INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Smash

Simulation, Modeling and Analysis of Heterogeneous Systems in mechanical engineering

Sophia Antipolis

THEME NUM

Activity Report

2006

Table of contents

1. Team

Head of project-team
Hervé Guillard [Research Director, HdR]

Administrative assistant
Montserrat Argente

Staff members (INRIA)
Alain Dervieux [Research Director, HdR]
Marie-Hélène Lallemand [Research scientist]

Staff members (University of Provence)
Eric Daniel [Professor, HdR]
Serguey Gavrilyuk [Professor, University Aix-Marseille III, HdR]
Jacques Massoni [Teaching Assistant]
Richard Saurel [Professor, HdR]

Post-doctoral fellows
Thibaud Kloczko
Erwin Franquet [From December 1st 2006]

Ph. D. students
Roxanna Panescu
Olivier Basset
Anne-Cécile Lesage
Erwin Franquet
Nicholas Favrie
Fabien Petipas
Youssef Mesri
Mathieu Labois
Damien Guegan

Project technical staff
David Rey

External collaborators
Thierry Coupez [Professor, ENSMP]
Philippe Helluy [Professor, University Louis Pasteur Strasbourg]

Graduate Student intern
Nicholas Favrie
Fabien Petipas
Florent Guignery [Master 2, University of Provence]

2. Overall Objectives

2.1. Overall Objectives

SMASH is a common project between INRIA and the University of Provence. The main topic of our project focuses on problems related to mathematical and numerical modeling of heterogeneous flows such as multiphase media, granular materials or reactive flows with mass transfer. The scientific themes in concern are the design and improvements of models for these flows as well as the definition and analysis of discretization methods and schemes for their numerical simulation. The final aim is to implement the resulting algorithms on parallel machines for solving large scale problems of industrial or pre-industrial interest.

One of the main original features of the SMASH researches on heterogeneous flows lies in the way we deal with multi-fluid flows (interface problems). We use an Eulerian approach with a diffuse interface model. The two different media are not modeled separately (using adequate scheme for each phase) nor the interface needs to be defined explicitly. On the opposite, the diffuse interface zone is considered as a true multiphase region and described with a two-phase model. With such an Eulerian approach, numerical problems related to the discontinuities of the state equations through the interface, which occur when using separate models for each phase, do not appear anymore.

The domains in which two-phase flows are of interest are widespread in the industry (nuclear industry, oil company industry, car engine technology, food industry ...) but also in environmental studies (forest fire, coast erosion, ...), biomedical engineering, detonation theory or astrophysics research areas.

3. Scientific Foundations

3.1. Modeling of multiphase media

Keywords: *Hamilton principle*, *Homogenization*, *Mixture models*, *Two-phase models*.

The microscopic description of an heterogeneous medium has to take into account the specific physical properties of each material component. For both practical and numerical reasons, it may be impossible to take into account all those microscopic features. As an illustration, one m^3 of water mist typically contains a range of about 10^8 to 10^{12} droplets! Modeling such an heterogeneous medium consists in replacing it by an artificial mixture that ideally would have the same averaged properties. The resulting *multiphase* models are very far from the classical Euler or Navier-Stokes models.

The definition and setting of such multiphase models may be based on different techniques.

The first formalism [38], is very similar to the techniques involved in the definition of statistical models of turbulence with the use of averaging operators. It leads to an open set of equations (that is there are more unknowns than there are available equations). A way to close that system is to take into account some physical assumptions concerning the behavior at the micro-scale level. This approach is certainly the most used in the industry but leads to difficult open questions in applied mathematics such as the hyperbolicity of the resulting models and the definition of non-conservative products. This methodology was the starting point of our studies in multiphase modeling and led us to promote the use of two-pressure, two-velocity *hyperbolic* models [7].

However, with this type of modeling, closure assumptions concerning the micro-scale behavior have to be formulated. This is an extremely difficult task. Therefore, we are also investigating a modeling formalism based on the Hamilton principle of least action [43]. The advantage of this formalism is that the only assumptions are on the definition of the potential energy associated to the flow.

Using either technique results in a set of non linear partial differential equations (PDE). Then, we need to discretize it by some numerical scheme in order to get a set of algebraic equations that in turn will provide the discrete solution. We are therefore faced with mainly two classes of difficulties: the first class of difficulties consists in finding the good set of PDE's to model the multiphase flow we want to study; the second class comes from the choice of the discretization scheme.

To avoid this addition of difficulties, we have recently introduced an original modeling technique [1]. In this approach, we start with the continuous equations defined at the micro-scale level but instead of averaging it, we *first* discretize those micro-scale continuous equations *before* filtering the resulting set of discrete equations. With this technique, we end up directly with a macro-scale discrete model.

3.2. Modeling of interface and multi-fluid problems

Keywords: *Diffuse interface*, *Eulerian Models*, *Front Capturing*, *Multi-fluid mixtures*.

An important part of CFD is to get a detailed description of the interaction between two different fluids at the scale of the interface between them. This is what we will call a *multi-fluid* problem. At the present time, tracking methods are certainly the most used technologies to treat this problem.

For compressible fluids, “capturing” or diffuse interface approaches, where the interface is not defined explicitly as a discontinuity surface but as non-zero thickness mixing zone (where the physical quantities are continuously varying) are just beginning to be used. Actually, before the original work of Abgrall [37] the capturing methods were plagued by the difficulty of computing the pressure in the mixing zone. Abgrall shows the feasibility of interface capturing methods provided that one partially gives up the conservative form of the equations. Improving upon this contribution, our project develops an original diffuse interface method where the artificial numerical zone is considered as a true two-phase flow region. Although seemingly artificial, this allows to consider a model that can handle huge density ratio and very different thermodynamics.

This front capturing - diffuse interface technique has proven its ability of solving interface flow problems more simply than usually and moreover offers the possibility to treat not only interface problems between pure fluids but also interfaces between mixtures (as for instance the boundaries of a cloud) in the same formalism.

3.3. Approximation methods

Keywords: *Finite Volume methods*, *Low Mach Compressible flows*, *Riemann Solvers*.

All the mathematical models considered and studied in SMASH consist in either a hyperbolic or parabolic system of PDE’s. The discretization techniques applied to these PDE should respect the properties of the continuous model such as conservativity, positiveness preserving (e.g. pressure, density), jump conditions, maximum principle or entropy inequality. Most of our numerical methods are based on finite volume discretizations [39]. That indeed allows us to keep the full description of the physics of the media by solving local *Riemann problems* [44] corresponding to the evolution of the medium variables through a plane interface separating two physical states. SMASH focuses its efforts into the development of approximation methods using either exact or approximate Riemann solvers.
When the resulting model is non conservative, which occurs as a “mechanical” consequence when using an averaging process, additional mathematical and numerical difficulties arise. From a theoretical point of view, it is known since the works of Schwartz [42] that the product of two distributions is not defined. Therefore, the question of giving a sense to this product arises and as a consequence, the numerical approximation of non-conservative terms is unclear. For contact discontinuities, our discretization methods are based on the principle that both velocities and pressures should remain constant. The resulting discretization schemes respecting that principle appear to be both robust and efficient for interface flow problems compared to most existing methods. For shocks, we investigate formulations where the Rankine-Hugoniot relations are imposed via some physical analysis of the internal structure of the relaxation zone.

Another difficulty encountered in solving two-phase flow problems comes from the high disparity between the wave speeds of each existing fluid material. In particular, one of the fluids may be very close to the incompressibility limit. In that case, we face up the problem of very low Mach number flows. The numerical treatment of these flows is still a problem and involves non trivial modifications of the original upwind schemes [5], [4]. Our investigations in that domain concern both acoustic and incompressible aspects in methodologies for setting up suitable numerical methods.

3.4. Solution algorithms

Keywords: *Grid Computing*, *Multi-grid methods*, *Multilevel methods*, *Parallelism*.

The approximation step generates large algebraic systems that have to be solved. The problems that the team is studying can result in systems that can have several tenth of millions of unknowns. The choice of appropriate solution methods is therefore fundamental. The team concentrates its investigations on multi-level and multi-grid methods. In this domain, since the meshes used for industrial applications can be totally non-structured, an important point is to be able to construct a hierarchy of meshes describing the problem with different levels of resolution. In this direction, the team studies both purely algebraic approaches as aggregation/agglomeration methods [6] as well as geometrical methods where a hierarchy of non-structured meshes is constructed by coarsening algorithms.

For the largest problems that we are currently considering, the use of modern parallel computers is mandatory. This requires a careful examination or adaptation of the numerical solvers. Nowadays, the usual way to parallelize large mesh-based scientific application relies on partitioning the computational domain. Then, a simple SPMD (Single Program Multiple Data) strategy using a message passing programming model (such as MPI "Message Passing Interface") can be used to parallelize these applications.

The SMASH team is also involved in some experiments in Grid computing using the same parallelization model (http://www-sop.inria.fr/smash/mecagrid/public/mainFrame.htm). Actually, the possibility to construct large scale computing platforms like the Grid5000 project is very attractive for solving some fundamental problems in engineering like multi-fluid applications or turbulence studies. However additional problems such as the heterogeneity of the computing nodes and of the interconnection networks or the multi-site localization of the computing or data storage resources have to be solved to make the concept of Grid effective in high performance computing.

4. Application Domains

4.1. Panorama

With a large experience in working on numerical fluid mechanics problems, SMASH focuses its particular interests on compressible multiphase or multiform flows; the application domains involves energy and transport industries: aeronautics, car engine combustion research, space research, oil company research, research on electricity and nuclear centers hazards, but involves also other various domains such as astrophysics and detonation studies.

4.2. Transport industry

Automotive industry : In Diesel engines, the new generation injection system technology use high pressure spray injection techniques. Our Eulerian modeling techniques may be used to describe the first steps of atomization of the spray. These phenomena are preceded by a dynamic liquid-vapor transition phase during which the compressibility feature of the flow appears to be crucial. Figure 1 shows the vapor volume fraction in a two dimensional model of fuel injector The dark area represents the location where the vapor volume fraction is high. This study has been performed in the framework of an "ARC" (Action Concertée de Recherche) of CNRS, whose industrial partners were Peugeot and Renault.

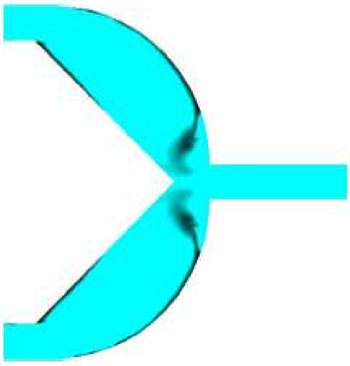

Figure 1. Vapor volume fraction in a two dimensional model of fuel injector

Aeronautics : The main needs in that area concern external aerodynamics, where turbulence has to be taken into account to model external complex flows around a complete geometry profile since the numerical simulations are still too costly to be a true part of the optimization process. SMASH is interested in defining suitable multi-grid solvers for the Navier Stokes equations using unstructured finite volume discretization grids. In addition, the unsteady feature of turbulent flow problems encountered e.g. in vibration of some material structure and damaged material problems requires the need of LES type models ("Large Eddy Simulation" techniques).

Space industry : Another application area we are concerned with is the behavior of a space launcher engine using liquid fuel or powder propellants. Since the media involve very heterogeneous ingredients, two-phase modelings as well as the study of free surface problems are needed

4.3. Energy industry

The needs in numerical modeling are concerned with thermo-hydraulics for nuclear energy production centers (CEA and EDF), flow problems in pipe lines for oil company industry (extraction, oil transport and refining) and all other industries related to energy production or chemical engineering.

In these industrial domains, turbines, boilers and pipes involve very complex flows which often evolve either violently and/or at high speed, or on the contrary evolve very slowly with a large stabilization time. Describing those phenomena which are intrinsically two-phase type flow problems appears to be fundamental in studies of security issues against hazards (nuclear industry, oil-chemical industry or chemical engineering industry). When dealing with very low Mach number flows, the numerical complexities and difficulties are even higher. The ability of a CFD code to treat efficiently and accurately the different phase flow regimes (gas/liquid flows, bubbling flows, packet flows, liquid film and droplet flows, supersonic, very subsonic) is still problematic. These difficulties are amplified in some research program on controlled Fusion like ITER, where the generated heat flux can be as high as $20MW/m^2$. To cope with such high fluxes, the design of relevant two-phase models and of the associated numerical methods is of primary importance.

4.4. Other application issues

Multiphase modeling techniques may also find a place in other various application domains. That is for instance the case in astrophysics for modeling keplerian type flows in a proto-planetary system composed of gas and particles. This type of study is currently done in the team in collaboration with astrophysicists to validate some assumptions on the process of planet formation in accretion disks. Figure 2 taken from [40] shows for instance the development of a non-linear instability in a gas flow around a star leading to the formation of vortices. The formation of such vortices is involved in some scenarii of planet formation.

Another interesting application domain concerns multiphase flow problems in highly energy-giving granular media. Most of the existing CFD codes that aim to simulate those types of multiphase flows uses the Euler equation model closed by an equation of state defined for the fluid mixture. That necessarily implies that the phase temperatures (or phase density ...) equilibrium holds without making sure that such assumption remains relevant to this type of flow problems. The project-team works on the definition of two-temperature models in which the physics is more accurately described for such media.

5. New Results

5.1. Mathematical Modeling in CFD

5.1.1. Shock relations for non-conservative hyperbolic systems

Participants: Sergey Gavrilyuk, Olivier Le Metayer, Jacques Massoni, Richard Saurel.

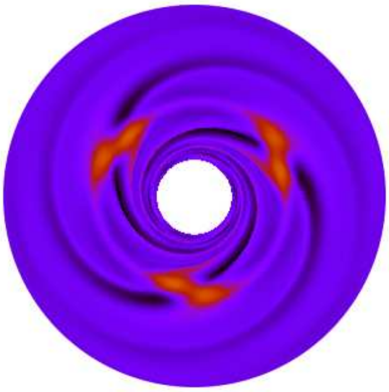

Figure 2. Pressure field after 2.7 orbital revolution

The conservation of mass, momentum and energy are not sufficient to close the system of jump relations for shocks propagating in heterogeneous media. Several aspects of this closure problem are currently studied in the project :

Shock relations for multiphase mixtures with stiff mechanical relaxation : Examples of multiphase mixtures for which velocity and pressure relaxation is a stiff phenomenon are involved in many practical applications dealing with condensed phase mixtures, solid alloys, propellants and solid explosives, specific composite materials, micro- and nano-structured mixtures etc. Shock relations for the mixture necessitate the determination of the volume fraction jump or any other thermodynamic variable jump. Examination of the shock dispersion mechanism suggests such jump relations. These relations are the phase Hugoniots which are compatible with the mixture energy equation. The corresponding model is conservative and symmetric. It fulfills the single-phase limit and guarantees volume fraction positivity. The shock relations are validated over a large set of experimental data and provide a remarkable agreement. A paper presented this work has been accepted in Int J. Shock Waves [26]

Shock relations in turbulent flows : The simplest model of isotropic compressible turbulence consists of the Euler equations augmented by the equation for the turbulent energy. This model can also be viewed as the Euler equations for a continuum with two independent entropies. One of them is a conventional thermodynamic entropy, and the other is associated with the turbulent energy. We have examined the shock relations for this model [15] It is shown that the turbulent entropy can not exceed some critical value. We propose a closed set of Rankine-Hugoniot relations for the description of shock waves in such a media based on this estimation.

Jump relations in heterogeneous mixtures : We propose here [16] a closed set of relations corresponding to a two-stage structure of shock fronts. At the first stage, a “micro-kinetic energy” due to the relative motion of mixture components forms at shock front. At the second stage, this “micro-kinetic energy” disappears inducing strong variations of the thermodynamical states that reach mechanical equilibrium. The “micro-kinetic energy” produced at the shock front is estimated by using an idea described in the previous paragraph. The relaxation zone between the shocked state and the equilibrium state is integrated by a thermodynamic path whose justification is provided. Comparisons with experiments on shock propagation in a mixture of condensed materials confirm the proposed theory.

5.1.2. *Modeling of bubbly flows*

Participants: Fabien Duval [IRSN], Hervé Guillard, Jean-Claude Latché [IRSN], Roxanna Panescu.

The simulation of disperse bubbly flows is very often done with the use of the so-called “drift flux” model where the slip velocity between the dispersed and the continuous phases is specified by an algebraic relationship. This simple approach suffers from a severe drawback : depending on the flow regime, the slip relationship can change and with it, the mathematical nature of the model that can switch from an hyperbolic to a non-hyperbolic system. Using a Chapman-Enskog asymptotic analysis, we have derived a model for bubbly flow where the slip velocity is expressed by a Darcy type relation. This model is always hyperbolic with a clear mathematical structure. Numerical approximation for this model have been devised and applications to several test cases have been realized. A paper has been submitted to J. Comp. Physics.

5.1.3. *Interface and multi-fluid low speed computations*

Keywords: *Capillarity fluids*, *Level Set*, *Low Mach multi-fluid problems*, *incompressible flows*.

Participants: Alain Dervieux, Herve Guillard, Bruno Koobus [université de Montpellier 2], Frédéric Alauzet [Projet Gamma, INRIA-Rocquencourt], Stephen Wornom [Lemma], Olivier Allain [Lemma], Anne-Cécile Lesage, Damien Guégan, Olivier Basset.

SMASH has developed a 3-D multi-fluid research code based on one pressure, one velocity model [41]. This code has received recent improvements in positivity numerical control published in [12] and new computational results are published in [20].
In parallel with these studies that use a multiphase modeling of the numerical mixing zone at the interface, the team also develops several activities where the level set technique is used to capture the interface zone. These studies are done in collaboration with Cemef for incompressible models where they are mainly used as benchmark computations for parallel and grid computing [8] and in partnership with Société Lemma. In particular new Level Set methods are studied for capillarity low gravity applications with small contact angle [31]. The thesis of Damien Guegan supported in partnership with Lemma, CNES and EADS, focuses this year on mesh adaption methods for interface computation, in cooperation with Frédéric Alauzet. A part of this work contributes to the ARC LNM "Combiner efficacement techniques d’adaptation de maillages et méthodes de lignes de niveaux".

5.1.4. *Turbulence modeling*

Keywords: *Large Eddy Simulation*, *Variational Multi-scale*, *hybrid models*, *unstructured meshes*, *vortex shedding*.

Participants: Bruno Koobus [université de Montpellier 2], Hilde Ouvrard [université de Montpellier 2], Alain Dervieux, Herve Guillard, Stephen Wornom [Lemma], Charbel Farhat [Stanford], Simone Camarri [Pise], Maria-Vittoria Salvetti [Pise], Eric Schall [Pau], Kamal El Omari [Pau], Yacine Bentaleb [Pau].

The purpose of our works in LES/LNS is to develop new approaches for industrial applications of LES-based analysis. In the mean term foreseen applications (aeronautics), the Reynolds number is several tenth millions, a too large number for pure LES models. However, certain regions in the flow can be much better predicted with LES than with usual statistical RANS (Reynolds averaged Navier-Stokes)models. These are mainly vortical separated regions as assumed in one of the most popular hybrid models, the Detached Eddy Simulation model. It is hybrid in the sense that a blending is applied between LES and RANS. Complex applications require unstructured meshes and the sixth-order dissipation previously developed on tetrahedrizations is intensively used and also extended to a new non-linear formulation which enjoy accuracy up to 6th order on Cartesian mesh subregions. The French-Italian team considered first the blending of Batten-Golberg-Chakravarthy, the LNS (Limited Numerical Scale) method. A new approach has then been developed. It relies on a Variational Multi-scale LES component and a low-Reynolds K-eps[33][36]. Although combined with several mechanisms of hybridization and scale selection, the LES component remains important. In her thesis starting end of 2006, Hilde Ouvrard will compare our Smagorinsky model with new ideas. Applications to vortex flows around circular and square cylinder show the improvement with respect to previous versions.

A particular application addresses shapes involving edges for which the backscatter of small scales towards larger ones is important and well accounted for by the Variational Multi-scale method, see [34]. Concerning statistical turbulence models, cubic low Reynolds extensions are studied in cooperation with University of Pau, see [32],[29].

5.1.5. Acoustics in high speed flows

Participants: Ilya Abalakin [IMM-Moscow], Alain Dervieux, Tatiana Kozubskaya [IMM-Moscow].

Previous works of this troika addressed the development of a new version of NLDE, and of super-convergent techniques for noise propagation with linear and nonlinear hyperbolic models. The interest of the Russian-French team is concentrating on nonlinear phenomena in a resonance-type liner. During the visit of T. Kozubskaya, a reflexion has been developed for a further improvement of our numerical scheme. This work is still in progress.

5.1.6. Laser ablation front

Participants: Olivier LeMetayer, Richard Saurel.

When a laser beam of high intensity interacts with a dense material, an ablation front appears in the high-temperature plasma resulting from the interaction. Such a front can be used to accelerate and compress the dense material. The dynamics of the ablation front is strongly coupled to that of the absorption front where the laser energy is absorbed. In this work [21] we have determined analytical solutions of the front internal structure in the fully compressible case .

5.1.7. Modeling of liquid nanofilms

Participants: Sergey Gavrilyuk, I Akhatov [North Dakota State University].

Van der Waals attractive forces drastically change the material properties of thin liquid layers several nanometers when in contact with a solid. At this scale, the fluid is no longer homogeneous. Moreover, it has properties which analogous to those of solids. In particular, in equilibrium the stress tensor is no longer spherical. For such fluids, we use in this work [14] a long-wave approximation to derive the evolution of a liquid nanofilm on a substrate. We establish that the driving pressure in nanofilm should be associated with the mean value of the component of the pressure tensor tangential to the liquid interface (along the substrate). Finally, we derive the equation for nanofilm dynamics by using mass conservation formulation. This is not a conventional, conservative equation for the position of the free surface normally used in the theory of thick films where the density is homogeneous, but rather a conservative equation for the liquid mass. The equation turns out to be a nonlinear parabolic equation with a diffusion coefficient of a ”good” sign.

5.1.8. Modeling of triple contact line

Participants: Sergey Gavrilyuk, V. S. Nikolayev, Henri Gouin [Laboratoire de Modelisation en Mecanique et Thermodynamique, Marseille].

We propose a model of the triple fluid-gas-solid contact line motion that takes into account the influence of the fluid inertia [23]. The viscous dissipation in the bulk of the fluid is assumed to be negligible comparing to the dissipation in the vicinity of the contact line. The equations of motion and the boundary condition at the contact line are derived from the Hamilton principle. The dissipation at the contact line is introduced using the dissipation functional method. As an example, the capillary rise along a vertical non homogeneous surface is solved. This approach is especially suitable to describe the fast motion of a low-viscosity fluid coupled with a slower motion of the contact line.

5.1.9. Dissipative two-fluid models

Participants: Sergey Gavrilyuk, Henri Gouin [Laboratoire de Modelisation en Mecanique et Thermodynamique, Marseille].

In this work, [17], the governing equations of two-fluid mixtures are derived from Hamilton’s principle of stationary action, the model is then extended to the dissipative case without chemical reactions. The governing system is hyperbolic for small relative velocity of phases.

5.1.10. Modeling of three-dimensional water waves

Participants: Sergey Gavrilyuk, Vladimir Teshukov [Lawrentiev Institute of Hydrodynamics, Novosibirsk].

This work [27] considers the Green-Naghdi equations describing three-dimensional water waves. Assuming that transverse variations of the flow occur at a much shorter length-scale than variations along the wave propagation direction, we derive simplified asymptotic equations from the Green-Naghdi model. For steady flows, we show that the approximate model reduces to a one-dimensional Hamiltonian system along each stream line. Exact solutions describing a wide class of free boundary flows depending on several arbitrary functions of one argument are found. The numerical results showing different patterns of steady three-dimensional waves are presented.

5.1.11. Modeling of spherical waves explosions

Participants: Jacques Massoni, Richard Saurel, A. Lefrancois [DGA Centre d'Etudes de Gramat], G Baudin [DGA Centre d'Etudes de Gramat].

This work [22] deals with the numerical solution and validation of a reactive flow model dedicated to the study of spherical explosions with an aluminized energetic material. Situations related to air blast as well as underwater explosions are examined. Such situations involve multi-scale phenomena associated with the detonation reaction zone, the aluminium reaction zone, the shock propagation distance and the bubble oscillation period. A detonation tracking method is developed in order to avoid the detonation structure computation. An ALE formulation is combined to the detonation tracking method in order to solve the material interface between detonation products and the environment as well as shock propagation. The model and the algorithm are then validated over a wide range of spherical explosions involving several types of explosives, both in air and liquid water environment. Large scale experiments have been done in order to determine the blast wave effects with explosive compositions of variable aluminium content. In all situations the agreement between computed and experimental results is very good.

5.2. Approximation Methods

5.2.1. Mesh adaptation

Keywords: *anisotropic meshes*, *continuous metrics*.

Participants: Frederic Alauzet [Projet Gamma, INRIA-Rocquencourt], Alain Dervieux, Bruno Koobus, Adrien Loseille [Projet Gamma, INRIA-Rocquencourt], Youssef Mesri.

This subject is addressed inside the three projects Gamma (Rocquencourt), Tropics, Smash. An approximative description of each role in this collaboration is as follows: Gamma brings mesh and approximation expertise, Tropics contributes to adjoint methods, Smash works on approximation and CFD applications.
We have mentioned the mesh adaptation action for unsteady interface calculations. The team has continued his reflexion on steady CFD. Smart mesh adaptation for increasing the convergence order of a series of adapted computation. The continuous metric method ([13],[28]) is extensively used. This is the focus of a cooperation with project-team Gamma at INRIA-Rocquencourt (Frédéric Alauzet, Adrien Loseille) for the INRIA contribution to the HISAC IP European project in association with 30 other partners in aeronautics, [35]. Part of this work is also done in the framework of the INRIA ARC LNM "combiner efficacement techniques d'adaptation de maillages et méthodes de lignes de niveaux". http://www-rocq.inria.fr/who/Frederic.Alauzet/arc/content.html

5.2.2. Relaxation-projection method for the Euler equations with real gas EOS

Participants: Richard Saurel, Erwin Franquet, Eric Daniel.

A new projection method [24] is developed for the Euler equations to determine the thermodynamic state in computational cells. It consists in the resolution of a mechanical relaxation problem between the various sub-volumes present in a computational cell. These sub-volumes correspond to the ones traveled by the various waves that produce states with different pressures, velocities, densities and temperatures. Contrarily to Godunov type schemes the relaxed state corresponds to mechanical equilibrium only and remains out of thermal equilibrium. The pressure computation with this relaxation process replaces the use of the conventional equation of state (EOS). A simplified relaxation method is also derived and provides a specific EOS (named the Numerical EOS). The use of the Numerical EOS gives a cure to spurious pressure oscillations that appear at contact discontinuities for fluids governed by real gas EOS. It is then extended to the computation of interface problems separating fluids with different EOS (liquid-gas interface for example) with the Euler equations. The resulting method is very robust, accurate, oscillation free and conservative. For the sake of simplicity and efficiency the method is developed in a Lagrange - Projection context and is validated over exact solutions.

5.2.3. Lagrange method for non-equilibrium multiphase flow models

Participants: Richard Saurel, Jacques Massoni, Francois Renaud.

This work [25] is devoted to the numerical approximation of a hyperbolic non-equilibrium multiphase flow model with several velocities on moving meshes. Such a goal poses several difficulties. The presence of different flow velocities in conjunction with cell velocities poses difficulties for upwinding fluxes. Another issue is related to the presence of non conservative terms. To solve these difficulties the Discrete Equations Method ([1]) is employed and generalized to the context of moving cells. The complementary conservation laws, available for the mixture, are used to determine the velocities of the cells boundaries. With these extensions an accurate and robust multiphase flow method on moving meshes is obtained and validated over several test problems having exact or experimental solutions.

5.3. Solution Algorithms, Parallelism and Grid Computing

5.3.1. Development of multi-grid algorithms on non-structured meshes

Participants: Hervé Guillard, Youssef Mesri, Ales Janka [Ecole Polytechnique Federale de Lausanne (Switzerland)].

The development of efficient multi-grid algorithms on non-structured meshes is a long-term objective of the project. It is considered both with geometrical methods as well as algebraic ones. This year the following works have been be done :

Mesh coarsening for anisotropic non-structured meshes : Multigrid methods needs a hierarchy of meshes able to filter the components of the solution at different levels of resolution. On the other hand the accurate computation of aerodynamical problems including turbulence modeling have to use extremely anisotropic meshes in the boundary layers where the ratio of the mesh size in the direction perpendicular and parallel to the wall can be as small as 10^{-5}. For this type of anisotropic meshes, an efficient use of multi-grid techniques requires a semi-coarsening strategy where the fine grids are progressively coarsened in the direction perpendicular to the wall. In this work, we study such semi-coarsening strategies using the notion of metrics to normalize the mesh size specification. Specifically, at each node of the fine mesh is associated a metric in which the elements are equilateral, then a new metric field is defined corresponding to a semi-coarsening in the direction perpendicular to the wall and a new mesh optimizing this new metric field is generated. This strategy implied to solve difficult problems related to the interpolation and smoothing of a metric field. The current work aims at validating this approach on industrial test cases.

Algebraic Aggregation method : Here [19] we give a convergence estimate for a Petrov-Galerkin Algebraic Multigrid method. In this method, the prolongations are defined using the concept of smoothed aggregation while the restrictions are simple aggregation operators. The analysis is carried out by showing that these methods can be interpreted as variational Ritz-Galerkin ones using modified transfer and smoothing operators. The estimate depends only on a weak approximation property for the aggregation operators. For a scalar second order elliptic problem using linear elements, this assumption is shown to hold using simple geometrical arguments on the aggregates.

5.3.2. Grid-enabled application codes

Participants: Alain Dervieux, Bruno Koobus, Steve Wornom, David Rey, Thibaud Kloczko, Hervé Guillard.

In the context of the MecaGRID initiative, (http://www-sop.inria.fr/smash/mecagrid/public/mainFrame.htm). the SMASH team has developed a set of computational tools for demonstrations in Grid Computing. The central kernel is a CFD code derived from the synthesis of research developed by the SMASH Team in collaboration with the University of Colorado at Boulder. This code have been also used on the parallel SGI O3800 of CINES and is now used in the context of the GRID-5000@sophia initiative . See [20] for a recent publication. This code executes in parallel using MPI and is naturally suited for MPI Grid computing. However, the absence of dynamic memory allocation penalizes FORTRAN 77 codes in an environment made of heterogeneous computing resources. A re-writing of the code using FORTRAN 95 has therefore been performed and has shown significant improvment on the previous version of the code. Preliminary experiments with up to 256 processors and unstructured meshes of 10 Millions of elements have been performed.

6. Contracts and Grants with Industry

6.1. Modeling of bubbly flows

Participants: Hervé Guillard, Roxanna Panescu.

In the framework of a preliminary program to study convective pattern in bubbly flows, IRSN and SMASH have engaged a common initiative for the numerical modeling of bubbly flows.

6.2. Level-Set software

Participants: Alain Dervieux, Anne-Cécile Lesage.

The subject of this partnership with the technological company LEMMA is to develop a level-set based multi-fluid software for applications in the aerospace industry.

6.3. Multiphase Algorithms for high energy material

Participants: Jacques Massoni, Richard Saurel, Olivier Le Metayer, Eric Daniel.

This study realized with the support of DGA, deals with the development of multiphase algorithms to compute the dispersion of a multiphase mixture in air and its interaction with detonation products.

6.4. Coarsening Algorithms for Multi-grid applications

Participants: Hervé Guillard, Youssef Mesri.

This contract with Dassault-Aviation supports a 18 month study devoted to the design of semi-coarsening algorithms for 3-D anisotropic meshes for multi-grid applications.

6.5. Modeling of nano-structured explosives

Participants: Richard Saurel, Eric Daniel, Sergey Gavrilyuk, Olivier Le Metayer, Erwin Franquet, Jacques Massoni.

This work supported by DGA addresses the modeling of the micro-scale physics in nano-structured explosives.

6.6. Modeling heterogeneous explosions and particles dispersion

Participants: Richard Saurel, Eric Daniel, Sergey Gavrilyuk, Olivier Le Metayer, Erwin Franquet, Jacques Massoni.

This project with DGA is aimed to model particles bed compaction and dispersion under shock waves. When dispersion and mixing with air is obtained, ignition and reaction of the mixture may occur.

6.7. Modeling of heterogeneous compressible flows

Participants: Richard Saurel, Olivier Le Metayer.

This project with Airbus is aimed to model a high gas flow into a complex medium for which it is not possible to solve 2D or 3D gas dynamics equations. A homogeneous model is built as well as an appropriate numerical method.

6.8. Dust-Gas flow modeling in ITER

Participants: Hervé Guillard, Thibaud Kloczko.

This contract with CEA - Saclay supports the post-doctoral contract of Thibaud Kloczko and is devoted to the modeling of dust-gas flows for security application in nuclear fusion reactors.

7. Other Grants and Activities

7.1. National and Regional initiatives

7.1.1. ANR Calcul intensif et Grilles de calcul

Participants: Hervé Guillard, Youssef Mesri.

The project is part of the three-year DiscoGrid project that have been selected by ANR in the 2005 call for projects of the program *Calcul intensif et Grilles de calcul*. In this project, following the works done in the MECAGRID (http://www-sop.inria.fr/smash/mecagrid/public/mainFrame.htm) project, the team studies mesh partitioning for heterogeneous computing architectures and the design of parallel numerical algorithms to efficiently exploit a computational grid.

7.1.2. ARC LMN

The ARC LMN *Combiner efficacement techniques d'adaptation de maillages et méthodes de lignes de niveaux* gathers researchers from INRIA (team-projects Gamma and Smash), University Paris VI (Laboratoire Jacques Louis Lions), Orsay University (Math Dpt) and CNAM (Math Dpt). It aims at studying the coupling of level set methods and mesh adaptation for efficient multi-fluid computations.

7.2. Bilateral international relation

- Collaboration with the University of Pisa

  Initiated through a support program of the "Conseil regional de la région PACA" in 2005, the collaboration with the University of Pisa on turbulence modeling and the development of numerical models for two-phase flows is going on.
- Scientific exchanges with IMM-Moscow (I. Abalakin, T. Kozubskaya) continue with common communications and papers on Acoustics.
- French-German collaboration DFG/CNRS: Micro and macro modeling and simulation of liquid - vapor flows (FOR 563). This collaboration aims to improve two-phase flows models and associated numerical methods. French participants: F. Coquel, T. Gallouet, P. Helluy, J.M. Hérard, P. Josserand, S. Zaleski, R. Abgrall, C. Berthon, B. Nkonga, R. Saurel, S. Benzoni-Gavage, D. Jamet, A. Dervieux, P. Le Floch, V. Perrier. German Participants: C. Rohde, Ohlberger, S. Muller, Ballman, Lauterborn, Kurz, N. Peters, Binninger, Warnecke, D. Kroner, W. Dreyer, M. Hermann, J. Haink, C. Kraus, R. Dahms, M. Ferch, C. Merkle.

- A scientific collaboration with North Dakota University (IAkhatov) on multifluid modeling have been initiated.

8. Dissemination

8.1. Teaching

In the academic year 2005-2006, project members have taught the following courses :

Olivier Le Metayer : University of Provence : 192 h, First and second years and third years of engineering school.

Sergey Gavrilyuk : Univ Aix Marseille 3 192h First year of Mastere M1 “Mecanique physique et modelisation” and second year of Mastere M2 “Energetique et combustion’.

Eric Daniel : University of Provence : 20h in Mastere 2 “Energetique et combustion”

Jacques Massoni : University of Provence : 192 h, First and second years and third years of engineering school. “Scientific computations” course

Richard Saurel : University of Provence : 100h, Second year of engineering school and mastère. Richard Saurel is also director of the Mastère “Energétique et Combustion”.

8.2. Ph. D thesis and Masters Thesis

This year, the project has harbored the following Ph. D Students :

ROXANNA PANESCU University of Nice-Sophia-Antipolis, "Méthodes de volumes-Eléments finis pour les écoulements de liquides à bulles"

ANNE-CÉCILE LESAGE University of Nice-Sophia-Antipolis, “Méthodes Level Set pour les écoulements bi-fluides incompressibles avec tension de surface et angle de contact sur maillages non-structurés”

OLIVIER BASSET ENSMP, "Simulation numérique d’écoulements diphasiques sur grille de calcul"

YOUSSEF MESRI, University of Nice-Sophia-Antipolis,"Adaptation for anisotropic non-structured meshes"

ERWIN FRANQUET, University of Provence, "Modeling of nano-structured explosives"

MATHIEU LABOIS, University of Provence, "Développement de modèles diphasiques à sept équations"

DAMIEN GUEGAN, University of Nice-Sophia-Antipolis, "Modèles pour les fluides capillaires en faible gravité"

The following masters thesis have taken place :

NICHOLAS FAVRIE

FABIEN PETIPAS

FLORENT GUIGNERY "Simulation directe d’écoulements multiphasiques hétérogènes par des approches euleriennes: détermination de polaires de choc d’alliages" Stage de Master 2, de l’Université de Provence, Master "Mécanique, Physique et Modélisation", Spécialité Energétique et Combustion.

8.3. Conferences and workshops

Members of the team have delivered lectures in the following conferences and seminars (see the bibliography) :

- R. Saurel, Séminaire CEA-GAMNI-SMAI Mécanique des Fluides Numérique le 30/01/2006 "Méthode de projection relaxation pour les écoulements compressibles, monophasiques et diphasiques"
- R. Saurel, Invited conference in the mini symposium Multiphase flows. Eleventh International Conference on Numerical Combustion, SIAM Numerical Combustion, April 23-26, Granada, Spain. "Multiphase shocks and related numerical methods".
- H. Guillard, Seminar at University of Nice Sophia-Antipolis
- H. Guillard, Key-notes lecture in the mini-symposium "Computational methods for compressible two-fluid flows", ECCOMAS CFD Conference, September 2006, The Netherlands.
- A-C. Lesage, , "Incompressible multi-fluid problems", ECCOMAS CFD Conference, September 2006, The Netherlands.

9. Bibliography

Major publications by the team in recent years

[1] R. ABGRALL, R. SAUREL. *Discrete equations for physical and numerical compressible multiphase mixtures*, in "J. Computational. Phys.", vol. 186 No 2, 2003, p. 361-396.

[2] S. CAMARRI, M. SALVETTI, B. KOOBUS, A. DERVIEUX. *A low-diffusion MUSCL scheme for LES on unstructured grids*, in "Computers and Fluids", vol. 33, n^{o} 9, 2004, p. 1101-1129.

[3] A. CHINNAYYA, E. DANIEL, R. SAUREL. *Computation of detonation waves in heterogeneous energetic materials*, in "J. of Computational Physics", vol. 196, 2004, p. 490-538.

[4] H. GUILLARD, A. MURRONE. *On the behavior of upwind schemes in the low Mach number limit : II. Godunov type schemes*, in "Computers and Fluids", vol. 33, n^{o} 4, 2004, p. 655-675.

[5] H. GUILLARD, C. VIOZAT. *On the behaviour of upwind schemes in the low Mach number limit*, in "Comput. Fluids", vol. 28, 1999, p. 63-86.

[6] B. KOOBUS, M.-H. LALLEMAND, A. DERVIEUX. *Agglomeration multigrid for two-dimensional viscous flows*, in "Int. J. Numer. Meth. Fluids", vol. 18, 1994, p. 27-42.

[7] R. SAUREL, R. ABGRALL. *A Multiphase Godunov method for compressible Multifluid and Multiphase flows*, in "J. Compu. Phys.", vol. 150, 1999, p. 1-43.

Year Publications

Doctoral dissertations and Habilitation theses

[8] O. BASSET. *Simulation numérique d'écoulements multifluide sur grille de calcul*, Ph. D. Thesis, Ecole des Mines de Paris, 2006.

[9] E. FRANQUET. , Ph. D. Thesis, University of Provence, 2006.

[10] A. LESAGE. *Méthodes Level Set pour les écoulements bi-fluides incompressibles avec tension de surface et angle de contact sur maillages non-structurés*, Ph. D. Thesis, University of Nice Sophia-Antipolis, 2006.

[11] R. PANESCU. *Modélisation Eulerienne d'écoulements diphasiques à phase dispersée et simulation numérique par une méthode volumes-éléments finis*, Ph. D. Thesis, University of Nice Sophia-Antipolis, 2006.

Articles in refereed journals and book chapters

[12] P.-H. COURNEDE, B. KOOBUS, A. DERVIEUX. *Positivity statements for a Mixed-Element-Volume scheme on fixed and moving grids*, in "Revue Européenne de Mécanique Numérique", vol. 15:7-8, 2006, p. 767-799.

[13] F. COURTY, D. LESERVOISIER, P.-L. GEORGE, A. DERVIEUX. *Continuous metrics and mesh optimization*, in "Applied Numerical Mathematics", vol. 56, n$^{\text{o}}$ 2, 2006.

[14] S. GAVRILYUK, I. AKHATOV. *Model of a liquid nanofilm on a solid substrate based on the van der Waals concept of capillarity*, in "Physical Review E", vol. 73, 2006.

[15] S. L. GAVRILYUK, R. SAUREL. *Estimation of the turbulent energy production across a shock wave*, in "Journal of Fluid Mechanics", vol. 549, 2006, p. 131–139.

[16] S. L. GAVRILYUK, R. SAUREL. *Rankine-Hugoniot relations for shocks in heterogeneous mixtures*, in "Journal of Fluid Mechanics", to appear, 2006.

[17] H. GOUIN, S. L. GAVRILYUK. *Dissipative two-fluid models*, in "Rendiconti del Circolo Matematico di Palermo", vol. series II, No 78, 2006, p. 133–145.

[18] H. GUILLARD. *Recent developments in the computation of compressible low Mach number flows*, in "Flow, Turbulence and Combustion", vol. 76, 2006, p. 363–369, http://dx.doi.org/10.1007/s10494-006-9024-8.

[19] H. GUILLARD, A. JANKA, P. VANEK. *Analysis of an Algebraic Petrov-Galerkin Smoothed Aggregation Multigrid Method*, in "Applied Numerical Mathematics", to appear, 2006.

[20] B. KOOBUS, S. CAMARRI, M. SALVETTI, S. WORNOM, A. DERVIEUX. *Parallel simulation of three-dimensional flows: application to turbulent wakes and two-phase compressible flows*, in "Advances in Engineering Software", to appear, 2006.

[21] O. LE METAYER, R. SAUREL. *Compressible exact solutions for one-dimensional laser ablation fronts ICF*, in "Journal of Fluid Mechanics", vol. 561, 2006, p. 465–475.

[22] J. MASSONI, R. SAUREL, A. LEFRANCOIS, G. BAUDIN. *Modeling spherical explosions with aluminized energetic materials*, in "Int. J of Shock waves", to appear, 2006.

[23] V. S. NIKOLAYEV, S. L. GAVRILYUK, H. GOUIN. *Modeling of the moving deformed triple contact line: influence of the fluid inertia*, in "Journal of Colloid and Interface Science", vol. 302, 2006, p. 605–612.

[24] R. SAUREL, E. FRANQUET, E. DANIEL. *A relaxation-projection method for compressible flows. Part I : The numerical equation of state for the Euler equations*, in "Journal of Computational Physics", to appear, 2006.

[25] R. SAUREL, J. MASSONI, F. RENAUD. *A Lagrangian numerical method for compressible multiphase flows*, in "Int. J. Numerical Methods in Fluids", to appear, 2006.

[26] R. SAUREL, O. LE METAYER, J. MASSONI, S. GAVRILYUK. *Shock jump relations for multiphase mixtures with stiff mechanical relaxation*, in "Shock Waves", to appear, 2006.

[27] V.M. TESHUKOV, S. L. GAVRILYUK. *Three-dimensional nonlinear dispersive waves on shear flows*, in "Studies in Applied Mathematics", vol. 116, 2006, p. 241–255.

Publications in Conferences and Workshops

[28] F. ALAUZET, A. LOSEILLE, A. DERVIEUX, P. FREY. *Multi-dimensional continuous metric for mesh adaptation*, in "Proc. 15th International Meshing Roundtable, Birmingham, AL, USA, 2006", 2006.

[29] Y. BENTALEB, E. SCHALL, B. KOOBUS, A. DERVIEUX, M. AMARA. *A Numerical Method for Simulating turbulent shear flows with low-Reynolds k-eps models*, in "9th Conference of Applied Mathematics and Statistics, Jaca, Spain, september 19-21, 2005. Monografias del Seminario Matematico García del Galdeano", 2006.

[30] H. GUILLARD, M. LABOIS. *Numerical modelling of compressible two-phase flows*, in "European Conference on Computational Fluid Dynamics ECCOMAS CFD 2006", 2006.

[31] A.-C. LESAGE, A. DERVIEUX, O. ALLAIN. *A local mass conservation Method for the Level Set Method applied to capillary incompressible flow*, in "European Conference on Computational Fluid Dynamics ECCOMAS CFD 2006", 2006.

[32] K. E. OMARI, E. SCHALL, B. KOOBUS, A. DERVIEUX, M. AMARA, J.-P. DUMAS. *Fluid-structure coupling of a turbulent flow and a generic blimp structure at hight angle of attack*, in "9th Conference of Applied Mathematics and Statistics, Jaca, Spain, september 19-21, 2005. Monografias del Seminario Matematico García del Galdeano", 2006.

[33] M. SALVETTI, S. CAMARRI, B. KOOBUS, A. DERVIEUX. *A locally superconvergent scheme for the simulation of turbulent flows in complex geometries*, in "ICCFD4, The Fourth International Conference on Computational Fluid Dynamics, Ghent, Belgium, July 10-14", 2006.

[34] S. SIRNIVAS, S. WORNOM, A. DERVIEUX, B. KOOBUS, O. ALLAIN. *A study of LES models for the simulation of a turbulent flow around a truss spar geometry, OMAE2006-92355*, in "Proceedings of OMAE'06, 25th International Conference on Offshore and Arctic Engineering, 4-9 June, 2006, Hamburg, Germany", 2006.

Internal Reports

[35] F. ALAUZET, A. LOSEILLE, A. DERVIEUX. *Mesh adaptation for Sonic Boom*, HISAC 18th Month 2.2 Report, 10 2006.

[36] G. PAGANO, S. CAMARRI, M.-V. SALVETTI, B. KOOBUS, A. DERVIEUX. *Strategies for RANS/VMS-LES coupling*, Research Report, n^o 5954, INRIA, 07 2006, https://hal.inria.fr/inria-00088040.

References in notes

[37] R. ABGRALL. *How to prevent pressure oscillations in multicomponent flow calculations: A quasi-conservative approach*, in "Journal of Computational physics", vol. 125, 1996, p. 150-160.

[38] D. A. DREW, S. PASSMAN. *Theory of Multicomponent Fluids*, Springer, New-York, 1998.

[39] R. EYMARD, T. GALLOUET, R. HERBIN. *Finite Volume Methods, Handbook for numerical analysis,Vol. VII,*, Springer, 1999.

[40] S. INABA, P. BARGE, E. DANIEL, H. GUILLARD. *A two-phase code for protoplanetary disks*, in "Astronomy & Astrophysics", vol. 431, n^{o} 1, 2005, p. 365-379.

[41] A. MURRONE, H. GUILLARD. *A five equation reduced model for compressible two-phase flow computations*, in "J. Comput. Phys.", vol. 202 No 2, 2005, p. 664-698.

[42] L. SCHWARTZ. *Sur l'impossibilité de la multiplication des distributions*, in "C.R.A.S. Paris", vol. I-239, 1954, p. 847-848.

[43] D. SERRE. *Sur le principe variationnel des équations de la mécanique des fluides compressibles*, in "M2AN", vol. 27, No 6, 1993, p. 739-758.

[44] E. TORO. *Riemann solvers and numerical methods for fluid dynamics*, Springer-Verlag, Berlin, 1997.