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Mathematical Physics

Hybrid kinetic/fluid models for nonequilibrium systems

Modèles hybrides cinétiques-fluides pour les systèmes hors équilibre

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Abstract

Our purpose is to derive a model describing the evolution of particles at various scales following their kinetic energy. Fast particles will be described through a collisional kinetic equation of Boltzmann-BGK type. This equation will be coupled with a fluid model (Euler equations) that describes the evolution of slower particles. The main interest of this approach is to reduce the cost of numerical simulations. ***To cite this article: N. Crouseilles et al., C. R. Acad. Sci. Paris, Ser. I 336 (2003).***

Résumé

Dans cette Note, nous proposons un modèle permettant de décrire différemment l'évolution de particules suivant leurs énergies cinétiques. Les particules rapides seront décrites par une équation cinétique de type Boltzmann-BGK. Cette dernière sera couplée à un modèle fluide (équations d'Euler) destiné à modéliser l'évolution des particules lentes. Un des intérêts de ce type d'approche est la réduction du coût des simulations numériques. ***Pour citer cet article : N. Crouseilles et al., C. R. Acad. Sci. Paris, Ser. I 336 (2003).***

Version française abrégée

L'étude et la simulation de systèmes de particules hors équilibre sont des problèmes complexes. De tels régimes ne peuvent être décrits correctement par des modèles fluides de type Euler ou Navier–Stokes ; en effet, ces modèles supposent que le système dévie peu de l'équilibre, hypothèse qui n'est pas vérifiée lorsqu'une forte proportion de particules suprathermiques est présente. D'autre part, les modèles cinétiques qui seuls peuvent rendre compte du déséquilibre, nécessitent la discrétisation de l'espace des phases (position et vitesse), ce qui est prohibitif.

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Pour décrire des systèmes hors équilibre, nous proposons dans cette Note un modèle hybride qui modélise différemment les particules rapides et les particules lentes : les premières seront modélisées par un modèle cinétique de type Boltzmann-BGK, tandis que les secondes le seront à travers les équations d'Euler (régime fluide).

Un schéma numérique conservatif est alors construit à partir duquel des simulations sont effectuées. Des comparaisons avec des modèles existants sont présentées.

1. Introduction

Kinetic theories describe a gas through the evolution of a nonnegative density $f = f(t, x, v)$ over the particle phase space $\mathbb{R}^d \times \mathbb{R}^d$ (with $t \geqslant 0,\ x \in \mathbb{R}^d,\ v \in \mathbb{R}^d,\ d = 1, 2, 3$). In our case, this evolution is governed by the BGK equation:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\varepsilon}(\mathcal{M}_{[f]} - f), \quad \text{with } \mathcal{M}_{[f]}(v) = \frac{n}{(2\pi T)^{d/2}} \exp\left[-\frac{|v-u|^2}{2T}\right], \tag{1}$$

with $\varepsilon > 0$ the relaxation time and where n, u, T (density, mean velocity and temperature) satisfy $n = \int_{\mathbb{R}^d} f(v)\,\mathrm{d}v$, $nu = \int_{\mathbb{R}^d} vf(v)\,\mathrm{d}v$, $\int_{\mathbb{R}^d} |v|^2 f(v)\,\mathrm{d}v = n|u|^2 + dnT,\ d = 1, 2, 3$. Far outside fluid dynamical regimes, one may abandon fluid dynamics in favor of the full kinetic model, which may be effectively solved *via* molecular dynamics, Monte Carlo methods, deterministic methods, etc. [1,5]. However, because of its phase space description and numerical stiffness, the computational cost of doing so in regimes near the fluid dynamical limit becomes too prohibitive in both time and storage requirements to allow for general usage. Consequently, we propose to describe differently fast particles and slower particles (see [2]). Slow ones, which do not deviate far from equilibrium, can be modelized through a fluid equation of Euler type, whereas the Boltzmann-BGK model (1) will take into account fast particles. More precisely, we consider a ball $B_1 = \{v \in \mathbb{R}^d \mid |v - \underline{u}| \leqslant R\sqrt{\underline{T}}\}$, where $\underline{u}$ and $\underline{T}$ are a velocity and a temperature (supposed to depend on t and x), while R is a constant parameter. This ball represents the velocities which are slow relatively to $\underline{u}(t, x)$. In the same way, $v \in B_2 = \mathbb{R}^d \setminus B_1$ will be the velocities set of relatively fast particles.

The remainder of the paper is organized as follows. Section 2 is devoted to the derivation of the hybrid fluid/kinetic model. Section 3 indicates a numerical scheme for the hybrid model and presents some simulations. Finally, Section 4 gives a concluding discussion.

2. Obtention of the coupled model

Our starting point is (1) which takes account of all the velocities $v \in \mathbb{R}^d$. Let us introduce some notations relative to $B_1 = \{v \in \mathbb{R}^d \mid |v - \underline{u}| \leqslant R\sqrt{\underline{T}}\}$ and $B_2 = \mathbb{R}^d \setminus B_1$:

Definition 2.1. For any function $g : \mathbb{R}^d \to \mathbb{R}$, we set for $i = 1, 2$: $g_i(v) = g(v)$ if $v \in B_i$ and $g_i(v) = 0$ otherwise.

Our goal is to appoach (1) by a fluid/kinetic model. Associated to f, solution to (1), f_2 will be the unknown of the kinetic part of the hybrid model. On the other hand, the fluid part must be a closed system of $d + 2$ equations satisfied by $U_1 = (n_1, P_1, W_1)^{\mathrm{T}}$, with n_1 the density, P_1 the momentum and W_1 the energy of f on B_1. The closure distribution function will be imposed by the minimization entropy principle (see [4]). However, since B_1 is a bounded set, the situation is slightly different. We choose for the entropy functional: $H_1(g) = \int_{B_1} g(v) \log(g(v))\,\mathrm{d}v,\ g \geqslant 0$.

Let us now summarize this closure strategy applied to our case. Here, the minimization entropy principle with prescribed moments U_1 can be written, with $m(v) = (1, v, |v|^2)^{\mathrm{T}}$:

$$\text{Find } \mathcal{M}_1 \geqslant 0 \text{ s.t. } H_1(\mathcal{M}_1) = \mathrm{Min}\left\{ H_1(g),\ g \geqslant 0 \text{ s.t. } \int_{B_1} g(v) m(v)\,\mathrm{d}v = U_1 \right\}. \tag{2}$$

If (2) has a solution $\mathcal{M}_1$, then the system of moments U_1 derived from (1) on B_1 can be closed by a distribution function that coincides with $\mathcal{M}_1$. This closure strategy, introduced by Levermore [4], ensures the hyperbolicity of the so-obtained system (here, if $\underline{u}$ and $\underline{T}$ are chosen *a priori*). Next, we prove that (2) has a unique solution provided that the prescribed moments satisfy some constraints that will be precised later on. Before going to this statement, we first define the moment realizability problem: what necessary and sufficient conditions have to be satisfied by the prescribed moments $U_1 = (n_1, P_1, W_1)^{\mathrm{T}}$ such that the moment problem:

$$\text{Find } \mathcal{M}_1 \geqslant 0 \text{ s.t. } \int_{B_1} \mathcal{M}_1(v) m(v)\,\mathrm{d}v = U_1, \quad \text{where } m(v) = \left(1, v, |v|^2\right)^{\mathrm{T}}, \tag{3}$$

admits at least one solution? When (3) is solvable, the question is then: what are the necessary and sufficient conditions on (n_1, P_1, W_1) so that (2) admits a solution? The following proposition answers these questions (following results in [3]):

Proposition 2.2. *The minimization entropy problem* (2) *admits a solution if and only if the moments problem* (3) *has a solution, if and only if*:

$$|P_1|^2 \leqslant n_1 W_1, \qquad \frac{n_1 W_1 - |P_1|^2}{n_1^2} + \left| \underline{u} - \frac{P_1}{n_1} \right|^2 \leqslant R^2 \underline{T}. \tag{4}$$

Moreover, under conditions (4)*, the solution is unique and is a Maxwellian function*:

$$\mathcal{M}_1(v) = \exp\left(\lambda_0 + \lambda_1 \cdot v + \lambda_2 |v|^2\right), \quad \textit{with } (\lambda_0, \lambda_1, \lambda_2)^{\mathrm{T}} \in \mathbb{R}^{d+2},\ d = 1, 2, 3, \tag{5}$$

where $\lambda = (\lambda_0, \lambda_1, \lambda_2)^{\mathrm{T}} \in \mathbb{R}^{d+2}$ *is uniquely determined by relation* (3)*.*

As mentioned above, the so-obtained distribution function (5) will close our system of moments. Let us now introduce some notations which enable us to write the hybrid model:

$$\begin{pmatrix} \psi_{n_1} \\ \psi_{P_1} \\ \psi_{W_1} \end{pmatrix} = \int_{B_1} v \mathcal{M}_1(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \mathrm{d}v, \qquad \vec{F}(v) = \mathcal{D}\left(\frac{v - \underline{u}}{R\sqrt{\underline{T}}} \right) \quad \left(\text{with } \mathcal{D} = \frac{\partial}{\partial t} + v \cdot \nabla_x \right), \tag{6}$$

are respectively the moments fluxes, and a force which modelizes the space and time variations of B_1. Now, if we note $\mathbb{S}(\underline{u}, R\sqrt{\underline{T}})$ the boundary (sphere) of B_1, we can introduce the following sets:

$$\mathbb{S}_+ = \left\{ v \in \mathbb{S}(\underline{u}, R\sqrt{\underline{T}}) \text{ s.t. } \vec{F}(v) \cdot \vec{\nu} > 0 \right\}, \qquad \mathbb{S}_- = \left\{ v \in \mathbb{S}(\underline{u}, R\sqrt{\underline{T}}) \text{ s.t. } \vec{F}(v) \cdot \vec{\nu} < 0 \right\}, \tag{7}$$

where $\vec{\nu}$ is the outgoing normal to $\mathbb{S}(\underline{u}, R\sqrt{\underline{T}})$. If $\mathrm{d}S$ is the surface measure, then we can define the boundary semi-fluxes (outgoing and incoming semi-fluxes respectively):

$$\begin{pmatrix} L_{n_1} \\ L_{P_1} \\ L_{W_1} \end{pmatrix} = \int_{\mathbb{S}_+} \vec{F}(v) \cdot \vec{\nu} \mathcal{M}_1(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \mathrm{d}S, \qquad \begin{pmatrix} G_{n_1} \\ G_{P_1} \\ G_{W_1} \end{pmatrix} = \int_{\mathbb{S}_-} \left| \vec{F}(v) \cdot \vec{\nu} \right| f_2(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \mathrm{d}S.$$

Then, if we take the moments of (1) on B_1, use the closure $\mathcal{M}_1$ given by (5), and if we restrict (1) to B_2, then we obtain:

Proposition 2.3. *With the previous notations, the hybrid fluid/kinetic model of unknowns* (n_1, P_1, W_1, f_2) *writes*:

$$\begin{aligned}
&\frac{\partial}{\partial t}\begin{pmatrix} n_1 \\ P_1 \\ W_1 \end{pmatrix} + \nabla_x \cdot \begin{pmatrix} \psi_{n_1} \\ \psi_{P_1} \\ \psi_{W_1} \end{pmatrix} = -\frac{1}{\varepsilon}\begin{pmatrix} n^{(2)} - n_2 \\ P^{(2)} - P_2 \\ W^{(2)} - W_2 \end{pmatrix} - \begin{pmatrix} L_{n_1} \\ L_{P_1} \\ L_{W_1} \end{pmatrix} + \begin{pmatrix} G_{n_1} \\ G_{P_1} \\ G_{W_1} \end{pmatrix}, \\
&\frac{\partial f_2}{\partial t} + v \cdot \nabla_x f_2 = \frac{1}{\varepsilon} Q_2(f_2, \mathcal{M}_1) \quad \text{on } B_2
\end{aligned} \tag{8}$$

with the boundary conditions $f_2(v) = \mathcal{M}_1(v)$, $\forall v \in \mathbb{S}_+$. *Moreover,* $Q_2(f_2, \mathcal{M}_1) = (\mathcal{M}_{[\mathcal{M}_1+f_2],2} - f_2)(v)$, $v \in B_2$, *where* $\mathcal{M}_{[\mathcal{M}_1+f_2]}$ *satisfies* $\int_{\mathbb{R}^d} m(v)\ \mathcal{M}_{[\mathcal{M}_1+f_2]}(v)\,\mathrm{d}v = \int_{\mathbb{R}^d} m(v)(\mathcal{M}_1 + f_2)(v)\,\mathrm{d}v$, *with* $m(v) = (1, v, |v|^2)^{\mathrm{T}}$, *and*:

$$\begin{pmatrix} n^{(2)} \\ P^{(2)} \\ W^{(2)} \end{pmatrix} = \int_{B_2} \mathcal{M}_{[\mathcal{M}_1+f_2],2}(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \mathrm{d}v, \qquad \begin{pmatrix} n_2 \\ P_2 \\ W_2 \end{pmatrix} = \int_{B_2} f_2(v) \begin{pmatrix} 1 \\ v \\ |v|^2 \end{pmatrix} \mathrm{d}v.$$

3. Numerical schemes for the hybrid model

In this section, we present a numerical scheme for the hybrid model (8). The main difficulty of the discretization of such a model comes from the dependence of B_1 on both time and space. To overcome this problem, we follow a splitting method: in a first step, we only take into account the space variations of B_1; its time variations will be considered in a second step. Let us construct the numerical scheme.

For the sake of simplicity, we present a 1-D scheme, with a Cartesian grid $x_i = i\Delta x$, $v_k = k\Delta v$, $i, k \in \mathbb{Z}$; $t^n = n\Delta t$ is the time discretization, $n \in \mathbb{N}$. Like in the continuous case (see Section 2), our starting point is the BGK equation. To discretize (1), we follow the strategy developped in [5]. We approximate $f(t^n, x_i, v_k)$ by $f^n_{i,k}$ such that:

$$f^{n+1}_{i,k} = f^n_{i,k} - v_k^+ \frac{\Delta t}{\Delta x}\big[f^n_{i,k} - f^n_{i-1,k}\big] - v_k^- \frac{\Delta t}{\Delta x}\big[f^n_{i+1,k} - f^n_{i,k}\big] + \frac{\Delta t}{\varepsilon}\big[\mathcal{E}^n_{i,k} - f^n_{i,k}\big], \tag{9}$$

with $v_k^{\pm} = \frac{1}{2}(v_k \pm |v_k|)$ and where $(\mathcal{E}^n_{i,k})_{k\in\mathbb{Z}}$ realizes the following minimum:

$$\mathrm{Min}\left\{ \sum_{k\in\mathbb{Z}} g_k \log(g_k)\Delta v,\ g_k \geqslant 0 \text{ s.t. } \sum_{k\in\mathbb{Z}} m_k g_k \Delta v = U^n_i \right\}, \tag{10}$$

with $U^n_i = \sum_{k\in\mathbb{Z}} f^n_{i,k} m_k \Delta v$ and $m_k = (1, v_k, |v_k|^2)$. Thanks to [5], the computation of $(\mathcal{E}^n_{i,k})_{k\in\mathbb{Z}}$ does not require to solve (10). Instead, we only have to compute $\alpha^n_i \in \mathbb{R}^3$ such that $\mathcal{E}^n_{i,k} = \exp(\alpha^n_i \cdot m_k)$, $\forall k \in \mathbb{Z}$ holds.

Now, in order to decompose the velocity domain, we have to define a discretized version of the ball $B_1 = B_1(t, x)$. We consider a special case where $\underline{u}$ and $\underline{T}$ are chosen as the global mean velocity $u(t, x)$ and temperature $T(t, x)$ respectively. They are approximated by:

$$\underline{u}^n_i = \frac{U^n_i(2)}{U^n_i(1)}, \qquad \underline{T}^n_i = \frac{U^n_i(3)U^n_i(1) - (U^n_i(2))^2}{(U^n_i(1))^2},$$

where $U^n_i(j)$ is the j-th component of U^n_i, R remains an arbitrary parameter. Then, $B_1(t^n, x_i) \simeq \mathcal{K}^n_i = \{v_k = k\Delta v,\ k \in \mathbb{Z} \text{ s.t. } |v_k - \underline{u}^n_i| \leqslant R\sqrt{\underline{T}^n_i}\}$. We introduce the approximation unknowns of the hybrid model (8),

$$U^n_{1,i} = \sum_{k\in\mathcal{K}^n_i} m_k f^n_{i,k} \Delta v \quad \text{and} \quad f^n_{2,i,k} = \begin{cases} f^n_{i,k} & \text{if } k \in \mathbb{Z} \setminus \mathcal{K}^n_i, \\ 0 & \text{otherwise.} \end{cases}$$

We denote by $\phi^n_{1,i,\pm}(g) = \sum_{k\in\mathcal{K}^n_i} v^{\pm}_k m_k g_k \Delta v$, the discrete fluxes; $U^n_{(1),i} = \sum_{k\in\mathcal{K}^n_i} m_k \mathcal{E}^n_{i,k}\Delta v$ are the moments of $(\mathcal{E}^n_{i,k})_k$ on $\mathcal{K}^n_i$. Afterwards, we approximate $(f^n_{i,k})_{k\in\mathbb{Z}}$, $\forall k \in \mathcal{K}^n_i$, by the solution $(\mathcal{M}^n_{1,i,k})_{k\in\mathcal{K}^n_i}$ of the following minimization problem:

$$\mathrm{Min}\left\{ \sum_{k\in\mathcal{K}^n_i} g_k \log(g_k)\Delta v,\ g_k \geqslant 0 \text{ s.t. } \sum_{k\in\mathcal{K}^n_i} m_k g_k \Delta v = U^n_{1,i} \right\}. \tag{11}$$

This problem is solved in the same way as (10). Taking the moments of (9) on $\mathcal{K}^n_i$ and, on the other hand, restricting (9) to $\mathbb{Z}\setminus\mathcal{K}^n_i$ yields:

$$\begin{aligned} U^{n+1/2}_{1,i} &= U^n_{1,i} - \frac{\Delta t}{\Delta x}\left[\phi^n_{1,i,+}\left(\mathcal{M}^n_{1,i}\right) - \phi^n_{1,i,+}\left(\mathcal{M}^n_{1,i-1} + f^n_{2,i-1}\right)\right] \\ &\quad - \frac{\Delta t}{\Delta x}\left[\phi^n_{1,i,-}\left(\mathcal{M}^n_{1,i+1} + f^n_{2,i+1}\right) - \phi^n_{1,i,-}\left(\mathcal{M}^n_{1,i}\right)\right] + \frac{\Delta t}{\varepsilon}\left[U^n_{(1),i} - U^n_{1,i}\right], \end{aligned} \tag{12}$$

$$\begin{aligned} f^{n+1/2}_{2,i,k} &= f^n_{2,i,k} - v^+_k \frac{\Delta t}{\Delta x}\left[f^n_{2,i,k} - \mathcal{M}^n_{1,i-1,k} - f^n_{2,i-1,k}\right] \\ &\quad - v^-_k \frac{\Delta t}{\Delta x}\left[\mathcal{M}^n_{1,i+1,k} + f^n_{2,i+1,k} - f^n_{2,i,k}\right] + \frac{\Delta t}{\varepsilon}\left[\mathcal{E}^n_{i,k} - f^n_{2,i,k}\right], \end{aligned} \tag{13}$$

where $U^{n+1/2}_{1,i}$ and $f^{n+1/2}_{2,i,k}$ are intermediate variables that only take account of the space variation of $\mathcal{K}^n_i$ through the fluxes.

The next step of the splitting is to consider time variations of $\mathcal{K}^n_i$. To that purpose, we construct $(\mathcal{M}^{n+1/2}_{1,i,k})_{k\in\mathcal{K}^n_i}$ the Maxwellian realizing the minimum of (11) with the prescribed moments equal to $U^{n+1/2}_{1,i}$. Then we define $g^{n+1}_{i,k} = f^{n+1/2}_{2,i,k} + \mathcal{M}^{n+1/2}_{1,i,k}$, $\forall k \in \mathbb{Z}$, the moments of which are an approximation of U^{n+1}_i. At this level, $\mathcal{K}^{n+1}_i$ can be defined. The unknowns at the next time step are finally: $U^{n+1}_{1,i} = \sum_{k\in\mathcal{K}^{n+1}_i} m_k g^{n+1}_{i,k}\Delta v$, $f^{n+1}_{2,i,k} = g^{n+1}_{i,k}|_{\mathbb{Z}\setminus\mathcal{K}^{n+1}_i}$. The following proposition ensures the conservativity of the above scheme.

Proposition 3.1. *Eqs.* (12), (13) *together with the splitting procedure, give a numerical scheme that preserves the total mass, momentum and energy.*

Now, we present some numerical results. We compare the discrete hybrid model to the discrete BGK model (9) and to the exact solution of the Sod shock tube problem. The initial conditions are: $(\rho_L, u_L, p_L) = (1., 0., 1.)$, $(\rho_R, u_R, p_R) = (0.125, 0., 0.1)$. The numerical parameters are: 100 cells in space ($\Delta x = 1/100$), 80 cells in velocity ($\Delta v = 0.25$) and $\Delta t = 3.33 \times 10^{-4}$. Moreover $\varepsilon = 10^{-3}$ and $R = 2$. The solution is observed at 0.18 s.

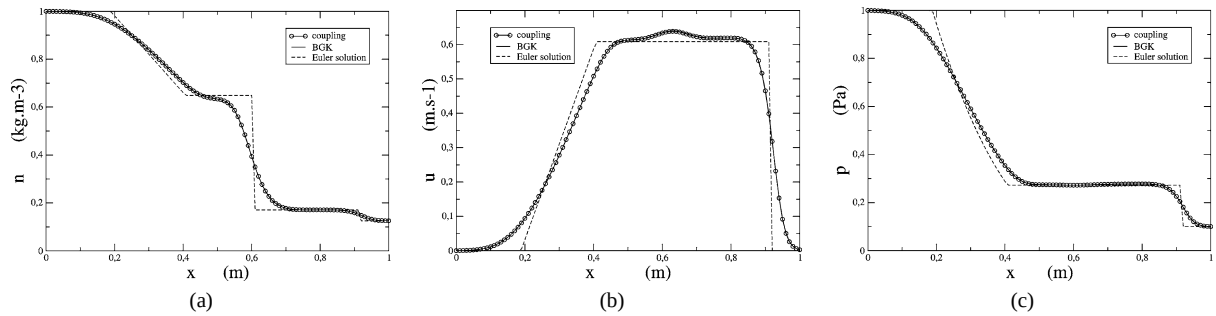

Fig. 1. (a) Density; (b) velocity; (c) pressure.

Fig. 1. (a) Densité ; (b) vélocité ; (c) pression.

Figs. 1(a)–(c) represent respectively the density, velocity and pressure (circle curves) profiles with the above conservative scheme as a function of the space variable x. We have also plotted the numerical solution of the BGK model (continuous curves) and the exact solution of the Euler equations (discontinuous curves). The hybrid numerical solution is nearly superposed on the BGK solution; the rarefaction, the contact discontinuity and the shock are well described by the hybrid model.

4. Conclusion

We have presented a new model for the description of particles far from equilibrium. A velocity domain decomposition enables us to consider differently fast and low particles. Then we used a closure strategy (only for slow particles) based on the minimization entropy principle. An explicit scheme of this model, which satisfies the conservation laws is then presented. Our results appear to compare favorably with the BGK numerical solution. Nevertheless, the method has to be extended to more realistic relaxation time, or collision operator. A second order scheme can also be written.

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