Hybrid multiscale methods for hyperbolic and kinetic equations

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Outline

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Introduction
Multiscale problems

- A broad range of scientific problems involve multiple scales and multi-scale phenomena (material science, chemistry, fluid dynamics, biology...). These involve different physical laws which govern the processes at different scales.
- On the computational side, several important classes of numerical methods have been developed which address explicitly the multiscale nature of the solutions (wavelets, multigrid, domain decomposition, stiff solvers, adaptive mesh refinements...).
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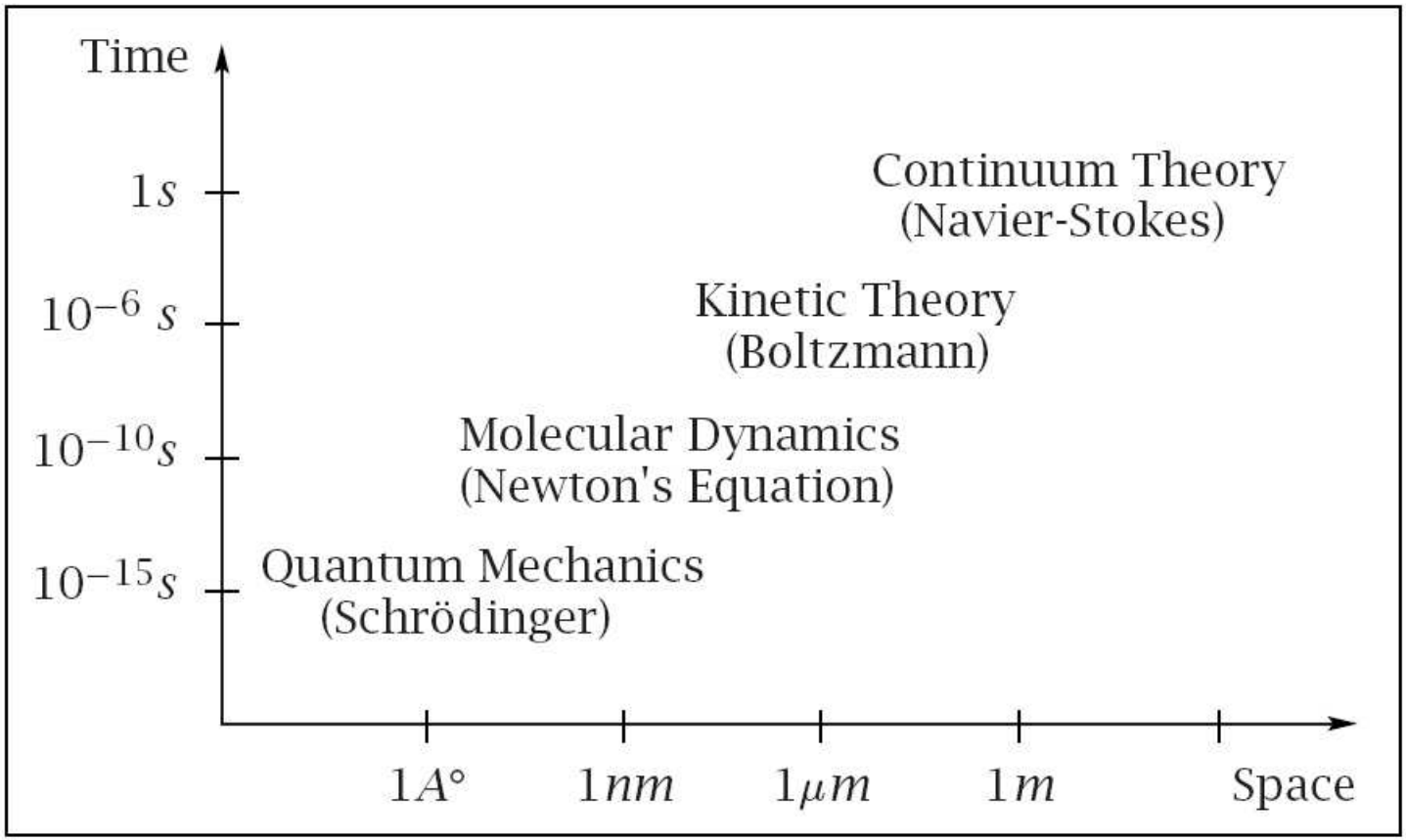
The different scales



Multiscale methods

- Couplings of atomistic or molecular, and more generally microscopic stochastic models, to macroscopic deterministic models based on ODEs and PDEs is highly desirable in many applications. Similar arguments apply also to numerical methods[1].
- A classical field where this coupling play an important rule is that of hyperbolic system with relaxation and kinetic equations. In such system the time scale is proportional to the relaxation time ε and a strong model (and dimension) reduction is obtained when $\varepsilon \to 0$.

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Jin-Xin system

A simple prototype example of relaxation system is given by

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$$\begin{cases} \partial_t u + \partial_x v &= 0, \\ \partial_t v + \partial_x a u &= -\frac{1}{\varepsilon}(v - f(u)), \end{cases} \qquad \text{(microscale)}$$

where $u = u(x,t)$, $v = v(x,t)$, $(x,t) \in \mathbb{R} \times \mathbb{R}_+$.

For small values of ε we get the local equilibrium

$$v = f(u)$$

and (subcharacteristic condition $a > f'(u)^2$) we obtain at $O(\varepsilon)$

$$\partial_t u + \partial_x f(u) = \varepsilon \partial_x ((a - f'(u)^2)\partial_x u). \qquad \text{(macroscale)}$$

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Broadwell model

A simple kinetic model for a gas was introduced by Broadwell

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$$\begin{cases} \partial_t f + \partial_x f = \frac{1}{\varepsilon}(h^2 - fg), \\ \partial_t g + \partial_x g = \frac{1}{\varepsilon}(h^2 - fg), \\ \partial_t h = -\frac{1}{\varepsilon}(h^2 - fg), \end{cases} \qquad \text{(microscale)}$$

Here f, h, and g denote the mass densities of particles with speed 1, 0, and -1, respectively.
The fluid variables are density $\varrho = f + 2h + g$ and momentum $\rho u = f - g$. In addition we define $z = f + g$.

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A local equilibrium is obtained when the state variables satisfy

$$\varrho^2 + (\rho u)^2 - 2\varrho z = 0, \Rightarrow z = \frac{1}{2}\varrho(1+u^2)$$

Thus as $\varepsilon \to 0$ one gets the set of Euler equations

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Hyperbolic relaxation systems

We consider the general case of hyperbolic relaxation systems

[G.Chen, D.Levermore, T.P.Liu, CPAM '94]

$$\partial_t U + \partial_x F(U) = \frac{1}{\varepsilon} R(U), \quad x \in \mathbb{R}, \qquad \text{(microscale)}$$

where $R : \mathbb{R}^N \to \mathbb{R}^N$ is a relaxation operator if there exists a $n \times N$ matrix Q with $rank(Q) = n < N$ such that $QR(U) = 0 \quad \forall\, U \in \mathbb{R}^N$.

This gives n independent "conserved" quantities $u = QU$ that uniquely determine a local equilibrium

$$U = \mathcal{E}(u), \qquad R(\mathcal{E}(u)) = 0.$$

For $\varepsilon \to 0 \Rightarrow R(U) = 0 \Rightarrow U = \mathcal{E}(u)$ and under a suitable subcharacteristic condition on $\mathcal{F}(u)$ we have

$$\partial_t u + \partial_x \mathcal{F}(u) = 0, \qquad \mathcal{F}(u) = QF(\mathcal{E}(u)). \qquad \text{(macroscale)}$$

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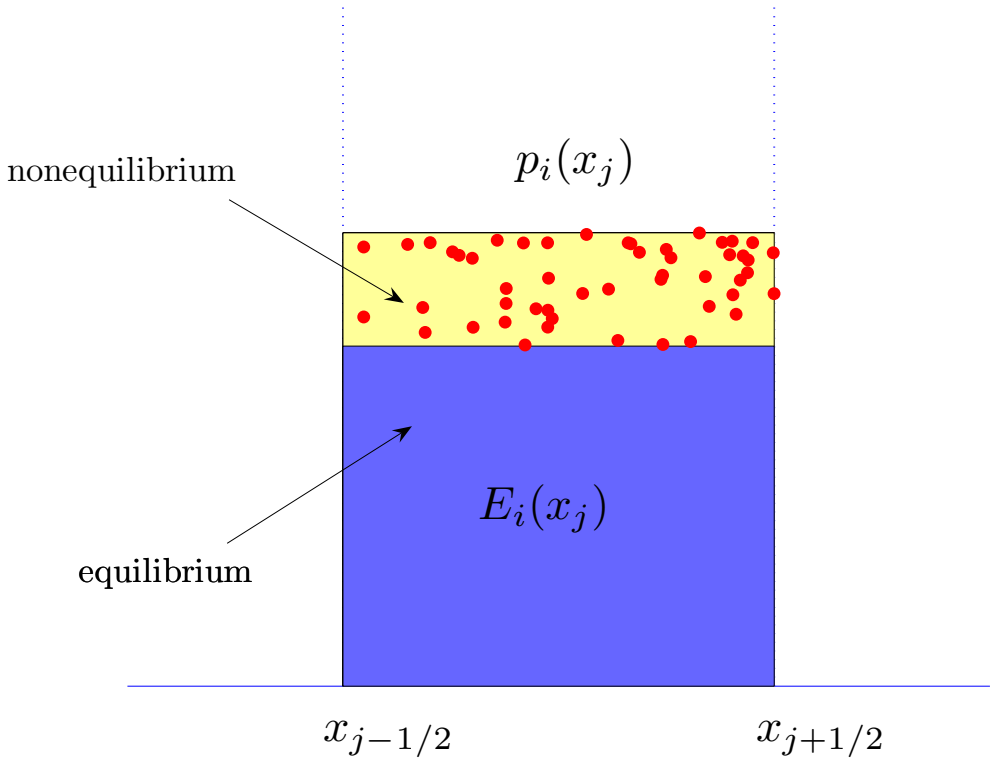
The Hybrid Method

Hybrid cell representation

The solution in each space cell is represented as a combination of a nonequilibrium part (microscale) and an equilibrium part (macroscale)



The starting point in the construction of the methods is the following[2]

Definition (I-hybrid function)

Given a discrete probability density p_i, $i = 1, \dots, N$ (i.e. $p_i \geq 0$, $\sum_i p_i = 1$) and a discrete probability density E_i, $i = 1, \dots, N$ called equilibrium density, we define $w_i \in [0, 1]$ and $\tilde{p}_i \geq 0$ in the following way

$$w_i = \begin{cases} \dfrac{p_i}{E_i}, & p_i \leq E_i \neq 0 \\ 1, & p_i \geq E_i \end{cases}$$

and $\tilde{p}_i = p_i - w_i E_i$. Thus p_i can be represented as

$$p_i = \tilde{p}_i + w_i E_i .$$

[2] L.P. ESAIM '05, G.Dimarco, L.P. CMS '06

Note that if we take $\beta = \min_i\{w_i\}$, and $\tilde{p}_i = p_i - \beta E_i$, we have

$$\sum_i \tilde{p}_i = 1 - \beta.$$

Let us define for $\beta \neq 1$ the discrete probability density

$$p_i^p = \frac{\tilde{p}_i}{1-\beta}.$$

The case $\beta = 1$ is trivial since it implies $p_i = E_i$, $i = 1, \ldots, N$. Thus the discrete probability density p_i, $i = 1, \ldots, N$ can be written as a convex combination of two probability densities[3]

$$p_i = (1-\beta)p_i^p + \beta E_i.$$

[3] R.E.Caflisch, L.P. JCP'99

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The general methodology

For hyperbolic system with relaxation we recall that $U(x,t) \in \mathbb{R}^N$ denotes the solution and $\mathcal{E}(v(x,t)) \in \mathbb{R}^N$ denotes the equilibrium state where $v(x,t) \in \mathbb{R}^n$ are the conserved variables.

We have the following representation

$$U(x,t) = \underbrace{\tilde{U}(x,t)}_{nonequilibrium} + \underbrace{W(x,t)\mathcal{E}(v(x,t))}_{equilibrium},$$

where $W(x,t) = \mathrm{diag}(w_1(x,t), w_2(x,t), \ldots, w_N(x,t))$, $0 \leq w_i(x,t) \leq 1$ is a $N \times N$ matrix that characterizes the equilibrium fraction and $\tilde{U}(x,t)$ the non equilibrium part of the solution.

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The nonequilibrium part is represented stochastically, whereas the equilibrium part deterministically. The general methodology is the following.

- Solve the evolution of the non equilibrium part by Monte Carlo methods. Thus $\tilde{U}(x,t)$ will be represented by a set of samples (particles) in the computational domain.
- Solve the evolution of the equilibrium part by deterministic methods. Thus $W(x,t)\mathcal{E}(v(x,t))$ will be represented on a suitable grid in the computational domain.

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A simple example: Jin-Xin system

We rewrite the system in diagonal form

$$\begin{aligned} \partial_t f + \sqrt{a}\partial_x f &= -\frac{1}{\varepsilon}(f - E_f(u)) \\ \partial_t g - \sqrt{a}\partial_x g &= -\frac{1}{\varepsilon}(g - E_g(u)). \end{aligned}$$

$$f = \frac{\sqrt{a}u + v}{2\sqrt{a}},\ g = \frac{\sqrt{a}u - v}{2\sqrt{a}},\ E_f(u) = \frac{\sqrt{a}u + F(u)}{2\sqrt{a}},\ E_g(u) = \frac{\sqrt{a}u - F(u)}{2\sqrt{a}}.$$

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$$\text{(R)} \begin{cases} \partial_t f^r &= -\frac{1}{\varepsilon}(f^r - E_f(u^r)) \\ \partial_t g^r &= -\frac{1}{\varepsilon}(g^r - E_g(u^r)) \end{cases} \qquad \text{(C)} \begin{cases} \partial_t f^c + \sqrt{a}\partial_x f^c &= 0 \\ \partial_t g^c - \sqrt{a}\partial_x g^c &= 0 \end{cases}$$

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"Ansatz" on the solution structure

$$\begin{aligned} f(x,t) &= \tilde{f}(x,t) + w_f(x,t)E_f(u(x,t)), \\ g(x,t) &= \tilde{g}(x,t) + w_g(x,t)E_g(u(x,t)). \end{aligned}$$

The relaxation step (R) preserves the solution structure (the local equilibrium state is unchanged) and we obtain

$$\begin{aligned} \tilde{f}^r(x,t) &= e^{-t/\varepsilon}\tilde{f}(x,0), \quad w_f^r(x,t) = e^{-t/\varepsilon}w_f(x,0) + 1 - e^{-t/\varepsilon}, \\ \tilde{g}^r(x,t) &= e^{-t/\varepsilon}\tilde{g}(x,0), \quad w_g^r(x,t) = e^{-t/\varepsilon}w_g(x,0) + 1 - e^{-t/\varepsilon}. \end{aligned}$$

The convection step (C) destroys the structure of the solution since we have the deterministic fractions

$$w_f^r(x-\sqrt{a}t,t)E_f(u(x-\sqrt{a}t,0)), \quad w_g^r(x+\sqrt{a}t,t)E_g(u(x+\sqrt{a}t,0)).$$

Starting from the above terms we construct the new values of $w_f^c(x,t)$, $\tilde{f}^c(x,t)$, $w_g^c(x,t)$ and $\tilde{g}^c(x,t)$ using the Definition of discrete hybrid function.

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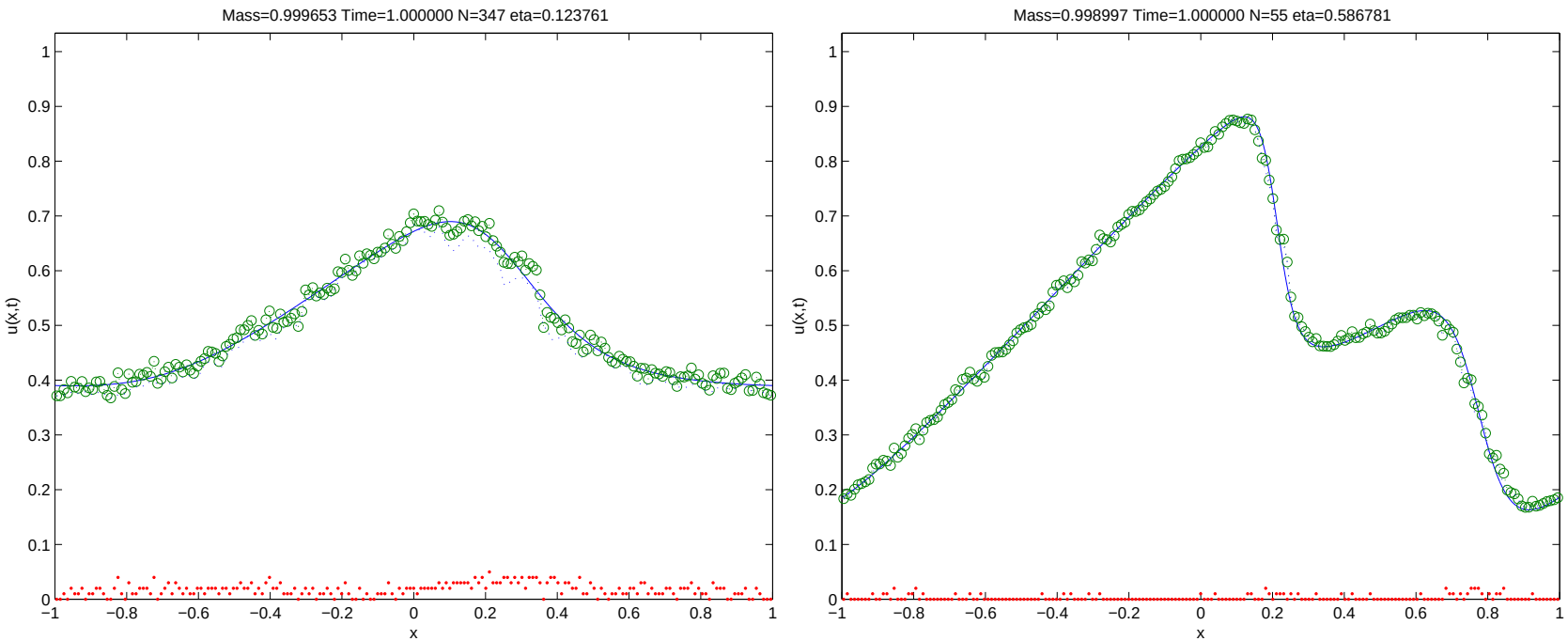
1D Example: Jin-Xin model

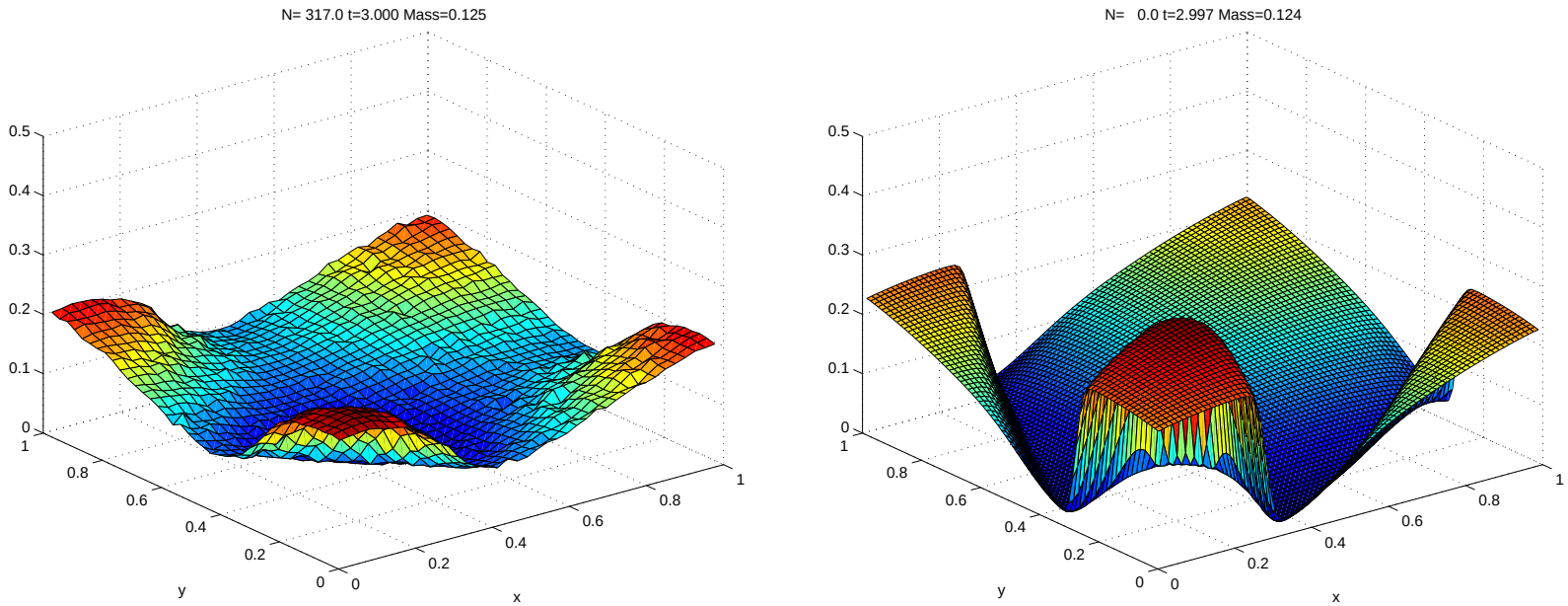
Initial data sum of sines and $w_f, w_g = 0$, with $F(u) = u^2/2$.



Solution at $t = 1$ for $\varepsilon = 0.1$ (left) and $\varepsilon = 0.01$ (right).

2D Example: Jin-Xin model

Initial data sine square and $w_f, w_g = 0$, with $F(u) = u^2/2$.



Solution at $t = 3.0$ for $\varepsilon = 0.01$ (left) and $\varepsilon = 10^{-6}$ (right).

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Remarks

- The methods developed for hyperbolic systems with relaxation can be directly extended to general discrete velocity models (DVM) of the Boltzmann equation.
- The limiting scheme $\varepsilon \to 0$ is by construction a relaxation scheme (kinetic scheme) for the equilibrium system of conservation laws (Euler equations).
- For more general kinetic equations it is desirable to have a scheme that can deal with the infinite velocity range of the model and that are based on an arbitrary fluid solver.
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Kinetic equations

Kinetic equations

$$\partial_t f + v\nabla_x f = \frac{1}{\varepsilon} Q(f,f), \quad x, v \in \mathbb{R}^d, d \geq 1$$

Here $f = f(x,v,t) \geq 0$ is the particle density and $Q(f,f)$ describes the particle interactions. In rarefied gas dynamics the equilibrium functions M for which $Q(M,M) = 0$ are local Maxwellian

$$M(\rho,u,T)(v) = \frac{\rho}{(2\pi T)^{d/2}} \exp\left(-\frac{|u-v|^2}{2T}\right),$$

$$\rho = \int_{\mathbb{R}^d} f\,dv, \qquad u = \frac{1}{\rho}\int_{\mathbb{R}^d} vf\,dv, \qquad T = \frac{1}{d\,\rho}\int_{\mathbb{R}^d} [v-u]^2 f\,dv.$$

As $\varepsilon \to 0$ the distribution function approaches M. Higher order moments can be computed as function of ρ, u, and T. To the leading order we obtain the compressible Euler equations.

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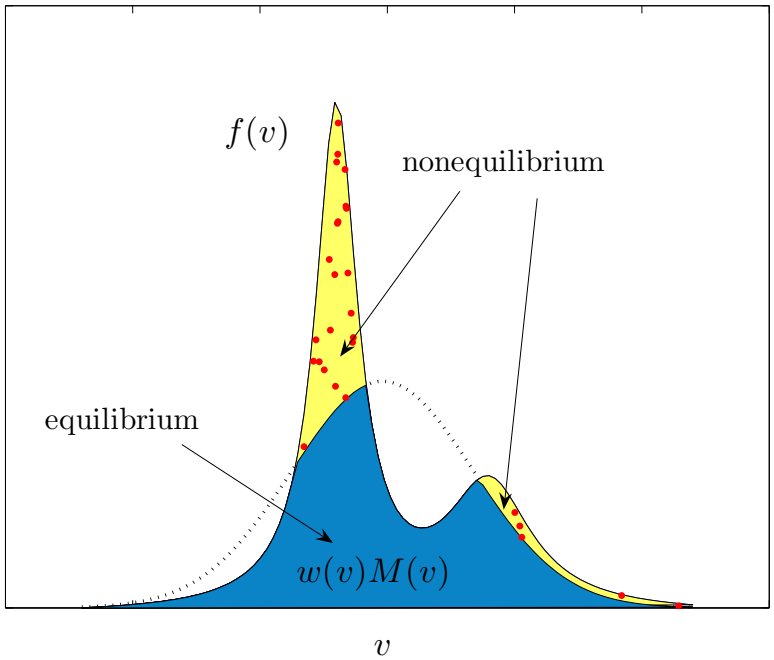
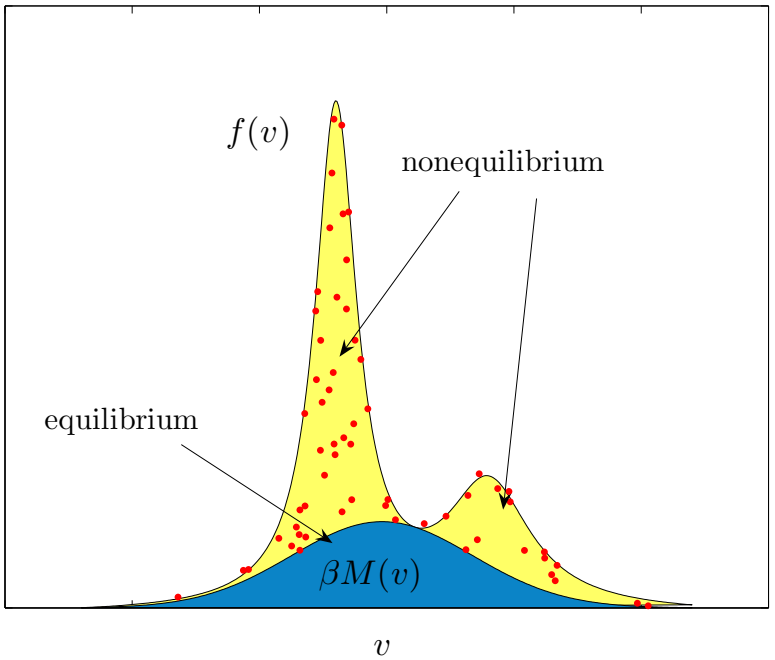
Hybrid representation

The solution is represented at each space point as a combination of a nonequilibrium part (microscale) and an equilibrium part (macroscale)





The starting point is the following[7]

Definition II - hybrid function

Given a probability density $f(v)$, $v \in \mathbb{R}^d$ (i.e. $f(v) \geq 0$, $\int f(v)dv = 1$) and a probability density $M(v)$, $v \in \mathbb{R}^d$ called equilibrium density, we define $w(v) \in [0,1]$ and $\tilde{f}(v) \geq 0$ in the following way

$$w(v) = \begin{cases} \dfrac{f(v)}{M(v)}, & f(v) \leq M(v) \neq 0 \\ 1, & f(v) \geq M(v) \end{cases}$$

and $\tilde{f}(v) = f(v) - w(v)M(v)$. Thus $f(v)$ can be represented as

$$f(v) = \tilde{f}(v) + w(v)M(v).$$

[7] L.P. ESAIM '05, L.P., G.Dimarco CMS '06

Taking $\beta = \min_v\{w(v)\}$, and $\tilde{f}(v) = f(v) - \beta M(v)$, we have

$$\int \tilde{f}(v)dv = 1 - \beta.$$

Let us define for $\beta \neq 1$ the probability density

$$f_p(v) = \frac{\tilde{f}(v)}{1-\beta}.$$

The case $\beta = 1$ is trivial since it implies $f \equiv M$. Thus we recover the hybrid representation[8] as

$$f(v) = (1-\beta)f_p(v) + \beta M(v).$$

[8] R.E.Caflisch, L.P. JCP '99

Outline

The hybrid method

Again the methods are based on a time splitting of the equation and on the hybrid representation

$$f(x,v,t) = \underbrace{\tilde{f}(x,v,t)}_{\text{nonequilibrium}} + \underbrace{w(x,v,t)M(f)(x,v,t)}_{\text{equilibrium}}.$$

The main difference is that the continuum part requires a grid (and artificial boundaries) in the velocity space (i.e. a kinetic scheme). The sample values can then take any value of the velocity grid.

Except for BGK-like models where the collision term has the form $Q(f,f) = M(f) - f$, one needs a suitable solver for the stiff nonlinear collision operator[9].

[9] E.Gabetta, L.P., G.Toscani SINUM '97

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Outline

Generalization

- The macroscale process is described by the conserved quantities $U = (\rho, u, T)$ whereas the microscale process is described by f. The two processes and state variables are related by compression and reconstruction operators P and R, such that $P(f) = U$ and $R(U) = f$, with the property $PR = I$, where I is the identity operator.
- The compression operator is a projection to low order moments). The reconstruction operator does the opposite and it is under-determined, except close to the local equilibrium state when $Q(f, f) = 0$ implies $f = M(U)$.

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We use the following decomposition on the averaged quantities

$$P(f) = U = \underbrace{P(f - M(U))}_{\text{nonequilibrium}} + \underbrace{PM(U)}_{\text{equilibrium}} = U_p + \beta U_E,$$

where U_p is obtained by standard Monte Carlo and the equilibrium part U_E is computed by any deterministic scheme.

This is obtained by solving the whole microscopic scale for f by Monte Carlo (and then computing averaged quantities) and the macroscopic scale for $PM(U)$ both by Monte Carlo and the deterministic scheme.

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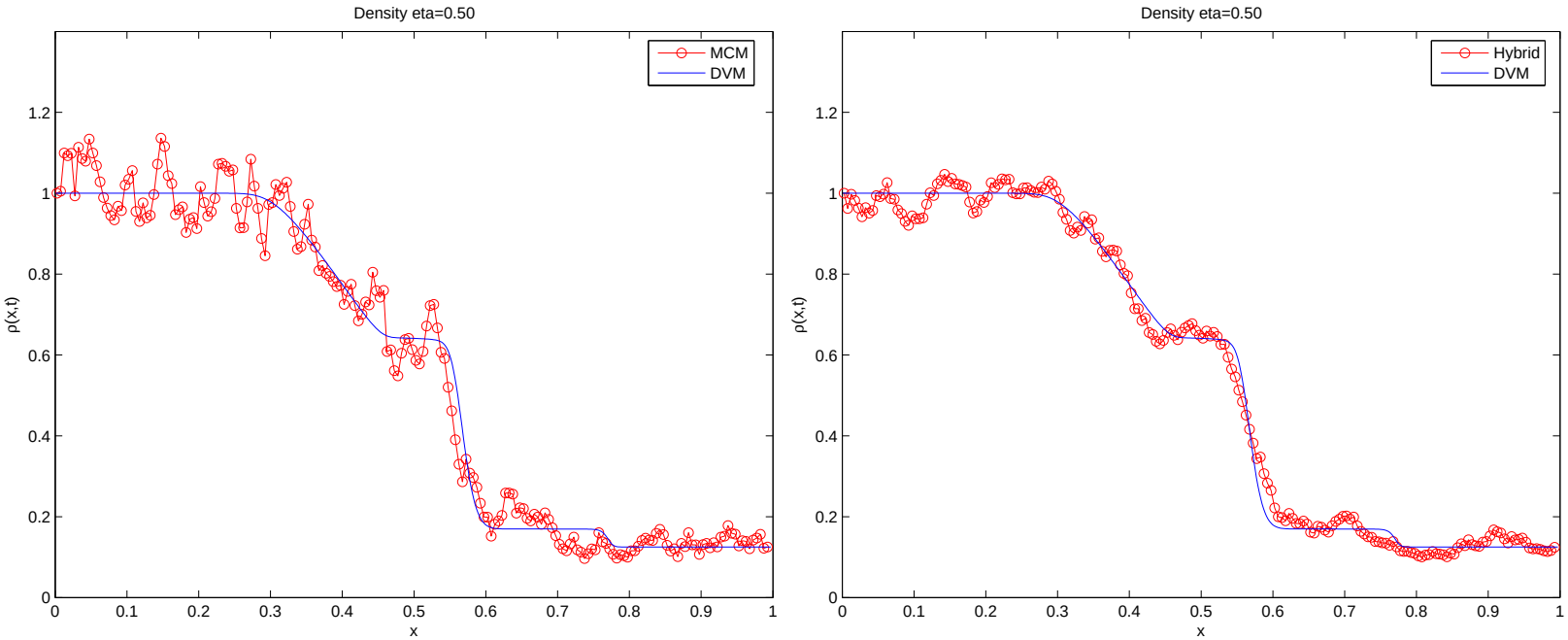
Sketch of the method

1. Solve the relaxation process by DSMC
   1. with probability $e^{-t/\varepsilon}$ the samples are unchanged
   2. with probability $1 - e^{-t/\varepsilon}$ the samples are replaced with equilibrium samples.
   3. Compute the effective $\beta = 1 - \frac{N^p}{N}$
2. Compute the macroscopic quantities U
3. Solve the Euler equations for U to obtain U_E
4. Transport the ”particle fraction”
5. Compute the stochastic term U_p using particles that were not in equilibrium before the transport
6. Compute the new solution $U = U_p + \beta U_E$

Outline

Sod test

Comparison of results for ρ, DSMC (left), HMC (right)[10].



ε is such that 50% of the solution is represented by particles in HMC.

[10] G.Dimarco, L.P. '06

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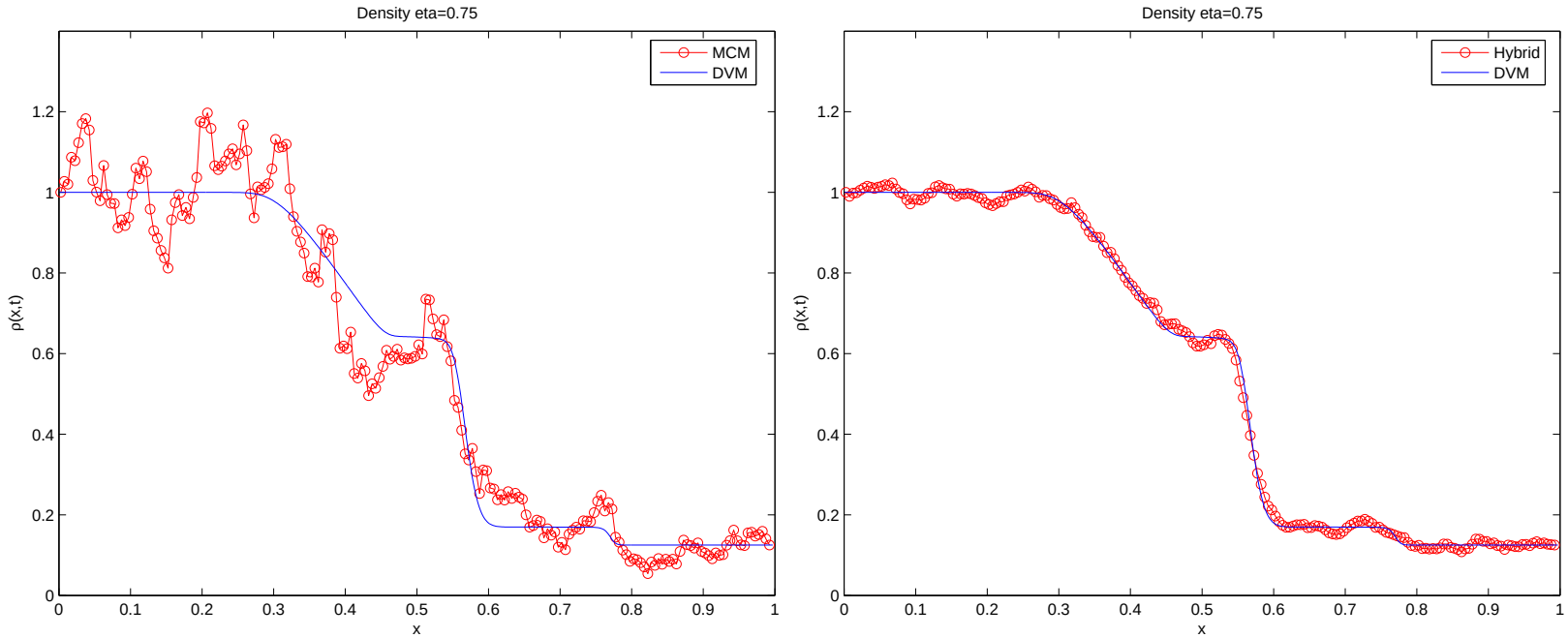
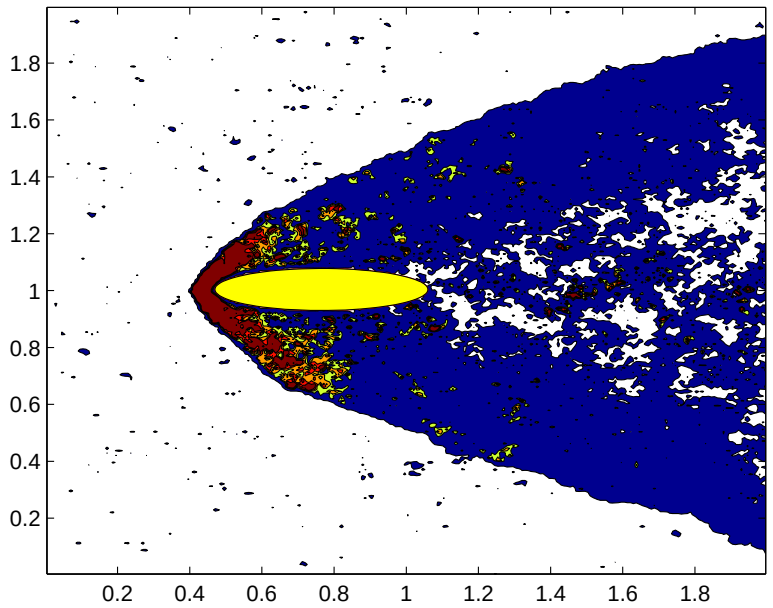
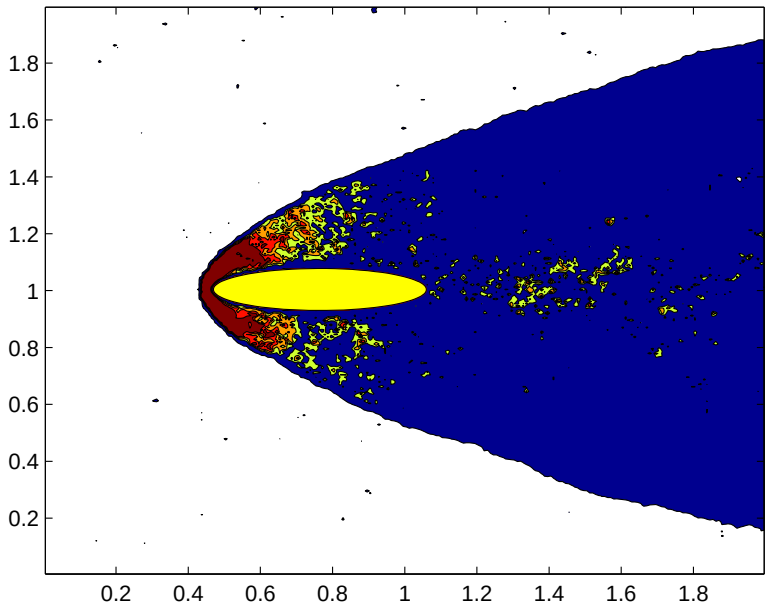


ε is such that 25% of the solution is represented by particles in HMC.

BGK equation: flow past an ellipse

Comparison of results for T, DSMC (left), HMC (right).





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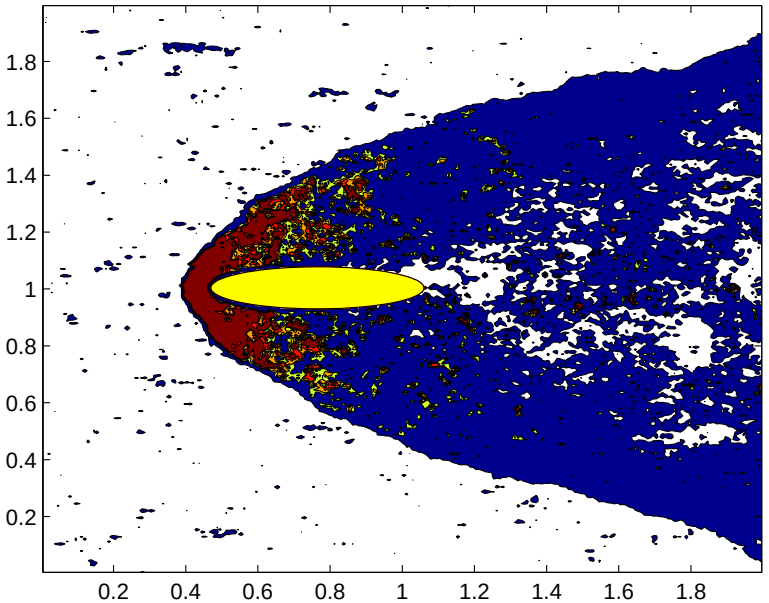
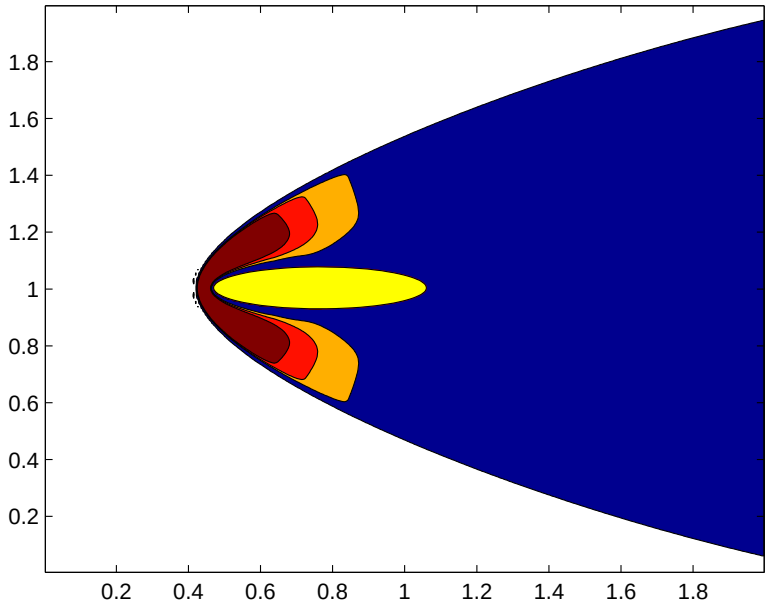
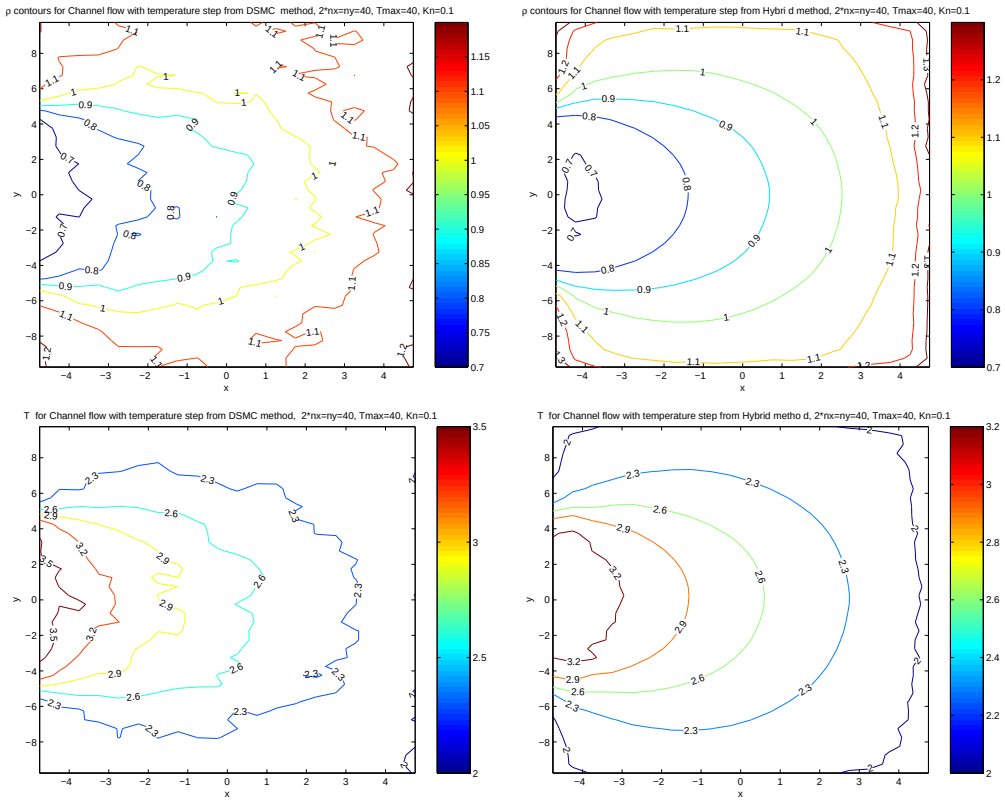




The fluid limit $\varepsilon \longrightarrow 0$.

Boltzmann equation: 2D channel flow

Comparison of results for ρ (left), T (right), DSMC (left), HMC (right)[10].



[10] R.Caflisch, H.Chen, E.Luo, L.P. AIAA '06

Conclusions

- Hybrid multiscale methods can be applied successfully to hyperbolic relaxation systems and kinetic equations.
- They have better efficiency and accuracy property with respect to standard Monte Carlo or particle methods.
- For systems with a finite number of components such as hyperbolic relaxation system and discrete velocity models a componentwise strategy permits to maximize the deterministic fraction of the solution.
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