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CNRS

**Université Nice - Sophia
Antipolis**

Activity Report 2017

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

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

Keywords:

Computer Science and Digital Science:

- A6.1.1. - Continuous Modeling (PDE, ODE)
- A6.1.4. - Multiscale modeling
- A6.1.5. - Multiphysics modeling
- A6.2.1. - Numerical analysis of PDE and ODE
- A6.2.7. - High performance computing

Other Research Topics and Application Domains:

- B1.1.10. - Mathematical biology
- B3.3.1. - Earth and subsoil
- B4.1. - Fossil energy production (oil, gas)
- B4.2. - Nuclear Energy Production
- B7.1. - Traffic management

1. Personnel

Research Scientists

Thierry Goudon [Team leader, Inria, Senior Researcher, HDR]
Laurent Monasse [Inria, Researcher, from Sep 2017]

Faculty Members

Florent Berthelin [Univ de Nice - Sophia Antipolis, Associate Professor, HDR]
Konstantin Brenner [Univ de Nice - Sophia Antipolis, Associate Professor]
Stéphane Junca [Univ de Nice - Sophia Antipolis, Associate Professor, HDR]
Stella Krell [Univ de Nice - Sophia Antipolis, Associate Professor]
Roland Masson [Univ de Nice - Sophia Antipolis, Professor, HDR]

Post-Doctoral Fellows

Joubine Aghili [Inria, from Oct 2017]
Nabil Birgile [Inria]

PhD Students

Kevin Atsou [Inria, from Oct 2017]
Laurence Beaude [Univ. Côte d'Azur]
Billel Guelmame [Univ. Côte d'Azur, from Oct 2017]
Julian Hennicker [Univ. Côte d'Azur, until May 2017]
Thi Huong Le [Univ. Côte d'Azur, until Jun 2017]
Giulia Lissoni [Univ. Côte d'Azur]
Julie Llobell [Univ. Côte d'Azur]
Leo Vivion [Univ. Côte d'Azur, from Sep 2017]

Administrative Assistant

Marie-Cécile Lafont [Inria]

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

Our research focuses on the numerical modeling of multiphase porous media flows accounting for complex geology and for nonlinear and multi-physics couplings. It is applied to various problems in the field of energy such as the simulation of geothermal systems in collaboration with BRGM, of nuclear waste repositories in collaboration with Andra, and of oil and gas recovery in collaboration with Total. Our research directions include the development of advanced numerical schemes adapted to polyhedral meshes and highly heterogeneous media in order to represent more accurately complex geologies. A special focus is made on the modeling of multiphase flows in network of faults or fractures represented as interfaces of co-dimension one coupled to the surrounding matrix. We also investigate nonlinear solvers adapted to the nonlinear couplings between gravity, capillary and viscous forces in highly heterogeneous porous media. In the same line, we study new domain decomposition algorithms to couple non-isothermal compositional liquid gas flows in a porous medium with free gas flows occurring at the interface between the ventilation gallery and the nuclear waste repository or between a geothermal reservoir and the atmosphere.

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 was supported by a ANR-project, led by M. Ribot, and it was the main topic of the PhD thesis of B. Polizzi.

5. New Software and Platforms

5.1. AP_PartFlow

FUNCTIONAL DESCRIPTION: 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.

- Contact: Thierry Goudon

5.2. Compass

Computing Architecture to Speed up Simulation

KEYWORDS: Finite volume methods - Porous media - High performance computing

FUNCTIONAL DESCRIPTION: Compass is a parallel code initiated in 2012 and co-developed by LJAD-Inria Coffee and BRGM since 2015. It is devoted to the simulation of multiphase flows in porous media, it accounts for non isothermal and compositional flows and includes complex network of fractures or faults represented as interfaces of co-dimension one coupled to the surrounding matrix. The discretization is based on vertex and cell unknowns and is adapted to polyhedral meshes and heterogeneous media. The ComPASS code is co-developed since december 2016 by the partners of the ANR CHARMS project including BGRM, LJAD-Inria Coffee, Storengy, MdS and LJLL with the objective to develop a new generation simulator for geothermal systems focusing on fluids and accounting for complex fault networks and wells.

- Participants: Chang Yang, Cindy Guichard, Robert Eymard, Roland Masson and Thierry Goudon
- Partners: Université de Nice Sophia Antipolis (UNS) - BRGM
- Contact: Roland Masson

5.3. NS2DDV

2D Navier-Stokes equations with variable density

KEYWORDS: Partial differential equation - Finite volume methods - Finite element modelling

FUNCTIONAL DESCRIPTION: The NS2DDV Matlab toolbox is an open-source program written in Matlab for simulating 2D viscous, incompressible and inhomogeneous flows. The computation kernel of the code is based on Finite Elements - Finite Volumes hybrid methods applied on the 2D Navier-Stokes equations. It works on unstructured meshes and can include mesh refinements strategies. We develop and freely distribute a new version of the Matlab code NS2DDV-M (equipped with a graphic interface and an accurate documentation) to promote new collaborations in the domain, allow some easy comparisons with concurrent codes on the same benchmark cases, and compare alternative numerical solution methods.

- Partner: Laboratoire Paul Painlevé
- Contact: Creusé Emmanuel
- URL: <https://wikis.univ-lille1.fr/painleve/ns2ddv>

5.4. SimBiof

KEYWORDS: Bioinformatics - Chemistry

FUNCTIONAL DESCRIPTION: 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.

- Contact: Thierry Goudon

5.5. CELIA3D

KEYWORDS: Fluid mechanics - Multi-physics simulation

FUNCTIONAL DESCRIPTION: The CELIA3D code simulates the coupling between a compressible fluid flow and a deformable structure. The fluid is handled by a Finite Volume method on a structured Cartesian grid. The solid is handled by a Discrete Element method (Mka3d scheme). The solid overlaps the fluid grid and the coupling is carried out with immersed boundaries (cut cells) in a conservative way.

- Partners: Ecole des Ponts ParisTech - CEA
- Contact: Laurent Monasse
- URL: <http://cermics.enpc.fr/~monassel/CELIA3D/>

5.6. Mka3d

KEYWORDS: Scientific computing - Elasticity - Elastodynamic equations

FUNCTIONAL DESCRIPTION: The Mka3d method simulates an elastic solid by discretizing the solid into rigid particles. An adequate choice of forces and torques between particles allows to recover the equations of elastodynamics.

- Partners: Ecole des Ponts ParisTech - CEA
- Contact: Laurent Monasse
- URL: <http://cermics.enpc.fr/~monassel/Mka3D/>

6. New Results

6.1. A few words on the results of the year

- Analysis of models with constraints: existence of solutions for a multidimensional model [1].
- Analysis of the convergence of a particle approximation for a traffic flow model with constraints [2].
- Numerical study of a traffic flow model with constraints [3]
- Existence of martingale solutions for the stochastic isentropic Euler model [4]
- New approach to accelerate convergence of Newton's methods applied to highly nonlinear and heterogeneous porous media flow problems [5], [6]
- We provide the numerical analysis of Discrete Duality Finite Volume (DDFV) schemes on general meshes for the (linear) Stokes problem with Neumann boundary conditions (on a fraction of the boundary). We prove well-posedness for a stabilized version of the scheme and we derive some error estimates. Finally, our theoretical results are illustrated with numerical simulations and stabilized and unstabilized schemes are compared. [26]
- A new domain decomposition algorithm to couple a non-isothermal compositional liquid gas Darcy flow and a free gas flow occurring at the interface between the nuclear waste repository and the ventilation galleries. [16], [22]
- A new two-phase Darcy flow model in fractured porous medium with fractures represented as interfaces of co-dimension one coupled to the surrounding matrix. The model accounts accurately for highly discontinuous capillary pressures, for gravity in the fracture width and both for fractures acting as drains or barriers. [7], [18]
- Use of the code COMPASS at BRGM to study the hydrothermal system of Lamentin Bay in Martinique during the PhD thesis of Yannis Labeau from University of Martinique [14], [21]
- New explicit energy-momentum conserving scheme for Hamiltonian systems [28].
- L. Monasse obtained an ANR JCJC grant.
- Through the PhD of J. Llobell, progress have been made to set up new schemes on staggered grids for solving the Euler system of gas dynamics (full Euler equations, MUSCL version on MAC grids, Low Mach regimes).

7. Bilateral Contracts and Grants with Industry

7.1. Bilateral Contracts with Industry

- Contract with Andra financing the two years postdoctoral position of Nabil Birgile (april 2016- march 2018) and dealing with domain decomposition algorithms to couple the non-isothermal liquid gas Darcy flow and the free gas flow occurring at the interface between the nuclear waste repository and the ventilation galleries. Supervision Roland Masson from LJAD-Inria and Laurent Trenty from Andra.
- Contract with Andra financing the two year postdoctoral position of Joubine Aghili (october 2017 - september 2019) and dealing with the simulation of compositional liquid gas Darcy flows in highly heterogeneous porous medium with network of fractures using Discrete Fracture Matrix models (DFM). It is applied to the simulation of the desaturation of the nuclear waste storage in the neighbourhood of the galleries. Supervision Roland Masson and Konstantin Brenner from LJAD-Inria, Jean-Raynald de Dreuzy from Geosciences Rennes and Laurent Trenty from Andra.

8. Partnerships and Cooperations

8.1. Regional Initiatives

The team is involved in the IDEX project UCA-JEDI.

- PhD of Laurence Beaudé (october 2015 - december 2018) co-funded by BRGM and Region PACA and dealing with the simulation of geothermal systems, supervised by Roland Masson, Konstantin Brenner from LJAD-Inria and by Simon Lopez, Farid Smai from BRGM.

8.2. National Initiatives

8.2.1. ANR

- ANR CHARMS (Quantitative Reservoir Models for Complex Hydrothermal Systems): december 2016 - december 2020, partners BRGM (leader), LJAD-Inria, Storengy, M&S, LJLL.

8.2.2. National and European networks

- GdR MANU.
The research group MANU 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 GdR 3437 DYNOLIN “Dynamique non linéaire” and GdR MecaWave.
- LJAD-Inria and BRGM are the French partners of the Norwegian, German French project InSPiRE “International Open Source Simulation Software Partnership in Research and Education” which has just been accepted by the Research Council of Norway with the code COMPASS as one of the softwares of this project together with Dune, Dumux and OPM.

8.3. International Research Visitors

8.3.1. Visits of International Scientists

- Felix Kwok, one month in may 2017: nonlinear domain decomposition methods for the Richards equation with Roland Masson and Victorita Dolean.

8.3.1.1. Internships

- Internship of Willy Bonneuil (March 2017-August 2017) funded by EDF Chatou on nonlinear solvers based on variable switches for the Richards equation, supervision Konstantin Brenner and Roland Masson from LJAD-Inria and Jerome Bonnelle and Raphael Lamouroux from EDF.

9. Dissemination

9.1. Promoting Scientific Activities

9.1.1. Scientific Events Organisation

9.1.1.1. General Chair, Scientific Chair

We do not keep track of such activities.

9.1.1.2. Member of the Organizing Committees

- Co-organisation of the conference FVCA8 june 2017 in Lille

9.1.2. Scientific Events Selection

9.1.2.1. Chair of Conference Program Committees

We do not keep track of such activities.

9.1.2.2. Member of the Conference Program Committees

We do not keep track of such activities.

9.1.2.3. Reviewer

We do not keep track of such activities.

9.1.3. Journal

9.1.3.1. Member of the Editorial Boards

T. Goudon is founding editor and co-Editor in chief of SMAI-J. Computational Mathematics

9.1.3.2. Reviewer - Reviewing Activities

We do not keep track of such activities.

9.1.4. Invited Talks

We do not keep track of such activities.

9.1.5. Leadership within the Scientific Community

We do not keep track of such activities.

9.1.6. Scientific Expertise

Thierry Goudon is member of the scientific board of CIRM and of FSMP.

9.1.7. Research Administration

Roland Masson is the head of the team PDE and Numerical Analysis of the laboratory J.A. Dieudonné.

Roland Masson is a member of the scientific committee of CERFACS.

Roland Masson is scientific advisor at the scientific direction of Total.

Thierry Goudon is member of the Evaluation Committee of Inria.

Thierry Goudon is Scientific Officer at the French Ministry of Education and Research.

9.2. Teaching - Supervision - Juries

9.2.1. Teaching

Members of the team are faculties of University Nice Sophia Antipolis and they teach in all degrees of the University.

Florent Berthelin, Master 2 Agrégation, Université Nice Sophia Antipolis.

Florent Berthelin, Chair of the Master 2 Agrégation, Université Nice Sophia Antipolis.

Thierry Goudon is President of the national competition to hire teachers (agrégation de mathématiques).

Stella Krell, Linear Algebra, Master 1 enseignement, ESPE Nice, 23h.

Stella Krell, Didactics of mathematics, Master 1 EEF, Université Nice Sophia Antipolis, 43h.

Stella Krell, Theses and placement supervision, Master 2 EEF, Université Nice Sophia Antipolis, 12h.

Stella Krell, Preparation to mathematics agrégation interne, Université Nice Sophia Antipolis, 18h.

Stella Krell, Intervention, Master 2 enseignement, Université Nice Sophia Antipolis, 3h.

Laurent Monasse, Introduction to analysis and dynamical systems, Ecole des Ponts ParisTech, 20h.

Thierry Goudon is President of the jury of agrégation.

9.2.2. Supervision

PhD: Julian Hennicker, Hybrid dimensional modeling of multi-phase Darcy flows in fractured porous media, Univ Nice - Sophia Antipolis, 10 July 2017, Roland Masson and Konstantin Brenner

PhD: Thi Huong Le, On some periodic solutions of discrete vibro-impact systems with a unilateral contact condition, Univ Nice - Sophia Antipolis, 16 June 2017, Stéphane Junca

PhD in progress: Kevin Atsou, Mathematical modeling of tumor growth, analysis and simulation, 01 October 2017, Thierry Goudon

PhD in progress: Laurence Beaude, Discretization of high energy geothermal systems in faulted porous media, 01 October 2015, Roland Masson, Konstantin Brenner, Simon Lopez and Farid Smai

PhD in progress: Billel Guelmame, Conservation laws in mechanics, 01 October 2017, Stéphane Junca

PhD in progress: Giulia Lissonni, DDFV methods and domain decomposition: applications in fluid mechanics, 01 September 2016, Stella Krell and Thierry Goudon.

PhD in progress: Julie Llobell, Numerical schemes on staggered grids for conservation laws, 01 September 2015, Thierry Goudon and Sebastian Minjeaud

PhD in progress: Leo Vivion, Dynamical model of a Lorentz gas : kinetic approach, analysis and asymptotic issues, 01 September 2017, Thierry Goudon

PhD in progress: Frédéric Marazzato, Modeling of fracture and fragmentation using a Discrete Element method, 01 October 2016, Alexandre Ern, Karam Sab and Laurent Monasse.

9.2.3. *Juries*

- Laurent Monasse, Examiner, PhD defense Julien Ridoux, Université Paris 6, 4 October 2017.
- Thierry Goudon, Pdt HDR defese F. Laurent-Nègre, “Méthodes de moments pour la description de sprays et d’aérosols : modélisations et simulations num’eriques”, ECParis, Mars 2017.
- Thierry Goudon, referee PhD defense T. Blanc, “Étude mathématique des problèmes paraboliques fortement anisotropes”, Marseille, Déc. 2017.

10. Bibliography

Publications of the year

Articles in International Peer-Reviewed Journals

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- [2] F. BERTHELIN, P. GOATIN. *Particle approximation of a constrained model for traffic flow*, in "NoDEA : Nonlinear Differential Equations and Applications", 2017, vol. 24, n^o 5, pp. 24-55, <https://hal.archives-ouvertes.fr/hal-01437867>
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- [10] P. CASTELLI, S. JUNCA. *On the maximal smoothing effect for multidimensional scalar conservation laws*, in "Nonlinear Analysis: Theory, Methods and Applications", May 2017, vol. 155, pp. 207-218 [DOI : 10.1016/J.NA.2017.01.018], <https://hal.archives-ouvertes.fr/hal-01290871>
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International Conferences with Proceedings

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