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 : Computational models and simulation

Activity Report

2009

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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. It was previously located at both locations (till 2008) and is now uniquely located at Marseille. As a matter of fact, Hervé Guillard and Alain Dervieux are creating a new INRIA project team* PUMAS, *focuses on plasma physics modelling and have therefore left* SMASH *this year.*
Two new associate professors have been recently hired :

- *Fabien Petitpas : has got a University–CNES chair, September 1, 2009;*
- *Nicolas Favrie : has got an associate professor position at the Civil Engineering Department of Polytech'Marseille school, Aix–Marseille I University, September 1, 2009.*

1. Team

Research Scientist

Marie-Hélène Lallemand [Research associate (CR) – located at IUSTI (Marseille)]

Faculty Member

Richard Saurel [Team Leader - Professor – Aix-Marseille University, located at IUSTI (Marseille), in delegation at INRIA since September 2009, HdR]
Eric Daniel [Professor – Aix-Marseille University, located at IUSTI (Marseille), HdR]
Sergey Gavrilyuk [Professor – Aix-Marseille University, located at IUSTI (Marseille), HdR]
Olivier Le Métayer [Associate Professor – Aix-Marseille University, located at IUSTI (Marseille)]
Jacques Massoni [Associate Professor – Aix-Marseille University, located at IUSTI (Marseille)]
Nicolas Favrie [Associate Professor, Aix-Marseille University, located at IUSTI (Marseille)]
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Gregory Huber [RS2N-Region PACA, since 2008, Aix-Marseille University, located at IUSTI (Marseille)]
Julien Verhaegen [DGA, Aix-Marseille University, since 2007]
Sarah Hank [MRE grant, Aix-Marseille University, located at IUSTI, since 2009]
Gaël Richard [salaried, Aix-Marseille University, since 2009]
Laurent Munier [DGA salaried, since 2005, DGA Gramat – Aix-Marseille University, located at the Gramat Center (France)]

Administrative Assistant

Montserrat Argente [Part time in SMASH, located at INRIA–Sophia Antipolis–Méditerranée]

2. Overall Objectives

2.1. Presentation

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.

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

The second issue deals with the *design* of *appropriate numerical schemes*. These models are not known as well 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* questions such as, *shock wave existence in multiphase mixture*, *cell averages of non–conservative variables*, *Chapman–Jouguet detonation conditions for heterogenous explosives* and so on.

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.

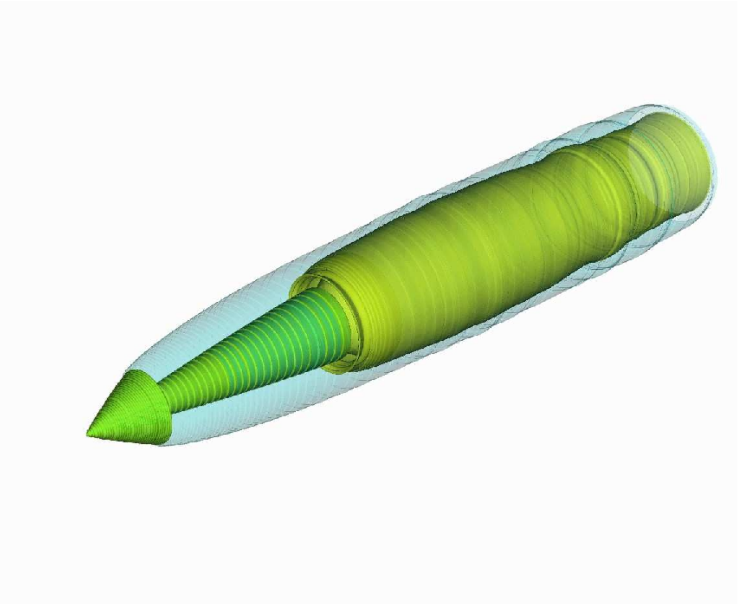

Figure 1. Numerical simulation of an underwater missile flying at 600 m/s. Three fluids are present : liquid water, steam and propulsion gases. Two different types of interfaces are present : a contact interface separates steam and combustion gases while an evaporating interface separates metastable expanded liquid and steam. To deal with metastable phase transition, the novel approach of [51] is used. The numerical approximation of the non-conservative hyperbolic system with stiff relaxation is achieved by the method of [16].

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, ADD, Korea).

3. Scientific Foundations

3.1. Modeling of Multiphase Media

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 [55] and subtle remedy was given by [26]. 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 [50] 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 [3]. 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) :

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

Only the equations for phase 1 are written, since those of phase 2 are symmetric. General closure relations for this system need the determination of :

- 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, either 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 of the pure fluid equations (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 with 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 [7], [27] 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 plasma mixtures, granular materials, chemical reactions, continuum media with elastic-plastic effects. An example is shown in the Figures 2-3.

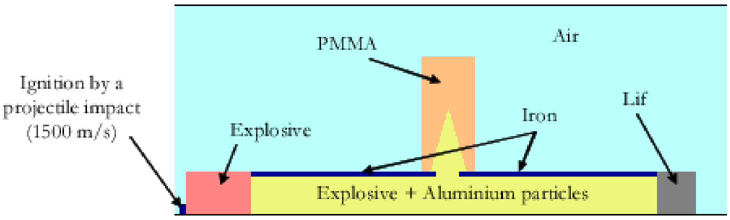

Figure 2. A steel tube is filled with a heterogeneous explosive. A high velocity impactor creates a shock wave transmitted to the explosive, that becomes a detonation wave.

Most of these extensions are done with the help of the Hamilton principle of least action [54], [2] 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

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 in relaxing 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.

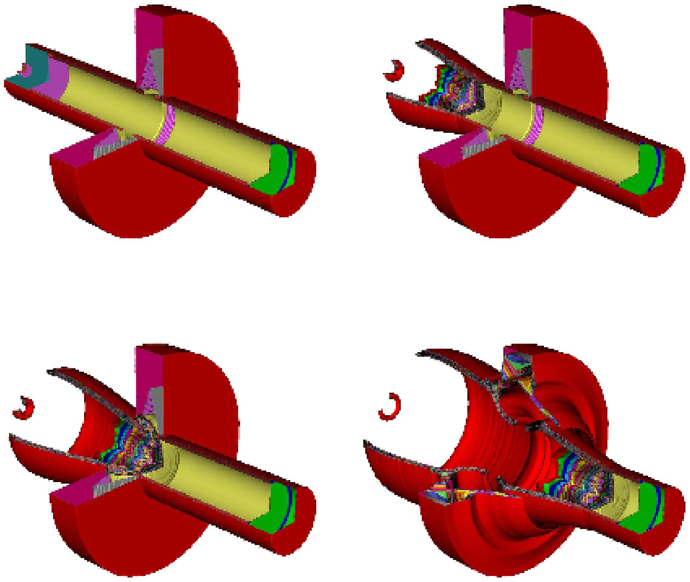

Figure 3. After a short period of time the shock wave becomes a detonation wave that produces gas and solid products at very high pressure. They set into intense motion solid tube walls. Two different types of mixture are present in this type of application : a physical one, corresponding to the mixture 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 [16]. Moreover, the detonation dynamics is checked against generalized CJ solutions [13], specifically determined for this temperature non-equilibrium model.

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 [40], [37] : 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 [30], nor interface reconstruction and so on. The same equations are solved everywhere [41], [42] and the interface is captured with the 5 equation 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* [47]. 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 at) have shown its excellent accuracy, as shown in the Figure 4;

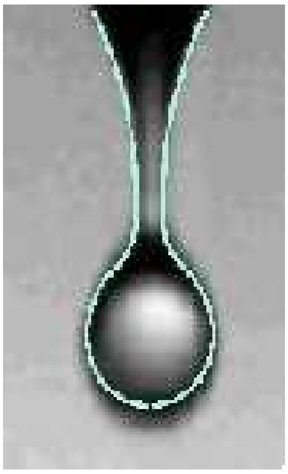

Figure 4. Comparison of the drop shape during formation (experiment in grey area, computations in lines). No interface tracking nor interface reconstruction method are used. The same equations are solved at each mesh point. The model accounts for compressible, viscous and capillary effects. The compressible 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 phenomena.

- *phase transition* in *metastable liquids* [51]. 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, several contracts with CNES and SNECMA have been concluded to model phase transition and multiphase flows in the Ariane VI 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 [52], [33] and [32]. Opposite 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. Consequently, 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 both *weak* and *very strong* shocks.

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

- *restoration of drift effects* : a dissipative one-pressure, one-velocity model has been studied in [44], and implemented in a parallel, three-dimensional code [43]. This model is able to reproduce phase separation and other complex phenomena [36];
- extending the approach to deal with *fluid-structure interactions*. A non-linear elastic model for compressible materials has been built [31]. 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 was the aim of Nicolas Favrie's PhD thesis [29], that has been persued this year [9];
- 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 [51], closed by appropriate shock conditions [52], 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 [13].

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

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 equation model for non-equilibrium mixtures and the 5 equation 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 in particular) cannot be cast under conservative form. From a theoretical point of view, it is known since the works of Schwartz [53] 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 [28], [39]. 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 moreover a numerical method that solves non-conservative products for the 7 equation 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], [7], [5], [27].

The second numerical method deals with the numerical approximation of the *five equation 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 meaning. 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 [16]. This method uses *two main ideas*.

The first one is to *transform* one of the *non-conservative products* into 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 [3], there is no difficulty neither to derive entropy preserving and positive relaxation solvers.

The second idea deals with the *management of the phase's energy equations*, which are also present under *non-conservative form*. These equations are able to compute regular/smooth solutions, such as expansion waves, but are inaccurate for shocks. Thus they are only used at shocks to predict the solution. 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 however. Its numerical approximation is obvious even in the presence of shocks since it is a conservation law. With the help of the mixture energy and predicted volume fraction, the *mixture pressure* is now computed, therefore 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 [52]. To ensure the numerical solution strictly follows the phase's Hugoniot curves, the poles of these curves are transported [13]. 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 arising for elastic materials in large deformations. The fluid-solid coupling via diffuse interfaces with extreme density ratios was done efficiently, as shown in Figure 5.

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

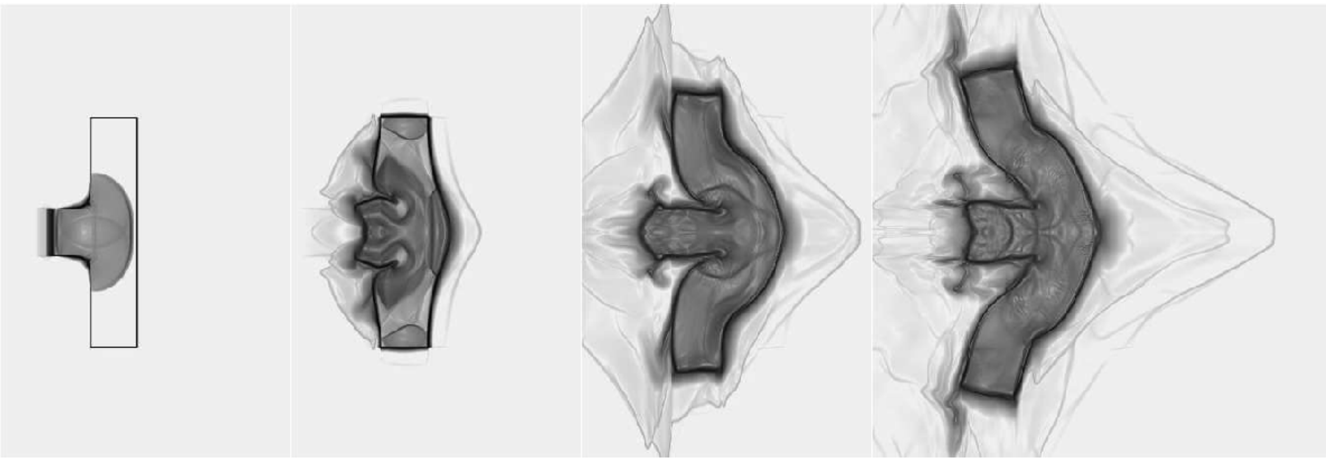

Figure 5. A copper projectile impacts a copper plate at the velocity of 800 m/s. Both materials are considered compressible and elastic, and are surrounded by air at atmospheric pressure.

schemes [38], [37]. Our investigations in that domain concern both acoustic and incompressible aspects in methodologies for setting up suitable numerical methods.

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 have started with the US and Korea.

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 Allègre.

4.2. Defense Applications

4.2.1. Explosions

Four 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 2M€ for 6 years work. They will end in 2013.

4.2.2. 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 2011.

4.2.3. Hypervelocity underwater missile

A contract with Chungnam National University (South Korea) is starting in order to model supercavitation around a high velocity topedo, propulsed by underwater solid rocket motor. The total amount is 100 K$ for one year work. It will end in 2010, but will possibly continue.

4.3. Space Industry

CNES and SNECMA have joined their support and efforts to ask SMASH for the development of flow solvers to study the restart stage of cryogenic engine under microgravity.

A three year project plan has been validated during 2009 for the total amount of 650 K€. In addition, Richard Saurel has been asked by SNECMA to make different expertise works in other areas, such as cavitation and system codes.

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].

The dynamics of the Reynolds stress tensor is described with an evolution equation coupling both geometric effects and turbulent source terms. The effects of the mean flow geometry are shown up when the source terms are neglected : the Reynolds stress tensor is then expressed as the sum of three tensor products of vector fields which are governed by a distorted gyroscopic equation. Along the mean flow trajectories and in the directions of the vector fields, the fluctuations of velocity are described by differential equations whose coefficients only depend on the mean flow deformation. If the mean flow vorticity is small enough, an approximate turbulence model is derived, and its application to shear shallow water flows is proposed. In particular, it is proven that the approximate turbulence model admits a variational formulation [10].

5.1.2. A numerical scheme for the Green-Naghdi model

Participants: Olivier Le Métayer, Sergey Gavrilyuk, Sarah Hank.

For this work, a hybrid numerical method using a Godunov type scheme is proposed to solve the Green-Naghdi model describing dispersive *shallow water* waves. The corresponding equations are rewritten in terms of new variables adapted for numerical studies. In particular, the numerical scheme preserves the dynamics of solitary waves. Some numerical results are shown and compared to exact and/or experimental ones in different and significant configurations. A dam break problem and an impact problem where a liquid cylinder is falling to a rigid wall are solved numerically. This last configuration is also compared with experiments leading to a good qualitative agreement [11].

5.1.3. Shallow water model for lakes with friction and penetration

Participants: Nikolay V. Chemetov, Fernanda Cipriano, Sergey Gavrilyuk.

We consider the flow of an ideal fluid in a 2D-bounded domain, admitting flows through the boundary of this domain. The flow is described by the Euler equations with *non-homogeneous* Navier slip boundary conditions. We establish the solvability of this problem in the class of solutions with L_p-bounded vorticity, $p \in (2, \infty]$. To prove the solvability we realize the passage to the limit in Navier-Stokes equations with vanishing viscosity [8].

5.1.4. 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 [40], [46], [25], [48], [16]. Elastic effects are included following the Eulerian conservative formulation proposed by Godunov in 1978 [34]), by Miller and Colella (2001) [45], Godunov and Romenskii (2003) [35], Plohr and Plohr (2005) [49], Gavrilyuk *et al.* (2008) [31]. 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 [9].

5.1.5. Modelling 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 [40]. 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 [51]. With the help of the shock relations given in [52] 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) [57]. 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, [56]).

Multidimensional 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 [16] 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 [13].

5.1.6. Reduced models for compaction

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 [44].

We are reporting the present study in [24].

5.1.7. Modeling dynamic and irreversible powder compaction

Participants: Richard Saurel, Nicolas Favrie, Fabien Petitpas, Marie-Hélène Lallemand, Sergey Gavrilyuk.

A multiphase hyperbolic model for dynamic and irreversible powder compaction is built. Three major issues have to be addressed in this aim. The first one is related to the irreversible character of powder compaction. When a granular media is subjected to a loading-unloading cycle the final volume is lower than the initial one. To deal with this hysteresis phenomenon a multiphase model with relaxation is built. During loading, mechanical equilibrium is assumed corresponding to stiff mechanical relaxation, while during unloading non-equilibrium mechanical transformation is assumed. Consequently, the sound speeds of the limit models are very different during loading and unloading. These differences in acoustic properties are responsible for irreversibility in the compaction process. The second issue is related to dynamic effects where pressure and shock waves play important role. Wave dynamics is guaranteed by the hyperbolic character of the equations. Phases compressibility is considered, as well as configuration pressure and energy. The third issue is related to multidimensional situations that involve material interfaces. Indeed, most processes with powder compaction entail free surfaces . Consequently the model has to be able to solve interfaces separating pure fluids and granular mixtures. These various issues are solved by a unique model fitting the frame of multiphase theory of diffuse interfaces (Saurel and Abgrall, 1999, Kapila et al., 2001, Saurel et al., 2009). Model s ability to deal with these various effects is validated on basic situations, where each phenomenon is considered separately. Special attention is paid to the validation of the hysteresis phenomenon that occurs during powder compaction. Basic experiments on energetic material (granular HMX) and granular NaCl compaction are considered and are perfectly reproduced by the model. Excepting the materials equations of state (hydrodynamic and granular pressures and energies) that are determined on the basis of separate experiments found in the literature, the model is free of adjustable parameter. Its ability to reproduce the hysteresis phenomenon is due to a relaxation parameter that tends either to infinity in the loading regime, or to zero in the unloading stage. Discontinuous evolution of this relaxation parameter is explained [15].

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

Participants: François Renaud [CEA / DAM, Bruyères le Châtel, France], Richard Saurel, Georges Jourdan, 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 [14].

5.1.9. 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 [12].

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) [40] 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 ([46], [25], [48]). 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 [6], 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 [48] is adapted to the present formulation [16].

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, Eric 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, Jacques Massoni, Fabien Petitpas.

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.

7. Dissemination

7.1. Teaching

In the academic year 2008–2009, 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*.
- **Nicolas Favrie :** Aix-Marseille I University : 70 h,
  - **Polytech Engineering School :** Second year in *Structure modeling in civil engineering*.
- **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*.
- **Fabien Petitpas :** Aix-Marseille I University : 64 h,
  - **Polytech Engineering School :** First and Second year in *Simulation and Modelling methods for gas flows* and *C-programming language*.
- **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*.

7.2. Responsabilities

Éric Daniel : has been elected this year as the Director of the Mechanical Engineering Department of Polytech Engineering School of Marseille. He has also got a promotion and is now a first class professor.

Sergey Gavrilyuk : is Director of the Master M2 *Diphasic flows, 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.

7.3. Ph.D thesis

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

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

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

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

Sarah Hank : Aix-Marseille University, MRE support,
Modélisation et simulation numérique de la dispersion de fluides dans un milieu fortement hétérogène, since 2009.

Gaël Richard : Aix-Marseille University, salaried, (professor at the CPGE of "Lycée Notre Dame de Sion", Marseille,
Écoulements des eaux peu profondes avec effet de cisaillement, since 2009.

7.4. Invited Conferences

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

Sergey Gavrilyuk and Richard Saurel :

- *International Conference honoring S. K. Godunov*, Novosibirsk, Russia, July 2009;
- *EUROTHERM 84 - Thermodynamics of phase changes*, Namur, Belgium, May 2009; (http://www.term.ucl.ac.be/eurotherm84/)
- *New Mathematical Models of Continuum Mechanics : Construction and Investigation*, devoted to the 90-years anniversary of the Academician L. V. Ovsyannikov, Novosibirsk, Russia, April 23–28, 2009 (Sergey Gavrilyuk only).

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