ECCOMAS Thematic Conference on Multi-scale
Computational Methods for Solids and Fluids
A. Ibrahimbegovic, F. Dias, H. Matthies, P. Wriggers (eds.)
Cachan, France, November 28-30, 2007

SOME ASPECTS OF THE MODELING AT DIFFERENT SCALES OF MULTIPHASE FLOWS

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Keywords: Multiphase flows, Eulerian-Eulerian, Eulerian-Lagrangian, Sprays

Abstract. *We present the various levels of possible modeling for multiphase flows: coupling of fluid equations in different domains with a free boundary; coupling (in the same domain) of a fluid equation and a kinetic (Vlasov or Vlasov-Boltzmann) equation; coupling (in the same domain) of two (or more) fluid equations. We briefly present the mathematical results relative to the passage from one of these approaches to another approach, and we give some ideas of how to use those different models on a specific practical example*

1 THE CONTEXT

We are interested in complex flows of spray type, in which a dispersed phase constituted of liquid droplets lies in a surrounding gas. The typical radius of droplets is assumed to be small in front of the typical length of the flow under study.

The approach presented here is related to works done in the framework of a long term collaboration with the CEA-DAM.

We begin by presenting the basics of the possible levels of modeling and simulation of such flows.

2 DIFFERENT LEVELS OF MODELING

2.1 Microscopic level

A first possibility consists in writing a system of Navier-Stokes equations inside and outside the droplets, the boundary (surface of the droplets) being free (that is, part of the unknown), together with boundary conditions at the interface, and rules of coalescence/dissociation of the droplets. In the case of an incompressible gas and liquid, it writes (with Ω_g the domain occupied by the gas and Ω_p the domain occupied by the droplets, the rest of the notations being transparent):

$$\partial_t u + \nabla_x \cdot (u \otimes u) + \nabla_x p = \nu_g \, \Delta_x u \quad \text{for} \quad x \in \Omega_g, \tag{1}$$

$$\partial_t u + \nabla_x \cdot (u \otimes u) + \nabla_x p = \nu_p \, \Delta_x u \quad \text{for} \quad x \in \Omega_p, \tag{2}$$

$$\nabla_x \cdot u = 0, \quad \text{for} \quad x \in \Omega_g \cap \Omega_p, \tag{3}$$

$$\text{boundary conditions on the free interface} \quad \partial\Omega_g = \partial\Omega_p. \tag{4}$$

Such a model can be discretized and simulated thanks to adapted methods (Cf. [15] for example), but of course there is a strong limitation on the number of droplets which can be simulated. Note that this model can be simplified by assuming that the droplets are rigid and spherical, but even in this case only a reasonable number of droplets can be put in a simulation.

2.2 Mesoscopic level

When a lot of droplets of very small size are present in the spray, one can try to write an equation on the pdf (Particle Distribution Function) $f(t, x, u_p, r_p)$, density of droplets which at time t and point x have a velocity u_p and a radius r_p, having in mind that the force acting on the (spherical) droplets will be of the following type:

$$m_p \, F(t, x, u_p, r_p) = -\frac{4}{3} \, \pi \, r_p^3 \, \nabla_x p(t, x) - D \, (u_p - u_g(t, x)), \tag{5}$$

where u_g is the velocity of the gas, m_p is the mass of a droplet, D is the drag coefficient, and p is the pressure.

Such a way of modeling the spray, first introduced by Williams ([16]), leads to the so-called "gas-particles", or "Eulerian-Lagrangian" models. From the point of view of mathematics, it consists in coupling a kinetic equation of Vlasov (or Vlasov-Boltzmann) type with an hyperbolic (or Navier-Stokes) system.

According to a classification due to O'Rourke (Cf. [13]), it is possible to distinguish between the thin sprays, which correspond to a volume occupied by (the totality of) the droplets negligeable in front of the volume occupied by the gas; and the thick sprays in which the volume

fraction $1-\alpha(t,x)$ of the droplets has to be taken into account, together with the effect of the collisions between droplets (modeled here by an operator $Q(f)$).

We consider the simplest case, in which the gas is inviscid and incompressible. One obtains for thin sprays the following set of equations (with the density of gas being $\rho_g = 1$, and $u_g(t,x)$, $p(t,x)$ being respectively the velocity and pressure of the gas):

$$\nabla_x \cdot u_g = 0, \tag{6}$$

$$\partial_t u_g + \nabla_x \cdot (u_g \otimes u_g) + \nabla_x p = \int\int_{u_p, r_p} -m_p \, F \, f \, du_p dr_p, \tag{7}$$

$$\partial_t f + u_p \cdot \nabla_x f + \nabla_{u_p}(F\, f) = 0. \tag{8}$$

For thick sprays, the equations become sensibly more complicated, since the coupling is also done through the volume fraction:

$$\partial_t \alpha + \nabla_x \cdot (\alpha \, u_g) = 0, \tag{9}$$

$$\partial_t (\alpha \, u_g) + \nabla_x \cdot (\alpha \, u_g \otimes u_g) + \nabla_x p = \int\int_{u_p, r_p} -m_p \, F \, f \, du_p dr_p, \tag{10}$$

$$1 - \alpha = \int\int_{u_p, r_p} \frac{4}{3} \, \pi \, r_p^3 \, f \, du_p dr_p, \tag{11}$$

$$\partial_t f + u_p \cdot \nabla_x f + \nabla_{u_p}(F\, f) = Q(f). \tag{12}$$

At the numerical level, one usually performs a splitting in time, first solving the equation of the gas thanks to a finite volume method (at least when the gas is inviscid), and secondly using a particle method (PIC) for solving the Vlasov equation. This means that f is discretized using a sum of Dirac masses.

$$f \simeq \sum_i \omega_i \, \delta_{x_i(t^n), v_i(t^n), r_i(t^n)}. \tag{13}$$

Note that the presence of the collision term (which can include the phenomena of coalescence and breakup of droplets) leads to specific numerical problems (Cf. [14]). We refer to [2] for a complete description of a Lagrangian-Eulerian numerical code.

2.3 Macroscopic level

When the volume fraction of droplets becomes sufficently large, the mesoscopic description can be replaced by the so-called Eulerian-Eulerian modeling (Cf. [10]), in which one introduces two coupled Euler (or Navier-Stokes) equations. Note however the difference of point of view with respect to the microscopic description: here the unknows are defined on the whole domain of computation, and the interface between the two fluids has become invisible because at the scale at which the fluid is looked at, it is microscopic. This interface is now completely described by the volume fraction α of gas. We denote by ρ_p, u_p the density and velocity of the liquid, and by p the common pressure of both phases. A typical set of equations is the following (still for a mixture of an incompressible inviscid gas of density $\rho_g = 1$, but for a compressible isotherm inviscid liquid):

$$\partial_t \alpha + \nabla_x \cdot (\alpha \; u_g) = 0, \tag{14}$$

$$\partial_t (\alpha \, u_g) + \nabla_x \cdot (\alpha \, u_g \otimes u_g) + \alpha \, \nabla_x p = D \, (u_p - u_g), \tag{15}$$

$$\partial_t((1-\alpha)\,\rho_p) + \nabla_x \cdot ((1-\alpha)\,\rho_p\,u_p) = 0, \tag{16}$$

$$\partial_t((1-\alpha)\,\rho_p\,u_p) + \nabla_x \cdot ((1-\alpha)\,\rho_p\,u_p \otimes u_p) + (1-\alpha)\nabla_x p = -D\,(u_p - u_g), \tag{17}$$

where $D\,(u_p - u_g)$ is the drag between the phases and the pressure law of the isothermal liquid is taken into account:

$$p = p_2(\rho_p). \tag{18}$$

The numerics of such a system is complex since the equations are not conservative (because of terms like $\alpha\,\nabla_x p$) and not hyperbolic. Finite volumes schemes especially designed for those systems can be used (Cf. [1]).

3 LINKS BETWEEN THE DIFFERENT LEVELS OF MODELING : THEORETICAL RESULTS

The passage from the microscopic equations to the mesoscopic equations is a difficult problem in which methods from statistical physics and from fluid mechanics have to be brought together. Passing rigorously from equations including a free boundary to Eulerian/Lagrangian models seems out of reach with the existing techniques, and one starts therefore from a simpler model, such as the union of N rigid balls of radius $\varepsilon \sim 1/N$ in a Stokes or Navier-Stokes flow. Even when considering such a simple situation, it has only been proven (Cf. [6]) that (a viscous version of) eq. (6), (7) can be rigorously recovered in the limit when $N \to \infty$. The coupling with eq. (8) remains a challenge, since the limiting equation are known to have solutions only in particular situations (Stokes or Burgers approximation, small time solutions, etc.: Cf. [7], [9], [3]).

The passage from the mesoscopic to the macroscopic model is quite different for various reasons: first, the macroscopic equations are known to be linearly unstable and there is therefore no hope to establish an asymptotic theorem in which the limit satisfies those equations, even in a "small time" regime. Secondly, the mesoscopic and macroscopic models are both written in terms of standard systems of PDEs (without moving boundary), so that the "statistical physics" aspect which was present in the passage from the microscopic model to the mesoscopic model is not relevant here.

As a consequence, the idea is rather to identify a small parameter in the mesoscopic equations, and to perform a *formal* asymptotics leading to the macroscopic model. This has been done in [12]: the small parameter is the Knudsen number (mean free path of a droplet divided by a characteristic length of the flow), and the asymptotics is reminiscent of the Hilbert expansion of the classical fluid mechanics (Cf. [5]). One of the main differences is that (at least in the applications which are interesting us) the collisions between droplets do not conserve the kinetic energy (part of it is released as oscillation energy of the droplets). We also note that the result of [12] holds only (at the formal level) for monodisperse sprays (that is, when all droplets have the same radius).

4 LINKS BETWEEN THE DIFFERENT LEVELS OF MODELING : PRACTICAL APPLICATIONS

We briefly describe here what could be the possible use of the various levels of modeling at the practical level for a given problem. What we propose below has not yet been implemented

in totality in the framework of the collaboration of the CEA-DAM, and some of the issues are still under discussion.

First, one cannot hope to obtain in a rigorous (or even rigorous at the formal level) way all the coefficients entering the mesoscopic description from an asymptotic analysis based on the microscopic description (even the value of the drag coefficient can be obtained only under very stringent assumptions which are not satisfied in general in practical computations). Many coefficients used in the industrial codes (coefficients related e.g. to the complex phenomena involving droplets such as collisions, coalescence, breakup, interaction with the wall) are based on experimental results or (less often) numerical results taken in the litterature (Cf. [8]). In order to improve the precision of the computations which are sometimes done for physical situations which are not close to the experimental or numerical situations described in the litterature, one would like to perform auxiliary computations at the microscopic scale (direct numerical simulation) allowing to obtain the coefficients used in the averaged (mesoscopic) simulation. Note that this is far from being possible for the whole range of interesting physical parameters (such as large Reynolds numbers, large ratios of density for the liquid and gas, etc.).

Secondly, it happens that in some situations, the Knudsen number (of the droplets) can become quite small and make the mesoscopic simulation much too expensive. One needs then to transit to the macroscopic simulation. This can be done in a certain region of space, or everywhere at a given time. It leads to problems comparable to the problem encoutered in the study of rarefied gases when one wishes to couple a Boltzmann simulation with a Navier-Stokes simulation (Cf. [11]). In particular, one needs to identify the zones in which this transition is justified, and then to "create" the new unknowns using the discretization (particles) of the pdf defined in the mesoscopic description.

The previous approaches have to be incorporated in a code which is often already quite complicated. Here are some of the difficulties which have to be taken in account in the simulations of the sprays that we have investigated with the CEA-DAM: the gas as well as the droplets can be compressible (Cf. [4]); the pressure and energy laws are given by tables and can be quite complex, the collisions between droplets do not conserve the kinetic energy and lead to an exchange of temperature (Cf. [12]).

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