INRIA Project **COFFEE**

**CO**mplex **F**lows **F**or **E**nergy and **E**nvironment

Theme 1: Applied Mathematics, Computational Models and Simulation
Sub–Theme: Modeling, Simulation and Numerical Analysis

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# 1 Aims and Scopes

The project aims at studying mathematical models issued from environmental and energy management questions. We consider systems of PDEs of hydrodynamic type (where the unknowns depend on the time and space variables) or hybrid fluid/kinetic systems (where a part of the unknowns depends on additional variables: microscopic velocity, internal energy, varying radius...). The problems we wish to address involve unusual coupling, which in turn leads to challenging difficulties for mathematical analysis and the need of original numerical solutions. Moreover, by nature many different scales arise in the problems, which introduces stiffness within the equations but which allows, under certain circumstances, to seek hierarchies of reduced models based on asymptotic arguments. The research program requires 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.

# 2 Context

The proposal arises from the following favorable circumstances:

- The existence in the math. department of the University of Nice Sophia Antipolis (UNS) of a well-identified group working on the mathematical modeling of various phenomena related to biological degradation. The activity of the group, led by Magali Ribot and which contains Florent Berthelin and Stéphane Junca, is partly based on a strong collaboration with the team of Roberto Natalini in Roma. The visibility of the research is attested by the grant attributed by the National Agency for Research (ANR).

- The arrivals in Nice of

  - Roland Masson, formerly the head of the Applied Math. Department at IFP Energies Nouvelles, as a UNS Professor

  - Thierry Goudon, Inria Senior Research Scientist, formerly the head of the team Simpaf in the Lille Nord Europe Research Centre,

- Stella Krell, hired as UNS Assistant Professor, after a PhD in Marseilles devoted to modern FV methods for fluid mechanics and a successful post doc in Lille concerned with the numerical homogenization of flows in porous media.

The combination of these expertises leads to propose the creation of a Inria team focused on the mathematical study of PDEs systems motivated by environmental issues, and the design of specific schemes mainly based on the Finite Volume framework. The proposal is supported by the laboratory J.-A. Dieudonné, a joint CNRS–UNS research unit[2], which will host the project. The team mainly involves people from the "PDE and Numerical Analysis" group of the laboratory J.-A. Dieudonné but it will have natural connections with the groups "Probability", "Dynamical systems and interfaces" and "Numerical models and fluid dynamics".

The regional environment is rich of potential opportunities in strong connection with the scientific aims and scopes of the project. First of all, the Group "PDE and Numerical Analysis" of the laboratory of Marseilles (LATP) is definitely a privileged partner, with a well-established collaboration on:

- the design and the analysis of FV schemes, a subject on which Marseilles' group has a leading position, with F. Boyer, T. Gallouët, R. Herbin, F. Hubert [B81, B47, B46, B67, B66, B65, B68, B45].
- the analysis of kinetic models, with M. Bostan, A. Nouri [B53, B52].
- the modeling, analysis and simulation of wave propagation in heterogeneous media, with B. Lombard [B85, B84].

The activity of the Group "Numerical Models" of the University of Toulon, led by C. Galusinski, is potentially subject to fruitful interactions, because the group is developing a quite ambitious numerical library for certain multidimensional multiphase flows (the code `CM2`), including elaborated mesh refinements strategies. Interactions with this group could be very helpful because of its skills and experience in the development of large scale computational codes.

[2]Information can be found at the URL `http://math.unice.fr/`

Second of all, various initiatives towards scientific studies motivated by environmental issues are supported by local government agencies. For instance, the University of Nice has recently created IMREDD (Institut Méditerranéen du Risque, de l'Ecologie et du Développement Durable) an Institute which aims at fostering local expertises on topics related to sustainable development. It contains both formation and research programs and it involves academic and industrial partners; we are already organizing scientific events in this context[3] . It is also worth mentioning the project "Campus Sophia Tech" (Sophia Institute for Technologies), supported by Conseil Général des Alpes-Maritimes, with its specific program devoted to "Modeling, Simulation and Technologies for Environment, Risks and Sustainable Development". Beyond the organization of specific scientific events and of oriented masters studies, "Campus Sophia Tech" also fosters interactions between the academic partners. In this context, discussions with members of the laboratory GeoAzur[4], a research unit devoted to geosciences, look promising. Similarly, it is worth mentioning discussions with INRA teams concerning the modeling of formation of biofilms of pathogenic cells involved in plant infections[5].

The activity of the team COFFEE can also take place in Regional Competitiveness Clusters. Participating to such clusters can be decisive to develop regionally non academic partnerships, to valor our research and to discover new problems. We mention with this respect the Innovative Cluster in Risk Management with connections with the axis "management of industrial waste" , "$CO2$ storage", and "prevention of environmental failures", and the Innovative Cluster Capenergies, which is dedicated to energy sources that do not produce greenhouse gases: energy efficiency, renewable and nuclear energy.

Finally it is worth mentioning that the Center of Cadarache offers natural industrial partners in a neighboring area. In particular we wish to develop collaboration with IRSN, a research institute for nuclear safety, and with CEA in connection with the ITER project.

[3] `http://math.unice.fr/~reynaudb/RDimredd.html`

[4] `https://geoazur.oca.eu/`

[5] see `http://www.sophia.inra.fr/`, especially the UMR Interactions Biotiques et Santé Végétale, and and the joint INRA/CNRS/Inria team MODEMIC `http://www-sop.inria.fr/teams/modemic/`

# 3 Members

The list of members has been kept short so as to include only researchers committed to take an active part towards the objectives of the project. For the time being the team is rather theoretically-oriented. Hence it will be a high priority to complete the team as soon as possible with at least one young expert of scientific computing. Since all junior members have permanent affiliations at the University, we aim at proposing to them temporary positions free of teaching duties, in order to strengthen their participation to the project, and to help them in deepening their current research.

The list of members, with their affiliations, is as follows, short vitae being given in the Appendix:

- Thierry Goudon (Senior Researcher INRIA, HDR[6]), Head of the team
- Florent Berthelin (Ass. Professor Univ. Nice, HDR)
- Stéphane Junca (Ass. Professor Univ. Nice)
- Stella Krell (Ass. Prof. Univ. Nice)
- Roland Masson (Prof. Univ. Nice, HDR)
- Magali Ribot (Ass. Professor Univ. Nice)

The team itself is a collection of well trained researchers, with quite different background and scientific skills. It is worth emphasizing that this composition is one of the originality of the project, which is precisely based on the scientific bet that, having identified a series of common technical difficulties, we will be able to propose innovative and efficient solutions by merging the different viewpoints. Proceeding that way, we clearly expect that the team will be more than the sum of its parts. Besides, we wish to have an overall balanced activity between the discussion of the modeling issues, the analysis of PDEs and numerical schemes and their implementation for simulating flows of practical interest.

The project aims at welcoming numerous PhD students, especially working on applied subjects, in collaboration with academic or industrial partners.

[6]the French acronym for the habilitation to conduct research

We are faced with the difficulty of attracting students because of the small number of students specialized in Mathematics and Scientific Computing at the University of Nice. Therefore, we plan to develop an active policy towards MSc students, proposing training periods with industrial partners to them, and offering research subjects to students of other universities and of the Ecoles Normales Supérieures. Thanks to international research networks, we are also involved in the thesis of students from abroad and we plan to welcome them within the INRIA Internship programs.

For the academic year 2011-12, the PhD students involved in the scientific activity of the team are:

- Martin Parisot, advised by T. Goudon, jointly with the SIMPAF team in Lille. He works on hierarchies of non local models for the Spitzer-Härm regime, a question motivated by the simulation of ICF devices, in collaboration with CEA/DAM. Martin Parisot defended the PhD by the end of 2011; he is currently on a post-doc position at EdF (Chatou) and he works on sediments transport.

- Léon M. Tiné, advised by T. Goudon, F. Lagoutière (Orsay) jointly with the SIMPAF team in Lille and Univ. Gaston Berger in Saint Louis, Senegal. He works on coagulation–fragmentation models. Léon M. Tiné defended the PhD by the end of 2011; he is currently on a post-doc position at Paris 5/Paris 11 and he works on inverse problems arising in biology.

- Cristina Di Russo, advised by M. Ribot with R. Natalini (Roma). She is working on the analysis and simulations of hydrodynamical models of biological movements. She defended in 2011 and she is currently post-doc in Lyon.

- Monika Twarogowska, advised by M. Ribot and R. Natalini (Roma). She works on the modeling of cells displacements and chemotaxis phenomena. She defended the PhD beginning of 2012; she is currently on a post-doc position in the Inria team Opale.

- Damien Broizat, advised by F. Berthelin and P.-E. Jabin (Maryland). He is working on kinetic models describing coagulation and break–up phenomena and PDEs systems for traffic flows.

As of 2012, we welcome several Internships: Riad Sanchez from EPU Nice (6 months, working on the simulation of the incompressible Euler system by hybrid FV/FE methods) and Florian Danard from ENS (8 months, working on DDFV schemes for flows in porous media).

Cindy Guichard from Univ. Marne-la-Vallée arrives in the team for a post-doc, supported by Total and devoted to the simulation of oil recovery problems by FV methods.

We are proposing a research project in the forthcoming edition of CEMRACS, devoted to HPC issues[7], and, as far as it will be permitted by the selected topics, we will try to participate to the future editions.

We are already participating to the Internships, doc, and post-doc markets, with several positions subject to funding by our industrial partners. We consider as a very high priority to be able to attract and welcome new PhD students.

# 4 Overview

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.

[7] `http://smai.emath.fr/cemracs/cemracs12/`

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 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 wish to acquire a solid and large enough background which will allow us to tackle these issues, which all appear in the series of problems discussed

below. We expect that dealing with different problems will lead us to develop a large set of techniques, numerical and analytical, which will cross-fertilize through the exchanges within the team.

A substantial part of the efforts of the project is concerned with the identification of relevant mathematical structures of the models. We think that an important task consists in establishing which models are well-posed and in investigating the qualitative properties of the solutions. The question should not be seen as a pure mathematical exercise; on the contrary the mathematical analysis is necessary to provide solid basis to the models and it can help to decide whether or not the models are relevant. For instance, some multi-phase models that look reasonable at first sight can be shown to be ill-posed, developing unrealistic instabilities and are therefore completely useless. The following quote from [A41] can motivate our approach: *If the numerical methods currently available are not ideal, a point to keep in mind is that uncertainties in the correct formulation of the equations and the modeling of source terms may ultimately have a bigger impact on the result than the particular numerical method adopted.* Despite the potentially high technical content we bear in mind both the modeling issues at the basis of the equations under consideration, and the will to serve the construction of simulation tools. Indeed, this information is helpful for designing numerical methods: preserving conservation and dissipative properties of the equations as well as the stability of specific equilibria can be used as basic requirements in the design of a numerical scheme. In particular we believe that understanding their derivation from a microscopic viewpoint can shed some light on the macroscopic models. In turn, it can guide the design of numerical schemes based on "Asymptotic Preserving" approaches or on splitting methods.

To be more precise on the technical content, we distinguish the following domains, where we mention the researchers mainly interested in these topics.

- **Analysis of PDEs**

  Main contributors: F. Berthelin, T. Goudon, S. Junca, M. Ribot

  We are led to consider coupled non linear systems of PDEs. We are mainly interested here in systems exhibiting hyperbolic structures, possibly with (partial) diffusive corrections. It includes non linear kinetic equations (of Vlasov-Fokker-Planck or Vlasov-Boltzmann type, say). It is also possible that the coefficients depend on the unknown in a non–local way. Generally speaking, we are concerned in the project

with flows where the multiphase character is crucial and makes part of the difficulty. Models involve PDEs systems of hybrid type, and we expect to be able to exhibit common structures between several models coming from different physical motivation. In turn, it will foster fruitful exchanges between the technical skills and experiences present within the team. We do not favor any technical approach: approximation/compactness techniques, energy methods for classical solutions close to equilibrium, fixed point arguments... can be used as well. We point out that several models we are interested in, while , share common structure.

- **Numerical analysis of FV methods**

  Main contributors: F. Berthelin, T. Goudon, S. Krell, R. Masson, M. Ribot

  We wish to design and analyze new numerical schemes, mostly in the FV framework. For hyperbolic systems the theory is well-advanced, but there remain many challenging questions, of crucial relevance for the applications:

  - While the general FV framework is clear for conservation laws, the design of numerical fluxes and the discussion of stability issues can be "application-dependent". In particular, we wish to use the underlying microscopic description of particulate and mixtures flows to design dedicated kinetic schemes [A7, A40]. We will be particularly interested in the analysis of "close-packing" terms which are intended to impose bounds on the particle volume fraction.
  - Stability issues become more intricate when we try to increase the consistency accuracy and when we deal with complex meshes. For instance preserving positivity of certain fields could be absolutely crucial not only for physical reasons, but also to preserve the stability of the simulation of a coupled system. We will therefore continue our work on MUSCL-like methods working on vertex-based discretization, with limiters defined by using multislope analysis [B56, B58]. We will certainly make some attempts with the RD framework introduced by R. Abgrall [A2], because it looks appropriate for our purposes, especially for dealing with 3D simulations.

– Finally, source terms have to be considered appropriately, in particular in order to preserve equilibrium states and to capture correct asymptotic regimes. It requires to UpWind the numerical fluxes by taking into account the source terms. Well-balanced schemes have known very active developments in the recent years [A6, A7, A26]. Among others, we are particularly interested in Asymptotic High Order (AHO) schemes [A5], that we have successfully used for chemotaxis problems [B86].

Besides, the conception of new methods based on Finite Volume discretizations for diffusion has known very intense activities after pioneering works at the beginning of the '00s [A13, A15]. The FV framework, dealing with very general meshes, is very appropriate to deal with complex flows in highly heterogeneous media. The difficulty consists in defining additional unknowns to evaluate diffusion fluxes on the interfaces of the control volumes: using as unique numerical unknown the cell average of the continuous unknown requires unrealistic conditions on the mesh geometry. We are highly involved in the developments of such methods, which are strongly motivated by industrial needs (and our research is enhanced by a 12 years-long experience in the industrial context). We plan to investigate in particular the VAG (Vertex Approximate Gradient) method [B67, B66], based on cell center discretizations involving additional unknowns stored at the vertices, and the DDFV (Discrete Duality Finite Volume) method, which uses a dual mesh [B47, B81, B82, B83, B46].

- **Asymptotic analysis**

  Main contributors: F. Berthelin, T. Goudon, S. Junca, M. Ribot

  Asymptotic analysis has a crucial role in our activity. We are interested in the derivation of hierarchies of models based on asymptotic arguments: it allows to design reduced models, that can be relevant under well-identified assumptions of the physical coefficients. In particular, the discussion of hydrodynamic regimes which start from kinetic equations and lead to macroscopic equations will be the object of a specific attention. We plan to study in details models for mixtures flows where disperse and dense phases interact [B59, B70, B71]. Similar techniques apply also in plasma physics. This topic also includes the

design and analysis of schemes that preserve the asymptotic behavior [A19, A29, B60, B72, B76].

- **Interface problems**

  Main contributors: T. Goudon, F. Berthelin, S. Junca, M. Ribot, S. Krell, R. Masson

  We are faced difficulties related to the coupling of models, methods and codes at interfaces. We distinguish several questions, which are nevertheless intimately connected on the technical viewpoint.

  - As far as we consider flows in porous media, interface conditions and domain decomposition methods have been thoroughly investigated. However, the question of their numerical treatment left many questions open, which naturally depend on the underlying discretization techniques. A typical question, which is strongly motivated by collaborations with our industrial partners, relies on the simulations of mass and heat exchanges between a porous medium and an adjacent free-flow region. Different models are used in the two subdomains: the Navier-Stokes equations apply in the free-flow region while Darcy's law is used in the porous medium. Suitable coupling conditions have to be specified at the interface and thermodynamic properties might lead to discontinuities and jump conditions. Note that some of these conditions can be derived through homogenization arguments [A28]. So far, existing approaches are mostly restricted to single-phase flow and using FE schemes [A14]. It is also remarkable that, despite the existing literature on the subject, techniques have still a reduced spreading out of the academics: in many industrial simulations, two different (commercial) codes are used and the interface coupling is managed more or less "manually" at each time step! Therefore, the challenge consists in dealing with compositional non-isothermal two-phase systems [A36], including vaporization effects, and, again, the application fields make the use of FV schemes in the porous media more appropriate.
  - The situation is a bit different for hyperbolic problems because the design of the interface condition itself is less clear. We are concerned with the coupling of hyperbolic systems involving different

propagation properties, and possibly different set of unknowns. It raises modeling issues in order to design the coupling condition, problems of mathematical analysis, as well as complicated questions in order to match numerical methods. The framework of kinetic schemes might be a possible way to define consistent numerical fluxes. The problem is again strongly motivated by industrial needs, with the additional constraint of not to modify too much existing computational tools; we refer to [A11] and [A8] for recent overviews. We are involved in a collaboration with physicists specifically dedicated to such problems of wave propagations through complex interfaces [B85, B84].

– Fluid/Kinetic coupling. Very closely related to the previous item, we are concerned with applications which naturally lead to consider the coupling through interfaces of kinetic and macroscopic models: algae proliferation, domain decomposition between transparent and opaque domains in radiative transfer... The theory only covers linear situations with simple collision operators [A12, A24, A44], and several numerical issues remain unclear for evolution problems [B51].

# 5 Application domains

The proposal is also "application–driven" since the project is concerned with models motivated by applications in energy production and environmental issues. Despite the variety of the subjects, the unity comes from the common (sometimes surprising, though) features of the underlying models so that we expect that all questions we address will naturally have fruitful connections. Beyond the naive appearance, it should not be seen as a patchy catalog. We have clearly identified a set of problems with common technical bottlenecks, which echoes to the discussion on technical issues above. In particular, for all these problems we are faced with:

- heterogeneous flows, where either the media or the flow itself present high contrasts,

- nonlinear systems of PDEs of hybrid types, with possible coupling through interface conditions,

- multiscale aspects motivating both the design of adequate splitting techniques and the discussion of asymptotic issues.

- *Polyphasic flows in heterogeneous media*

  Main contributors: T. Goudon, S. Krell, R. Masson, M. Ribot

  Polyphasic flows involving several constituents occur in many problems motivated by environmental issues in connection with geosciences: oil and gas recovery, CO2 storage, nuclear waste disposal... Details of the model and technical difficulties depend on the considered application. Nevertheless, there are many common features, which motivate that we can try to design a general numerical strategy.

  The models involve a pression-like unknown which satisfies an equation of elliptic or parabolic type. It is coupled to equations governing the evolution of the volume and molar fractions of the different phases, which are of hyperbolic type, or parabolic type with degeneracies. Furthermore, the system is closed by thermodynamic conditions and phase transition relation. Therefore, the conception of numerical schemes for these problems faces with the following difficulties, that we wish to address:

  - The structure of the discrete formulation highly depends on the choice of unknowns: thermodynamic equilibrium, mass conservation and phase transition relations can be used to reduce the number of unknowns, but the choice impacts the structure of the discrete coupling and might influence the stability of the computation.
  - By definition the flows take place in media with strong contrasts and complex heterogeneities. In turn, computations need adapted (and complex!) tessellations, and the numerical methods should be designed on general unstructured meshes, possibly non conformal. It turns out that Darcy solver for obtaining the pressure is often the main source of computational cost. We develop FV methods for such diffusion problems; in particular by using the VAG, and DDFV frameworks.

    Preliminary tests with both methods look promising and deserve further developments, as described below: we can simulate 2D and 3D flows, with cell centered MPFA schemes, the vertex centered VAG scheme or the DDFV discretization using both cell centers and vertices. We are also currently investigating the adaption of VAG schemes to models with discontinuous capillary pressure,

which is essential to deal with highly contrasted rock types in practical reservoirs and basins.

- Since one has to solve non linear equations with terms of different nature (convection, diffusion and reaction), with potentially stiff terms, a direct approach might lead to quite intricate solvers, or penalizing stability conditions. Therefore, we develop suitable splitting techniques in order to reduce the computational cost.
- Finally, intricate coupling can also arise through interface conditions, describing mass and/or heat exchanges between different domains. This situation occurs for instance in the modeling of ventilation devices in nuclear waste disposal: the evolution is driven by such exchanges between the free medium in the ventilation channel and the porous medium. The flows are described by different equations in the two domains (Darcy vs. Navier-Stokes); derivation of the interface conditions relies either on continuum mechanics principles or asymptotics arguments (or a combination of both), it then raises the questions of the well-posedness of the coupled system and of its numerical treatment.

We wish to design quite general tools, which can be adapted with flexibility to different situations. Indeed, it turns out that many of the available simulation codes are restricted, either in terms of the models that can be addressed, or in terms of the numerical method to evaluate the solutions. For instance, numerical methods for oil recovery engineering are usually based on structured meshes, which make them quite inappropriate for the simulation of CO2 storage [A10]. For this reason, we propose to design a versatile Open Source code, allowing the simulation of a wide range of multiphase flows in porous media, with the potential use of different numerical schemes and technical options. This specific project, refered to as `FV_MULTIP`, is detailed in Section 6.2. Definitely such a tool would be quite unique, it would have a strong impact in the community and it would be a strong asset in our industrial partnerships.

- *Particulate flows, Mixture flows.*

  Main contributors: F. Berthelin, T. Goudon, R. Masson, S. Junca, M. Ribot

We will investigate fluid mechanics models referred to as "multi–fluids" flows 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 modeling of fluidized beds, the dynamic of sprays and in particular biosprays with medical applications, engine fine particles emission... There are many possible modeling 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, see e. g. [A37, A34, A35, A39, A38, A43]. 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 deserves further analysis and dedicated numerical schemes. 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 [B59, B70, B71, B55, B54], while they share some common features of the porous media problems. For instance we can derive that way models for mixtures, like for describing powder–snow avalanches [A3, A17], which look like the Navier–Stokes equation but where the divergence free condition is replaced by a constraint involving derivatives of the density [A42, A30]. The mathematical analysis of these models, known as the Graffi [A21, A22, A25] and Smagulov-Kazhikov [A31] equations, remains in its infancy, despite recent progress in [A33] or [A9], the latter work exploiting a very specific dependence of the viscosity with respect to the density. The constraint introduces new and non trivial difficulties. The treatment of these difficulties certainly requires a clear understanding of the underlying modeling issues (for miscible flows it relies on the distinction between the mean mass velocity and the mean volume velocity) and coming back to a microscopic description might help. At the numeri-

cal level, the constraint cannot be treated by a mere adaptation from the incompressible case. For instance it induces a complex interplay between the regularity of the approximation to be used for the density and the velocity so that the naive approaches rapidly exhibit instability phenomena. We are beginning with models describing powder-snow avalanches, for which we plan to extend the hybrid VF/FE methods we have designed for the usual Navier-Stokes equations [B57, B56]: the key of the method relies on the definition of suitable footbridges between the two discretizations in order to approximate the mass conservation and the momentum equation consistently. The scheme, which is maximum principle preserving and second order accurate, supports unstructured meshes and can be coupled to mesh refinements strategies in order to track front evolution. It already allows to simulate complex incompressible viscous flows with high density contrasts, and it provides an efficient basis to consider more intricate models.

It turns out that models issued from combustion and radiative transfer theory lead to similar issues. A relevant example is given by particulate flows models accounting for energy exchanges, as arising in combustion theory: unusual coupling terms appear in the hydrodynamic regime, that can be interpreted as convection-diffusion terms, with coefficients depending in a complex way on density and temperature (this is related to the so–called Soret and Dufour terms). For such limit models, there is no "natural" scheme; hence coming back to the microscopic modeling might be useful to guide the conception of numerical schemes: designing an Asymptotic Preserving scheme can be an relevant way to simulate the macroscopic model, defining numerical fluxes in the spirit of kinetic schemes [B60, B72, B76]. Similarly, in Low Mach regimes, non standard constraints appear on the velocity field, like for the Mixtures models. Furthermore, for many applications, like for instance the description of fire in tunnels, the validation of fire prevention strategies, the design of industrial furnaces [A23]... it makes sense to couple the Zero Mach system to a kinetic equation describing energy exchanges by radiation. Finally, the derivation of interface conditions to be used between opaque and transparent domains in radiative transfer is also a challenging question. It leads to half–space kinetic problems, the analysis of which is usually quite delicate, and left open the question of finding a numerical counterpart to the analytical statement. Hence

this subject is appealing for the project, both in terms of potential applications and of interesting technical developments [B75, B63].

- *Biological degradation.*

  Main contributors: F. Berthelin, T. Goudon, S. Junca, S. Krell, M. Ribot

  Members of the team have started an original research program devoted to the modeling and simulation of biological damage on monuments and algae proliferation in the Mediterranean Sea, [B61, B62]. Indeed, the biodegradation of monuments is due, in part, to the formation of biofilms, namely a colony of bacteria embedded within an extra-cellular matrix. Biofilms can also be used a a protection device against corrosion of well cement in CO2 storage reservoir [A16]. More generally the formation of biofilms is a common feature of the behavior of bacteria and has potentially many applications in medical and industrial settings; for instance, the cyanobacteria are seriously considered in order to produce energy as bio-fuel[8] and there are also researches to set up bio-devices to avoid human or plant diseases. We are particularly interested in mathematical models of such phenomena based on arguments coming from mixture theory [A4, A18, A32, A42, A30] (thus with a natural connection to the previous item); it leads to a complex multi-dimensional hydrodynamic-type system, with polyphasic features.

  Besides, when considering proliferation of micro-algae in a large domain, it is relevant to distinguish two phases : a development one on the sea bed as a biofilm and a spreading one in water which can be described thanks to kinetic equations subject to coagulation-fragmentation dynamics (see related works [B73, B74]). We wish to derive a complete system, describing the two phases, including the design of coupling interface conditions. This is definitely an interesting and original modeling challenge. We also wish to identify scaling parameters which will allow to bring out hierarchies of reduced models. Of course, the program has to be completed with the conception of the corresponding numerical schemes, so that we will be able to validate, at least on qualitative grounds, our approach, which, in turn, will be decisive to strengthen the collaborations with biologists.

[8] see e. g. `http://biofuels.asu.edu/tubes.shtml`

Another question, which is equally related technically to the other problems addressed in the project, is concerned with the analysis and simulation of equations of hyperbolic type in inhomogeneous media, like porous media or networks [B80, B64, B86]. This is a direction to improve the existing models in biology and it can give rise in analytical and numerical viewpoints to fruitful exchanges between the biological domain and the environmental one. We are particularly interested in PDEs describing chemotactic behaviors, namely the movement of cells in response to a chemical signal and have potential applications, for example to model the movement of fibroblasts on scaffold [B86, B80, B64].

- *Plasmas Physics.*

  Main contributors: F. Berthelin, T. Goudon, S. Junca

  Several members of the team have been trained to deal with equations motivated by plasma physics [B53, B52, B48, B79, B78, B77]. The development of magnetic and inertial confinement fusion makes this subject quite appealing for the team. Again, it naturally leads to multiscale, non linear problems, with unusual coupling. Compared to other research teams already working on this subject, our main purpose will be to work on the derivation, analysis and simulation of reduced models, that can be used for instance for routine computations, and to address questions related to the coupling of different models through domain decomposition. However, the management of the plasma physics research activities within the Institute is quite unclear right now, so that we are not able to make our commitment to the subject precise.

# 6 Software

As far as possible, we plan to make our software activity visible, in particular through "Numerical galleries" showing the "know-how" of the team. However, we distinguish two kinds of software produced within the team: we have advanced softwares proposed as Open-Source that are expected to become references for benchmarking activities, and prototype codes, mostly reserved for internal use. Clearly, having an Open Source policy requires specific efforts in order to maintain the codes, to make them as visible as possible, and to add continuously new functionalities.

## 6.1 NS2DDV

`NS2DDV` is a joint program with the project SIMPAF in Lille. The code simulates non homogeneous viscous flows. The current version works in 2D. It is based on an original hybrid FV/FE method, presented in [B57, B56]. The code works on unstructured meshes and it can incorporate mesh refinements strategies (using BAMG [A1]). In fact there are two versions

- a `Matlab` version, allowing fast experiments of new ideas,
- a `C++` optimized version, devoted to more ambitious simulations.

The `Matlab` version is the object of a APP deposit and it is proposed as an Open Source code[9], together with a series of test cases and a documentation. The `C++` version is rather a prototype, for internal use. Such a "dual" strategy can be compared to the project MRST, devoted to the simulation of flows in porous media, developed by the SINTEF Applied Math team[10]. The originality of the method allows to treat non homogeneous flows with high density ratio (typically 1:1000 for the falling droplet test-case). By working on unstructured meshes, the scheme can be combined to mesh refinements strategies and front tracking techniques (used mostly as blackboxes). The working plan is two–fold, which leads to tasks of various difficulties; to reach these objectives we are proposing, both in Lille and Nice, several training positions at various levels:

- on the one hand, the codes can be optimized in several ways, and we wish to explore further discretization options (like the use of Residual Distributed schemes);
- on the other hand, we plan to extend the physical content and to apply the method for a large variety of flows. It implies to develop the set of test cases, and we also plan to apply the method for the incompressible Euler system. More ambitious research objectives are concerned with more complex models and applications like avalanches, mixture flows and pollutants transport, as well as certain combustion problems.

[9] `math.univ-lille1.fr/~simpaf/SITE-NS2DDV/home.html`
[10] `www.sintef.no/Projectweb/MRST/`

## 6.2 Project FV_MULTIP

The community of experts of FV approaches is well-organized both at the national and the international level, with a strong commitment of industrial partners[11], who express a strong demand on the development of new and adapted FV schemes, dealing with general polyhedral meshes (see the Section on Industrial Partnerships). These networks have permitted the design of several relevant benchmarks.

Our objective is to develop a generic simulator, offering an Open Source version of the code, for multiphase Darcy flows which will be versatile both in terms of discretization methods and meshes. On the technical side, the project includes both cell centered and vertex centered schemes as well as hybrid discretizations using both cell and vertex unknowns. The multiphase Darcy flow models that we address include an arbitrary number of phases (typically from 1 to 4), miscible and immiscible models, compositional models taking into account thermodynamical equilibrium and thermal models accounting for the coupling with an energy conservation equation. The simulator will contain parallel procedures. On this aspect, the ambition depends on our capacity to be reinforced by an expert on parallel computing. The simulator will be applied to several types of industrial applications including CO2 storage, reservoir simulation and nuclear waste repository. It is likely that the code will naturally use and take place into the `Num3sis` platform developed at the Sophia Antipolis Méditerranée Inria research Centre.

We expect that such a tool can be used as a reference benchmark by a large community, and we think that it would be quite unique and it would have a strong impact. As far as one considers the specific application to CO2 storage, the objective competes with the project `Dumux` developed at Stuttgart University by the team of Rainer Helmig [A20] or the project `Pflotran` developed at LANL by Peter Lichtner [A27]. We already have a prototype version of the code, and the development is the object of a very active policy, already made visible through a CEMRACS project, in collaboration with BRGM and the Internship program of F. Danard. We expect the project will be rapidly mature enough to obtain the support of the specific ADT Inria program which allows the temporary support of engineers, especially to deal with aspects related to parallel computing. On the same token, we plan to apply for a specific support to be able to make use of the potentialities of the `Num3sis` platform.

[11] see e. g. `http://fvca6.fs.cvut.cz/` and `http://www.gdrmomas.org`

The project is detailed in the Appendix. It is based on the significant experience of the team on the numerical simulation of polyphasic flows, including in the industrial context. As said above, the goal is to provide a general tool for FV methods, working on quite arbitrary polyhedral grids. The initializing step of the project is already advanced, and the preliminary version will be used and developed during CEMRACS 2012. The code already manages with conformal meshes made of general polyhedra, and with numerical unknowns stored on cells, vertices and faces. The next step will be to include parallel procedures. We shall start with basic MPI routines, using static domain decomposition. Clearly, we will need to reinforce the team to go beyond this basic objective, which nevertheless, will be enough to start dealing with most of our applications of interest. We will also rapidly include performing preconditioner and solver, certainly by starting with a library like `PETSc`, and visualisation tools. Certainly this could be subject for fruitful interactions with the team SAGE (see below). Hence, we will be able to use a 3D code on distributed grids, and progressively we will increase the physical contents. Clearly, progress are expected through the commitment of PhD students, post-docs and through collaborations with our partners.

## 6.3 Comp_Algae

In order to validate the original models derived for describing biofilms formation and algae proliferation, a Finite Difference code has been developed, that includes the treatment of 3 dimensional geometries. 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 [B62].

## 6.4 AP_PartFlow

We are developing experimental codes, mainly based on Finite Differences or Finite Volumes, for the simulation of particulate flows, in dimension 1 and 2. A particular attention is paid to guarantee the asymptotic properties of the scheme, with respect to relaxation parameters [B60, B72, B76].

# 7 Positioning and Scientific Interactions

## 7.1 Positioning and Interaction With Other INRIA Teams

There are numerous Inria teams with a scientific scope more or less related to ours. It is not possible to be exhaustive and to mention all subjects of potential interactions. Below, we clarify the positioning or mention the ongoing collaborations.

• *Positioning.* There are a couple of teams interested in numerical simulations of flows in porous media belonging to the scientific theme "Sciences and Technologies for Information and Communication for Life Sciences and Environment" of the Inria organisation. At least, we are quite complementary with the POMDAPI project in Rocquencourt, led by J. Jaffré and the project SAGE, in Rennes led by J. Erhel. Note however, as a mark of the different positioning, that we feel more closely related to the scientific theme "Applied Mathematics, Computational Models and Simulation", and we already have advanced contacts with several teams belonging to this theme. (For the time being the only deep interaction with a team of the "STIC for Life Science and Environment" theme is the interaction with the NUMED project mentioned below.) SAGE's expertise is neatly focused on numerical linear algebra and parallel computing with, indeed, geophysical flows as main application. The research of POMDAPI is mainly dedicated to flows in porous media, including reactive flows, with a strong content on optimization solvers and programming techniques, a set of questions that we do not address. Concerning PDEs' approximation POMDAPI is mostly working on the framework of mixed Finite Elements methods. COFFEE is rather interested in a large spectrum of FV schemes and, maybe, it is slightly more oriented on the theoretical side. Hence, the approaches are complementary which can be certainly subject to fruitful exchanges, the strength of each project being quite distinct and the discretization techniques being different. In particular the know-how developed by SAGE on parallel computing and solvers can be a real boost for our project `FV_MULTIP` (detailed above). For our industrial partners, there is a well identified need of developing simulation tools for transient state of liquid/vapor flows (for instance, ANDRA is interested in the simulation of gas emission from corroded confining devices and its interaction with water contained in the surrounding rocks). Com-

mercial codes, like `Tough2` are limited both in terms of performances and versatility of the methods, which are not well-adapted to the use of complex meshes. Therefore, in a near future, it might be an interesting opportunity to foster stronger relations between all INRIA teams working in this direction.

Another question concerns the positioning of COFFEE with respect to the scientific activities devoted to plasma physics. For Inria, it has been a very active subject until quite recently with the leading role of the CALVI Project in Nancy/Strasbourg and the Action d'Envergure FUSION, both led by E. Sonnendrucker, which have had a decisive role in the development of the code `GYSELA` used at CEA for the kinetic simulation for ITER. As of 2012, CALVI is subject to important evolution and we cannot anticipate the future positioning of Inria concerning the modeling and simulation of magnetized plasma; the policy of the scientific board of Inria being quite unclear on this subject. It is likely that a new Action d'Envergure will start soon, with new Inria teams that are supposed to be created in the forthcoming years. In particular the XXX team in Sophia, led by J. Blum, the YYY team in Lyon/Grenoble led by F. Filbet and the ZZZ team in Strasbourg could be natural scientific partners. We have also regular contact and working sessions with the group in Univ. Paris 6 led by B. Després, which is by now one of the more advanced academic research team on plasma physics in France. But the current situation does not allow us to evaluate what could be our commitment to plasma physics subjects in a near future.

- *Main Collaborations with INRIA Teams.*

  - The SIMPAF project and the lab. P. Painlevé in Lille.

    SIMPAF was the previous team of the team leader who is just moving to Nice. Naturally, many collaborations are still on–going. But, because of this departure, combined to other evolutions in the memberships, the scientific foundations of SIMPAF will substantially change in the near future. The kinetic formalism was a natural bridge between the different topics addressed by SIMPAF but there is currently no expert of this framework in the team. Nevertheless, many interactions will be maintained on the developments of numerical methods for fluid mechanics. With C. Calgaro and E. Creusé, T. Goudon has an intense collaboration on the simulations of heterogeneous viscous flows, in con-

nections to the development of the software NS2DDV[12]. With P. Lafitte, T. Goudon has many different subjects of interest (particulate flows, free boundary problems...), while S. Krell started a collaboration with C. Chainais and A. Mouton on the analysis of FV schemes for flows in porous media.

- The BANG Project in Rocquencourt/ENS Paris led by B. Perthame:

  The BANG project mainly deals with modeling and simulations for biology and medicine. The subjects are therefore completely distinct; however we share common methodology approaches with B. Perthame and his coworkers. We have also collaborations with M. Doumic about coagulation-fragmentation models applied to biology.

- The NUMED Project in Lyon led by E. Grenier:

  The NUMED project aims at providing numerical simulation and analysis for biomedical purposes, as, for example, the modeling of the complex process of angiogenesis, using multi-scale techniques. The members of this project study in particular equations for chemotaxis of parabolic type, but also of hyperbolic or kinetic type. These equations are closely related to the ones which compose the models we consider and common reflexions on the strategies about analysis and simulations of them will be of great interest.

## 7.2 Collaborations in France and Abroad

As it is completely clear from the vitae, the members of the team have a solid and well–established network of both nation–wide and international collaborations. The currently most active collaborations are summarized as follows

**In France:**
LATP Marseille: F. Boyer, T. Gallouët, R. Herbin, F. Hubert. M. Bostan, A. Nouri, B. Lombard
As mentioned in the Introduction there exists a strong and natural partnership with the colleagues in Marseilles, by both geographical proximity and common scientific interests. We also include in this informal network R. Eymard (Marne-la-Vallée).

[12] see http://math.univ-lille1.fr/ simpaf/SITE-NS2DDV/home.html

MIP Toulouse: P. Degond
We have many common subjects of interest with P. Degond and the Applied Math Team in Toulouse, with a quite well-established collaboration: plasmas physics, transport of charge, traffic–flows modeling, design of Asymptotic Preserving schemes....

Laboratoire de Mathématiques Paris Sud: F. Lagoutière
We have on–going collaboration on the design of (low–order) FV schemes for conservation laws, with application to particulate flows and coagulation-fragmentation problems [B73, B74].

ENS Lyon and Institut Camille Jordan, Université de Lyon: J. Vovelle, F. Filbet, V. Calvez
F. Filbet is interested in the numerical treatment of collision terms in kinetic models, and applications for plasmas (ITER and ICF), microfluidics and some aspects of astrophysics. Clearly we share common interests, definitely subject to fruitful collaborations. In particular we have in mind to apply jointly to the AYAME program for elaborating a new collaboration with the team of K. Aoki in Kyoto University. We have also on–going works with J. Vovelle about kinetic models, macroscopic limit and properties of the kinetic approximations. A collaboration with V. Calvez just began a few months ago on the analysis of hyperbolic and kinetic equations for chemotaxis and eventually on their numerical simulations taking into account the kinetic bases of the modeling.

Labo. de Math. Appliquées, Université de Savoie: C.Bourdarias, M. Gisclon
The long–standing collaboration is concerned with the study of hyperbolic systems motivated by many different applications. In particular, there are joint works on the analysis of macroscopic polyphasic models for fluidized beds [B55, B54].

**Abroad:**
Universitat Autonoma Barcelona-ICREA (and Imperial College, London): J. A. Carrillo.
The collaboration with J. A. Carrillo is well–established, since it started ten years ago, and it has led to a couple of papers. We aim at studying further kinetic models for fluid/particles interaction and coagulation-fragmentation

models.

UT-Austin: A. Vasseur, I. Gamba
The collaboration with A. Vasseur started also a long time ago, when he was Junior CNRS Researcher in Nice. It has continued at University of Texas in Austin. We work on many aspects of kinetic fluid coupling, in particular on the analysis of hydrodynamic regimes, applied to both the continuous or the discrete kinetic framework by using compactness or relative entropy methods [B50, B49], and fluid/kinetic matching conditions. We have also several projects with A. Gamba about kinetic theory for charged particles [B52].

CNR, Roma : R. Natalini
The collaboration with R. Natalini's team in Roma began five years ago and deals mostly with biological purposes. Several domains are under consideration : modeling of the formation and movement of biofilms, study of hyperbolic equations for chemotaxis... Present and future directions to this collaboration include the analytical and numerical study of hyperbolic equations on a network or in an inhomogeneous medium [B80, B61, B64, B62].

UW–Madison & Shanghai Jiao Tang Univ.: S. Jin
A collaboration with S. Jin and his team in UW Madison has started very recently on the design of Asymptotic Preserving schemes for particulate flows. We have many on–going projects on numerical analysis and simulation of hydrodynamic regimes [B72, B76].

University of Maryland : P-E. Jabin
P-E Jabin will be on leave of the University of Nice from September 2011 to the University of Maryland. The collaboration with him deals mostly with the modeling of algae proliferation in the sea thanks to coagulation-fragmentation equations coupled with hydrodynamic equations.

Finally, let us mention a few prospective, but well-identifed, projects:

- R. Masson is going to teach in the Subterranean Reservoir of Energies master, in Kazasthan, organized by NPL by ENSG.
- In 2006, Th. Goudon has been invited thanks to a specific funding of the European and International Affairs Department of INRIA at

the University Gaston Berger of Saint Louis du Senegal for lectures on Fluid Mechanics. This preliminary step has permitted to co–advise the PhD thesis of Léon M. Tiné. We expect to maintain this fruitful collaboration and to attract other students from UGB.

- As mentioned above, we plan to organize a collaboration with the group of K. Aoki from Kyoto University, jointly with F. Filbet. The simulation and experiments performed by this team have brought out many fascinating effects in plasma physics and gas dynamics; they are open to collaboration with mathematicians in order to improve the understanding of these intriguing phenomena.

- A. Christlieb is a numerical analyst from Michigan State University. He is working on multiscale problems coming from physics and he is particularly interested in the construction of efficient time discretization. We started discussions during a recent thematic semester in UCLA and it would be very interesting to strengthen our contacts since we have complementary viewpoints on the problems.

## 7.3 Industrial Partnerships

We wish to develop activities towards industrial partners. It includes collaborations with state organisms with industrial and commercial vocations (EPIC legal status). The main (more or less advanced) contacts are the following:

• ANDRA: we have participated to the INRIA–ANDRA call for projects. In 2011, S. Krell and T. Goudon, with A. Gloria, have worked on the development of homogenization methods for the simulation of the transport of radionucleides in porous media [B69]. A new numerical method has been proposed, based on Reduced Basis techniques which allows efficient computation of the (space-dependent) effective coefficients. In the new 2012 call, the proposal is devoted to the modeling and simulation of ventilation devices in nuclear waste disposal. This is a long–term project which aims at solving numerically systems of PDEs describing mass and heat transfer between porous media and ventilation channels. Generally speaking ANDRA has strong needs of numerical tools for simulating transient water/gas flows (with typical applications to understand gas flows emanating from corroded

confining devices in nuclear waste disposal and mass/heat exchanges in circulation channels). The performances and flexibility of the commercial code `Tough2` are definitely too restricted. It is likely that fostering the skills of several Inria teams working on these topics can be decisive to design new two-phase codes using modern schemes and complex meshes, with domain decomposition methods and parallel procedures.

• Total: R. Masson is scientific consultant of the recently created team "Nouveau Simulateur de Réservoir", led by B. Fayssat. The team is concerned with the development of new research codes for oil recovery problems, based on FV methods. The collaboration provides post-doc fundings and C. Guichard is currently appointed by such a post-doc position, working on the simulation of two-phases flows with a code based on the VAG scheme on tetrahedral meshes. The workplan includes the treatment of discontinuous capillary pressures as well as the simulation of vaporization effects and gas dissolution. We will also consider schemes working with sub-time steps, defined locally in order to deal with well/reservoir coupling.

• GdF–Suez: We have established collaborations with both the GdF–Suez EP (Exploration/Production) team and the GdF–Storengy team. In particular, we have opening post-doc programs devoted to the control of rock permeability by polymer injections, and to the simulation of flows in tight rocks, with weak permeabilities. These questions lead to consider highly heterogeneous and fractured media; in turn simulations should use highly unstructured meshes. Another common features is the presence of disparate time scales.

• BRGM: It is a public institution concerned with Earth science and applications for the management of surface and subsurface resources and risks (mine safety, mineral resources, geological CO2 storage, geothermal energy...). For simulation, BRGM is currently using the software `Tough` for their CO2 storage studies, but this code is not open source, it is limited to orthogonal meshes, and not efficient in parallel. This is why BRGM is interested in the perspective of using our future simulator that could progressively replace `Tough` for CO2 storage studies at BRGM. Preliminary joint studies start with the support for a CEMRACS project in the 2012 edition, devoted to HPC.

• The CEA: the French Atomic Energy Agency is a quite natural partner for COFFEE, with all of four centers in Saclay, Bruyères, Bordeaux and Cadarache. We are just finishing a program devoted to the simulation of diffusion models issued from plasma physics for ICF modeling [B79, B78, B77]. We are currently starting a collaboration on particulate flows with

Bruyères (R. Motte) and Bordeaux (J. Mathiaud).
• IRSN develops numerical codes (the library `PELICANS`) for the simulation of inhomogeneous flows, low Mach and mixtures models. It is a natural partner both in terms of applications and numerical techniques.

## 7.4 Further Comments on Positioning

On the one hand, the team is kept small, with well identified aims and scopes, and on the other hand it is intended to mix various profiles, with overall objectives balanced between modeling, analysis and simulation. Naturally, scientific groups with comparable backgrounds and activities can be found among our collaborators. However, as such, the project might look quite original because one can easily find much more specialized teams, e.g. focused on a specific application (like oil recovery or CO2 storage or particulate flows...) with a substantial task force devoted to the development of codes or teams mainly concerned with the design and analysis of (quite general) numerical methods, with a weaker commitment to applications, or larger groups, that could be regroupment of several teams affiliated to different universities or institutes. In this sense our positioning might be interpreted as quite hybrid. Nevertheless, it can make sense to mention a few research projects because some aspects of their activity can be compared to our own aims and scopes, even though, as explained above, a direct comparison would not be fair.

- The Multiphase Flow Group[13] led by G. Tryggvason, from the Mechanical Engineering Department at Worcester Polytechnic Institute. This is a leading group in the development of numerical methods for direct simulations of multiphase flows (partly through collaboration with DoE, NASA, AFOSR...). The team has introduced front tracking techniques based on FV discretizations.

- The team of A. Prosperetti[14], from the Department of Mechanical Engineering at Johns Hopkins University has been pioneering in the modeling of fluid–particles flows. It proposes the code PHYSALIS, which is based on FD methods to perform direct numerical simulations of fluid-particles interactions in complex geometry.

[13] `http://www.me.wpi.edu/research/MFG/`
[14] `http://www.me.jhu.edu/prosper/`

- The Workgroup on Complex Dynamical Systems from the Department of Mathematics, at Politecnico di Torino[15] has a highly visible activity devoted to the modeling of natural phenomena inspired from concepts of continuum and statistical mechanics (biological systems, tumor growth...).

- The NUPUS program[16] fosters research activities of several teams from Germany, ths Netherlands and Norway. This is a big interdisciplinary group of scientists working on the modeling and simulation of flows in porous media. In particular, the group led by P. Bastian from Heidelberg, is among the core developers of DUNE, a very ambitious numerical toolbox for solving PDEs and is has a project with P. Helming (from Dept. of Hydromechanics and Modeling of Hydrosystems, Univ. Stuttgart) devoted to the development of an Open Source code for the simulation of CO2 storage scenario.

# 8 Conclusions and Mid–Term Perspectives

As said above the team composition is quite original, with a wide spectrum of technical skills, and the success of the project precisely relies on the ability to work together and to combine viewpoints and expertises. Considering the academic positioning of the team, a natural objective will be to present well–ranked publications records: our progress on modeling and analysis issues, as well as on the design of new numerical schemes will be the object of publications in the journals of the Applied Math and Scientific Computing community. However, we clearly wish to go beyond this basic objective:

- In the mid–term perspective, we wish to be clearly identified for our specific activity towards environmental and energy–related issues. To our mind, this objective implies that we will able to strengthen our scientific interactions beyond our natural "applied mathematics" community. The objective is two–fold. On the one–hand a part of the team activity will be concerned with industrial partnerships and we expect to be able to deliver mature simulation tools, useful for industrial applications. On the other hand, we develop new models in order to bring

[15] `http://calvino.polito.it/fismat/poli/`
[16] `http://www.nupus.uni-stuttgart.de/`

out remarkable biological phenomena; this approach needs to be validated through feedbacks from other scientific communities (biologists, engineers, physicists...). Definitely, the quest of such interactions is a major objective of the team.

- We plan to follow an active policy in order to valor the development of numerical codes within the team. Definitely we wish to go beyond the design of prototype versions restricted to internal use. To this end, we wish to participate to the benchmarking activities already organized in the community (GdR MOMAS, conferences FVCA...). Efforts (in particular through our hiring policy) will be specifically devoted to develop Open Source versions of (a selection of) our numerical schemes. Such efforts are important in our strategy on the one hand because we expect it will allow us to have a leading position in the benchmarking activity, on the other hand it will permit to foster our collaboration programs. We point out that such a policy is somehow original in our community. Through our experience, we measure the gap between a prototype code and a cleaned-up and optimized version, accessible to other research teams and we measure how such an objective can be time and energy consuming [17]. In particular the success depends on our capabilities to attract people working on the development steps.

Concerning specific scientific targets, we can summarize our major objectives as follows:

- Conception and analysis of FV methods for flows in porous media. We wish to consider polyphasic flows and general polyhedral meshes. Complementary to the numerical analysis, we wish to develop an Open Source code allowing the comparizon of various discretization options (VAG, DDFV) and containing relevant physics.

- Modeling, analysis and simulation of mixtures flows. Many models in this field are quite unusual and deserve further mathematical analysis. We will derive hierarchies of reduced models and study their numerical treatment. We will develop dedicated simulation tools for coupled fluid/kinetic models and their hydrodynamic versions.

[17] For instance the `CentPack` library `http://www.cscamm.umd.edu/centpack/` devoted to 1D and 2D conservation laws, and `ClawPack`, see `http://depts.washington.edu/clawpack/`, started in the mid '90s

- Biological degradation. We will perform a substantial modeling effort in order to describe by a set of PDEs both the degradation dynamics in the substrate layer and the transport/coagulation phenomena in the free flow. It will be completed by further analysis and simulation.

# References

## Selection of relevant references


[A1] Bamg mesh generator. `http://www.ann.jussieu.fr/hecht/ftp/bamg/`.

[A2] R. Abgrall, A. Larat, and M. Ricchiuto. Construction of very high order residual distribution schemes for steady inviscid flow problems on hybrid unstructured meshes. *J. Comput. Physics*, 230(11):4103–4136, 2011.

[A3] C. Acary-Robert, D. Bresch, and D. Dutykh. Mathematical modeling of powder-snow avalanche flows. Technical report, LAMA–UMR 5127, CNRS & Univ. Savoie, 2010.

[A4] E. Alpkvist and I. Klapper. A multidimensional multispecies continuum model for heterogeneous biofilm development. *Bull. Math. Biol.*, 69:765–789, 2007.

[A5] D. Argeba-Driollet, M. Briani, and R. Natalini. Asymptotic high-order schemes for $2 \times 2$ dissipative hyperbolic systems. *SIAM J. Num. Anal.*, 46(2):869–894, 2008.

[A6] R. Botchorishvili, B. Perthame, and A. Vasseur. Equilibrium schemes for scalar conservation laws with stiff sources. *Math. Comput.*, 72:131–157, 2003.

[A7] F. Bouchut. *Nonlinear stability of finite volume methods for hyperbolic conservation laws and well-balanced schemes for sources.* Frontiers in Math. Birkhauser, 2000.

[A8] B. Boutin. *Etude mathématique et numérique d'équations hyperboliques non-linéaires: couplage de modè & chocs non-classiques*. PhD thesis, Univ. Paris 6, 2009.

[A9] D. Bresch, E. H. Essoufi, and M. Sy. Effect of density dependent viscosities on multiphasic incompressible fluid models. *J. Math. Fluid Mech.*, 9(3):377–397, 2007.

[A10] H. Class et al. A benchmark study on problems related to $CO2$ storage in geologic formations. *Computational Geosciences*, 13:409–434, 2009.

[A11] F. Coquel. Couplage de systèmes hyperboliques : Interface mince versus interface épaisse. In *Congrès National d'Analyse Numérique, Guidel*. SMAI, 2011.

[A12] F. Coron, F. Golse, and C. Sulem. A classification of well-posed kinetic layer problems. *Comm. Pure Appl. Math.*, 41(4):409–435, 1988.

[A13] Y. Coudière, J.-P. Vila, and P. Villedieu. Convergence rate of a finite volume scheme for a two dimensional diffusion convection problem. *Math. Model. Numer. Anal. (M2AN)*, 33(3):493–516, 1999.

[A14] M. Discacciati and A. Quarteroni. Navier-Stokes/Darcy coupling: Modeling, analysis, and numerical approximation. *Rev. Mat. Complutense*, 22:315–426, 2009.

[A15] K. Domelevo and P. Omnes. A finite volume method for the Laplace equation on almost arbitrary two-dimensional grids. *Math. Model. Numer. Anal. (M2AN)*, 39(6):1203–1249, 2005.

[A16] A. Ebigbo, R. Helmig, A.B. Cunningham, H. Class, and R. Gerlach. Modelling biofilm growth in the presence of carbon dioxide and water flow in the subsurface. *Advances in Water Resources*, 33(7):762–781, 2010.

[A17] J. Etienne, P. Saramito, and J. Hopfinger, E. Numerical simulations of dense clouds on steep slopes: application to powder-snow avalanches. *Annals of Glaciology*, 38:379–383, 2004. Presented at IGS International Symposium on Snow and Avalanches. Davos, Switzerland 2-6 June 2003.

[A18] A. Farina and L. Preziosi. On Darcy's law for growing porous media. *Int. J. Nonlinear Mech.*, 37:485–491, 2001.

[A19] J. Filbet and S. Jin. A class of asymptotic–preserving schemes for kinetic equations and related problems with stiff sources. *J. Comp. Phys.*, 229(20):7625–7648, 2010.

[A20] B. Flemish, B. Fritz, R. Helmig, J. Niessner, and B. Wohlmuth. `DUMUX`: a multi- scale, multi-physics toolbox for flow and transport processes in porous media. In *Proceedings of ECCOMAS*, 2007.

[A21] F. Franchi and B. Straughan. A comparison of Graffi and Kazhikov–Smagulov models for top heavy pollution instability. *Adv. in Water Resources*, 24:585–594, 2001.

[A22] F. Franchi and B. Straughan. Convection, diffusion and pollution: The model of Dario Graffi. In *Proceedings of the Conference: Nuovi Progressi nella Fisica Matematica dall'Eredità di Dario Graffi, Roma*, volume 177 of *Atti dei Convegni Lincei*, pages 257–265, 2002.

[A23] I. Gasser, J. Struckmeier, and I. Teleaga. Modelling and simulation of fires in vehicle tunnels. *Internat. J. Numer. Methods Fluids*, 44(3):277–296, 2004.

[A24] F. Golse, S. Jin, and C. D. Levermore. A domain decomposition analysis for a two-scale linear transport problem. *M2AN Math. Model. Numer. Anal.*, 37(6):869–892, 2003.

[A25] D. Graffi. Il teorema di unicitá per i fluidi incompressibili, perfetti, eterogenei. *Rev. Unione Mat. Argentina*, 17:73–77, 1955.

[A26] J. M. Greenberg and A.-Y. Le Roux. A well-balanced scheme for the numerical processing of source terms in hyperbolic equations. *SIAM J. Numer. Anal.*, 33(1):1–16, 1996.

[A27] G. Hammond, P. Lichtner, and C. Lu. Subsurface multiphase flow and multicomponent reactive transport modelling using high performance computing. *J. of Physics Conference Series*, 78, 2007.

[A28] W. Jäger and A. Mikelic. Modeling effective interface laws for transport phenomena between an unconfined fluid and a porous medium using homogenization. *Transp. Porous Media*, 78:489–508, 2009.

[A29] S. Jin. Efficient asymptotic–preserving (AP) schemes for some multiscale kinetic equations. *SIAM J. Sci. Comput.*, 21(2):441–454, 1999.

[A30] D. D. Joseph and Y. Y. Renardy. *Fundamentals of two-fluid dynamics. Part II: Lubricated Transport, Drops and Miscible Liquids*, volume 3 of *Interdisciplinary Applied Mathematics*. Springer-Verlag, New York, 1993. Mathematical theory and applications.

[A31] A. V. Kazhikhov and S. Smagulov. The correctness of boundary value problems in a diffusion model in an inhomogeneous fluid. *Sov. Phys. Dokl.*, 22:249–250, 1977.

[A32] I. Klapper and J. Dockery. Mathematical description of microbial biofilms. *SIAM Review*, 2009.

[A33] P.-L. Lions. *Mathematical topics in fluid mechanics. Vol. 2: Compressible models*, volume 10 of *Oxford Lecture Series in Mathematics and its Applications*. The Clarendon Press Oxford University Press, New York, 1998. Oxford Science Publications.

[A34] H. Liu, Z. Wang, and R. Fox. A level set approach for dilute non-collisional fluid-particle flows. *J. Comput. Physics*, 230:920–936, 2011.

[A35] J. Mathiaud. *Etude de systèmes de type gaz-particules*. PhD thesis, ENS Cachan, 2006.

[A36] K. Mosthaf, K. Baber, B. Flemisch, A. Helmig, A. Leijnse, I. Rybak, and B. Wohlmuth. A coupling concept for two-phase compositional porous-medium and single-phase compositional free flow. Technical report, SimTech–Univ. Stuttgart, 2012.

[A37] P. J. O'Rourke. *Collective drop effects on vaporizing liquid sprays*. PhD thesis, Princeton University, NJ, 1981.

[A38] N. A. Patankar and D. D. Joseph. Lagrangian numerical simulation of particulate flows. *Int. J. Multiphase Flow*, 27:1685–1706, 2001.

[A39] N. A. Patankar and D. D. Joseph. Modeling and numerical simulation of particulate flows by the Eulerian–Lagrangian approach. *Int. J. Multiphase Flow*, 27:1659–1684, 2001.

[A40] B. Perthame. *Kinetic formulation of conservation laws.* Oxford Lecture Series in Math. and its Appl. Oxford University Press, 2003.

[A41] A. Prosperetti and G. Tryggvason. *Computational methods for multiphase flows.* Cambridge University Press, 2007.

[A42] K. R. Rajagopal and L. Tao. *Mechanics of mixtures*, volume 35 of *Series on Advances in Math. for Appl. Sci.* World Scientific, 1985.

[A43] D. M. Snider, P. J. O'Rourke, and M. J. Andrews. Sediment flow in inclined vessels calculated using a multiphase particle-in-cell model for dense particle flows. *Int. J. Multiphase Flow*, 24:1359–1382, 1998.

[A44] X. Yang, F. Golse, Z. Huang, and S. Jin. Numerical study of a domain decomposition method for a two-scale linear transport equation. *Netw. Heterog. Media*, 1(1):143–166 (electronic), 2006.

## Selected publications of the team members

[B45] L. Agelas, D.A. Di Pietro, R. Eymard, and R. Masson. An abstract analysis framework for nonconforming approximations of the single phase Darcy equation. *Int. J. F.V.*, 2010.

[B46] B. Andreianov, M. Bendahmane, Hubert F., and S. Krell. On 3D DDFV discretization of gradient and divergence operators. I. Meshing, operators and discrete duality. *IMA J. Numer. Anal.*, 2012. To appear. Available online at http://hal.archives-ouvertes.fr/hal-00355212/en/.

[B47] B. Andreianov, F. Hubert, and S. Krell. Benchmark 3D: a version of the DDFV scheme with cell/vertex unknowns on general meshes. In J. Fort, J. Furst, J. Halama, R. Herbin, and F. Hubert, editors, *Finite Volumes for Complex Applications VI Problems and Perspectives*, volume 4 of *Springer Proceedings in Mathematics*, pages 937–948. Springer Berlin Heidelberg, 2011.

[B48] F. Berthelin and S. Junca. Averaging lemmas with a force term in the transport equation. *J. de Math. Pures et Appl.*, 93(2):113–131, 2010.

[B49] F. Berthelin, A. Tzavaras, and A. Vasseur. From discrete velocity Boltzmann equations to gas dynamics before shocks. *J. Stat. Phys.*, 135:151–173, 2009.

[B50] F. Berthelin and A. Vasseur. From kinetic equations to multidimensional isentropic gas dynamics before shocks. *SIAM J. Math. Anal.*, 36(6):1807–1835, 2005.

[B51] C. Besse, S. Borghol, J.-P. Dudon, T. Goudon, and I. Lacroix-Violet. Hydrodynamic regimes, Knudsen layer, numerical schemes: Definition of boundary fluxes. *Adv. Appl. Math. Mech. (AAMM)*, 3:519–561, 2011.

[B52] M. Bostan, I. Gamba, T. Goudon, and A. Vasseur. Boundary value problems for the linear Boltzmann equation involving a variable force field. *Indiana Univ. Math. J.*, 59(5):1629–1660, 2010.

[B53] M. Bostan and T. Goudon. High-electric-field limit for the Vlasov-Maxwell-Fokker-Planck system. *Ann. IHP Non Linear Anal.*, 25:1221–1251, 2008.

[B54] C. Bourdarias, M. Gisclon, and Junca. S. Blow up at the hyperbolic boundary for a $2 \times 2$ system arising from chemical engineering. *J. of Hyperbolic Diff. Eq.*, 7(2):297–316, 2010.

[B55] C. Bourdarias, M. Gisclon, and Junca. S. Strong stability with respect to weak limit for a hyperbolic system arising from gas chromatography. *Methods and Applications of Analysis*, 17(3):301–330, 2010.

[B56] C. Calgaro, E. Chane-Kane, E. Creusé, and T. Goudon. $L^\infty$ stability of vertex-based MUSCL finite volume schemes on unstructured grids; simulation of incompressible flows with high density ratios. *J. Comput. Phys.*, 229(17):6027–6046, 2010.

[B57] C. Calgaro, E. Creusé, and T. Goudon. An hybrid finite volume-finite element method for variable density incompressible flows. *J. Comput. Phys.*, 227(9):4671–4696, 2008.

[B58] C. Calgaro, E. Creusé, T. Goudon, and Y. Penel. Positivity-preserving schemes for Euler equations: sharp and practical CFL conditions. Technical report, INRIA, 2012.

[B59] J. A. Carrillo and T. Goudon. Stability and asymptotic analysis of a fluid-particle interaction model. *Comm. PDE.*, 31(9):1349–1379, 2006.

[B60] J. A Carrillo, T. Goudon, and P. Lafitte. Simulation of fluid & particles flows: Asymptotic preserving schemes for bubbling and flowing regimes. *J. Comput. Phys.*, 227(16):7929–7951, 2008.

[B61] F. Clarelli, C. Di Russo, R. Natalini, and M. Ribot. Mathematical models for biofilms on the surface of monuments. In *Applied and Industrial Mathematics in Italy III, proceedings of the 9th Conference SIMAI*, volume 82 of *Series on Advances in Mathematics for Applied Sciences*. World Scientific, 2009.

[B62] F. Clarelli, C. Di Russo, R. Natalini, and M. Ribot. A fluid dynamics model of the growth of phototrophic biofilms. Technical report, CNRS, 2012.

[B63] J.-F. Coulombel, T. Goudon, P. Lafitte, and C. Lin. Analysis of large amplitude shock profiles for non-equilibrium radiative hydrodynamics: formation of Zeldovich spikes. Technical report, CNRS & Inria, 2011.

[B64] C. Di Russo, R. Natalini, and M. Ribot. Global existence of smooth solutions to a two-dimensional hyperbolic model of chemotaxis. In *CAIM, Perspective on Applied Mathematics in Italy*, 2010.

[B65] R. Eymard, C. Guichard, R. Herbin, and R. Masson. Convergence analysis of the vertex centred discretization of two-phase Darcy flows on general meshes. Technical report, CNRS, 2011.

[B66] R. Eymard, C. Guichard, R. Herbin, and R. Masson. Vertex-centred discretization of compositional Darcy flows on general meshes. *Computational Geosciences*, 2011.

[B67] R. Eymard, C. Guichard, R. Herbin, and R. Masson. Vertex centred discretization of two-phase Darcy flows on general meshes. In *Proceedings of the SMAI conference 2011*. ESAIM Proceedings, 2011.

[B68] R. Eymard, C. Guichard, and R. Masson. Grid orientation effect in coupled finite volume schemes. Technical report, CNRS, 2011.

[B69] A. Gloria, T. Goudon, and S. Krell. Numerical homogenization of a nonlinearly coupled elliptic-parabolic system, reduced basis method, and application to nuclear waste storage. Technical report, Andra & Inria, 2011.

[B70] T. Goudon, P.-E. Jabin, and A. Vasseur. Hydrodynamic limit for the Vlasov-Navier-Stokes equations. I. Light particles regime. *Indiana Univ. Math. J.*, 53(6):1495–1515, 2004.

[B71] T. Goudon, P.-E. Jabin, and A. Vasseur. Hydrodynamic limit for the Vlasov-Navier-Stokes equations. II. Fine particles regime. *Indiana Univ. Math. J.*, 53(6):1517–1536, 2004.

[B72] T. Goudon, S. Jin, and B. Yan. Simulation of fluid–particles flows: heavy particles, flowing regime and asymptotic–preserving schemes. *Comm. Math. Sci.*, 10(1):355–385, 2011.

[B73] T. Goudon, F. Lagoutière, and L. M. Tiné. The Lifschitz-Slyozov equation with space-diffusion of monomers. Technical report, CNRS & Inria, 2011.

[B74] T. Goudon, F. Lagoutière, and L. M. Tiné. Simulations of the lifshitz-slyozov equations: the role of coagulation terms in the asymptotic behavior. Technical report, CNRS & Inria, 2011.

[B75] T. Goudon and C. Lin. Global existence to the equilibrium diffusion model in radiative hydrodynamics. *Chinese Annals of Math-B., Series B*, 32(4):549–568, 2011.

[B76] T. Goudon, J.-G. Liu, S. Jin, and B. B. Yan. Asymptotic-preserving schemes for kinetic–fluid modeling of disperse two–phase flows. Technical report, Inria, 2011.

[B77] T. Goudon and M. Parisot. Finite volume schemes on unstructured grids for non-local models: Application to the simulation of heat transport in plasmas. Technical report, Inria, 2011.

[B78] T. Goudon and M. Parisot. Non–local macroscopic models based on Gaussian closures for the Spitzer–Härm regime. *AIMS–Kinetic and Related Models*, 4(3):735–766, 2011.

[B79] T. Goudon and M. Parisot. On the Spitzer-Härm regime and non local approximations: modeling, analysis and numerical simulations. *SIAM Multiscale Modeling and Simulation*, 9:568–600, 2011.

[B80] F.R. Guarguaglini, C. Mascia, R. Natalini, and M. Ribot. Global stability of constant states and qualitative behavior of solutions to a one dimensional hyperbolic model of chemotaxis. *Discrete Contin. Dyn. Syst. Ser. B*, 12(1):39–76, 2009.

[B81] S. Krell. Stabilized DDFV schemes for the incompressible Navier-Stokes equations. In J. Fort, J. Furst, J. Halama, R. Herbin, and F. Hubert, editors, *Finite Volumes for Complex Applications VI Problems and Perspectives*, volume 4 of *Springer Proceedings in Mathematics*, pages 605–612. Springer Berlin Heidelberg, 2011.

[B82] S. Krell. Finite volume method for general multifluid flows governed by the interface Stokes problem. *Mathematical Models and Methods in Applied Sciences*, 2012. to appear. Available online at http://hal.archives-ouvertes.fr/hal-00473783/fr/.

[B83] S. Krell and G. Manzini. The Discrete Duality Finite Volume method for the Stokes equation on 3D polyhedral meshes. *SIAM Journal on Numerical Analysis*, 2012. To appear. Available online at http://hal.archives-ouvertes.fr/hal-00448465/fr/.

[B84] B. Lombard and S. Junca. Dilatation of a one-dimensional nonlinear crack impacted by a periodic elastic wave. *SIAM J. on Appl. Math.*, 70(3):735–761, 2009.

[B85] B. Lombard and S. Junca. Interaction between periodic elastic waves and two contact nonlinearities. *Math. Models and Methods in Appl. Sc.*, 2012. to appear.

[B86] R. Natalini and M. Ribot. An asymptotic high order mass-preserving scheme for a hyperbolic model of chemotaxis. *SIAM J. Num. Anal*, 2012. to appear.

# Vita of the PI: Thierry GOUDON

Born January 1st, 1969, Aix-en-Provence, France

**Employments and Education**

• 2011– Senior Research Scientist INRIA, Sophia Antipolis Research Centre
Head of the Team COFFEE; Fellowship DMA, ENS

• 2007–2011 Senior Research Scientist INRIA, Lille Nord Europe Research Centre
R. Dautray Prize (SMAI–CEA) for works on Radiative Transfer, 2008
Head of the Project-Team SIMPAF (SImulation and Models for Particles And Fluids).

• 2003-2007 : Professor at University of Sciences and Technologies of Lille
with a CNRS appointment as Senior Research Scientist, in charge of the animation of the Numerical Analysis/PDE group of the laboratory P. Painlevé
Head of the CNRS Research Network "Interacting Particles"

• 1997–2003 : UNS , Laboratory J. A. Dieudonné, Associate Professor
Habilitation à diriger les recherches '01, reports by G. Allaire, F. Golse, M. Slemrod

• 1994–1997 : University Bordeaux 1, Laboratory of Applied Math. of Bordeaux
Instructor, Grant of the French Ministry of Research
PhD, '97, adv.: K. Hamdache, with reports by P. Gérard, B. Perthame, G. Toscani.

• 1994 : Military Service

• 1991–1993 : University Bordeaux 1,
Magistère MATMECA, Pluridisciplinary formation in Applied Mathematics, and Mechanics, based on modeling, scientific computing and analysis of complex phenomena, Ranked 1st & MSc in Applied Mathematics and Scientific Computing

**Academic activities**

Member of the Committee for the Blaise Pascal Award 2011 & 2012.
Member of the Scientific Board of CIRM since 2012.
Member of the Scientific Committee of Allistene on Scientific Computing
Co-organisation of the National Meeting of Numerical Analysis '08, Head of the Scientific Committee
Steering Committee of SMAI since 2008.
Member of the Evaluation Committee at INRIA, 2008–2011.
Member of the National Evaluation Committee of Universities in Applied Math, 2007–11.
Member of the jury of "agrégation", since 2005, in charge of the Modeling exams.
Responsible of doctoral studies in applied math. at Lille 2005–2010.
Co-organization of CEMRACS '03 "Numerical Methods for Kinetic and Hyperbolic Equations"

**Publications**

More than 70 publications in refereed journals like J. Comput. Physics, J. Sci. Comput., Comm. in Comput. Phys., SIAM J. Math. Anal., Ann. Sci. ENS, Comm. Math. Phys., J. Stat. Phys., Indiana Univ. Math. J... The research activity is concerned with the analysis of kinetic equations, the investigation of hydrodynamic regimes, the study of homogenization problems, in both deterministic or stochastic framework, the design of numerical schemes for complex flows. Complete list of references available at `http://math.univ-lille1.fr/~goudon`

**Editorial Activities**

Coagulation-fragmentation, Comm. Math. Sci., 2004.
Numerical Methods for Hyperbolic and Kinetic Problems, EMS, 2005
Simulation of transport phenomena, particles methods, ESAIM-Proc, 2005.
Analysis and Simulation of Fluid Dynamics, Birkhauser, 2007.
Proc. of CANUM, ESAIM-Proc. 2008
Math. models and numerical methods for radiative transfer, Panoramas et Synthèses, SMF, 2009

**Industrial Partnerships**

Collaborations with Thales (since '04) and CEA (since '09) on plasmas physics, with ANDRA (since '10) on flows in porous media.

**Main invitations abroad**

Invitations for research projects:
Shanghai Jiao Tong University' 12, Kyoto University'11, UW-Madison'10, Isaac Newton Institute–Cambridge Univ.'10, DAM– Brown Univ. Providence'09, Texas A&M College Station'07, ICES Univ. of Texas Austin'03-'07, CSCAMM Univ. Maryland College Park'05, IMA Univ. Minneapolis'00, Erwin Schrödinger Institute Vienna, Chalmers Institute–Göteborg Univ.'96;
with, in some occasions, the opportunity to give lectures:

Morningside Institute Beijing (lectures on math. tools for kinetic eq.'09), UCLA (IPAM tutorials on Math. analysis of kinetic eq.'09), Fudan University Shanghai (lectures on Charge transport), Univ. Gaston Berger Saint Louis in Sénégal (lectures on Hyperbolic systems'06), CRM Barcelona (lectures on Hydrodynamic limits'06), Univ. Granada (lectures on Kinetic eq.'06), Wolfgang Pauli Institute Vienna (lectures on Homogenization techniques'05)

# Vita of the Project Members

- **Magali RIBOT**
  - `http://math.unice.fr/~ribot/`
  - Born Sept. 3rd, 1977
  - Ass. Prof. Univ. Nice, since 2004
  - 2011: PI of the ANR project "Monumentalg" devoted to the modeling and simulation of biological damage on monuments and algae proliferation
  - 2003: PhD Lyon 1 (adv. M. Schatzman)
  - 1997–01: Scholarship at ENS Lyon
  - 7 publications in referred journals: DCDS B, Numerische Math., Methods Appl. of Analysis, SIAM J. Num. Anal.
  - M. R. is an expert on the numerical analysis of methods for transport–reaction–diffusion systems and the modeling thanks to hydrodynamic-type and kinetic equations of various biological phenomena that lead to aggregation phenomena and front displacement. She is also studying the behavior of solutions for hyperbolic models of chemotaxis in various situations, for example on a network or in porous media.

- **Florent BERTHELIN**
  - `http://math.unice.fr/~bertheli/`
  - Born Nov. 13rd, 1973
  - Ass. Prof. Univ. Nice, since 2003
  - 2009: HDR Nice
  - 2001: PhD Orléans (adv. F. Bouchut)
  - 1998: Agrégation de Mathématiques (ranked 21).
  - 1995–01: Scholarship at Univ. Orléans
  - 18 publications in referred journals: JMPA, SIAM J. Math. Anal., M2AN, Numerische Math., J. Diff. Eq...
  - F. B. is an expert on the analysis of kinetic models and systems of conservation laws, and of their connection through relaxation phenomena. He is also studying conservation laws with constraints.

- **Stéphane JUNCA**
  - `http://math.unice.fr/~junca/`
  - Born Dec. 10th, 1968
  - Ass. Prof. Univ. Nice, since 2006 (formerly affiliated at IUFM Nice 1996-2006)
  - 1995 : PhD Nice (adv. A. Piriou and M. Rascle)
  - 1994: Military Service and Agrégation de Mathématiques (ranked 43).
  - 1986–1991: Scholarship at Universities of Nice, Rennes and Grenoble, ranked 1st or 2nd.
  - 16 publications in referred journals: J. Math. Pures et Appl., J. Differential Eq., Comm. Math. Sci., J. Math. Anal. Appl., SIAM J. Appl. Math., Comm. Partial Differential Equations, Asymptot. Anal, Methods Appl. Anal...
  - S. J. is an expert on the analysis of nonlinear PDEs, with a specific interest on hyperbolic systems and asymptotic analysis of singularly perturbed problems.

- **Stella KRELL**
  - `http://math.unice.fr/~krell/`
  - Born March, 16th, 1983
  - Ass. Prof. Univ. Nice, since 2011
  - 2011 : Post Doc INRIA Lille (SIMPAF)
  - 2010 : PhD Marseille (adv. F. Boyer, F. Hubert)
  - 2006: Agrégation de Mathématiques.
  - 2005–2007: Scholarship at ENS Cachan–Ker Lann
  - 2 publications in referred journals: IMA J. Num. Anal., Num. Meth. for PDEs.
  - S. K. is an expert on the analysis of numerical methods of finite volume type for fluid dynamics (viscous flows, porous media), including domain decomposition techniques.

- **Roland MASSON**
  - `http://math.unice.fr/~masson/`
  - Born May 3rd, 1967
  - Prof. Univ. Nice, since 2011.
  - Member of the Scientific Board of the 2012 European Conference of Mathematics of Oil Recovery.
  - Engineer at IFP (Institut Français du Pétrole, Head of the Applied Math Department (2001-11)
  - 2006: HDR Univ. Marne-la Vallée
  - 1999 : PhD Paris 6 (adv. A. Cohen)
  - 1996: Engineer "Corps des Mines"
  - 1990–1993: Scholarship at Ecole Polytechnique
  - 1987-1990: Scholarship at ENSAM
  - 9 PhD students since 1996.
  - 29 publications in referred journals: J. Comput. Physics, Int. J. Finite Volumes, Comput. Geoscience, Inverse problems, SINUM,...
  - R. M. is an expert on Finite Volumes methods, with a specific interest for applications to porous media. He has developed 3D codes for multiphases flows, using FV methods on unstructured and non conformal meshes.

# A Details on the FV_MULTIP project

## A.1 Objectives

- To develop a simulator implementing advanced finite volume discretizations on general polyhedral meshes for heterogeneous anisotropic media, as well as a generic compositional multiphase Darcy flow model with adaptive implicit time integration. Current simulators are limited to structured CPG geometries not adapted to complex basin and reservoir models.

- To develop a simulator more efficient in parallel distributed architectures than existing reference industrial software (`Tough` and `Eclipse`) for CO2, reservoir, and nuclear waste repository simulations. On this aspect it is likely that the project can be strongly connected to the aims and scope of the new AE devoted to HPC.

- This simulator will enable our team to capitalize our research and developments in order to simulate more advanced reservoir and basin geometries (faults, erosions, complex wells, etc.) and more advanced models (formation damage, poromechanical couplings, chemical couplings, etc.).

- To foster our collaborations with BRGM, ANDRA, TOTAL, GDFSuez, based on this new tool.

## A.2 Description

Our simulator should be able to deal with general 3D unstructured meshes with polyhedral cells on heterogeneous, anisotropic media. It will incorporate cell centered finite volume schemes such as the MPFA O scheme, vertex centered schemes such as the Vertex Approximate Gradient (VAG) scheme, and hybrid schemes such as DDFV discretizations. The code will implement a general formulation for compositional multiphase flows in porous media with an arbitrary number of phases (typically from 1 to 4), an arbitrary number of components (typically from 1 to 10), the coupling with the thermodynamic equilibrium and a global energy conservation equation for the mixture. The data set will be at this stage kept simple and in particular the physical laws will be analytically defined as functions of the main set of unknowns (pressure, temperature, saturations, molar compositions). The integration scheme will be semi implicit, with the possibility to choose between explicit and implicit variables in each cell of the domain (adaptive implicit schemes). The code will be able to run in parallel on distributed architectures, the first

target is, say, about a hundred cores, then it will be extended to around a thousand cores. Good scalability should be obtained provided the number of cells per processor is large enough (weak scalability) since the bottleneck of scalability for such implicit systems is governed by the preconditioned iterative linear solver requiring between 10000 and 50000 cells per node for a good scalability. The validation will include a range of test cases from single to multiphase and compositional test cases which are already running on our current scalar prototype (for instance the 3D nearwell simulation of the injection of CO2 in a saline aquifer, 2D thermal recovery of heavy oil by the SAGD process (steam assisted gravity drainage), 3D black oil reservoir simulation in a five spot pattern, etc.).

We do not aim to include as many physical options as simulators like `Tough2` or `Eclipse` but rather to focus on possibilities offered by more advanced schemes on unstructured meshes, and by a code more adapted for the coupling of different physical models and numerical schemes.

## A.3 WorkPlan

We split the workplan into several tasks.

- Task "preprocessor": computation of the finite volume schemes, input=mesh, output=graphs of transmissibilities. At this stage this computation is kept outside the simulator and will not be parallel. A large part of the simulator will be already developed at the beginning of CEMRACS 2012.

- Task "partitioning and distributed graphs": data structure of the distributed graphs, choice of a library for the graph and the graph partitioner, developments. `Scotch` is a possible choice to be investigated.

- Task "sparse linear (possibly nonlinear) algebra": choice of a library(ies) for assembly of the Jacobian, basic sparse linear algebra, preconditioner and solver, could possibly include the nonlinear solver (depending on the library), `PETSc` is the most probable choice, to be investigated.

- Task "definition of the data set and its use in the simulator": BC, IC, physical laws and their derivatives, unknowns management, time management

- Task "developments of physical laws and their derivative": computations, fluxes and residual computations, Jacobian computation and assembly.
- Task "algebraic operations on the Jacobian before solving" (scaling, Schur complements for explicit unknowns elimination, etc.), preconditioner and solver.
- Task "integration of a distributed mesh data structure and connection with the computation of the distributed graphs".
- Task "numerical specifications, test case definition, validation".

  Note that we distinguish tasks with a content of mathematical modeling and task oriented to scientific computing.

## A.4 ManPower

R. Masson and S. Krell, permanent members of the team, will be the leaders of this activity, with more or less punctual commitment of T. Goudon, and M. Ribot. Generally speaking, members of the team will be privileged users of the code for their own applications.

The team hosts and will host internships at various levels working on the program (ideally twice 6 month/year for Master2 or Engineer). PhD students and post-doc will be strongly involved in the development of the code. We also need additional support, in particular concerning the development of parallel procedures. At least, we need a 2 year-support of an engineer for the development of the code.