Numerical methods for multiscale kinetic equations: asymptotic-preserving and hybrid methods

Lecture 4: Fluid-kinetic coupling and hybrid methods

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Lecture 6 Outline

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Multiscale methods

- Couplings of atomistic or molecular, and more generally microscopic stochastic models, to macroscopic deterministic models is highly desirable in many applications [1].
- A classical field where this coupling play an important rule is that of kinetic equations. In such system the time scale is proportional to a relaxation time ε and a strong model (and dimension) reduction is obtained when $\varepsilon \to 0$.
- The amount of literature in this direction is enormous [2]. Several different techniques are possible and often the implementation details are of fundamental importance for the effective understanding of the methods.
- Here we limit ourselves to illustrate some *examples*, that we consider to be representative of some common ideas used in this context [3].

[1] W.E, B.Engquist '03

[2] J. Burt, I. Boyd '09; T. Homolle, N. Hadjiconstantinou '07; P. Degond, G. Dimarco, L. Mieussens '07; ...

[3] G. Dimarco, L. Pareschi '07-'08, P. Degond, G. Dimarco, L. Pareschi '11

Kinetic equations

Kinetic equations

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

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

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

where we define the density, mean velocity and temperature as

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

Fluid limit

If we multiply the kinetic equation by its collision invariants $(1, v, |v|^2)$ and integrate the result in velocity space we obtain five equations that describe the balance of mass, momentum and energy.
As $\varepsilon \to 0$ we have $Q(f) \to 0$ and thus f approaches the local Maxwellian $M[f]$. Higher order moments of f can be computed as function of ρ, u, and T and we obtain the closed system

Compressible Euler equations

$$\begin{cases} \partial_t \varrho + \nabla_x \cdot (\varrho u) = 0, \\ \partial_t \varrho u + \nabla_x \cdot (\varrho u \otimes u + p) = 0, \\ \partial_t E + \nabla_x \cdot (u(E + p)) = 0, \end{cases} \qquad \text{(macroscale)}$$

where p is the gas pressure.

Generalizations

- 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

$$P(f) = U, \qquad R(U) = f,$$

  with the property $PR = I$, where I is the identity operator.

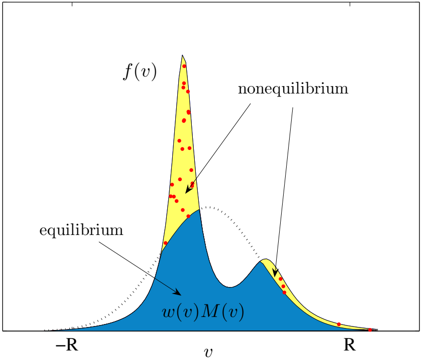
- The compression operator is a projection to low order moments

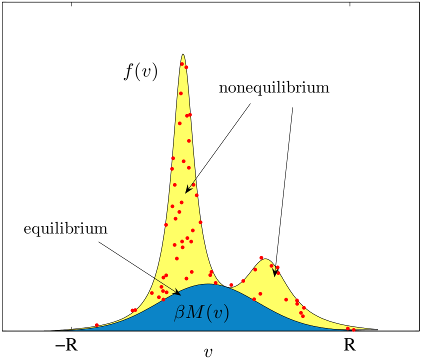
$$P(f) = \int_{\mathbb{R}^d} f \left(\begin{array}{c} 1 \\ \frac{v}{\rho} \\ \frac{|v-u|^2}{d\rho} \end{array} \right) dv.$$

  The reconstruction operator does the opposite and it is *under-determined*, except close to the local equilibrium state when $Q(f) = 0$ implies $f = M[f](U)$.

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[4]

Definition - 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

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

[4] L.P. '05, L.P., G.Dimarco '06, '08

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[5] as

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

[5] R.E.Caflisch, L.P. '99

The general methodology

Now we consider the following general representation

Hybrid decomposition

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

The nonequilibrium part $\tilde{f}(x,v,t)$ is represented stochastically, whereas the equilibrium part $w(x,v,t)M(\rho(x,t),u(x,t),T(x,t))(v)$ deterministically. The general methodology is the following.

- Solve the evolution of the non equilibrium part by Monte Carlo methods. Thus $\tilde{f}(x,v,t)$ is represented by a set of samples (particles) in the computational domain.
- Solve the evolution of the equilibrium part by deterministic methods. Thus $w(x,v,t)M(\rho(x,t),u(x,t),T(x,t))(v)$ is obtained from a suitable grid in the computational domain.

The general methodology

The starting point of the method is the classical operator splitting which consists in solving first a homogeneous collision step

$$(C) \quad \partial_t f^r(x,v,t) = \frac{1}{\varepsilon} Q(f^r, f^r)(x,v,t)$$

and then a free trasport step

$$(T) \quad \partial_t f^c(x,v,t) + v \cdot \nabla_x f^c(x,v,t) = 0.$$

Except for BGK-like models where the collision term has the form $Q(f,f) = M - f$, one needs a suitable solver for the stiff nonlinear collision operator[4].

[4] E.Gabetta, L.P., G.Toscani '97; G. Dimarco, L.P. '13

Sketch of the basic method

C: Starting from a hybrid function $f(t) = \tilde{f}(t) + w(t)M(t)$ solve the collision step $f^r(t+\Delta t) = \lambda f(t) + (1-\lambda)M(t)$ with $\lambda = e^{-\Delta t/\varepsilon}$.

1. The new value $\tilde{f}^r(t+\Delta t) = \lambda \tilde{f}(t)$ is computed by particles.
2. Set $w^r(t+\Delta t) = \lambda w(t) + 1 - \lambda$.
3. Discard a fraction of Monte Carlo samples since $w^r(t+\Delta t) \geq w(t)$.

T: Starting from the hybrid function $f^r(t+\Delta t)$ computed above solve the transport step $f(x,v,t+\Delta t) = f^r(x - v\Delta t, v, t+\Delta t)$.

1. Transport the particle fraction $\tilde{f}^r(x - v\Delta t, v, t+\Delta t)$ by simple particles shifts.
2. Transport the deterministic fraction $w^r(x - v\Delta t, v, t+\Delta t)M(x - v\Delta t, v, t)$ by a deterministic scheme.
3. Project the computed solution to the hybrid form $f(t+\Delta t) = \tilde{f}(t+\Delta t) + w(t+\Delta t)M(t+\Delta t)$.

Remarks

Note that point 2 of the transport corresponds to a Maxwellian shift analogous to that usually performed in the so called kinetic or Boltzmann schemes for the Euler equations[5].

Clearly point 3 after the transport step is crucial for the details of the hybrid method. We have considered three different possibile reconstructions

(0) We loose entirely equilibrium thus $w(x, v, t + \Delta t) = 0$.

(C) We compute the new equilibrium fraction from $w^r(x - v\Delta t, v, t + \Delta t)M(x - v\Delta t, v, t)$ using definition I.

(1) We compute the new equilibrium fraction from $w^r(x - v\Delta t, v, t + \Delta t)M(x - v\Delta t, v, t)$ using definition I and take the minimum $\beta = min_v\{w(x, v, t + \Delta t)\}$

Off course the different reconstructions are strictly connected to the choice of the macroscopic solver used in point 2.

[5] S.Deshpande '79, B.Perthame '90

Macroscopic solvers I

Methods based on discrete velocity model[6] (HM methods).

Main features

- Representation $f(v) = \tilde{f}(v) + w(v)M(v)$
- Discretize the velocity space.
- Solve the deterministic and stochastic part with a DVM.
- Compact support, equilibrium functions $\mathcal{E}_f$ differ from Maxwellian $\mathcal{E}_f \neq M_f$.
- We need to solve a non linear system for each cell at each time step.
- Time step restrictions from deterministic transport step.

[6] L. Mieussens'00, L.P. G.Dimarco '07

Macroscopic solvers II

II) Methods based on the full kinetic equation (BHM methods).

Main features

- Representation $f(v) = \tilde{f}_R(v) + w_R(v)M(v)$ where $w_R(v) = 0$ for $v \notin [-R, R]^d$.
- Discretize velocity space only in the central part $v \in [-R, R]^d$.
- Tails are treated by particles.
- Shorter computational time due to time step increase, no need of nonlinear iterations, and to less mesh points in velocity space.
- More fluctuations due to the the presence of the tails.

[7] L.P., G.Dimarco '08, P.Degond, G.Dimarco, L.Mieussens '07

Macroscopic solvers III

III) Methods independent from the fluid solver (FSI methods).

Main features

- Representation $f(v) = \tilde{f}(v) + \beta M(v)$, $\beta = \min_v\{w(v)\}$.
- Solve relaxation in the usual way to get $\beta^r(t)$.
- Solve the transport (equilibrium and nonequilibrium part) with a Monte Carlo method.
- Solve the Euler equations with initial data $U^E(t) = P(\beta^r(t)M(t))$ to get the moments $U^E(t+\Delta t)$. We have $P(\beta^r(x-v\Delta t,t)M(x-v\Delta t,v,t)) = U^E(t+\Delta t) + O(\Delta t^2)$.
- Apply a moment matching only to the advected equilibrium particles so that the above equation is satisfied exactly.
- Additional difficulties sin the reconstruction since the kinetic information are only available through particles.

[8] L.P., G.Dimarco '08

Accuracy test

Smooth solution in 1D (velocity and space) with periodic boundary conditions. L_1 norm of the errors for temperature respect to different value of the Knudsen number ε (in units of 10^{-2}).

	$\varepsilon = 10^{-2}$	$\varepsilon = 10^{-3}$	$\varepsilon = 10^{-4}$	$\varepsilon = 10^{-5}$	$\varepsilon = 10^{-6}$
MCM	3.2923	4.4354	6.2404	5.7733	6.1142
HM	2.9520	2.7893	2.6305	0.96996	0.2840
HM1	2.8437	2.5110	1.6132	0.6617	0.2053
CHM	1.8196	1.2004	0.5368	0.1310	0.0651
BHM	3.1869	3.0254	2.8536	2.1430	1.8134
BHM1	2.7132	2.6807	2.3756	2.0148	2.1010
BCHM	2.6210	2.3226	2.1498	1.9315	1.8849

$N = 1500$ particles for cell, $v \in [-15, 15]$ for HM schemes, $R = 5$ for BHM schemes, $\Delta v = 0.16$ and $\Delta x = 0.05$.

	$\varepsilon = 10^{-2}$	$\varepsilon = 10^{-3}$	$\varepsilon = 5 * 10^{-4}$	$\varepsilon = 10^{-4}$
MCM	6.762	7.611	7.578	7.316
FSI	7.007	6.022	4.500	0.641
FSI1	6.662	4.939	3.773	0.598

$N = 200$ particles for cell $\Delta x = 0.05$.

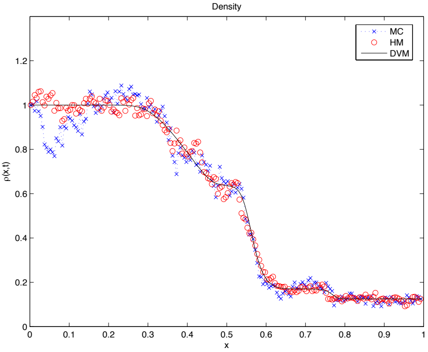
Computational cost

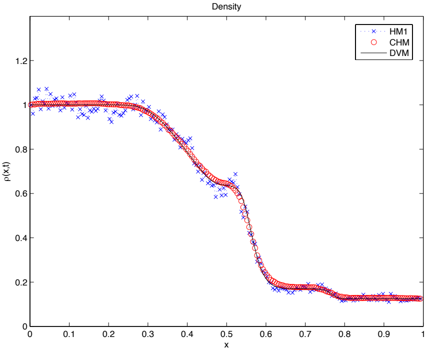
Smooth solution in 1D (velocity and space) with periodic boundary conditions.

	$\varepsilon = 10^{-2}$	$\varepsilon = 10^{-3}$	$\varepsilon = 10^{-4}$	$\varepsilon = 10^{-5}$
MCM N=1500	23 sec	25 sec	27 sec	26 sec
BHM N=1500	35 sec	25 sec	22 sec	22 sec
BHM1 N=1500	34 sec	20 sec	19 sec	20 sec
BCHM N=1500	15 sec	11 sec	17 sec	21 sec
FSI N=1500	25 sec	22 sec	3 sec	0.6 sec
FSI1 N=1500	18 sec	17 sec	2 sec	0.6 sec
FSI N=500	9 sec	8 sec	0.4 sec	0.3 sec
FSI N=500	7 sec	6 sec	0.4 sec	0.3 sec

Sod test

Comparison of results for ρ for HM and CHM with $\varepsilon = 10^{-3}$ [9].

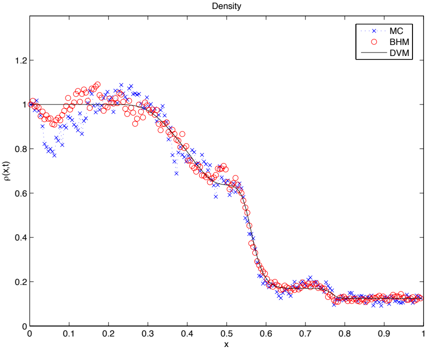


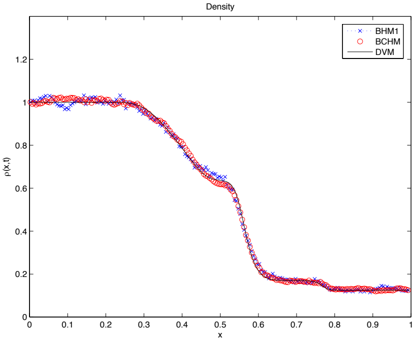


[9] G.Dimarco, L.P. '06

Sod test

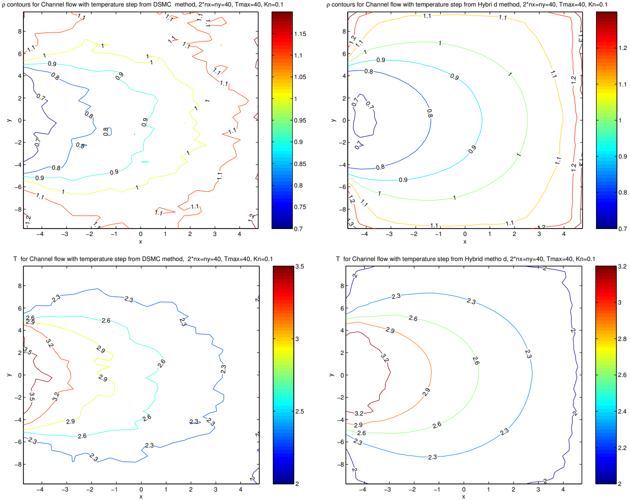
Comparison of results for ρ for BHM and BHM1 with $\varepsilon = 10^{-3}$.





Boltzmann equation: 2D channel flow

Comparison of results for ρ (left), T (right), DSMC (left), HM1 (right)[10].



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

Hydro-guided Monte Carlo: basic principles

- The basic idea consists in obtaining reduced variance Monte Carlo methods forcing particles to match prescribed sets of moments given by the solution of deterministic macroscopic fluid equations[6].
- These macroscopic models, in order to represent the correct physics for all range of Knudsen numbers include a kinetic correction term, which takes into account departures from thermodynamical equilibrium.
- We will focus on a basic matching technique between the first three moments of the macroscopic and microscopic equations. However, in principle, it is possible to force particles to match also higher order moments, which possibly can further diminish fluctuations.
- The general methodology described in the following is independent from the choice of the collisional kernel (Boltzmann, Fokker-Planck, BGK etc..).

[6] G.Dimarco, P.Degond, L.P., '09

The setting

Consider a kinetic equation of the form

$$\partial_t f + v \cdot \nabla_x f = Q(f,f)$$

The operator $Q(f,f)$ is assumed to satisfy

$$\int_{-\mathbb{R}^3} \phi(v) Q(f,f)(v) dv = 0$$

where $\phi(v) = (1, v, |v|^2)$ are the collision invariants.
We define

$$U = \int_{-\mathbb{R}^3} \phi(v) f(v) dv = (\rho, \rho u, 2E).$$

The HG method

The starting point of the methods is the following micro-macro decomposition

$$f(v) = M(v) + g(v).$$

The function $g(v)$ represents the non equilibrium part and it is not strictly positive. Now the moments vector U and $g = f - M$ satisfy the coupled system of equations

$$\partial_t U + \partial_x \int_{\mathbb{R}^3} v f \phi(v)\, dv + \partial_x \int_{\mathbb{R}^3} v g \phi(v)\, dv = 0$$

$$\partial_t f + v \partial_x f = Q(f, f).$$

Our scope is to solve the kinetic equation with a Monte Carlo method, and contemporaneously the fluid equation with any type of finite difference or finite volume scheme and than match the resulting moments. Similar decomposition strategies can be used also for low Mach number flows [7].

[7] N.Hadjiconstantinou, 05

The HG method

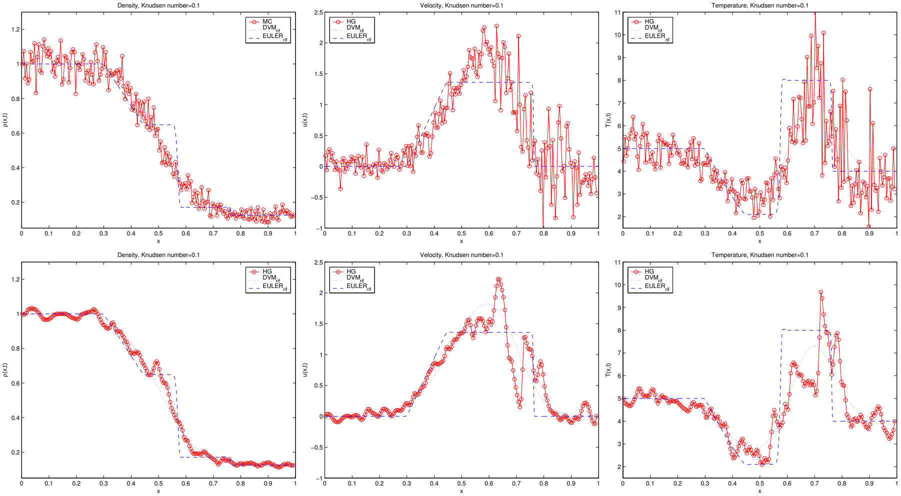
Note that the two systems, with the same initial data, furnish the same results in terms of macroscopic quantities apart from numerical fluctuations.
We summarize the method in the following way

1. Solve the kinetic equation and obtain a first set of moments.
2. Solve the fluid equation with the preferred finite volume/difference scheme.
3. Match the moments of the two models through a transformation of samples values.
4. Restart the computation for the next time step.

Step 3 of the above procedure requires great care. If we restrict to moments up to second order then a standard moment matching procedure based on a velocity (linear) transformation can be applied.
In the sequel we apply the method to the case of the BGK operator for an unsteady shock problem.

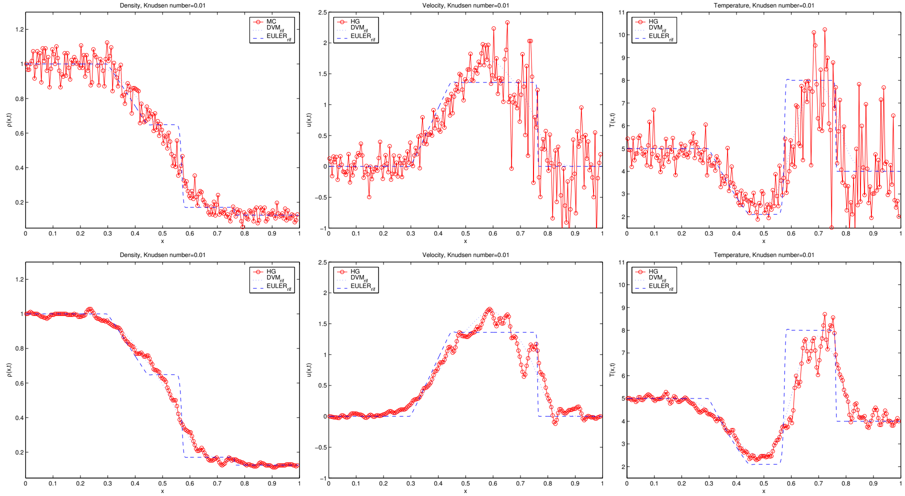
Sod's shock tube: $\varepsilon = 0.1$

BGK solution at $t = 0.05$ for density, velocity and temperature. MC method (top), Moment Guided MC method (bottom). Knudsen number $\varepsilon = 0.1$.



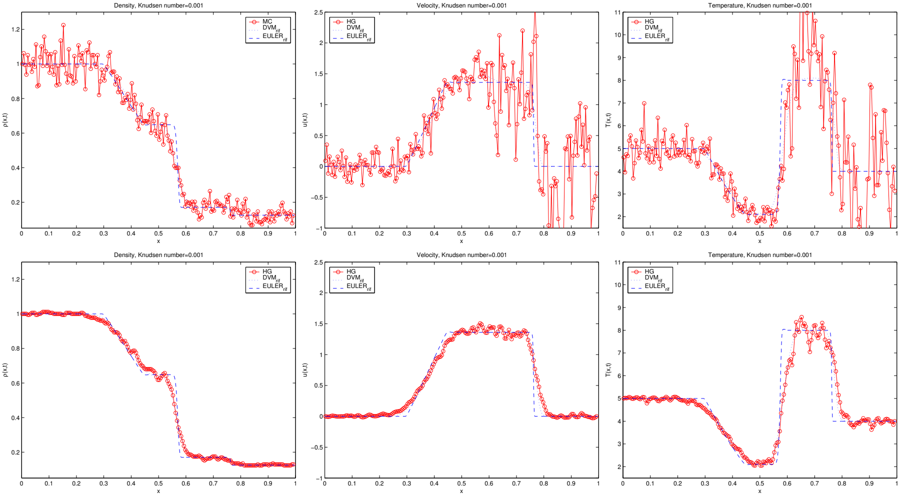
Sod's shock tube: $\varepsilon = 0.01$

BGK solution at $t = 0.05$ for density, velocity and temperature. MC method (top), Moment Guided MC method (bottom). Knudsen number $\varepsilon = 0.01$.



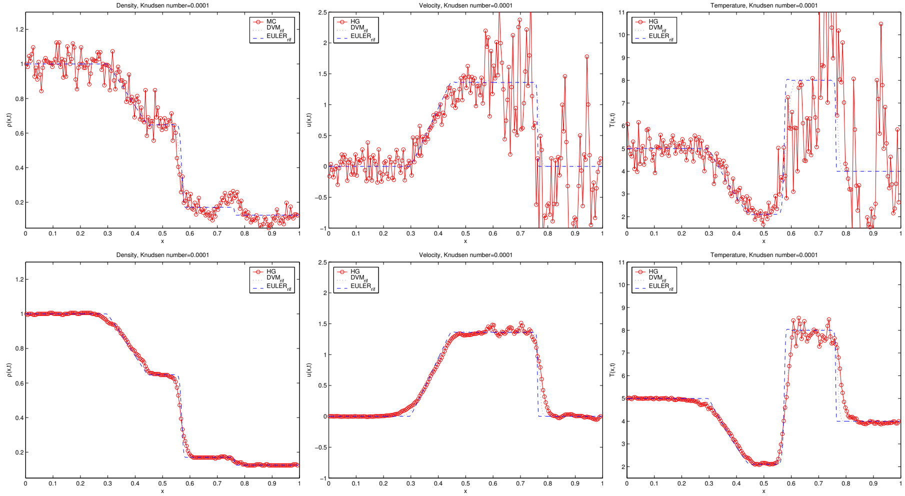
Sod's shock tube: $\varepsilon = 0.001$

BGK solution at $t = 0.05$ for density, velocity and temperature. MC method (top), Moment Guided MC method (bottom). Knudsen number $\varepsilon = 0.001$.



Sod's shock tube: $\varepsilon = 0.0001$

BGK solution at $t = 0.05$ for density, velocity and temperature. MC method (top), Moment Guided MC method (bottom). Knudsen number $\varepsilon = 0.0001$.



Further reading and conclusion remarks

- A survey of some hybrid approaches has been presented in
  - G. Radtke, J.-P. Péraud, N. Hadjiconstantinou (2013), 'On efficient simulations of multiscale kinetic transport', *Phil. Trans. R. Soc. A*
  - G. Dimarco, L. Pareschi (2014), 'Numerical methods for kinetic equations', *Acta Numerica*
- There are several important aspects concerning the numerical solution of kinetic equations that we skipped or quickly mentioned in the present survey:
  - Numerical discretization of the collision operator. The major difficulty is related to the high computational cost and the need to preserve some structural properties of the equation (conservations, entropy, steady state,...). Spectral methods are an affective way to overcome some of these difficulties..
  - Moment based methods. The problem of finding high order closures to the moment system for small and moderate Knudsen numbers has been tackled by several authors with the goal to avoid the expensive solution of the kinetic equation.
  - New emerging applications of kinetic models. Recently, kinetic equations have found applications in new areas like car traffic flows, tumor immune cells competition, bacterial movement, wealth distributions, opinion formation, flocking, ... In these new emerging fields the construction of accurate numerical methods for kinetic equations will play a major rule in the future.