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**Université Nice - Sophia
Antipolis**

Activity Report 2012

Project-Team COFFEE

COmplex Flows For Energy and Environment

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

RESEARCH CENTER
Sophia Antipolis - Méditerranée

THEME
Computational models and simulation

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Project-Team COFFEE

Keywords: Flow Modeling, Fluid Dynamics, Multiscale Analysis, Multiscale Models, Numerical Methods, Particles, Porous Media, Scientific Computation, Simulation

COFFEE is a joint team with the laboratory J. A. Dieudonné, University Nice Sophia Antipolis and CNRS (UMR 7351).

Creation of the Project-Team: July 01, 2011 .

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2. Overall Objectives

2.1. Overall Objectives

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

3. Scientific Foundations

3.1. Scientific Foundations

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 an unexpected fashion, many common features. The proposal is precisely based on the conviction that these subjects can mutually cross-fertilize and that they will both be a source of general technical developments, and a relevant way to demonstrate the skills of the methods we wish to design.

To be more specific:

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

4. Application Domains

4.1. Analysis of PDEs

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.

4.2. Numerical analysis of FV methods

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.
- 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.
- 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. Among others, we are particularly interested in Asymptotic High Order (AHO) schemes.

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. 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, 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.

4.3. Asymptotic analysis

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.

4.4. Particulate flows, Mixture flows

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

4.5. Interface problems

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. 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, 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 are involved in a collaboration with physicists specifically dedicated to such problems of wave propagations through complex interfaces.

4.6. Biological degradation

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 as a protection device against corrosion of well cement in CO₂ storage reservoir. 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 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 (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. 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.

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. 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

5. Software

5.1. NS2DDV

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

5.2. FV_PM

We are developing codes based on Finite Volume discretization, for the (2d and 3d) simulations of multiphase flows in porous media. For instance these methods apply to the simulation of problems motivated by CO₂ storage, oil recovery or nuclear waste depository. A preliminary version, the code ComPASS (Computing Parallel Architecture to Speed up Simulations), which includes parallel procedures, has been recently developed, through a successful CEMRACS project.

5.3. SimBiof

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

5.4. AP_PartFlow

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

6. Bilateral Contracts and Grants with Industry

6.1. Bilateral Contracts with Industry

- ANDRA

In 2011/12, S. Krell and T. Goudon, with A. Gloria, have worked on the development of homogenization methods for the simulation of the transport of radionuclides in porous media. A new numerical method has been proposed, based on Reduced Basis techniques which allows efficient computation of the (space-dependent) effective coefficients. In 2012/13 we start a new collaboration devoted to the modeling and simulation of ventilation devices in nuclear waste disposal. This is a long-term project (with the PhD of Y. Zhang) 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.

- CEA

We work on the simulation of two-phase flows described by Eulerian/Lagrangian models. To this end, A. Champmartin develops a new semi-Lagrangian algorithm for fluid-kinetic coupling, in collaboration with CEA/DAM and the LRC Manon.

- GDFSuez EP-Storengy - (Contract with UNS-CNRS)

The collaboration is 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. During her post-doc, C. Guichard develops new methods for diphasic flows in porous media, with application to tight gas and gas stockage.

- TOTAL (Contract with UNS-CNRS)

R. Masson is scientific consultant of the recently created team "Nouveau Simulateur de Réservoir", led by B. Faissat. The team is concerned with the development of new research codes for oil recovery problems, based on FV methods. Through the post doc of W. Kherriji, we develop new domain decomposition algorithm for the simulation of oil recovery, with local refinement, both in time and space. C. Guichard works on Finite Volumes methods on unstructured meshes.

7. Partnerships and Cooperations

7.1. National Initiatives

7.1.1. ANR

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

7.1.2. National and European networks

- GdR MoMas.

The research group MoMaS (Mathematical Modeling and Numerical Simulation for Nuclear Waste Management Problems) has activities centered around scientific computing, design of new numerical schemes and mathematical modelling (upscaling, homogenization, sensitivity studies, inverse problems,...). Its goal is to coordinate research in this area, as well as to promote the emergence of focused groups around specific projects. In particular, in 2012, R. Masson has been involved in the organization of two MoMaS workshop "Multiphasic flows", Oct. 8-9 2012, with Danielle Hilhorst, University of Orsay.

- S. Junca is involved in the GdR-e “Wave Propagation in Complex Media for Quantitative and non Destructive Evaluation”; in particular he organized the Workshop “Nonlinearities in Acoustics” Nice, March 22-23/2012.
- GdR EGRIN is a newly created CNRS-network, devoted to gravitational flows and natural risks; Coffee is among the members of this network.
- R. Masson, with Pierre Samier (Total) has been organizer of ECMOR XIII European Conference on the Mathematics of Oil Recovery, 10-13 september 2012, Biarritz, France, a scientific event of the European Association of Geoscientists and Engineers.

8. Dissemination

8.1. Teaching - Supervision - Juries

8.1.1. Teaching

Master : Th. Goudon, Scientific Computing, ENS Paris, France.

Master : F. Berthelin, PDEs and kinetic equations (M2), Nice, France

Master : F. Berthelin & M. Ribot, préparation to agrégation (M2), Nice, France.

Master : Th. Goudon & R. Masson, Mathematical modeling and Scientific Computing for biology (M2), Nice, France.

Master : S. Junca & S. Krell have their teaching duties at IUFM, being in charge of preparation of teachers.

Agrégation : T. Goudon is member of the jury of agrégation, the national competition to hire teachers, in charge of the scientific computing exams.

8.1.2. Supervision

Master & PhD

Master Nice, F. Berthelin, EDO for biological modeling.

Master Nice, S. Junca, Regularizing effect for scalar conservation laws.

Master EPU Nice, T. Goudon & C. Scheid, Simulation of 2D incompressible Euler equations in vortex simulation.

Master ENS Paris, R. Masson & S. Krell, Finite volumes methods for elliptic PDEs

PhD L'Aquila (Italy): M. Twarogowska, Numerical approximation and analysis of mathematical models arising in cells movement, advised by M. Ribot & R. Natalini (defended 02/14/2012).

PhD in progress : Y. Zhang, Modeling and simulation of mass and heat exchanges in nuclear waste storage, starting Sept. 2012, advised by Th. Goudon and R. Masson

8.1.3. Juries

S. Junca : PhD M. Hajjej, “Couches initiales et limites de relaxation aux systèmes d’Euler-Poisson et d’Euler-Maxwell”, Clermont-Ferrand, Mars 2012.

Th. Goudon : HDR of A. Gloria, “Propriétés qualitatives et quantitatives en homogénéisation périodique et stochastique”, Lille fev. 2012.

Th. Goudon : PhD of I. Guaraldo, “Some analytical results for hyperbolic chemotaxis model on networks”, Roma, July 2012 (referee).

Th. Goudon : HDR of R. Turpault, “Modélisation, analyse numérique et simulations de phénomènes complexes pour des systèmes hyperboliques de lois de conservation avec termes sources raides et en électrocardiologie”, Nantes, Oct. 2012 (Pdt.)

Th. Goudon : HDR of S. Mancini, “Modèles cinétiques. Applications en volcanologie et neurosciences”, Orléans, Nov. 2012 (Pdt.).

R. Masson, PhD of D. Chauveheid, “Ecoulements multi-matériaux et multi-physiques: solveur volumes finis eulérien co-localisé avec capture d’interfaces, analyse et simulations”, CMLA.

8.2. Popularization

Th. Goudon is in charge for SMAI, the french society for applied and industrial mathematics, of the animation of “2013, Mathematics of Planet Earth”, a event supported by UNESCO. In particular he is member of the Steering Committee of the operation “1 jour, 1 brève” which aims at publishing one text a day devoted to the topics of Mathematics of Planet Earth.

R. Masson is involved in the Atelier de Recherche Prospective MathsInTerre, led by D. Bresch: this network has been created in connection to the worldwide event "2013, Mathematics for the Planet Earth"; this project aims at bringing out several key subjects that deserve a specific attention for future researches.

9. Bibliography

Publications of the year

Doctoral Dissertations and Habilitation Theses

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Articles in International Peer-Reviewed Journals

- [2] B. ANDREIANOV, H. F. BENDAHMANE, S. KRELL. *On 3D DDFV discretization of gradient and divergence operators. I. Meshing, operators and discrete duality.*, in "IMA J. N. A.", 2012, vol. 32, n^o 4, p. 1574–1603 [DOI : 10.1093/IMANUM/DRR046], <http://hal.archives-ouvertes.fr/hal-00355212>.
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