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**Université Nice - Sophia  
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Activity Report 2014

**Project-Team COFFEE**

COmplex Flows For Energy and Environment

IN COLLABORATION WITH: Laboratoire Jean-Alexandre Dieudonné (JAD)

RESEARCH CENTER  
**Sophia Antipolis - Méditerranée**

THEME  
**Earth, Environmental and Energy  
Sciences**



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# Project-Team COFFEE

**Keywords:** Multiscale Analysis, Multiscale Models, Numerical Methods, Porous Media

*Coffee is a joint team with the laboratory J. A. Dieudonné, UNS-CNRS.*

*Creation of the Team: 2011 July 01, updated into Project-Team: 2013 January 01.*

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### Research Scientist

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## 2. Overall Objectives

### 2.1. Overall Objectives

The project aims at studying mathematical models issued from environmental and energy management questions. We consider systems of PDEs of hydrodynamic type or hybrid fluid/kinetic systems. The problems we have in mind involve unusual coupling, which in turn leads to challenging difficulties for mathematical analysis and the need of original numerical solutions. By nature many different scales arise in the problems, which allows to seek hierarchies of reduced models based on asymptotic arguments. The topics require a deep understanding of the modeling issues and, as far as possible boosted by the mathematical analysis of the equations and the identification of key structure properties, we wish to propose innovative and performing numerical schemes. To this end, the development of innovative Finite Volumes schemes with unstructured meshes on complex geometries will be a leading topic of the team activity.

## 3. Research Program

### 3.1. Research Program

Mathematical modeling and computer simulation are among the main research tools for environmental management, risks evaluation and sustainable development policy. Many aspects of the computer codes as well as the PDEs systems on which these codes are based can be considered as questionable regarding the established standards of applied mathematical modeling and numerical analysis. This is due to the intricate multiscale nature and tremendous complexity of those phenomena that require to set up new and appropriate tools. Our research group aims to contribute to bridging the gap by developing advanced abstract mathematical models as well as related computational techniques.

The scientific basis of the proposal is two-fold. On the one hand, the project is “technically-driven”: it has a strong content of mathematical analysis and design of general methodology tools. On the other hand, the project is also “application-driven”: we have identified a set of relevant problems motivated by environmental issues, which share, sometimes in a unexpected fashion, many common features. The proposal is precisely based on the conviction that these subjects can mutually cross-fertilize and that they will both be a source of general technical developments, and a relevant way to demonstrate the skills of the methods we wish to design.

To be more specific:

- We consider evolution problems describing highly heterogeneous flows (with different phases or with high density ratio). In turn, we are led to deal with non linear systems of PDEs of convection and/or convection–diffusion type.
- The nature of the coupling between the equations can be two-fold, which leads to different difficulties, both in terms of analysis and conception of numerical methods. For instance, the system can couple several equations of different types (elliptic/parabolic, parabolic/hyperbolic, parabolic or elliptic with algebraic constraints, parabolic with degenerate coefficients...). Furthermore, the unknowns can depend on different sets of variables, a typical example being the fluid/kinetic models for particulate flows. In turn, the simulation cannot use a single numerical approach to treat all the equations. Instead, hybrid methods have to be designed which raise the question of fitting them in an appropriate way, both in terms of consistency of the discretization and in terms of stability of the whole computation. For the problems under consideration, the coupling can also arise through interface conditions. It naturally occurs when the physical conditions are highly different in subdomains of the physical domain in which the flows takes place. Hence interface conditions are intended to describe the exchange (of mass, energy...) between the domains. Again it gives rise to rather unexplored mathematical questions, and for numerics it yields the question of defining a suitable matching at the discrete level, that is requested to preserve the properties of the continuous model.
- By nature the problems we wish to consider involve many different scales (of time or length basically). It raises two families of mathematical questions. In terms of numerical schemes, the multiscale feature induces the presence of stiff terms within the equations, which naturally leads to stability issues. A clear understanding of scale separation helps in designing efficient methods, based on suitable splitting techniques for instance. On the other hand asymptotic arguments can be used to derive hierarchy of models and to identify physical regimes in which a reduced set of equations can be used.

We can distinguish the following fields of expertise

- Numerical Analysis: Finite Volume Schemes, Well-Balanced and Asymptotic-Preserving Methods
  - Finite Volume Schemes for Diffusion Equations
  - Finite Volume Schemes for Conservation Laws
  - Well-Balanced and Asymptotic-Preserving Methods

- Modeling and Analysis of PDEs
  - Kinetic equations and hyperbolic systems
  - PDEs in random media
  - Interface problems

## 4. Application Domains

### 4.1. Porous Media

Clearly, the analysis and simulation of flows in porous media is a major theme in our team. It is strongly motivated by industrial partnerships, with Total, GdF-Suez, ANDRA, BRGM, etc. with direct applications in geothermy, geological storages, and oil and gas recovery.

Our research has first dealt with the discretization and convergence analysis of multiphase Darcy flows on general polyhedral meshes and for heterogeneous anisotropic media. We have investigated both the Vertex Approximate Gradient (VAG) scheme using both cell and vertex unknowns and the Hybrid Finite Volume (HFV) scheme using both cell and face unknowns. It is remarkable that the VAG scheme is much more accurate than existing nodal approaches (such as CVFE) for heterogeneous test cases: since it avoids the mixing of different rocktypes inside the control volumes, while preserving the low cost of nodal discretizations thanks to the elimination of cell unknowns without any fill-in. The convergence of the numerical discretizations has been studied for the problem of contaminant transport with adsorption in the case of HFV scheme and for two phase Darcy flows in global pressure formulation using particular VAG or HFV schemes, as well as the more general framework of gradient schemes. To reduce the Grid Orientation Effect, a general methodology is proposed in on general meshes. It is based on the recombination of given conservative fluxes to define new conservative fluxes on a richer stencil. On the same token, we have considered the transport of radionuclides by water in porous media. The question is naturally motivated by security studies of nuclear waste storage. We have dealt with the non linear Peaceman system, set on a heterogeneous domain, typically a layered geological medium. The system couples anisotropic diffusion equation and a diffusion-dispersion equation for the pollutant concentration. We have developed and analyzed a specific DDFV scheme to investigate such flows

### 4.2. Particulate and mixture flows

We investigate fluid mechanics models referred to as “multi-fluids” flows. A large part of our activity is more specifically concerned with the case where a disperse phase interacts with a dense phase. Such flows arise in numerous applications, like for pollutant transport and dispersion, the combustion of fuel particles in air, the modelling of fluidized beds, the dynamic of sprays and in particular biosprays with medical applications, engine fine particles emission... There are many possible modelings of such flows: microscopic models where the two phases occupy distinct domains and where the coupling arises through intricate interface conditions; macroscopic models which are of hydrodynamic (multiphase) type, involving non standard state laws, possibly with non conservative terms, and the so-called mesoscopic models. The latter are based on Eulerian-Lagrangian description where the disperse phase is described by a particle distribution function in phase space. Following this path we are led to a Vlasov-like equation coupled to a system describing the evolution of the dense phase that is either the Euler or the Navier-Stokes equations. It turns out that the leading effect in such models is the drag force. However, the role of other terms, of more or less phenomenological nature, deserves to be discussed (close packing terms, lift term, Basset force...). Of course the fluid/kinetic model is interesting in itself and needs further analysis and dedicated numerical schemes. In particular, in collaboration with the Atomic Energy Commission (CEA), we have proposed a semi-Lagrangian scheme for the simulation of particulate flows, extending the framework established in plasma physics to such flows.

We also think it is worthwhile to identify hydrodynamic regimes: it leads to discuss hierarchies of coupled hydrodynamic systems, the nature of which could be quite intriguing and original, while they share some common features of the porous media problems. We are particularly interested in revisiting the modeling of mixture flows through the viewpoint of kinetic models and hydrodynamic regimes. We propose to revisit the derivation of new mixture models, generalizing Kazhikov-Smagulov equations, through hydrodynamic asymptotics. The model is of “hybrid” type in the sense that the constraint reduces to the standard incompressibility condition when the disperse phase is absent, while it involves derivatives of the particle volume fraction when the disperse phase is present.

### 4.3. Biological degradation, biofilms formation and algae proliferation

Members of the team have started an original research program devoted to biofilms formation and algae proliferation. We started working on this subject through a collaboration with Roberto Natalini and a group of experts in Firenze interested in preventing damages on historical monuments. It is also motivated by *Ostreopsis* proliferation in the Mediterranean Sea. The multidisciplinary character of this research relies on discussions with researchers of the Oceanography Laboratory in Villefranche-sur-Mer, a leading marine research unit, and the Inria team BIOCORE, led by J-L Gouzé. This research is supported by a ANR-project, led by M. Ribot, and it is the main topic of the PhD thesis of B. Polizzi.

## 5. New Software and Platforms

### 5.1. NS2DDV

The code NS2DDV is developed jointly with the team SIMPAF, of the Inria Research Centre Lille Nord Europe. It is devoted to the simulation of non-homogeneous viscous flows, in two-dimensional geometries. The code is based on an original hybrid Finite Volume/Finite Element scheme; it works on unstructured meshes and can include mesh refinements strategies. Further details can be found in the research papers *J. Comput. Phys.*, 227, 4671–4696, 2008 and *J. Comput. Phys.*, 229 (17), 6027–6046, 2010. The code exists in two versions: a Matlab public version, a C++ prototype version allowing more ambitious simulations. Both versions are still subject to developments. The current versions is restricted to incompressible flows but on-going progress are concerned with the simulation of avalanches. The source code of the public version is downloadable and several benchmarks tests can be reproduced directly.

### 5.2. Compass

for Computing Parallel Architecture to Speed up Simulation is a parallel code for the discretization of polyphasic flows by Finite Volumes methods. The code is mainly devoted to applications in porous media. It works on quite general polyhedral meshes. A first step in the code development has been made during the 2012 edition of CEMRACS and then pursued by C. Guichard, R. Masson and R. Eymard in 2013. A first version of the code has been deposited at the Agency for the Protection of Programs (APP). This current version of ComPASS has been tested on a gas storage two phase flow benchmark with GDFSuez using the Vertex Approximate Gradient spatial discretization. The results have shown a very good parallel scalability on the CICADA Cluster at UNS with a few millions of cells and up to 1024 cores. The objective is to develop a generic simulator for multiphase Darcy flows. This simulator will implement advanced finite volume methods on general 3D meshes and on heterogeneous anisotropic media, taking into account discrete fracture networks represented as interfaces of codimension one and coupled with the surrounding matrix. It will be able to treat a large range of multiphase Darcy flow models accounting for thermodynamical equilibrium and the coupling with an energy conservation equation. The simulator will run on massively parallel architectures with a few thousands of cores. It will be applied to several type of industrial applications starting with the simulation of high energy geothermal systems as a carbon-free source of power production.



### 5.3. SimBiof

We are developing numerical methods, currently by using Finite Differences approaches, for the simulation of biofilms growth. The underlying system of PDEs takes the form of multiphase flows equations with conservation constraints and vanishing phases. The numerical experiments have permitted to bring out the influence of physical parameters on the multidimensional growth dynamics.

### 5.4. AP\_PartFlow

We are developing experimental codes, mainly based on Finite Differences, for the simulation of particulate flows. A particular attention is paid to guaranty the asymptotic properties of the scheme, with respect to relaxation parameters.

## 6. Bilateral Contracts and Grants with Industry

### 6.1. Bilateral Contracts with Industry

The project has industrial collaborations with Total, GDFSuez EP and Storengy on oil and gas recovery and gas storage.

The collaboration with Andra is concerned with the modelling and the simulation of mass and heat exchanges between porous media and ventilation channels. It leads to consider porous medium equations and hydrodynamic systems, coupled through intricate boundary conditions. Clearly one of the difficulties relies on the multiphase nature of the flows (at least water and air are present). We identify relevant physical scales, typical of the flows under consideration in nuclear waste engineering. We start by dealing with quite simple geometries, in order to discuss properly the order of magnitude of the different phenomena, and to design suitable schemes

## 7. Partnerships and Cooperations

### 7.1. National Initiatives

#### 7.1.1. ANR

The ANR-project Monumentalg, led by M. Ribot, is devoted to the modeling and simulation of biological damage on monuments and algae proliferation.

#### 7.1.2. National and European networks

- GdR MoMas.  
The research group MoMaS (Mathematical Modeling and Numerical Simulation for Nuclear Waste Management Problems ) has activities centered around scientific computing, design of new numerical schemes and mathematical modelling (upscaling, homogenization, sensitivity studies, inverse problems,...). Its goal is to coordinate research in this area, as well as to promote the emergence of focused groups around specific projects
- S. Junca is involved in the GdR-e “Wave Propagation in Complex Media for Quantitative and non Destructive Evaluation”.
- GdR EGRIN is a newly created CNRS-network, devoted to gravitational flows and natural risks; Coffee is among the members of this network.

## 7.2. International Initiatives

### 7.2.1. Inria Associate Teams

#### 7.2.1.1. COKLYCO

Title: Modeling, analysis and simulation of kinetic and fluid models for MEMS

International Partner (Institution - Laboratory - Researcher):

Kyoto (JAPON)

Duration: 2014 -

See also: [https://team.inria.fr/coffee/?page\\_id=323](https://team.inria.fr/coffee/?page_id=323)

The team led the project CoKLyCo, a collaborative program with Kyoto University and the team Khaliffe in Lyon. We wish to elaborate and analyse new models of microscopic and macroscopic type for Micro-Electro-Mechanical Systems (MEMS). The tiny scales of such technical devices induce new and challenging difficulties. A specific attention will be paid to the treatment of coupling conditions from moving boundaries, and to the multi-scale character of the problem. The project is based on a strong interplay between mathematical analysis, experiments and numerical simulations, made possible by the composition of the team.

#### 7.2.2. Participation In other International Programs

Quite recently, S. Junca has started a collaboration with Mathias Legrand, from the Mechanical Engineering department at Mc Gill, Montréal with the supervision of the internship of a master student (S. Heng, 6 months, June-Nov. 2013). Furthermore, S. Junca is an active member of the European network “Wave propagation in complex media for quantitative and non destructive evaluation” <http://www.gdre-us.cnrs-mrs.fr/spip.php?rubrique8>

S. Krell has a collaboration with Martin Gander (University of Geneva, Switzerland) on domain decomposition methods, adapted to DDFV discretizations.

M. Ribot started a collaboration with Roberto Natalini a couple of years ago. Connections with experts in Firenze was the starting point of the research on biofilm formation and algae proliferation. M. Ribot and R. Natalini have also worked on new well-balanced strategy — the so-called AHO schemes — in order to preserve equilibria and to capture correctly large time solutions for complex PDEs system, without knowing explicitly the equilibrium solution. They have co-advised 2 PhD thesis.

Finally, we have many international collaborations, with variable peaks of activity, in our research networks: A. Vasseur (U. T. Austin), P.E. Jabin (Univ. Maryland), J.-A. Carrillo (Imperial College London), S. Jin (U. W. Madison and Jiao Tong Univ.), R. Aavatsmark (Univ. of Bergen), etc.

## 8. Dissemination

### 8.1. Promoting Scientific Activities

#### 8.1.1. Journal

##### 8.1.1.1. SIAM J. Computational Math.

T. Goudon is founding editor of the SMAI J. of Computational Math.

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