Alloys and Compounds 769 (2018) 1121- 1131 - **doi:** pu.doi
- "Diffusion of interstitial species (H and O atoms) in fcc systems (Al, Cu, Co, Ni and Pd) : contribution of first and second order transition states.", D. Connétable and M. David, J. Alloys and Compounds 772 (2019) 280-287 - **doi:** pu.doi

Modélisation des nano-structures moléculaires auto-assemblées et de la réactivité sur surfaces

Projet démarré en 2006

CEMES - Centre d'Élaboration de Matériaux et d'Études Structurales (UPR 8011)
Porteur de projet: **Hao Tang**
The spontaneous self-organization of molecules would not only have a very large number of nano-components in a well defined architecture, but also to obtain specific properties related to the geometry of these structures. However, the mechanisms of these self-assembling are not yet totally well understood. In this project we propose to study the molecular nanostructures as two-dimensional whose formation is the result of balance between molecule-molecule interactions and molecule-substrate interactions. In addition, we will also study the electronic and magnetic properties at the interface molecule as well as to understand how these molecular self-assembled monolayers could stabilize some orientations during the growth of nanoparticles. To do this, we use both quantum methods (DFT, semi-empirical) and classical methods (molecular mechanics, molecular dynamics).

Dernières publications:

- Corrosion protection of Al(111) by 8-hydroxyquinoline: a comprehensive DFT study, Fatah Chiter, Marie-Laure Bonnet, Corinne Lacaze-Dufaure, Hao Tang, NFatah Chiter, Marie-Laure Bonnet, Corinne Lacaze-Dufaure, Hao Tang, Nadine Pébère, Phys. Chem. Chem. Phys., 20, 21474-21486 (2018).adine Pébère -

- One-dimensional molecular chains formed by Sierpinski triangles on Au(111)One-dimensional molecular chains formed by Sierpinski triangles on Au(111),X. Zhang, G. Gu, N. Li, H. Wang, H. Tang, Y. Zhang, S. Hou, Y. Wang, RSC. Adv., 8, 1852–1856 (2018). -

Simulations de systèmes quantiques fortement corrélés : propriétés magnétiques, supraconductrices et influence du désordre

Projet démarré en 2006

LPT - Laboratoire de Physique Théorique (UMR 5152)
Porteur de projet: **Fabien Alet**
This project is an ongoing continuation (started about 10 years ago) of our scientific activity, which belongs to the field of theoretical condensed matter physics. We are interested in understanding novel phenomena appearing in so-called strongly correlated systems. In other words, these are quantum many-body effects where both quantum fluctuations and interactions cannot be neglected. Quite interestingly, these models are relevant for a large variety of physical systems ranging from correlated materials (Mott insulators, exotic superconductors) to ultracold atomic gases on optical lattices. Our centers of interest have moved gradually from quantum magnetism, unconventional superconductivity towards new aspects in condensed matter, such as the topic of quantum entanglement, the phenomenon of many-body localization and relation to cold-atom experiments. We develop and use state-of-the-art algorithms to fight the exponential complexity of the quantum many-body problem: quantum Monte Carlo (QMC), exact diagonalization (ED), density matrix renormalization group (DMRG). We have produced several efforts in the last few years to adapt and/or develop new methods (such as shift-invert exact diagonalization, time evolution with Krylov techniques, or Time-Evolving Block Decimation), which put us in a leading position in the field of computational quantum many-body physics. This position is of course also due to the possibility of performing our large-scale computations on advanced supercomputers such as eos. This year, we present three projects on : 1) Dynamical correlations in quantum antiferromagnets 2) Glassy properties of the Bose glass phase 3) Many-Body Localization

Dernières publications:

- Many-body localization as a large family of localized groundstates, Maxime Dupont, Nicolas Laflorencie - **url:** pu.open_url
- Unified Phase Diagram of Antiferromagnetic SU(N) Spin Ladders, Andreas Weichselbaum, Sylvain Capponi, Philippe Lecheminant, Alexei M. Tsvelik, Andreas M. Läuchli, Phys. Rev. B 98, 085104 (2018) - **doi:** pu.doi **url:** pu.open_url

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4.8 Méthodes et algorithmes

AMAS4BigData

Projet démarré en 2018

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)
Porteur de projet: **Jean-Pierre Georgé**
-L'objectif est de tester le framework "AMAS4BigData" qui utilise une intelligence artificielle collective qui

analyse en temps réel et de manière dynamique les relations entre plusieurs sources de données. -Nécessite java 1.8+ (idéalement la dernière version 10.0.1) -Il s'agit d'un logiciel académique. -Le framework est développé sous java et génère beaucoup de threads (entre 800 et 1200 selon la taille du data).

Evaluation de méthodes d'imputation multiple par validation croisée

Projet démarré en 2018

LGP - Laboratoire Génie de Production (Tarbes)
Porteur de projet: **Kamal Medjaher**
Avant de pouvoir exploiter des données, la première étape consiste à vérifier leur pertinence. Dans notre cas, nous disposons de 148 mesures de 411 paramètres concernant la qualité de l'eau. Chaque variable et chaque observation comportent au moins une donnée non renseignée(donnée manquante), et le nombre total de données manquantes s'élève à plus de 80%. Ainsi, il n'est pas envisageable de supprimer les lignes/colonnes contenant des données manquantes. Une alternative consiste à deviner les valeurs manquantes. Ainsi, l'objectif du projet est d'évaluer la performance de plusieurs méthodes de traitement des données manquantes par imputation sur des données concernant la qualité de l'eau. Pour cela, une validation croisée est effectuée, ce qui demande une grande capacité de calcul. J'utilise Anaconda, une distribution open-source, le langage Python et sa librairie scikit-learn, et travaille sous Windows.

ECHOPPE, Economie du logement

Projet démarré en 2018

TSE-R - TSE-R UMR 5314
Porteur de projet: **celine parzani**
Housing is a critical target of public policy in France. The budget of housing policies devoted to transfers exceeded 40 billion euros in 2014 or approximately 2% of GDP. These policies include housing benefits, property taxes and construction subsidies and extend to social housing and rent controls. The goal of this project is to build up dynamic structural models of household inter-temporal decisions regarding their housing with an emphasis on life-cycle issues, and to calibrate these models using French data. There exists no such empirical model for France and only recently for the US. This core model will be used to assess the long-run impacts of housing public policies like housing benefits, means-tested zero-interest loans to first time owners etc. In particular, it would measure the order of magnitude of the reduction of housing inequalities that can be achieved by public policies, including general equilibrium effects through prices and rents. To do so, we consider a model in which households, who are stochastically ageing and changing their marginal productivity, choose, each year, whether to rent or to buy their house (or another one to rent it to other households), to consume and to save . A parametric utility function is assumed and there are institutional constraints added to the model : the tax system faced by the households and the borrowing constraints. The goal is to first estimate the value function of a given household which depends on its earnings, his wealth, his housing situation and, of course, on the parameters of the model. Once this value function is determined, we need to estimate the renting price and housing price by balancing the two sides of the markets (supply and demand). Ultimately, we aim at estimating the utility parameters by comparing some aggregate statistics estimated on the French Housing Survey and predicted by our model. The final results will be used for counterfactual analysis.

Modélisation de covariances d'erreur d'ébauche sur grille non-structurée

Projet démarré en 2018

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)
Porteur de projet: **Benjamin MENETRIER**
L'assimilation de données regroupe l'ensemble des techniques permettant d'initialiser les modèles numériques de prévision. Elle se base sur la combinaison d'informations provenant d'une ébauche (prévision récente) et d'observations du système. Le poids accordé à chaque source d'information dépend de leur incertitude, représentée sous la forme de matrices de covariances d'erreur. En raison de la taille des systèmes utilisés (de l'ordre du milliard de variables), les covariances d'erreur d'ébauche ne peuvent être estimées et stockées directement, et doivent être modélisées. La diversité croissante des grilles utilisées par les modèles de prévision pour l'atmosphère, l'océan et les milieux connexes nécessite le développement d'approches innovantes permettant de modéliser les covariances d'erreur d'ébauche sur des grilles non-structurées. C'est précisément l'objet du code BUMP (Background error covariance on Unstructured Mesh Package), développé conjointement par l'IRIT, Météo-France et le JCSDA (USA). Ce code est interfacé dans l'environnement OOPS (Object-Oriented Prediction System), développé conjointement par ECMWF (UK), Météo-France et le JCSDA, et dont l'objectif est de permettre de façon flexible le développement d'algorithmes d'assimilation de données, leur test puis leur mise en production. Un aspect important de modélisation des covariances d'erreur d'ébauche est l'efficacité et la scalabilité du code sur des calculateurs massivement parallèles. En effet, l'augmentation de résolution des modèles numériques et les contraintes horaires strictes de la production opérationnelle imposent une parallélisation efficace. Le code BUMP étant distribué sous licence libre, il est important de le tester sur un maximum de machines, afin d'en assurer la fiabilité pour tous les utilisateurs. L'installation et la validation du code sur le calculateur CALMIP permettra aux partenaires présents et futurs du projet d'envisager sereinement l'utilisation de ce calculateur pour leurs contributions au code.

Algorithmes parallèles pour la résolution de problèmes issus de la discrétisation d'équations aux dérivées partielles

Projet démarré en 2017

ISAE/DISC - Département d'Ingénierie des Systèmes Complexes
Porteur de projet: **Xavier Vasseur**
Efficient parallel algorithms for the numerical solution of partial differential equations are required for solving large-scale problems in Computational Science and Engineering. This project aims at tackling certain aspects of modern iterative solution methods for the solution of nonlinear systems issued from the discretization of partial differential equations. First, we focus on the analysis and implementation of time-parallel methods for the solution of time-dependent partial differential equations. Time parallelism can be combined indeed with space parallelization to further improve the scalability properties of the numerical solver. We especially focus on the Parareal algorithm with spatial coarsening used with explicit time integration schemes. In this context we study both theoretically and numerically its efficiency on relevant testcases in compressible fluid mechanics. Indeed the simulation of turbulent compressible flows offers a relevant testbed for the assessment of such time-parallel algorithms. Secondly, we focus on the analysis and implementation of stochastic preconditioners for the numerical solution of large-scale nonlinear systems of equations. We investigate if these algorithms which recently appeared in the numerical optimization literature can be beneficial as preconditioners of Krylov subspace methods in terms both of convergence rate and parallel efficiency. The application to a sequence of nonlinear systems will be considered.

Dernières publications:

- T. Lunet, J. Bodart, S. Gratton and X. Vasseur "Time-parallel simulation of the decay of homogeneous turbulence using Parareal with spatial coarsening". Comput. Vis. Sci., 19-1–2, pp. 31–44, 2018. - **doi:** pu.doi **url:** pu.open_url
- T. Lunet, Stratégies de parallélisation espace-temps pour la simulation des écoulements turbulents, Thèse de doctorat, ISAE-SUPAERO, thèse soutenue le 9 janvier 2018. - **url:** pu.open_url

Fast Kinetic Schemes for Boltzmann equation

Projet démarré en 2017

IMT - Institut de Mathématiques de Toulouse (UMR 5219)
Porteur de projet: **Jacek Narski**
The aim of the project is to develop an efficient parallel algorithm to perform deterministic numerical simulations of the rarefied gas dynamics on distributed memory systems. The rarefied gas dynamics described by a full Boltzmann equation defined in 7D (three coordinates in the physical space, three coordinates in the velocity space and time). The numerical scheme that is considered is an extension of the Fast Kinetic Scheme (FKS) [J. Comput. Phys., Vol. 255, 2013, pp 680-698] originally constructed for solving the BGK equation, to the more challenging case of the Boltzmann equation, where the collisions between particles are modeled by multiple integrals over the whole velocity space. The scheme combines a robust and fast method for treating the transport part based on an innovative Lagrangian technique supplemented with fast spectral schemes to treat the collisional operator by means of an operator splitting approach. The construction of the FKS makes it extremely well suited for parallelization on shared or distributed memory systems. The OpenMP and GPU parallization was the objective of a previous work [J. Comput. Phys., Vol. 284, 2015, pp 22-39]. The strong scaling obtained was close to ideal. However, due to the curse of dimensionality of the Boltzmann equation, the size of the problems that can be treated on a shared memory systems is very limited. The necessary next step is to move beyond shared memory system to distributed systems. The approach that is choosen for parallelization is the decomposition of the physical space: every computational node contains only a subset of the physical domain and a whole velocity space. This strategy allows to evaluate the Boltzmann collision operator (multiple integral over the velocity space) without any additional MPI communication required. Finally, computations on every node are performed in parallel using the OpenMP framework.

Dernières publications:

- Jacek Narski, Fast Kinetic Scheme: efficient MPI parallelization strategy for 3D Boltzmann equation, Commun. Comput. Phys., 25 (2019), pp. 361-389 - **doi:** pu.doi

Modelisation THCM des ouvrages en béton, béton armé et précontraint

Projet démarré en 2016

LMDC - Laboratoire Matériaux et Durabilité des Constructions de Toulouse
Porteur de projet: **Laurie Lacarriere**
The main objective of this project is to study the thermo-hydro-chemo-mechanical (THCM) behavior of concrete and reinforced concrete structures (confinement vessels, larges beams of bridges). The coupling between physico-chemical and mechanical behavior is studied for several applications (early age, ageing concrete, severe accident with high temperatures, chemical endogenous attack, ...).

Embryogenèse de créatures et de réseaux de neurones artificiels

Projet démarré en 2016

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)
Porteur de projet: **Sylvain Cussat-blanc**
Artificial embryogenesis aims to mimic or to take inspiration from the natural process of embryogenesis either to generate artificial creatures that populate virtual worlds or to simulate cell proliferation for biological matters. Embryogenesis is the process that grows a living being from a unique egg cell. This process implies extremely complex mechanisms such as cell division and cell specialization both orchestrated by genetic regulation. The aim of this project is to develop in-silico models of artificial embryogenesis, also named a evo-devo model, that simulate the cell in its chemical and/or physical environment and its internal control via an evolved artificial gene regulatory network. This latter generates the behavior of the cells: as in nature, by sensing the protein concentration of its direct neighborhood and inside its own membrane, the cell can decide between dividing, specializing, waiting for better environmental condition (quiescence), committing a suicide (apoptosis) or migrate. With these models, multiple objectives will be addressed. First, this model can be used to produce artificial creatures by evolving (with a genetic algorithm for example) the gene regulatory network of the cell. This allows the study of the evolutionary process of multicellular organisms under particular environmental conditions. Another goal of this model is to simulate the growth of neural networks in order to produce larger, scalable and adaptative behavior engines to control virtual robots in complex changing environments.

Dernières publications:

- Learning Aquatic Locomotion for Animats -
- A Comparison of Genetic Regulatory Network Dynamics and Encoding -

Algèbre Linéaire Creuse (MUMPS, Méthodes Hybrides)

Projet démarré en 2009

IRIT - Institut de Recherche en Informatique de Toulouse (UMR 5505)
Porteur de projet: **Patrick Amestoy**
Our project focusses on sparse parallel algorithms, more precisely on the parallel solution of large sparse linear systems based on both direct and hybrid methods (mixing direct and iterative methods). Our work can impact the performance of many applications, in particular simulations using finite element or finite difference methods as well as numerical optimization problems. Two main aspects of our research are the scalability of our methods on problems with millions of equations when increasing the number of processors and the use of so called block low rank approximation techniques to reduce both memory and floating point number complexity of our algorithms. To reduce the memory and flops complexity we are also investigating hybrid methods based on block Cimmino approach. Parallel spectral classification is our last domain of activity. Our project takes place in the context of a strong collaboration between IRIT (APO team), LIP (Team ROMA at ENS-Lyon) and CERFACS (through a joint lab with IRIT). On real large 3D problems of size few hundred million variables we want to analyse the potential and limit of both direct approaches and hybrid resolution methods. Our work is often based on one of the following software research platforms: http://mumps.enseeiht.fr http://buttari.perso.enseeiht.fr/qr_mumps/ http://abcd.enseeiht.fr/ All software are freely distributed and the improvement of the parallel behaviour of our solvers has a direct benefit for the scientific community.

Dernières publications:

- Amestoy, Patrick R. and L'Excellent, Jean-Yves and Moreau, Gilles Elimination Tree Flattening to Exploit Right-Hand Sides Sparsity 2 pages reviewed extended abstract at SIAM Workshop on Combinatorial Scientific Computing 2018, Bergen, Norway, June 2018 -
- Amestoy, Patrick and de la Kethulle de Ryhove, S\'ebastien and L'Excellent, Jean-Yves and Moreau, Gilles and Shantsev Daniil Fast direct solver for 3D marine controlled-source EM problems based on sparsity utilization and BLR approximation At the 24th EM Induction Workshop (EMIW2018), Helsingør, Denmark, Aug 2018 -