INRIA

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

Project-Team Smash

Simulation, Modeling and Analysis of Heterogeneous Systems in Continuum Mechanics

Sophia Antipolis - Méditerranée

THEME NUM

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SMASH *is a common project between INRIA–Sophia Antipolis–Méditerranée, and Aix-Marseille University. Its main topic is related to the mathematical and numerical modeling of heterogeneous flows such as multiphase media, granular materials and interface problems.*

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2. Overall Objectives

2.1. Presentation

SMASH is a common project between INRIA and Aix-Marseille University. Its main topic is related to the mathematical and numerical modeling of heterogeneous flows such as multiphase media, granular materials and interface problems.

The first issue deals with the *design* and *improvements* of *theoretical models* for these flows. Particular attention is paid to *well posedness* issues and *systems' hyperbolicity*.

The second issue deals with the *design* of *appropriate numerical schemes*. These models are not well known as conventional single fluid models and pose numerical challenges such as, for example, the numerical approximation of *non–conservative terms*. These numerical issues pose *theoretical* ones such as, *shock wave existence in multiphase mixture*, *cell averages of non–conservative variables*, *Chapman–Jouguet detonation conditions for heterogenous explosives* etc.

The final aim is to *implement* the resulting algorithms on *parallel machines* for solving *large scale problems* for the design of advanced technology systems in Space, Defense and Nuclear energy.

One of the main original features of the SMASH researches on heterogeneous flows lies in the way we deal with multiphase mixtures. Our aim is to solve the *same equations* everywhere with the *same numerical* method :

- in pure fluid,
- in multi-velocity mixtures,
- in artificial smearing zones at material interfaces or in mixture cells,
- in shocks, phase transition fronts, detonation waves,
- in elastic-plastic materials.

An example of such computations is given in the Figure 1.

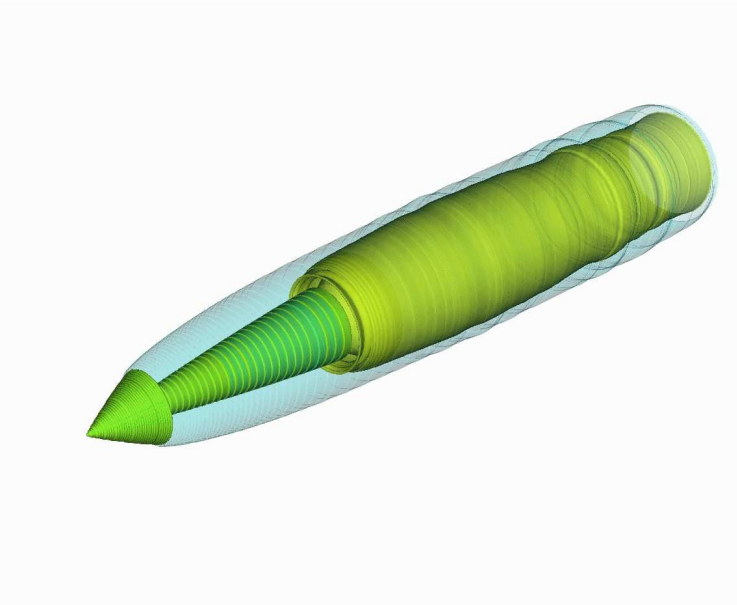

Figure 1. Numerical simulation of an underwater missile flying at 600 m/s. Three fluids are present : liquid water, steam and propulsion gases. Two different types of interfaces are present: A contact interface separates steam and combustion gases while an evaporating interface separates metastable expanded liquid and steam. To deal with metastable phase transition, the novel approach of [26] is used. The numerical approximation of the non-conservative hyperbolic system with stiff relaxation is achieved by the method of [27].

There are some advantages with this approach :

- the most obvious relies in the *coding simplicity* and *robustness* as a *unique algorithm* is used;
- *conservation principles* are guarantied *for the mixture*. Conventional algorithms are able to preserve mass conservation only when dealing with interfaces;
- *interface conditions are perfectly matched* even for the coupling of complex media (granular flows, capillary fluids, transition fronts) even in the presence of *shocks*;
- this approach is the *only one able to deal with dynamic appearance of interfaces* (cavitation, spallation);
- our methods allow the *coupling of multi-velocities, multi-temperatures mixtures* to macroscopic interfaces where a single velocity must be present. To illustrate this capability consider the example of a cloud of bubbles rising up in a liquid to the surface, where a free boundary is present. Two velocities have to be considered for the bubbles rising, while a single velocity must be present just after their crossing through the interface. This is also the only method able to deal with such situations.

Our approach rises increasing attention from the *scientific community* as well as *the industry*. As will be detailed further, many projects are currently under development with french oriented research centers (DGA, CNES, SNECMA) as well as foreign ones (Idaho National Laboratory - USA, General Electrics, USA).

3. Scientific Foundations

3.1. Modeling of Multiphase Media

Keywords: *Discrete Homogenization Method (DHM)*, *Hamilton Principle*, *Hyperbolic Models*.

Conventional models of two-phase mixtures having several velocities present under the form of partial differential systems with six equations: two mass, two momentum and two energy equations. These models are not hyperbolic and are consequently ill posed. It means that initial data and boundary conditions do not fully determine the solution at the next instant. In other words, wave propagation may have no physical sense, as the square sound speed may become negative.

This issue has been understood by [68] and subtle remedy was given by [42]. They proposed an extended model with seven equations. The extra differential equation replaced the pressure equilibrium assumption in the mixture. Thanks to this new equation, the model was correctly posed, unconditionnaly hyperbolic.

This model had little diffusion as it was presented in the context of a specific problem of detonation physics. Also, the model was difficult to solve at the numerical level, in particular with modern algorithms based on the Riemann problem solution. In [63] we developed the first Godunov type method for this model and derived accurate approximation formulas for the non-conservative terms. Moreover, a specific relaxation method was built in order to solve these equations in the presence of stiff relaxation terms. This issue was particularly important as,

- this model was involving two pressure and two velocities,
- at an interface the jump condition corresponds to continuous normal velocities and continuous pressures,
- in order to fulfill this condition it was necessary to relax the two pressures and velocities to unique equilibrium variables.

Such an issue was reached by using specific relaxation solvers, with infinite relaxation parameters like in [57]. With this solver, the model was able to solve interface problems (air/water for example) and multiphase mixtures with two velocities. Important applications of fundamental and applied physics were possible to solve. Financial supports from DGA and CEA helped us to pursue the investigations.

Denoting $p_r = p_1 - p_2$, $u_r = u_1 - u_2$, the two-phase flow model presents under the form (1) :

$$\begin{aligned}
&\frac{\partial \alpha_1}{\partial t} + u_I \frac{\partial \alpha_1}{\partial x} = \mu\, p_r \ , \\
&\frac{\partial \alpha_1 \rho_1}{\partial t} + \frac{\partial (\alpha_1 \rho_1 u_1)}{\partial x} = 0 \ , \\
&\frac{\partial \alpha_1 \rho_1 u_1}{\partial t} + \frac{\partial (\alpha_1 \rho_1 u_1^2 + \alpha_1 p_1)}{\partial x} = p_I \frac{\partial \alpha_1}{\partial x} - \lambda\, u_r \ , \\
&\frac{\partial \alpha_1 \rho_1 E_1}{\partial t} + \frac{\partial (\alpha_1 \rho_1 E_1 u_1 + \alpha_1 p_1 u_1)}{\partial x} = p_I\, u_I \frac{\partial \alpha_1}{\partial x} - \mu\, p_I^{'}\, p_r - \lambda\, u_I^{'}\, u_r \ .
\end{aligned} \tag{1}$$

The equations for phase 1 only are written, those of phase 2 being symmetric. General closure relations for this system need :

- the interface velocity u_I and pressure p_I that respectively represent the velocity and pressure that exert at the boundary of a cloud of bubbles or dropplets,
- the average interface velocity $u_I^{'}$ and pressure $p_I^{'}$ that exert in the bulk of a two-phase control volume,
- the relaxation parameters λ and μ that control the rate at which velocities and pressures relax to mechanical equilibrium respectively.

These relations were unknown, estimated in limit cases only, or determined by experimental means. In order to determine these closure relations a new homogenization method has been built in [1].

This new averaging method considers the mixture at the discrete level, with a stencil composed of three computational cells. In each cell, at each cell boundary and at each internal boundary separating the phases, the Riemann problem (RP) is solved. The RP solution provides all local interfacial information. These RP solutions are then averaged in the computational cell as done originally with the first version of the Godunov method, derived originally for the Euler equations. In our context, extra difficulties appear, due to the presence of internal material interfaces, material discontinuities at cell boundaries and variable sub-volumes, due to the phase presence in the cells. But the philosophy was the same as with the Godunov method : we are dealing with average RP solutions and not by discretized partial differential equations.

The resulting system of this averaging procedure is a quite complicated discrete system in algebraic form. It corresponds to the result of the Discrete Equations Method (DEM). The closure relations for the various interface variables have been obtained by reaching the continuous limit of these discrete equations [10], [44] that provide information easier to interprete than discrete formulas.

With this strong modeling foundations, it was possible to consider problems with extended physics : turbulence, phase transition, ions and electrons in plasmas mixtures, granular materials, chemical reactions, continuum media with elastic-plastic effects. An example is shown in the Figures 2-3.

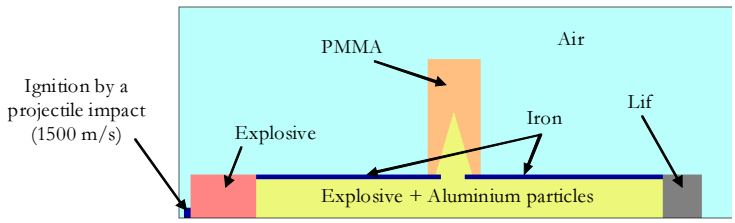

Figure 2. A steel tube is filled with a heterogenous explosive. A high velocity impactor creates a shock wave transmitted to the explosive, that becomes a detonation wave.

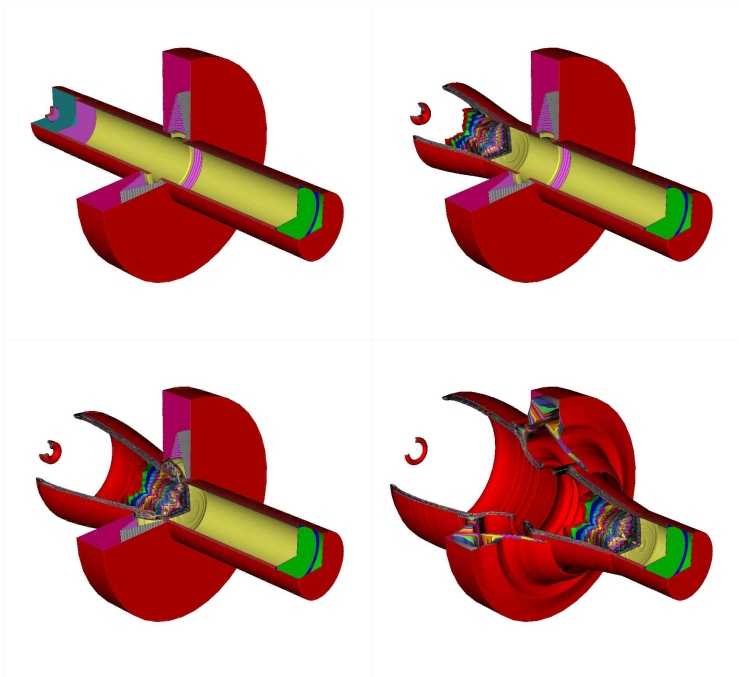

Figure 3. After a short period of time the shock wave becomes a detonation wave that produces gas and solid products at very high pressure. They set into intense motion solid tube walls. Two different types of mixture are present in this type of application : a physical one, corresponding to the mixture of gases and solid particles during the detonation dynamics, and artificial mixtures, corresponding to the ones that appear at material interfaces, here at the gas - steel tube boundary. Both types of mixture are solved by the same equations and the same numerical algorithm [27]. Moreover, the detonation dynamics is checked against generalized CJ solutions [23], specifically determined for this temperature non-equilibrium model.

Most of these extensions are done with the help of the Hamilton principle of least action [66], [3] to develop appropriate single phase material models that are then coupled with the DEM to form a multiphase flow model.

3.2. Modeling of Interface and Multi-Fluid Problems

Keywords: *Diffuse Interface*, *Eulerian Models*, *Front Capturing*, *Mixture Cells*, *Multi-Fluid Mixtures*.

In order to solve interfaces separating pure fluids or pure materials, two approaches have been developed. The first one has been described previously. It consits in solving a non-equilibrium flow model with two pressures and two velocities, and then relax instantaneously these variables to equilibrium ones. Such a method allows a perfect fulfillment of interface conditions in mixture cells, that appear as a result of numerical diffusion at material interfaces.

The second option consists in determining the *asymptotic model* that results from stiff mechanical relation. In the context of two fluids, it consists in a set of five partial differential equations [54], [4] : two masses, one mixture momentum, one mixture energy and one volume fraction equations. Such a system is obviously less general than the previous non-equilibrium system, but it is particularly interesting in solving interface problems, where a single velocity is present. More precisely, it is more appropriate and simpler, when considering extra physics extensions such as, phase transition, capillary effects, elastic-plastic effects.

Contrarily to conventional methods, there is no need to use a front tracking method, nor level set [46], nor interface reconstruction and so on. The interface is solved as any point of the flow [55], [56] with the 5 equations model. This model provides correct thermodynamic variables in artificial mixture zones. Although seemingly artificial, this model can handle huge density ratio, and materials governed by very different equations of state, in multi-dimensions. It is also able to describe multiphase mixtures where stiff mechanical relaxation effects are present, such as, for example, reactive powders, solid alloys, composite materials etc.

Several extentions have been done during these recent years by the SMASH team :

- a model involving *capillary*, *compressibility* and *viscous effects* [60]. This is the first time such effects are introduced in a hyperbolic model. Validations with experiments done at IUSTI (the laboratory where the group of Marseille is located) have shown its excellent accuracy, as shown in the Figure 4;
- *phase transition* in *metastable liquids* [26]. This is the first time a model solves the ill-posedness problem of spinodal zone in van der Waals fluids.

The combination of capillary and phase transition effects is under study in order to build a model to perform direct numerical simulation (DNS) of phase transition at interfaces, to study explosive evaporation of liquid drops, or bubble growth in severe heat flux conditions. This topic has important applications in *nuclear engineering* and *future reactors* (ITER for example). A collaboration is starting with the Idaho National Laboratory, General Electrics, and MIT (USA) in order to build codes and experiments on the basis of our models and numerical methods. In another application domain, extra support is coming form CNES and SNECMA to model phase transition in the Ariane V space launcher cryogenic engine.

In the presence of shocks, fundamental difficulties appear with multiphase flow modeling. Indeed, the volume fraction equation (or its variants) cannot be written under divergence form. It is thus necessary to determine appropriate jump relations.

In the limit of *weak* shocks, such relations have been determined by analysing the dispersive character of the shock structure in [64], [49] and [48]. Contrarily to single phase shocks, backward information is able to cross over the shock front in multiphase flows. Such phenomenon renders the shocks smooth enough so that analytical integration of the energy equations is possible. They provide the missing jump condition.

These shock conditions have been validated against all experimental data available in the various American and Russian databases, for *weak* and *very strong* shocks.

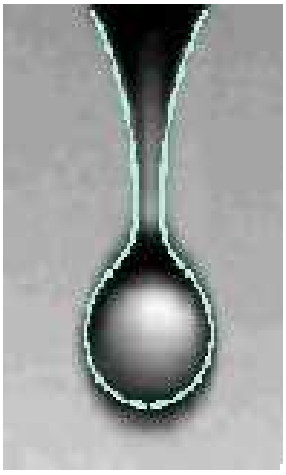

Figure 4. Comparison of the drop shape during formation. No interface tracking nor interface reconstruction method are used. The same equations are solved at each mesh point. The model accounts for compressible, viscous and capillary effects. The compressible effects are negligible in the present situation, but they become fundamental in other situations (phase transition for example) where the full thermodynamics of each fluid is mandatory. The method treats in a routinely manner both merging and fragmentation.

At this point, the theory of multiphase mixtures with single velocity was closed. Thanks to these ingredients we have done important extensions during the present year :

- *restoration of drift effects* : a dissipative one-pressure, one-velocity model has been studied in [13], and implemented in a parallel, three-dimensional code [32]. This model is able to reproduce phase separation and other complex phenomena [30];
- extending the approach to deal with *fluid-structure interactions*. A non-linear elastic model for compressible materials has been built [18]. It extends the preceding approach of Godunov to describe continuum media with conservative hyperbolic models. When embedded in our multiphase framework, fluid solid interactions are possible to solve in highly non-linear conditions with a single system of partial differential equations and a single algorithm. This is the aim of Nicolas Favrie's PhD thesis [11] and [17];
- determining the *Chapman–Jouguet conditions* for the detonation of *multiphase explosives*. The single velocity - single pressure model involves several temperatures and can be used to describe the non-equilibrium detonation reaction zone of condensed heterogenous energetic materials. Since the work of Zeldovich-Neumann and Doering (ZND model), the detonation dynamics of gaseous and condensed energetic materials is described by the ZND approach, assuming mixtures in thermal equilibrium. However, in condensed energetic materials, the mixture is not of molecular type and the thermal equilibrium assumption fails. With the help of the same model used for phase transition [26], closed by appropriate shock conditions [64], it is now possible to develop a ZND type model with temperature disequilibrium. This opens a new theory for the detonation of condensed materials. Successful computations of multidimensional detonation waves in heterogenous explosives have been done with an appropriate algorithm in [23].

Obviously, all these models are very different from the well studied gas dynamics equations and hyperbolic systems of conservation laws. The building of numerical schemes requires special attention as detailed hereafter.

3.3. Approximation methods

Keywords: *Discrete Equations Methods*, *Finite Volume Methods*, *Relaxation Methods*, *Riemann Solvers*.

All the mathematical models considered and studied in SMASH consist in hyperbolic systems of PDE's. Most of the attention is focused on the 7 equations model for non-equilibrium mixtures and the 5 equations model for mechanical equilibrium mixtures. The main difficulty with these models is that they cannot be written under divergence form. Obviously, the conservation principles and the entropy inequality are fulfilled, but some equations (the volume fraction equation for example) cannot be cast under conservative form. From a theoretical point of view, it is known since the works of Schwartz [65] 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 [45], [53]. Aware of this difficulty, we have developed two specific methods to solve such systems.

The first one is the discrete equations method (DEM) presented previously as a new homogenization method. It is also a numerical method that solves non-conservative products for the 7 equations model in the presence of shocks. With this method, Riemann problem solutions are averaged in each sub-volume corresponding to the phase volumes in a given computational cell. When a shock propagates inside a cell, each interaction with an interface, corresponds to the location where non-conservative products are undefined. However, at each interaction, a diffraction process appears. The shock discontinuity splits in several waves : a left facing reflected wave, a right facing transmitted wave and a contact wave. The interface position now corresponds to the one of the contact wave. Along its trajectory, the velocity and pressure are now continuous : this is a direct consequence of the diffraction process. The non-conservative products that appear in these equations are precisely those that involve velocity, pressure and characteristic function gradient. The characteristic function gradient remains discontinuous at each interface (it corresponds to the normal) but the other variables are now continuous. Corresponding non-conservative products are consequently perfectly defined : they correspond to the local solution of the Riemann problem with an incoming shock as initial data. This method has been successfully developed and validated in many applications [1], [10], [7], [44].

The second numerical method deals with the numerical approximation of the five equations model. Thanks to the shock relations previously determined, there is no difficulty to solve the Riemann problem. However, the next step is to average (or to project) the solution on the computational cell. Such a projection is not trivial when dealing with a non-conservative variable. For example, it is well known that pressure or temperature volume average has no physical sense. The same remark holds for the *cell average* of volume fraction and internal energy. To circumvent this difficulty a new relaxation method has been built [27]. This method uses *two main ideas*.

The first one is to *transform* one of the *non-conservative products* by a *relaxation term*. This is possible with the volume fraction equation, where the non conservative term corresponds to the asymptotic limit of a pressure relaxation term. Then, a splitting method is used to solve the corresponding volume fraction equation. During the hyperbolic step, there is no difficulty to derive a positivity preserving transport scheme. During the stiff relaxation step, following preceding analysis of pressure relaxation solvers [57], there is no difficulty to derive entropy preserving and positive relaxation solvers.

The second idea deals with the *management of the phase's energy equations*, that also present under *non-conservative form*. These equations are able to compute regular solutions, like expansion waves, but are inaccurate for shocks. They will be used at shocks to predict the solution only. With the predicted internal energies, phase's pressures are computed and then *relaxed to equilibrium*. It results in an *approximation* of the volume fraction at shocks. This approximation is then used in the *mixture equation of state*, that is unambiguously determined. This equation of state is based on the *mixture energy*, a supplementary equation. This equation, apparently redundant has to be fulfiled. Its numerical approximation is obvious even in the presence of shocks as it is a conservation law. With the help of the mixture energy and predicted volume fraction, the *mixture pressure* is now computed, closing the system. This treatment guarantees *correct*, *convergent* and *conservative wave transmission* across material interfaces separating pure media. When the interface separates a fluid and a mixture of materials, the correct partition of energies among phases is fulfiled

by replacing at the shock front the internal energy equations by their corresponding jumps [64]. To ensure the numerical solution strictly follows the phase's Hugoniot curves, the poles of these curves are transported [23]. With this treatment, the method also converges for multiphase shocks.

This method is very *efficient* and *simple to implement*. This also helped us considerably to solve very large systems of hyperbolic equations, like those of elastic materials in large deformations. The fluid-solid coupling via diffuse interfaces with extreme density ratios was done efficiently, as shown in Figure 5.

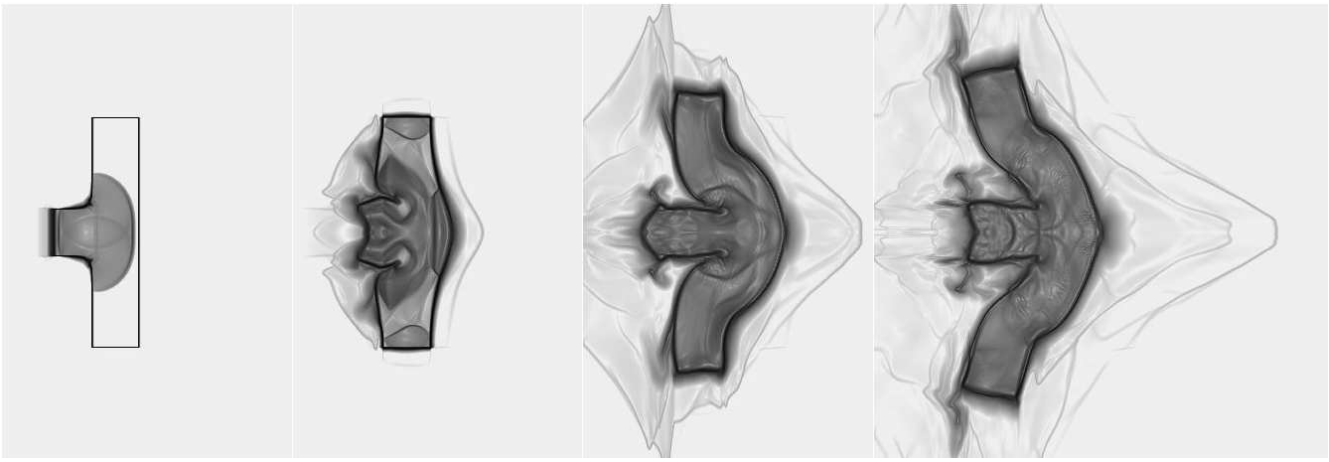

Figure 5. A copper projectile impacts a copper plate at the velocity of 800 m/s. Both materials are considered compressible and elastic, and are surrounded by air at atmospheric pressure.

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 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

About 15 years ago, working on the physics of detonation waves in highly energetic materials, we discovered a domain where flow conditions were extreme. Numerical simulations in detonation conditions were a true challenge. The mathematical models as well as numerical methods must be particularly well built. The presence of material interfaces was posing considerable difficulties.

During the years 90–95, we have investigated open and classified litterature in the domain of multimaterial shock-detonation physics codes. We came to the conclusion that nothing was clear regarding *mixture cells*. These *mixture cells* are a consequence of the numerical diffusion or cell projection of flow variables at contact discontinuites.

Thus, we have developed our own approach. On the basis of multiphase flow theory, revisited for a correct treatment of waves dynamics, we have proposed to solve mixture cells as true multiphase mixtures. These mixtures, initially out of equilibrium, were going to relax to mechanical equilibrium with a single pressure and velocity.

From this starting point, many extensions have been done, most times initiated by applications connected to the Defense domain. Collaborations have never stopped with these specialized laboratories since 1993. Applications have also been done with Space, Automotive, Oil, Nuclear engineering domains. International projects are now starting with the US.

From the technology developed in the Defense area, important applications are now coming for Space industry (CNES and SNECMA). The aim is to restart the Ariane cryogenic engine several times, for orbit change. Restarting a cryogenic engine is very challenging as the temperature difference between cryogenic liquid and walls is about 300K. Stiff phase change, cavitation, flashing in ducts and turbopumps are expected. These phenomena have to be particularly well computed as it is very important to determine the state of the fluids at the injection chamber. This is crucial for the engine ignition and combustion stability.

From a modeling point of view, our models and methods are aimed to replace the technology owned by space laboratories, taken 10 years ago from nuclear laboratories.

To deal with these industrial relations, the startup RS2N has been created in 2004 on the basis of the Innovation Law of the Minister Claude Allegre.

4.2. Defense Applications

4.2.1. Detonation physics

A contract with the Gramat Research Center (DGA) has been achieved in 2008 for the modelling of nano-structured energetic materials. The total amount was 250 K€ for 3 years work (2006-2008).

4.2.2. Explosions

Three contracts with the Gramat Research Center (DGA) are under realization for the modeling of explosions with liquid tanks, granular materials, combustion of particle clouds, phase change etc. The total amount is 1.5M€ for 6 years work. They will end in 2011.

4.2.3. Solid-fluid coupling

A contract with DGA (REI) is under realization for the modelling of solid-fluid coupling in extreme conditions. The diffuse interface theory is under extension to build equations which will be valid in pure solids, pure fluids as well as interfaces. The total amount is 300 K€ for 3 years work. It will end in 2010.

4.3. Space Industry

A contract has started with CNES to model multiphase flows in space launcher cryogenic engines for a 18 months period for the amount of 200 K€. A longer development plan for a 4 years work has been validated. Extra support from SNECMA is under discussion. A first contract of 30 K€ has been done to test the ability of our codes to deal with flows in space systems. A longer collaboration plan is under examination. In addition, a postdoc fellow (Vincent Deledicque) has already been supported by CNES.

4.4. Energy Industry

During the present year, a first contract (75 K $ for a 6 months period) has been done with Idaho National Laboratory (INL) to examine the capabilities of our formulation to model direct numerical simulation of bubble growth and phase change at liquid-gas interfaces. The aim is to model ebullition crisis at critical heat flux. This is very important for the design of the next generation of nuclear power plants. A visit to General Electrics (GE) in North Carolina has been done last september. They have been very convinced by our presentations. We plan to write a collaboration program including INL, GE and SMASH during next year and submit to DOE (Department of Energy) for funding.

4.5. Offshore Engineering

The project team is cooperating with the engineering company Lemma for the development of novel methods for modeling systems involving turbulent flows with interfaces (swell, sloshing), bluff bodies, and structures.

5. New Results

5.1. Mathematical Modeling

5.1.1. Geometric evolution of the Reynolds stress tensor in three-dimensional turbulence

Participants: Sergey Gavrilyuk, Henri Gouin [M2P2, Aix Marseille University, France].

In a turbulent flow, the Reynolds stress tensor is deduced from an equation of evolution separating geometrical effects and turbulent source terms. The effects of the mean flow geometry are shown up when the source terms are neglected. In this case, the Reynolds stress tensor is expressed as the sum of three tensor products of vector fields only associated with the mean flow. The vector fields are governed by differential equations similar to a distorted gyroscopic equation. Along the trajectories of mean flow, the fluctuations of velocity are determined by a differential equation whose coefficients only depend on the eigenvalues of the mean rate of deformation tensor [20].

5.1.2. An iso-pressure, iso-velocity dissipative system

Participants: Hervé Guillard, Mathieu Labois.

This work extends the results of [52] to two-temperature models. We have derived a five-equation dissipative model from the standard six-equation bifluid model using the Chapman-Enskog expansion technique. Developments to the first order lead to a hyperbolic system, and even if the model features only one velocity, dissipative second-order terms enable it to deal with velocity disequilibria. Indeed, terms that can be understood as differences between the phase velocities arise, which depend notably on the pressure gradient. They enable the model to obtain results closer to the seven-equation model that the reduced model without dissipative terms studied in [4].

In the PhD Thesis of Mathieu Labois [13] defended this year (http://tel.archives-ouvertes.fr/tel-00338818/fr/), numerical methods to approximate these dissipative terms have been developed. These schemes relie on a splitting of the dissipative operator in different terms that are approximated successively. Results obtained with this numerical method have been presented in [30].

The two-velocity, two-pressure model and the reduced model have also been implemented in the parallel, three-dimensional code Num3sis [32]. The results obtained with this model are compared with those obtained with some other two-phase models and codes (including the Genesis code of CEA). It shows that the dissipative one-pressure, one-velocity system is able to reproduce complex phenomena including phase separation (see [13]).

5.1.3. Fluid-Structure coupling methods

Keywords: *Geometric Conservation law*, *total energy conservation*.

Participants: Alain Dervieux, Bruno Koobus [University of Montpellier 2], Stephen Wornom [Lemma], Olivier Allain [Lemma].

The Geometric Conservation Law (GCL) expresses the exactness of an Arbitrary Lagrangian-Eulerian discretization for uniform flows. We have demonstrated that this is a necessary condition for total energy conservation. This also extends the GCL to boundaries in a canonical manner. Total energy conservation is a key property for numerical models of any mechanical system in which the internal energy of a compressible fluid is converted into mechanical energy transmitted to a structure. A new finite-volume scheme satisfying this condition has been built from our previous scheme, developed and tested. The stabilisation effect of this improvement has be put in evidence for a standard flutter test case. A paper written in cooperation with Charbel Farhat (Stanford) and Mariano Vàzquez (Barcelona Supercomputing Center) is submitted.

The coupling between a turbulent flow and the elastic fixation of an obstacle is the source of a number of experimental investigations in turbulence. Vortex induced motion or vortex induced vibration is a powerfull tool for measuring the strength of vortex shedding. This needs good structural models and an efficient fluid-structure coupling, which is continuously improved in AERO in order to validate our VMS and hybrid turbulence models (paper in preparation by Stephen Wornom, Olivier Allain, Bruno Koobus and Alain Dervieux).

5.1.4. Modeling Wave Dynamics of Compressible Elastic Materials

Participants: Sergey Gavrilyuk, Nicolas Favrie, Richard Saurel.

An Eulerian conservative hyperbolic model of isotropic elastic materials subjected to finite deformation is addressed. It was developed by Godunov (1978) and Miller and Colella (2001). Some modifications are made concerning a more suitable form of governing equations. They form a set of evolution equations for a local cobasis which is naturally related to the Almansi deformation tensor. Another novelty is that the equation of state is given in terms of invariants of the Almansi tensor in a form which separates hydrodynamic and shear effects. This model is compared with another hyperbolic non-conservative model which is widely used in engineering sciences. For this model we develop a Riemann solver and determine some reference solutions which are compared with the conservative model. The numerical results for different tests show good agreement of both models for waves of very small and very large amplitude. However, for waves of intermediate amplitude important discrepancies between results are clearly visible [18].

5.1.5. Diffuse solid-fluid interface model in cases of extreme deformations

Participants: Nicolas Favrie, Sergey Gavrilyuk, Richard Saurel.

A diffuse interface model for elastic solid – fluid coupling in Eulerian formulation is built. This formulation generalizes the diffuse interface models for compressible multi-fluid computations [54], [8], [41], [61], [27]. Elastic effects are included following the Eulerian conservative formulation proposed by Godunov in 1978 [50]), by Miller and Colella (2001) [59], Godunov and Romenskii (2003) [51], Plohr and Plohr (2005) [62], Gavrilyuk *et al*. (2008) [18]. The aim is to derive an extended system of hyperbolic partial differential equations, valid at each mesh point (pure fluid, pure elastic solid, and mixture cells) to be solved by a unique hyperbolic solver. The model is derived with the help of Hamilton's principle of stationary action. In the limit of vanishing volume fractions the Euler equations of compressible fluids and a conservative hyperelastic model are recovered. The model is hyperbolic and compatible with the entropy inequality. Special attention is paid to the approximation of geometrical equations, as well as the fulfilment of solid-fluid interface conditions. Capabilities of the model and methods are illustrated on hypervelocity impacts of solids [17].

5.1.6. Dynamics of liquid nanofilms

Participants: Henri Gouin [M2P2, Aix Marseille University, France], Sergey Gavrilyuk.

The van der Waals forces across a very thin liquid layer (nanofilm) in contact with a plane solid wall make the liquid non homogeneous. The dynamics of such flat liquid nanofilms is studied in isothermal case. The Navier-Stokes equations are unable to describe fluid motions in very thin films. The notion of surface free energy of a sharp interface separating gas and liquid layer is disqualified. The concept of disjoining pressure replaces the model of surface energy. In the nanofilm a supplementary free energy must be considered as a functional of the density. The equation of fluid motions along the nanofilm is obtained through the Hamilton variational principle by adding, to the conservative forces, the forces of viscosity in lubrication approximation. The evolution equation of the film thickness is deduced and takes into account the variation of the disjoining pressure along the layer [19].

5.1.7. Modeling phase transition in metastable liquids

Participants: Richard Saurel, Fabien Petitpas, Rémi Abgrall [EPI SCALAPPLIX, INRIA FUTURS (University of Bordeaux)].

A hyperbolic two-phase flow model involving five partial differential equations is built for liquid-gas interface modelling. The model is able to deal with interfaces of simple contact where normal velocity and pressure are continuous as well as transition fronts where heat and mass transfer occur, involving pressure and velocity jumps. These fronts correspond to extra waves into the system. The model involves two temperatures and entropies but a single pressure and a single velocity. The closure is achieved by two equations of state that reproduce the phase diagram when equilibrium is reached. Relaxation toward equilibrium is achieved by temperature and chemical potential relaxation terms whose kinetics is considered infinitely fast at specific locations only, typically at evaporation fronts. Doing so, metastable states are involved for locations far from these fronts. Computational results are compared to the experimental ones of [67] and show a good agreement. Situations involving complex wave patterns with up to 5 waves are reported. Moreover, the Chapman-Jouguet kinetic relation used to determine the evaporation front speed in cavitating system is recovered and explained as an expansion wave of the present model in the limit of stiff thermal and chemical relaxation [26].

5.1.8. Modeling detonation waves in condensed energetic materials: Multiphase CJ conditions and multidimensional computations

Participants: Fabien Petitpas, Richard Saurel, Erwin Franquet [University of Pau, France], Ashwin Chinnayya [University of Rouen, France].

A hyperbolic multiphase flow model with a single pressure and a single velocity but several temperatures is presented to deal with the detonation dynamics of condensed high energetic materials. Temperature non-equilibrium is mandatory in order to deal with realistic wave propagation (shocks, detonations) in heterogenous mixtures. The model is obtained as the asymptotic limit of a total non-equilibrium multiphase flow model in the limit of stiff mechanical relaxation only [54]. Special attention is given to mass transfer modeling, that is obtained with the help of entropy production analysis in each phase and in the system [26]. With the help of the shock relations given in [64] the model is closed and provides a generalized ZND formulation for condensed

energetic materials. In particular, generalized CJ conditions are obtained. They are based on a balance between the chemical reaction energy release and internal heat exchanges between phases. Moreover, the sound speed that appear at sonic surface corresponds to the non-monotonic one of Wood (1930) [70]. Therefore, non-conventional reaction zone structure is observed. When heat exchanges are absent, the conventional ZND model with conventional CJ conditions is recovered. When heat exchanges are involved, a behaviour similar to non-ideal explosives is observed, even in absence of front curvature effects (Wood and Kirkwood, 1954, [69]).

Multidimensionnal resolution of the corresponding model is then addressed. This poses serious difficulties related to the presence of material interfaces and shock propagation in multiphase mixtures. The first issue is solved by an extension of the method derived in [27] in the presence of heat and mass transfers. The second issue poses the difficult mathematical question of numerical approximation of non-conservative systems in the presence of shocks associated to the physical question of energy partition between phases for a multiphase shock. A novel approach is used, based on extra evolution equations used to retain the information of the material initial state. This method insure convergence of the method in the post-shock state.

Thanks to these various theoretical and numerical ingredients, one-dimensional and multidimensional unsteady detonation waves computations are done, eventually in the presence of material interfaces. Convergence of the numerical hyperbolic solver against ZND multiphase solution is reached. Material interfaces, shocks, detonations are solved with a unified formulation where the same equations are solved everywhere with the same numerical scheme. Method convergence is reached at material interfaces even in the presence of very high density and pressure ratios, as well as convergence in the multiphase detonation wave reaction zone [23].

5.1.9. Reduced models for compaction

Keywords: *asymptotic analysis*, *compaction model*.

Participants: Marie-Hélène Lallemand, Richard Saurel.

The aim of this study is to find a model that accounts for hysteresis effects due to compaction in multiphase flows where some of the phases are constituted by small solid grains (powder). Here, we are concerned with dynamic compaction, which means compaction is due to the pressure and velocity of the gas phase acting on the solid grains. We define an additional bulk pressure, assumed to represent the compaction pressure of the solid phase. That compaction pressure is supposed to represent the resulting forces due to material resistance of the solid phase under compression. This resistance is also first assumed to be in the elastic limit of the material. As a matter of fact, we first restrict our study to that limit, plasticity and rupture will be part of future work. For that purpose, an additional potential energy, the compaction energy, from which the compaction pressure is derived, is introduced. That energy is supposed to depend only on the volume fraction of the solid phase and will only act in a certain range of values (starting with a lower-limit value for which compaction begins to be effective, and ending with a upper-limit value depending on the elastic limit of the material). The parent model, written for two phases and in one dimension, is first introduced, and we derive several reduced models, resulting from asymptotic analysis around different equilibrium states (velocity equilibrium and pressure equilibrium), since we are interested in flows for which those mechanical equilibria are done in a very small time scale (dealing with very high gas pressure and velocity). Discussion about relaxation coefficients are also done together with links with the study done by M. Labois in [13]. We are reporting the present study in [39].

5.1.10. Shock-bubbles interaction : a test configuration for two-fluid modeling

Participants: François Renaud [CEA / DAM, Bruyères le Châtel, France], Richard Saurel, Lazhar Houas [IUSTI, Aix Marseille University].

Direct numerical simulation of two nonmiscible fluids mixing under shock waves is extremely expensive in computational resources. This is incompatible with design process. It is thus necessary to develop models of mixing in order to reduce this cost. This must be made on simple mixing flows representative of studied configurations. Doing so we can combine efficiently modeling and experimental validation. We illustrate this matter on the development of a one-dimensional two-fluid model [24].

5.1.11. Diffuse interface model for high speed cavitating underwater systems

Participants: Fabien Petitpas, Jacques Massoni, Richard Saurel, Emmanuel Lapébie [DGA, Centre d'Études de Gramat, France], Laurent Munier [DGA, Centre d'Études de Gramat, France].

High speed underwater systems involve many modeling and simulation difficulties related to shock, expansion waves and evaporation fronts. Modern propulsion systems like underwater solid rocket motors also involve extra difficulties related to non-condensable high speed gas flows. Such flows involve many continuous and discontinuous waves or fronts and the difficulty is to model and compute correctly jump conditions across them, particularly in unsteady regime and in multi-dimensions. To this end a new theory has been built that considers the various transformation fronts as *diffuse interfaces*. Inside these diffuse interfaces relaxation effects are solved in order to reproduce the correct jump conditions. For example, an interface separating a compressible non-condensable gas and compressible water is solved as a multiphase mixture where stiff mechanical relaxation effects are solved in order to match the jump conditions of equal pressure and equal normal velocities. When an interface separates a metastable liquid and its vapor, the situation becomes more complex as jump conditions involve pressure, velocity, temperature and entropy jumps. However, the same type of multiphase mixture can be considered in the diffuse interface and stiff velocity, pressure, temperature and Gibbs free energy relaxation are used to reproduce the dynamics of such fronts and corresponding jump conditions.

A general model, based on multiphase flow theory is thus built. It involves mixture energy and mixture momentum equations together with mass and volume fraction equations for each phase or constituent. For example, in high velocity flows around underwater missiles, three phases (or constituents) have to be considered: liquid, vapor and propulsion gas products. It results in a flow model with 8 partial differential equations. The model is strictly hyperbolic and involves waves speeds that vary under the degree of metastability. When none of the phase is metastable, the non-monotonic Wood (1930) sound speed is recovered. When phase transition occurs, the sound speed decreases and phase transition fronts become expansion waves of the equilibrium system.

The model is built on the basis of asymptotic analysis of a hyperbolic total non-equilibrium multiphase flow model, in the limit of stiff mechanical relaxation. Closure relations regarding heat and mass transfer are built under the examination of entropy production. The mixture equation of state (EOS) is based on energy conservation and mechanical equilibrium of the mixture. Pure phases EOS are used in the mixture EOS instead of cubic one in order to prevent loss of hyperbolicity in the spinodal zone of the phase diagram. The corresponding model is able to deal with metastable states without using Van der Waals representation.

The model's predictions are validated in multidimensions against experiments of high velocity projectile impact onto a liquid tank. Simulation are compared to experiments and reveal excellent quantitative agreement regarding shock and cavitation pocket dynamics as well as projectile deceleration versus time. Then model's capabilities are illustrated for flow computations around underwater missiles [22].

5.1.12. Turbulence models

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

Participants: Bruno Koobus [University of Montpellier 2, France], Hilde Ouvrard [University of Montpellier 2, France], Anca Belme [EPI Tropics, INRIA–Sophia Antipolis–Méditerranée], Alain Dervieux, Stephen Wornom [Lemma], Charbel Farhat [Stanford University], Simone Camarri [University of Pisa, Italy], Maria-Vittoria Salvetti [University of Pisa, Italy].

The purpose of our works in hybrid RANS/LES is to develop new approaches for industrial applications of LES-based analysis. In the mean term, foreseen applications (aeronautics, hydraulics), the Reynolds number can be as high as several tenth millions, a far 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 model, the hybrid Detached Eddy Simulation model. Here, *hybrid* means a blending is applied between LES and RANS. The french-italian team has designed a novel type of hybrid model.

The Continuous Correction Hybrid Model (CCHM) combines a Variational Multiscale LES component and a low-Reynolds K-epsilon model. The LES component is an important one. In her thesis, Hilde Ouvrard compared our Smagorinsky model with new models, namely the WALE model and Vreman's model. These three models yield LES turbulent viscosity models have been encapsulated into the Variational Multiscale (VMS) formulation of Koobus and Farhat, see [34], [33], [35]. The ability to modelize accurately back scatter is then importantly increased. Applications to vortex flows around circular and square cylinder show the improvement with respect to previous versions.

A particular attention has been paid to the extension of the method to lower Reynolds. In that case the boundary layer flow remains a laminar one, to be captured by Direct Numerical Simulation, which constrains to use a mesh which must be strongly stretched due to small spatial step normal to wall. The characteristic scale of the 3D spanwise instability can be much larger than the obstacle diameter, which constrains to use a mesh with large steps in spanwise direction, increasing further the stretching. The finite-volume approximation has been improve for this purpose by Stephen Wornom and Anca Belme (INRIA report in preparation), and by Anca Belme and Hilde Ouvrard (INRIA report in preparation). Concerning the global accuracy of the approximation, new high order extension are proposed in [38]. The new schemes were inspired by previous works in Aeroacoustics and extend them to nonlinear 3D models.

In contrast to many existing hybrid models, the CCHM hybrid model involves a hybridisation method able to combine a very large class of LES and RANS submodel since each component is directly weighted independantly of a common structure of turbulent viscosity [40], [36]. The CCHM method allows to address a second family of flows, flows with very high Reynolds number. For that purpose, we use the new improvement of the numerical scheme for stretched meshes, and we are improving the RANS model near the wall. Applications to supercritical bluff body flows, i.e. flows around bluff obstacles involving a fully turbulent boundary layer, have been developed.

5.1.13. Reduced order modeling

Keywords: *Proper Orthogonal Decomposition*, *turbulence*, *vortex shedding*.

Participants: Alain Dervieux, Marianna Braza [Institut de Mécanique des Fluides de Toulouse, France], Rémi Bourguet [Institut de Mécanique des Fluides de Toulouse, France].

Also in relation with unsteady turbulence models, a cooperation with IMFT (Marianna Braza and Rémi Bourguet) has continued on reduced order models. A novel parametrization of wing shape relying on the Hadamard formula has been introduced successfully in the Proper Orthogonal Decomposition compressible model developed during the two last years. This is one of the many ingredients of the thesis of Rémi Bourguet, [43].

5.1.14. Acoustics

Keywords: *aeroacoustics*.

Participants: Bruno Koobus [University of Montpellier 2, France], Alain Dervieux, Tatyana Kozubskaya [IMM-Moscow], ILya Abalakin [IMM-Moscow], Andrey Gorobets [IMM-Moscow].

Previous works in this cooperation addressed the development of a new version of the Non-Linear Disturbance Equation of Aeroacoustics. A method for the simulation of aeroacoustics on the basis of these models has been designed and developed by a cooperation between the Computational Aeroacoustics Laboratory (CAL) of Intitute for Mathematical Modeling at Moscow and Tropics ([28]). Further developments of the NOISETTE method and software have been started during the visit in december of Tatyana Kozubskaya head of the CAL and of Andrey Gorobets.

5.2. Approximation Methods

5.2.1. Simple and efficient relaxation for interfaces separating compressible fluids, cavitating flows and shocks in multiphase mixtures

Participants: Richard Saurel, Fabien Petitpas, Ray A. Berry [Idaho National Laboratory, USA].

Numerical approximation of the five-equation two-phase flow of Kapila et al. (2001) [54] is examined. This model has shown excellent capabilities for the numerical resolution of interfaces separating compressible fluids as well as wave propagation in compressible mixtures ([8], [41], [61]). However, its numerical approximation poses some serious difficulties. Among them, the non-monotonic behavior of the sound speed causes inaccuracies in wave's transmission across interfaces. Moreover, volume fraction variation across acoustic waves results in difficulties for the Riemann problem resolution, and in particular for the derivation of approximate solvers. Volume fraction positivity in the presence of shocks or strong expansion waves is another issue resulting in lack of robustness. To circumvent these difficulties, the pressure equilibrium assumption is relaxed and a pressure non-equilibrium model is developed. It results in a single velocity, non-conservative hyperbolic model with two energy equations involving relaxation terms. It fulfills the equation of state and energy conservation on both sides of interfaces and guaranties correct transmission of shocks across them. This formulation considerably simplifies numerical resolution. Following a strategy developed previously for another flow model [9], the hyperbolic part is first solved without relaxation terms with a simple, fast and robust algorithm, valid for unstructured meshes. Second, stiff relaxation terms are solved with a Newton method that also guaranties positivity and robustness. The algorithm and model are compared to exact solutions of the Euler equations as well as solutions of the five-equation model under extreme flow conditions, for interface computation and cavitating flows involving dynamics appearance of interfaces. In order to deal with correct dynamic of shock waves propagating through multiphase mixtures, the artificial heat exchange method [61] is adapted to the present formulation [27].

5.2.2. Approximation of gas-particle system

Participants: Hervé Guillard, Thibaud Kloczko.

The aim of this work has been to define a numerical model and the associated numerical methods that can be used to study dust explosion risks that can eventually occur in the vacuum chamber of the future fusion reactor ITER.

During the life of the plasma, dust (Beryllium, graphite) is accumulating at the bottom of the vacuum chamber. If air enters the vacuum chamber, strong expansion waves and shock wave structures will be generated and will interact with the deposited dust, mobilize it into the atmosphere leading eventually to an explosion.

The simulation of this scenario is a challenge for today numerical methods and models. The geometry of the vacuum chamber is three dimensional and of large dimensions. This study therefore requires computational ressources that can only be found on large parallel platforms. On the other hand, the chamber is initially near vacuum and the simulation of its pressurization by an accidental air entry requires robust numerical methods able to compute near vacuum flows that will occur in a large range of Mach number from very supersonic to very subsonic ones. This work has studied numerical algorithms able to deal with the approximation of the convective part of the equations both for the gas and the particle phase as well as some implicit numerical methods (Rosenbrock implicit time schemes) able to compute stiff source terms that represent in these models the interaction between the continuous and dispersed phases. These results have been presented in [31]. The numerical method have been implemented in the parallel code Numesis [32] and several numerical experiments with meshes up to 8 million nodes have been performed.

5.2.3. Mesh adaptation Methods

Keywords: *Anisotropic tetrahedrization*, *Continuous metric*.

Participants: Alain Dervieux, Frédéric Alauzet [EPI Gamma, INRIA–Rocquencourt], Adrien Loseille [EPI Gamma, INRIA–Rocquencourt], Damien Guégan [Lemma].

In a cooperation between Gamma, Tropics and SMASH, a new adjoint based on mesh adaptation criterion has been developed and applied to sonic boom mitigation, for the HISAC European project and to several other CFD problems [21]. See the comments of Tropics activity reports. A special effort was applied to mesh-adaptive capture discontinuities in CFD. Steady problems with compressible shocks and unsteady ones have been considered, in order to insure second-order convergence despite of the discontinuities. New results related to these are presented in the thesis of Adrien Loseille [58]. Unsteady discontinuities have been also considered, see the section on Level Set methods.

5.3. Solution Algorithms

5.3.1. Level set methods

Keywords: *Level Set*, *compressible*, *incompressible*.

Participants: Alain Dervieux, Hervé Guillard, Frédéric Alauzet [EPI Gamma, INRIA–Rocquencourt, France], Olivier Allain [Lemma], Damien Guégan [Lemma], Thomas Bouchérès [Lemma].

Level Set methods are studied by the team inside several partnerships. After the ARC LNM entitled *Combiner efficacement techniques d'adaptation de maillages et méthodes de lignes de niveaux* completed in 2007, the cooperation continues with Frédéric Alauzet of Project Gamma. Also, the cooperation with the software company Lemma continues after our Doctoral student Damien Guégan has been integrated in the Lemma R+D team. Let us note in passing that Thibaud Kloczko, post-doctoral student of Smash in 2008, has also been integrated in the Lemma R+D team. Two fields of applications are considered, the interaction of sea surface with obstacles, and the motion of fuel in spacial tanks. A first topic particularly addressed in 2008 is dedicated to the improvement of mass conservation in the Level Set method. In a forthcoming paper, the description and aplication of a new conservative formulation of Level Set, the Dual Level Set scheme, will be published. The main idea is to measure in a variational integral the defect of a predictor with respect to the advection of the discontinuous phase color function. This is possible thanks to the continuous test functions used in the level set approximation scheme. A second important topic is the combination of a Level Set based Navier-Stokes numerical model with the fixed point dynamic mesh adaptive algorithm. As a result of the collaboration between Lemma, Gamma, and Smash, a paper presenting a method for this combination is also in preparation. Several methods for controlling the accuracy of the interface advection, insuring the second-order convergence are developed and compared.

5.3.2. Mesh-partitioning for heterogeneous architectures

Participants: Hervé Guillard, Alexandre Moyer, Stéphane Lanteri [EPI Nachos, INRIA–Sophia Antipolis–Méditerranée].

In the context of the MecaGrid initiative
(http://www-sop.inria.fr/smash/mecagrid/public/mainFrame.htm),
the Smash project-team have developed a set of computational tools for Grid computing. In this work, the mesh partitioning strategies for heterogeneous architectures that have been studied during the MecaGrid initiative are revisited taking into account the hierarchical nature of grid architecture (clusters of clusters, themselves composed of multi-core processors). This work is performed in the framework of the DiscoGrid ANR action
(http://www-sop.inria.fr/nachos/team_members/Stephane.Lanteri/DiscoGrid/).

6. Contracts and Grants with Industry

6.1. DGA

6.1.1. Modeling detonation waves in nano-structured energetic materials

Participants: Richard Saurel, Fabien Petitpas.

This study realized under DGA grant deals with the development of models and computational tools for nano-structured explosives. Comparative experiments are done at Nuclear Federal Center, Sarov, Russia.

6.1.2. Modeling liquid and particle dispersion under explosion phenomena

Participants: Jacques Massoni, Richard Saurel, Olivier Le Métayer, Éric Daniel, Julien Verhaegen.

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

6.1.3. Multiphase modeling of fluid–solid interaction

Participants: Sergey Gavrilyuk, Nicolas Favrie, Richard Saurel.

This study realized under DGA grant, deals with the development of a conservative elastic-plastic-fluid flow model to deal with fluid-solid coupling in extreme deformations. A collaboration with Prof. S.K. Godunov is also active in this area.

6.2. CNES and SNECMA : Multiphase flows in cryogenic space launcher engines

Participants: Olivier Le Métayer, Richard Saurel, Erwin Franquet, Vincent Deledicque, Éric Daniel, Jacques Massoni.

Modeling and simulation of two-phase flows in cryogenic engine of space launchers (Ariane V) is the aim of this contract. A first contract is under realization with CNES. Another one with SNECMA. These two supports are aimed to continue during 4 years.

6.3. LEMMA engineering company

Keywords: *Turbulence modeling*, *free interfaces*, *mesh adaptation*.

Participants: Frédéric Alauzet [EPI Gamma, INRIA–Rocquencourt], Alain Dervieux, Damien Guégan [Boursier CNES-EADS/Lemma], Steve Wornom [Lemma].

In the terms of a grant between INRIA and Lemma on *Turbulence Modeling*, Steve Wornom (PhD, Research engineer at Lemma), is made available for research at INRIA and his hosting in SMASH project-team is partly supported by Lemma.

7. Other Grants and Activities

7.1. Idaho National Laboratory : DNS of multiphase flows and ebullition crisis

Participants: Ray A. Berry [Idaho National Laboratory, USA], Fabien Petitpas, Richard Saurel, Éric Daniel, Jacques Massoni, Sergey Gavrilyuk, Olivier Le Métayer.

A 6 month project has been done during the current year to examined the ability of our diffuse interface methods to deal with the direct numerical simulation of interfacial flows with heat and mass transfers coupled to capillary effects. A scientific collaboration with Dr. Ray A. Berry on numerical methods for DNS has been initiated [27]. A bigger project is in preparation with INL-General Electrics and SMASH.

7.2. Institute of Mathematical Modeling, Moscow : Acoustics

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

The long-term scientific collaboration with IMM on acoustics focusses now on superconvergent techniques for noise propagation with linear and nonlinear hyperbolic models.

7.3. Ingegneria Aerospaziale, University of Pisa : Turbulence Modeling

Participants: Hervé Guillard, Alain Dervieux, Bruno Koobus [University of Montpellier 2, France], Simone Camarri [University of Pisa, Italy], Maria-Vittoria Salvetti [University of Pisa, Italy].

The long-term scientific collaboration with the Department of Ingegneria Aerospaziale at university of Pisa (Italy), has concerned during last years complex fluid flows with cavitation, and continues with the development of hybrid models for turbulent flows.

7.4. North Dakota University : Nanofluids Modeling

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

A scientific collaboration with North Dakota University on nanofluids modelling have been initiated with I. Akhatov. A paper has been published in 2006 [47].

7.5. DFG/CNRS : Liquid-Vapor Flows

Participants: François Coquel, Thierry Gallouët, Philippe Helluy, Jean–Marc Hérard, P. Josserand, Stéphane Zaleski, Rémi Abgrall, Christophe Berthon, Boniface Nkonga, Richard Saurel, Sylvie Benzoni-Gavage, Didier Jamet, Alain Dervieux, Philippe Le Floch, Vincent Perrier, Christian Rohde, Mario Ohlberger, Stefan Müller, Werner Lauterborn, Wilfried Kurz, Norbert Peters, Richard Warnecke, Dietmar Kröner.

The French-German collaboration DFG/CNRS on micro and macro modeling and simulation of liquid-vapor flows (FOR 563), aims to improve two-phase flow models and associated numerical methods.

8. Dissemination

8.1. Teaching

In the academic year 2007–2008, project members have taught the following courses :

Éric Daniel : Aix-Marseille I University : 192 h,

Polytech Engineering School : first, second and third year in *mathematics in physics*, *fluid mechanics* and *programming languages*;

Master M2 : *two-phase dilute flows*.

Sergey Gavrilyuk : Aix-Marseille III University : 192 h,

Master M1 : *mathematics-physics*, *continuum media*;

Master M2 : *two-phase flows modeling*.

Olivier Le Métayer : Aix-Marseille I University : 192h,

Polytech Engineering School : First and second year in *mathematics*, *fluid mechanics* and *thermics*.

Jacques Massoni : Aix-Marseille I University : 192 h,

Polytech Engineering School : first, second and third year in *programming languages* and *fluid mechanics*;

Master M2 : *scientific programming with parallel machines*.

Richard Saurel : Aix-Marseille I University : 192h,

Master M1 : *Analysis and numerical resolution of unsteady flows*;

Master M2 : *Multiphase flows modeling, Interface problems, Numerical methods*;

Polytech Engineering School : First and second year in *Thermodynamics*.

8.2. Conference organization

Hervé Guillard has organized from September 8–12, 2008, the CEA-EDF-INRIA SUMMER SCHOOL intitled *Numerical Models for Controlled Fusion*. This school has gathered around 50 physicists, applied mathematicians and specialists of computer sciences, to review the main flow models used for controlled fusion.

8.3. Responsabilities

Éric Daniel : is Director of the Master M2 *Energetics and Combustion*.

Richard Saurel : is Director of the Doctoral School in Engineering Sciences, including all research units of Marseilles, Aix and Toulon in *Mechanics*, *Acoustics*, *Energetics*, *Macroscopic Physics*, *Micro and Nanoelectronics*. The laboratories are CNRS UMR and UPR units: LMA, IUSTI, IRPHE, M2P2, IM2NP. The doctoral school involves more than 300 researchers and 200 PhD students.

8.4. Ph.D and HDR defense

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

Nicolas Favrie : Aix-Marseille University, MRE-AMN Grant,
Multiphase modeling of interfaces separating fluids and elastic-plastic solids, PhD's defense December 1rst, 2008;

Damien Furfaro : Aix-Marseille University, MRE Grant,
Modeling plastic deformation in solids, since 2008.

Gregory Huber : Aix-Marseille University, RS2N-Region PACA grant ,
Modeling irreversible and dynamic compaction of powders, since 2008.

Mathieu Labois : Aix-Marseille University, CEA-Region PACA Grant,
Développement de modèles diphasiques en non-équilibre, PhD's defense October 31rst, 2008;

Laurent Munier : Aix-Marseille University and DGA Gramat, DGA financial support,
Experimental and numerical study of liquid and solid dispersion under explosion conditions.

Fabien Petitpas : Aix-Marseille University, MRE Grant,
DNS models and methods for liquid-vapor phase change, PhD's defense December 2nd, 2008;

Julien Verhaegen : Aix-Marseille University, DGA grant ,
Modeling multiphase explosions and dispersion phenomena, since 2007.

Bruno Koobus has defended his HDR last September 11th, 2008, at the University of Montpellier [12].

8.5. Invited Conferences

Members of the project team SMASH have delivered invited lectures in the following conferences and seminars :

Richard Saurel :

- *SUPERFAST2008 International Conference on Superfast marine vehicles moving above, under and in water surface*, Saint-Petersburg Branch of the Institute of Marine Engineering, Science and Technology (BIMarEST) and State Marine Technical University (SMTU), St Petersburg, Russia, 2-4 July 2008 : *Modelling liquid-gas interfaces in high speed compressible flows with or without phase transition*.
- *International Shock Interaction Symposium (18th ISIS)*, Rouen, France, July 15-18th : *Condensed energetic materials: Multiphase CJ conditions and multidimensional computations*.

8.6. Other meetings

Alain Dervieux :

- has visited *Stanford University*, last June 2008, for a cooperation (Prof. Charbel Farhat) based on *Fluid-Structure iteraction*;
- was member of the thesis juries of Rémi Bourguet (Toulouse), Raphaël Kuate (Paris 6), and Adrien Loseille (Paris 6);
- has also visited the *Barcelona Supercomputing Center* for a meeting with Pr Jose-Maria Cela, last November 27th, 2008;
- will receive, in December, two members of IMM-MOSCOW, Tatyana Kozubskaya and Andrey Gorobets.
- has received, several times this year, some members of the University of Pisa (mainly, Maria-Vittoria Salvetti and Simone Camarri).

9. Bibliography

Major publications by the team in recent years

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Year Publications

Doctoral Dissertations and Habilitation Theses

[11] N. FAVRIE. *Un modèle d'interfaces diffuses pour l'interaction solide–fluide dans le cas des grandes déformations*, Thèse de l'Université, Université de Provence, December 1rst, 2008.

[12] B. KOOBUS. *Contribution à la simulation numérique d'écoulements compressibles en maillages fixes dynamiques*, Habilitation à diriger des recherches, Université de Montpellier 2, September 11th, 2008.

[13] M. LABOIS. *Modélisation des déséquilibres mécaniques dans les écoulements diphasiques : approches par relaxation et par modèle réduit*, Ph. D. Thesis, Université de Provence, October 31rst, 2008.

[14] F. PETITPAS. *Contribution à la théorie des interfaces diffuses : interfaces matérielles, fronts de transition de phase et fronts de détonation*, Thèse de l'Université, Université de Provence, December 2nd, 2008.

Articles in International Peer-Reviewed Journal

[15] F. ALAUZET, S. BOREL-SANDOU, L. DAUMAS, A. DERVIEUX, Q. DINH, S. KLEINFELD, A. LOSEILLE, Y. MESRI, G. ROGÉ. *Multi-model and multi-scale optimization strategies*, in "European Journal for Computational Mechanics", vol. 17, n^{o} 1-2, 2008, p. 245–269.

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