ABOUT THE MODELLING OF COMPLEX FLOWS BY GAS-PARTICLE METHODS

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ABSTRACT. We wish to present to non–specialists some of the issues of the use of mixed fluid–kinetic equations (sometimes called Eulerian–Lagrangian, or gas–particles) in the context of complex flows. We discuss the modelling, the mathematical state of the art, and briefly describe the numerical methods.

1. Introduction

Most of the flows are modelled by a system of equations enabling one to compute quantities which are functions of the time t and the point x at which the flow is considered. Typically, those quantities are the density $\rho(t,x)$, the velocity $u(t,x)$, the temperature $T(t,x)$, the internal energy $e(t,x)$ and the pressure $p(t,x)$. For diphasic flows, such quantities are introduced for each phase (though some of them, like p for example, can be the same for the two phases), and the additional volume (or sometimes mass) fraction $\alpha(t,x)$ is added. Taking into account the turbulence can lead to consider yet other unknowns (like, for example, the usual turbulent quantities k, ε).

Equations describing the evolution of ρ, u, T (such as Euler or Navier–stokes equations, or their diphasic variants) will be refered as fluid equations in the sequel (Cf. [14]).

For rarefied gases, however, it is not possible to keep as unknowns functions of t and x only, and one has to come back to the density $f(t,x,v)$ of particles which at time t and point x move with velocity v (sometimes called density in the phase space). Note that for realistic gases (diatomic nitrogene for example), one even has to add one or more variables to f, in order to model the microscopic internal energy (Cf. [2]).

The equations used in this theory are variants of Boltzmann's equation of rarefied monoatomic gases, and are called kinetic equations. They are easily recognizable because their left–hand–side usually begins with the advection operator $\partial_t f + v \cdot \nabla_x f$, related to the inertia of the particles .

It many physical problems, one has to mix the two previous points of view and to couple fluid and kinetic equations. For example, the radiative hydrodynamics deals with photons which are modelled by a kinetic equation, whereas the underlying gas is described by fluid equations (Cf. [3]).

However, we are interested in this work only in the case when dispersed (macroscopic)particles (a spray) coexist with a fluid (liquid or gaseous) phase.

In such a case, an alternative to writing a system of fluid equations for the two phases consists in modelling the spray by a kinetic equation, usually a variant of the Boltzmann equation in which a force acting on the particles is due to the surrounding fluid. The fluid itself will be modelled by an Euler-type equation in which source terms represent the effect of the particles on the fluid.

Though many different physical situations can be handled in this way (bubbles of gas in a liquid, etc..), the examples given here rather refer to the case of liquid or solid particles (sometimes called droplets) in a gas.

In section 2, we derive a system of gas–particles equations, in a situation as simple as possible, and try to show the relationships between this system and the more classical equations of diphasic fluids. Some rigorous results are quoted in section 3, about the establishment of the equations and the mathematical study of their solutions. Finally, in section 4, we briefly describe the numerical methods adapted to the gas–particles equations.

2. Modelling

As announced in the introduction, the dispersed phase (spray) is described by its density in the phase space. At least an extra variable is added to the variables t, x, v of the standard kinetic theory, namely the radius r of the droplets of the spray. This density is denoted $f(t,x,v,r)$, it represents the number of particles (per unit of time, position, etc..) which at time t and point x move with velocity v and have a radius r.

The corresponding equation is a variant of Boltzmann's equation of rarefied gases (Cf. [2]), which is introduced for example in [23] or [17], and writes, in its simplest form

$$\partial_t f + v \cdot \nabla_x f + div_v(F\, f) = 0, \tag{1}$$

where $m_p\, F$ is the drag force of the gas on the droplets:

$$m_p\, F(t,x,v,r) = -\frac{4}{3}\,\pi\, r^3\, \nabla_x p(t,x) - D\,(v - u_g(t,x)), \tag{2}$$

and m_p is the mass of a droplet, p the pressure field of the gas, u_g its velocity field, and D a drag coefficient which depends in general on many variables (and at least r).

Equation (1) can be modified (and complexified) in many ways: the force $m_p\,F$ can include the added mass effect or Basset's history term (Cf. for example [21] and [19]); variables taking into account the temperature T_p of the droplets or their deformations are sometimes introduced (Cf. [12]); the radius r of the droplets can evolve because of abrasion, compressibility effects (Cf. [1]), evaporation or chemical reactions (Cf. [12]); the effect of turbulence is often represented by an extra diffusion (in both variables x and v) in equation (1) (Cf. [4], [18]); finally, many types of collisions between droplets can be taken into account, including fragmentation and coagulation (Cf. [12], [13] and [10]).

The underlying gas is described (once again in a situation which is as simplified as possible) by a set of two equations of Euler type, relative to the density $\rho_g(t,x)$, the velocity $u_g(t,x)$ and the volume fraction $\alpha(t,x)$ of the gas:

$$\partial_t(\alpha\,\rho_g) + div_x(\alpha\,\rho_g\,u_g) = 0, \tag{3}$$

$$\partial_t(\alpha\,\rho_g\,u_g) + div_x(\alpha\,\rho_g\,u_g \otimes u_g) + \nabla_x p = -\int m_p\,F\,f\,dvdr. \tag{4}$$

The right–hand–side of (4) models the transfer of impulsion from the droplets to the gas. It ensures the conservation of the global mass and impulsion of the mixture:

$$\partial_t\Big(\int \alpha\,\rho_g\,dx + \int m_p\,f\,dxdvdr\Big) = 0, \tag{5}$$

$$\partial_t\Big(\int \alpha\,\rho_g\,u_g\,dx + \int m_p\,f\,v\,dxdvdr\Big) = 0. \tag{6}$$

Note that equation (4) can also be written under the (maybe more familiar) form:

$$\partial_t(\alpha\,\rho_g\,u_g) + div_x(\alpha\,\rho_g\,u_g \otimes u_g) + \alpha\,\nabla_x p = \int D\,(v - u_g)\,f\,dvdr. \tag{7}$$

The system is then closed by imposing a pressure law

$$p = p(\rho_g), \tag{8}$$

and the relation between α and f:

$$1-\alpha = \int \frac{4}{3}\,\pi\, r^3\, f\, dvdr. \tag{9}$$

Once again, many variants or improvements of equations (3), (4), (8), (9) can be devised: introduction of the internal energy and compressibility of droplets (Cf. [1]), phase transitions and chemical reactions (Cf. [12]), etc..

In order to compare the set of equations (1) – (4), (8), (9) to classical diphasic equations, one can integrate (1) with respect to $m_p\, dvdr$ and $m_p\, vdvdr$. Denoting the mean density of the spray by

$$\bar{\rho}_p = \frac{\int m_p\, f\, dvdr}{\int \frac{4}{3}\,\pi\, r^3\, f\, dvdr}, \tag{10}$$

and its mean impulsion by

$$\bar{\rho}_p\, \bar{u}_p = \frac{\int m_p\, f\, v\, dvdr}{\int \frac{4}{3}\,\pi\, r^3\, f\, dvdr}, \tag{11}$$

we get

$$\partial_t((1-\alpha)\,\bar{\rho}_p) + div_x((1-\alpha)\,\bar{\rho}_p\,\bar{u}_p) = 0, \tag{12}$$

$$\partial_t((1-\alpha)\,\bar{\rho}_p\,\bar{u}_p) + div_x((1-\alpha)\,\bar{\rho}_p\,\bar{u}_p\otimes\bar{u}_p) + (1-\alpha)\nabla_x p + div_x p'$$

$$= -\int D\,(v-u_g)\, f\, dvdr, \tag{13}$$

where

$$p'(t,x) = \int m_p\,(v-\bar{u}_p(t,x))\otimes(v-\bar{u}_p(t,x))\, f(t,x,v,r)\, dvdr. \tag{14}$$

We now can compare the set of equations (12), (14), (3), (4), (8), (9) to the usual system of four diphasic equations. The main differences are the following:

1. The equation relating α to f replaces the equality of pressures,
2. The tensor p' is added to the pressure field,
3. The terms of exchange of momentum depend on the whole distribution f and not simply on the mean quantities $\bar{\rho}_p$, $\bar{u}_p$. In particular, the dependance of D with respect to r prevents to simplify the integral.

It is difficult to clearly understand which flows should be modelled by gas–particles rather than by diphasic equations. It seems that at least flows in which the dispersion in the variable r is very large (polydispersed flows) are better modelled in the gas–particles framework (Cf. [6]).

However, various authors have tried to compare the gas–particles and the diphasic approaches, at the level of numerical simulations (Cf. for example [15] and [8]).

3. Rigorous results

A rigorous establishment of the system (1) – (4), (8), (9) seems to be extremely difficult. However, such results exist when the flow underlying the particles is very simple (potential or Stokes flow). It is then possible to prove that the dipolar approximation of the flow around N particles leads, when N tends to infinity and under a suitable scaling of the size of the particles, to simplified versions of (1) – (4), (8), (9) (Cf. [11], [20], [22]). Those recent results seem very promising and improvements are expected in the future. One can also quote the study of the effect of turbulence on the droplets, leading to correcting diffusion terms in equation (1) (Cf. [4]).

Few mathematical studies of the behaviour of solutions of equations like (1) – (4), (8), (9) seem to exist. Existence and stability of travelling waves solutions are studied in [7] and [5] for a simplified 1D model where the fluid equation is of Bürger type. We also refer to the study of the Vlasov–Stokes system in [9].

4. Some remarks on the numerical simulation

Note first that particle–gas equations are not always written to be directly discretized and computed. They are sometimes used to derive fluid equations, which in turn will be discretized (Cf. for example [6] in the context of polydispersed flows).

Nevertheless, many academic and commercial codes have been developed, which directly simulate the gas–particles equations (Cf. for example [12], [16]). The fluid part of the equations is solved by standard methods (finite volumes for example). Like for the Boltzmann equation, however, it is not reasonable (except maybe for 1D simulations) to discretize with finite volumes or elements the phase space. In a 3D context, note that the dimension of this phase space is 7 (8 if the time is taken into account !). Therefore, a particle method is introduced for eq. (1). That is, f is discretized as (Cf. for example [10]):

$$f(t,x,v,r) = \sum_{i=1}^{N(t)} a_i(t)\, \delta_{x=x_i(t),v=v_i(t),r=r_i(t)}. \tag{15}$$

Then, when a value at some point of f is needed (for example if one wants to compute nonlinear functions of f such as the entropy), one uses the convolution of the sum of Dirac masses by a given nonnegative function $\chi(x,v,r)$ with compact support and such that $\int \chi dx dv dr = 1$. That is, eq. (15) is replaced by

$$f(t,x,v,r) = \sum_{i=1}^{N(t)} a_i(t)\, \chi(x - x_i(t), v - v_i(t), r - r_i(t)). \tag{16}$$

Taking for χ a characteristic function (in the x variable) leads to the notion of volume of control, which often coïncides with the mesh used to solve the fluid part of the equation.

Finally, note that the particle discretization enables sometimes to take into account complex phenomena (fragmentation of droplets, etc..) which are not always so easy to write down in the PDE formalism. As a consequence, some of the codes used in the industry do not necessarily refer to a given set of equations.

5. Conclusion

The gas–particles equations constitute an interesting alternative to the equations of diphasic fluids in certain circumstances (polydispersed flows for example). They can be solved at the numerical level by using a particle method for the kinetic part of the system, and (for example) a finite volume method for the fluid part.

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