

IN PARTNERSHIP WITH: CNRS

Université Nice - Sophia Antipolis

Activity Report 2019

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

A6.5. - Mathematical modeling for physical sciences

A6.5.2. - Fluid mechanics

A6.5.3. - Transport

Other Research Topics and Application Domains:

B1.1.8. - Mathematical biology

B3.3.1. - Earth and subsoil

B4.1. - Fossile energy production (oil, gas)

B4.2. - Nuclear Energy Production

B7.1. - Traffic management

1. Team, Visitors, External Collaborators

Research Scientists

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

Faculty Members

Florent Berthelin [Univ. Côte d'Azur, Associate Professor, HDR] Konstantin Brenner [Univ. Côte d'Azur, Associate Professor] Stéphane Junca [Univ. Côte d'Azur, Associate Professor, HDR] Stella Krell [Univ. Côte d'Azur, Associate Professor] Roland Masson [Univ. Côte d'Azur, Professor, HDR] Gilles Lebeau [Univ. Côte d'Azur, Professor, HDR]

Post-Doctoral Fellows

Joubine Aghili [Inria, Post-Doctoral Fellow, until Sep 2019] Laurence Beaude [Univ. Côte d'Azur, Post-Doctoral Fellow, until Dec. 2019] Francesco Bonaldi [Inria, Post-Doctoral Fellow, from Sep 2019] Daniel Castanon Quiroz [Univ. Côte d'Azur, Post-Doctoral Fellow, from Nov 2019] El Houssaine Quenjel [Univ Côte d'Azur, Post-Doctoral Fellow, from Feb 2019] Sean Mcgovern [Inria, Post-Doctoral Fellow, from Dec 2019]

PhD Students

Kevin Atsou [Inria, PhD Student] Nadine Dirani [Inria, PhD Student] Billel Guelmame [Univ. Côte d'Azur, PhD Student] Giulia Lissoni [Univ. Côte d'Azur, PhD Student, until Sep 2019] Leo Vivion [Univ. Côte d'Azur, PhD Student] Marie-Cécile Lafont [Inria, Administrative Assistant]

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 arises 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

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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 and Viscous Flows
 - Finite Volume Schemes for Conservation Laws
 - Well-Balanced and Asymptotic-Preserving Methods
 - Domain Decomposition Methods
- Modeling and Analysis of PDEs
 - Kinetic equations and hyperbolic systems
 - PDEs in random media
 - Interface problems

4. Application Domains

4.1. Multiphase porous media flows and multi-physics coupling

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. We have begun exploring the coupling between the multiphase flow in the porous matrix and the solid mechanics involved in opening fractures.

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. Fungal network growth

Members of the team have started an original research program devoted to fungal network growth. We started working on this subject through a collaboration with biologists and physicists at LIED (Université Paris Diderot) and probabilists in CMAP (Ecole Polytechnique) and Université Paris Sud, involving Rémi Catellier and Yves D'Angelo in LJAD in Nice. The motivation is to understand branching networks as an efficient space exploration strategy, with fungus *Podospora Anserina* being the biological model considered. This research is submitted as an ANR-project and has been supported by various local fundings.

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. 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/

5.3. 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: Simon Lopez, Farid Smai, Michel Kern, Yacine Ould Rouis, Nabil Birgle, Laurence Beaude, Konstantin Brenner and Roland Masson
- Partners: Université de Nice Sophia Antipolis (UNS) BRGM
- Contact: Roland Masson
- URL: http://www.anr-charms.org/page/compass-code

5.4. NS2DDV-M

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: Caterina Calgaro
- URL: https://wikis.univ-lille1.fr/painleve/ns2ddv

5.5. 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

5.6. 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/

6. Bilateral Contracts and Grants with Industry

6.1. Bilateral Contracts with Industry

- 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.
- The team has also on-going collaboration with Storengy (post-doc of Daniel Constantin-Quiroz).

7. Partnerships and Cooperations

7.1. Regional Initiatives

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

7.2. National Initiatives

7.2.1. ANR

- ANR CHARMS (Quantitative Reservoir Models for Complex Hydrothermal Systems), Roland Masson and Konstantin Brenner: december 2016 december 2020, partners BRGM (leader), LJAD-Inria, Storengy, MdS, LJLL.
- ANR JCJC PRECIS (Effect of a shock wave on a structure with contact using mesh refinement and parallelism), Laurent Monasse: april 2018 april 2021, partners Inria (leader), Ecole des Ponts, CEA, Université Paris-Est.

7.2.2. 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 Norvergian, 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.

7.3. International Initiatives

7.3.1. Inria Associate Teams Not Involved in an Inria International Labs

7.3.1.1. HDTHM

Title: Mathematical and numerical methods for thermo-hydro-mechanical models in porous media with discontinuities

International Partner (Institution - Laboratory - Researcher):

Monash University (Australia) - School of Mathematics - Jérome Droniou

Start year: 2019

See also: https://math.unice.fr/~massonr/HDTHM/HDTHM.html

The objective of this project is to extend a recent successful joint work between the two project leaders into a tight collaboration between the Monash and the Coffee teams involving several permanent members and students. The present project focuses on challenging directions of research related to the numerical simulation of thermo-hydro-mechanical models in fractured porous media that take advantage of the complementarity of both teams' expertise as well as of the recent arrival of Laurent Monasse in the Coffee team. It is an opportunity to extend our collaborations with the Coffee team industrial partners in geosciences as well as to submit in common a research project to the Australian Research Council toward the end of the project.

7.3.2. Inria International Partners

The team has many interactions abroad: UFRJ, Ut Austin, India, Geneva, ICL,...

7.3.3. Participation in Other International Programs

Coffee is member of the Interdisciplinary Union of Porous Media Research at the University of Stuttgart (NUPUS).

Principal areas of research cooperation to be pursued under this program include free flow and porous medla flow interaction, fracture and fluid flow interaction, fluid-solid phase change interaction, and simulation methods and tools.

7.4. International Research Visitors

7.4.1. Visits of International Scientists

The team has welcomed Paulo Amorim, from UFRJ, for research on the modeling of self-organization in f population dynamics, Corrado Mascia, from La Sapienza, on the analysis of hyperbolic systems and Martin Gander, from Univ. Geneva, for research on domain decomposition methods.

8. Dissemination

8.1. Promoting Scientific Activities

8.1.1. Journal

8.1.1.1. Member of the Editorial Boards

Thierry Goudon is Co-Ed. in Chief SMAI J. Comput. Math.

8.1.1.2. Reviewer - Reviewing Activities

The team members serve regularly as reviewers for journals in applied mathematics, scientific computing, numerical analysis, mathematical analysis.

8.1.2. Scientific Expertise

T. Goudon has been chair of the international panel of experts for the evaluation of all the Research Units of Mathematics in Portugal, nominated by the **Fundação para a Ciência e a Tecnologia**. Not only the panel had to write an assessment (see https://www.fct.pt/apoios/unidades/avaliacoes/2017/docs/Mathematics.pdf) on the scientific production and activities of the research units, but it was also in charge of the attribution of the funding, PhD and postdoc fellowships, for a total amount of 5.5 MEUR (see https://www.fct.pt/apoios/unidades/avaliacoes/2017/docs/Mathematics_table.pdf).

T. Goudon is Scientific Officer at the Ministry of Research.

T. Goudon is member of the scientific boards of CIRM and FSMP.

8.2. Teaching - Supervision - Juries

8.2.1. Teaching

Florent Berthelin, Master2 Mathématiques fondamentales, Université Côte d'Azur, 120h.

Florent Berthelin, Chair of the Master 2 Mathématiques fondamentales, Université Côte d'Azur.

Florent Berthelin, Analysis, L2, Université Nice Sophia Antipolis, 72h.

Laurent Monasse, Numerical analysis, L3, Université Nice Sophia Antipolis, 40h.

Thierry Goudon is President of the national competition to hire teachers (agregation de mathematiques).

8.2.2. Supervision

- PhD: Giulia Lissonni, DDFV methods and domain decomposition: applications in fluid mechanics, 04 October 2019, Stella Krell and Thierry Goudon.
- PhD in progress: Kevin Atsou, Mathematical modeling of tumor growth, analysis and simulation, 01 October 2017, Thierry Goudon
- PhD in progress: Billel Guelmame, Conservation laws in mechanics, 01 October 2017, Stéphane Junca
- 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.
- PhD in progress: Nadine Dirani, Effect of a shock wave on a structure with contact, 01 November 2018, Thierry Goudon and Laurent Monasse.

8.2.3. Juries

T. Goudon has been reviewer for the PhD theses:

- Z. Karaki, Équations cinétiques avec champ magnétique", Nantes, Dec. 2019.
- M. Mezache, "Processus oscillatoires lors de l'agrégation et la fragmentation des fibres amyloïdes", Sorbonne Univ., Dec. 2019.

9. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

[1] G. LISSONI. *DDFV method : applications to fluid mechanics and domain decomposition*, Université de Nice - Sophia Antipolis ; UCA, LJAD, October 2019, https://tel.archives-ouvertes.fr/tel-02309356

Articles in International Peer-Reviewed Journals

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- [3] P. AMORIM, T. GOUDON, F. PERUANI. An ant navigation model based on Weber's law, in "Journal of Mathematical Biology", 2019, https://hal.archives-ouvertes.fr/hal-01802998

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- [21] C. CANCÈS, C. CHAINAIS-HILLAIRET, M. HERDA, S. KRELL. Large time behavior of nonlinear finite volume schemes for convection-diffusion equations, November 2019, working paper or preprint, https://hal. archives-ouvertes.fr/hal-02360155
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