Implicit schemes for the equation of the BGK model

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Motivation for BGK model

The BGK model (Bhatnagar-Gross-Krook '54) approximates Boltzmann equation for the evolution of a rarefied gas for small and moderate Knudsen numbers:

$$\mathrm{Kn} = \frac{\text{mean free path}}{\text{characteristic length of the problem}}$$

Lately, interest in this model has increased because:

- Several desirable properties have been shown to hold for the BGK model and its variants, such as BGK-ES, (Perthame et al. from 1989 on)

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- The BGK model has been extended to include more general fluids and can now be applied to the flow of a polytropic gas (Mieussens) and to mixtures of reacting gases (Aoki et al.)

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Lately, interest in this model has increased because:

- New applications of kinetic models have appeared. For instance, fluid flow in nanostructures can be described by the BGK model, since it occures at moderate Knudsen numbers

Outline

The main topics of the talk

- The BGK equation and its properties

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- Numerical difficulties

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- Microscopically Implicit, Macroscopically Explicit (MiMe) schemes

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- Numerical examples
- Asymptotic properties of MiMe schemes

BGK model

The main variable is the mass density f of particles in the point $x \in \mathbb{R}^d$ with velocity $v \in \mathbb{R}^N$ at time t, thus $f = f(x, v, t)$. The evolution of f is given by:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\tau} \left(f_M - f \right),$$

with initial condition $f(x, v, 0) = f_0(x, v) \geq 0$. With this notation $f(x, v, t)$ becomes a probability density dividing by $\rho(x, t)$. Here τ is the collision time $\tau \simeq Kn$, so $\tau > 0$ and in the hydrodynamic regime τ can be very small.

The Maxwellian

f_M is the local Maxwellian function, and it is built starting from the macroscopic moments of f:

$$f_M(x,v,t) = \frac{\rho(x,t)}{(2\pi RT(x,t))^{N/2}} \exp\left(-\frac{||v-u(x,t)||^2}{2RT(x,t)}\right),$$

where ρ and u are the gas macroscopic density and velocity and T is the temperature. They are computed from f as:

$$\begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} = \left\langle f \begin{pmatrix} 1 \\ v \\ \frac{1}{2}||v||^2 \end{pmatrix} \right\rangle \qquad \text{where} \qquad \langle g \rangle = \int_{\mathbb{R}^N} g \, dv$$

E is total energy, and the temperature is: $NRT/2 = E - 1/2\rho u^2$, where N is the number of degrees of freedom in velocity

The Maxwellian

Thus the BGK equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\tau}\left(f_M - f\right),$$

describes the relaxation of f towards the local equilibrium Maxwellian f_M.
The local equilibrium is reached with a speed that is inversely proportional to τ. Thus the system is stiff for $\tau << 1$.

Conservation

Since

$$\begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix} = \left\langle f \begin{pmatrix} 1 \\ v \\ \frac{1}{2}||v||^2 \end{pmatrix} \right\rangle = \left\langle f_M \begin{pmatrix} 1 \\ v \\ \frac{1}{2}||v||^2 \end{pmatrix} \right\rangle$$

Conservation

As in Boltzmann equation, the first macroscopic moments of f are conserved:

$$\partial_t \langle f \rangle + \nabla_x \cdot \langle fv \rangle = 0,$$

$$\partial_t \langle fv \rangle + \nabla_x \cdot \langle v \otimes vf \rangle = 0,$$

$$\partial_t \left\langle \frac{1}{2}\|v\|^2 f \right\rangle + \nabla_x \cdot \left\langle \frac{1}{2}\|v\|^2 vf \right\rangle = 0.$$

Thus a numerical scheme for the BGK model must be conservative, and its numerical solution must converge to the Euler solution as $Kn \rightarrow 0$.

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Moreover, for $Kn \longrightarrow 0$ the macroscopic solution converges to the gas dynamic solution of Euler equations.

Entropy principle

The BGK model satisfies an entropy principle:

$$\partial_t \langle f \log f \rangle + \nabla_x \langle vf \log f \rangle \leq 0, \qquad \forall f \geq 0$$

where equality holds if and only if $f = f_M$. Thus the Maxwellian f_M is the equilibrium solution of the system.
The macroscopic entropy is:

$$S = \langle f \log f \rangle$$

Note that as $\tau \to 0$, entropy is conserved on smooth solutions, as for Euler solutions.

Numerical schemes for the BGK model

The development of numerical methods for the BGK model has started only recently.

- Yang, Huang '95
  This scheme is high order accurate in space, but only first order accurate in time

Numerical schemes for the BGK model

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- Aoki, Kanba, Takata '97
  This is a second order scheme, designed for smooth solutions

Numerical schemes for the BGK model

The development of numerical methods for the BGK model has started only recently.

- Mieussens, '00
  Second order schemes, where conservation is exactly enforced. Both explicit and implicit case are considered.
- Bennoune, Lemou, Mieussens, '08
  Micro-Macro decomposition

Numerical schemes for the BGK model

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- Andries, Bourgat, le Tallec, Perthame '02
  A stochastic Monte Carlo scheme

Numerical schemes for the BGK model

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- Pieraccini, Puppo SISC '06
  IMEX schemes for the BGK model. Non oscillatory high order schemes in space and time. The schemes are implicit in the relaxation part.
- Pieraccini, Puppo JCP '11
  Microscopically Implicit Macroscopically Explicit schemes for the BGK equation
- Alaia, Puppo, JCP '12
  A hybrid method for hydrodynamic and kinetic flow, Part II: Coupling of hydrodynamic and kinetic models

Numerical schemes for the BGK model

The development of numerical methods for the BGK model has started only recently.

- Russo, Santagati
  Lagrangian scheme
- Filbet, Jin, JCP 2010
  A class of asymptotic-preserving schemes for kinetic equations and related problems with stiff sources.
- F. Filbet and S. Jin, JSC 2011
  An asymptotic preserving scheme for the ES-BGK model of the Boltzmann equation

Numerical difficulties of BGK models

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- The BGK model is stiff both in the relaxation term and in the high microscopic speeds.
- The solution f must remain positive for all time, and should satisfy an entropy condition.
- It must reduce to free flow for $\mathrm{Kn} \to \infty$

Motivation for MiMe schemes for BGK models

In the following we will attempt the construction of a scheme which is implicit in the stiff source terms and in the fast convective modes, while still being explicit in the convective term on the macroscale, which determine the Maxwellian.

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1. The scheme is implicit in the relaxation and in the convective terms
2. The computation of the Maxwellian is still carried out explicitly. So the main non linearity of the BGK model is treated explicitly.
3. The stability condition which determines the timestep is dictated by the macroscopic modes

Structure of the implicit scheme

Let $f_{j,k}^n = f(x_j, v_k, t^n)$ and:

$$\Delta F(f^n)_{j,k} = F_{j+1/2}(f_k^n) - F_{j-1/2}(f_k^n)$$

be the convective flux difference. Then the first order discretized equation for f will be written as:

$$f_{j,k}^{n+1} = f_{j,k}^n - \lambda v_k \Delta F(f^{n+1})_{j,k} + \frac{\Delta t}{\tau_j^{n+1}} \left((f_M)_{j,k}^{n+1} - f_{j,k}^{n+1} \right)$$

The problem is that we cannot evaluate the moments at time level $n+1$ starting from known quantities, because the moments are not known at time t^{n+1}.

Computation of moments

We use an explicit discretization of the moments equations:

$$\partial_t \langle f \rangle + \nabla_x \cdot \langle fv \rangle = 0,$$

$$\partial_t \langle fv \rangle + \nabla_x \cdot \langle v \otimes vf \rangle = 0,$$

$$\partial_t \left\langle \frac{1}{2}\|v\|^2 f \right\rangle + \nabla_x \cdot \left\langle \frac{1}{2}\|v\|^2 vf \right\rangle = 0.$$

where the fluxes $\langle fv \rangle$, $\langle v \otimes vf \rangle$ and $\left\langle \frac{1}{2}\|v\|^2 vf \right\rangle$ are computed from f^n. From these equations we obtain ρ^{n+1}, u^{n+1} and T^{n+1}, under the macroscopic CFL:

$$\max\left(|u| + c\right) \Delta t \leq h$$

where c is the sound speed.

Numerical macroscopic fluxes

Write the macroscopic moment equations as:

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where $\mathbf{u}$ and $\mathbf{G}$ are

$$\mathbf{u} = \begin{pmatrix} \langle f \rangle \\ \langle fv \rangle \\ \left\langle \frac{1}{2} \|v\|^2 f \right\rangle \end{pmatrix} \qquad \mathbf{G} = \begin{pmatrix} \langle fv \rangle \\ \langle v \otimes vf \rangle \\ \left\langle \frac{1}{2} \|v\|^2 vf \right\rangle \end{pmatrix}$$

Numerical macroscopic fluxes

Write the macroscopic moment equations as:

$$\partial_t \mathbf{u}(f) = -\partial_x \mathbf{G}(f),$$

Then the equation can be discretized in space as

$$\partial_t \mathbf{u}(f) = -\frac{1}{h}\left(\mathcal{G}_{j+1/2}(\mathbf{u}) - \mathcal{G}_{j-1/2}(\mathbf{u})\right)$$

where the numerical flux $\mathcal{G}_{j+1/2} = \mathcal{G}(\mathbf{u}^-_{j+1/2}, \mathbf{u}^+_{j+1/2})$, and $\mathbf{u}^\pm_{j+1/2}$ are the left and right boundary extrapolated data at the cell interfaces, obtained from the reconstruction, applied to $\mathbf{u}$. As numerical flux, one can use the Lax Friedrichs flux splitting, or the HLL flux.

Time integration

We integrate in time the macroscopic equations with an explicit Runge-Kutta scheme:

$$\mathbf{u}(f)_j^{n+1} = \mathbf{u}(f)_j^n - \lambda \sum_l b_l \Delta \mathbf{G}_j(\mathbf{u}(f^{(l)})) \quad (1)$$

$$\mathbf{u}(f^{(l)})_j = \mathbf{u}(f)_j^n - \lambda \sum_{k=1}^{l-1} a_{l,k} \Delta \mathbf{G}_j(\mathbf{u}(f^{(k)})) \quad (2)$$

For the second order scheme, this requires to estimate $f^{(2)}$ at the new time level $t^n + \Delta t$. This is done solving the implicit equation for f with the implicit Euler scheme. We believe that this can be generalized to higher order schemes, because in all cases, the RK step is composed of first order Euler steps.

Second order integration for f

Implicit time integration can be very diffusive. For this reason, in the second order case, we choose the Crank Nicolson scheme.

$$f_{j,k}^{n+1} = f_{j,k}^{n} - \frac{\lambda}{2} v_k \left[\Delta F(f^{n+1})_{j,k} + \Delta F(f^{n})_{j,k}\right] + \frac{\Delta t}{2}\left[\frac{1}{\tau_j^{n+1}}\left((f_M)_{j,k}^{n+1} - f_{j,k}^{n+1}\right) + \frac{1}{\tau_j^{n}}\left((f_M)_{j,k}^{n} - f_{j,k}^{n}\right)\right]$$

Second order integration for f

1. The second order space discretization for f uses a second order upwind formula, which is based on the evaluation of limited slopes. This introduces non linearities in the system of equations for f^{n+1}.

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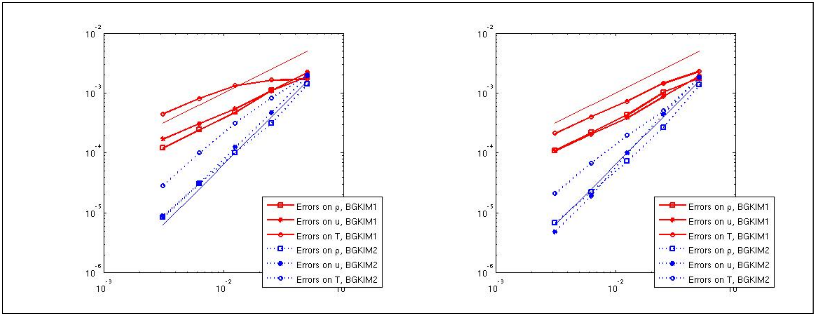
3. The same formula is used to compute the slopes of f^{n+1}, so that now the space discretization is linear in f^{n+1}.

Convergence rate



Convergence rate on macroscopic quantities for $\mathrm{Kn} = 10^{-1}$ and $\mathrm{Kn} = 10^{-2}$ in the L^1 norm, on a smooth profile.

Realigning moments

The integration of moments is conservative, because the numerical fluxes are conservative. However, f^{n+1} does not correspond exactly to the moments $\mathbf{u}^{n+1}$, which are only predicted from the old values f^n. In fact we can write:

$$\mathbf{u}^{n+1} = \mathcal{H}_u(\mathbf{u}^n, f^n)$$
$$f^{n+1} = \mathcal{H}_f(\mathbf{u}^{n+1}, f^n)$$

This effect becomes more important for large Knudsen numbers. So:

Realigning moments

1. Evaluate a local Knudsen number as: $\mathrm{Kn}_{\mathrm{loc}} = \mathrm{Kn}/\rho_x^{n+1}$. If $\mathrm{Kn}_{\mathrm{loc}} > 0.1$ in some cells, realign moments, i.e. set $\mathbf{u}^{n+1} = \langle f^{n+1}\phi(v)\rangle$.

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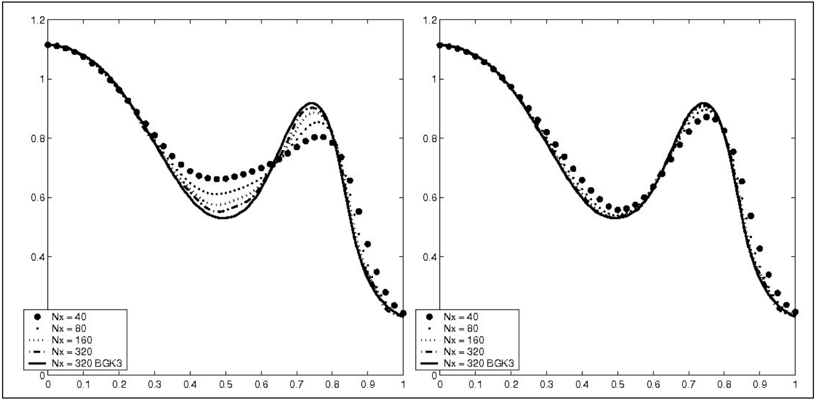
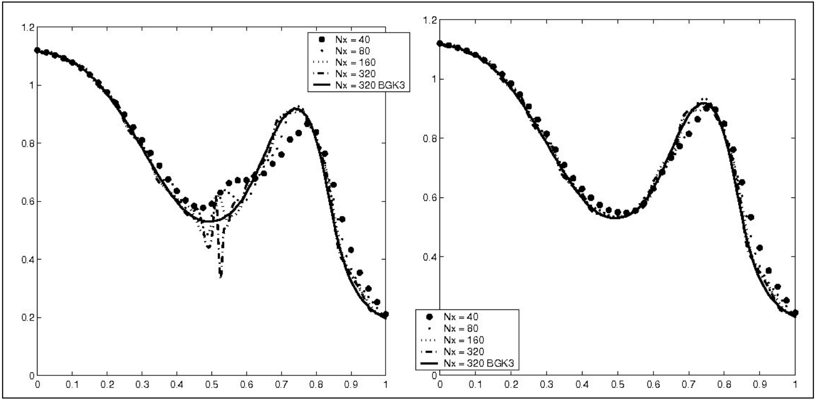
2. With this correction moments are corrected only in the first time steps for large Kn.
3. This device prevents instabilities and it accelerates the convergence rate in the kinetic regime.

Realignement of moments-1



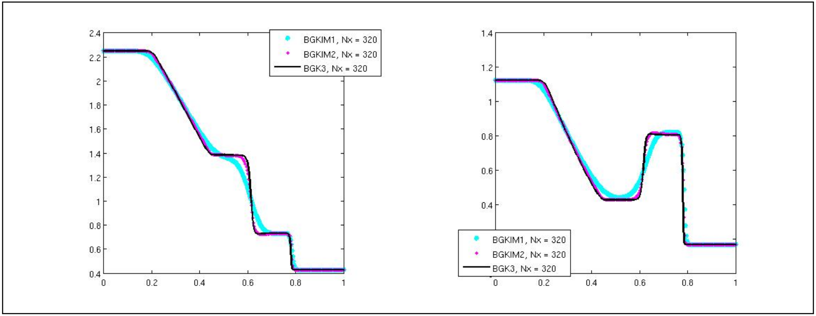
MiMe1, Kn $= 0.1$, temperature profile without (left) and with (right) realignement for several grids

Realignement of moments-2



MiMe2, Kn $= 0.1$, temperature profile without (left) and with (right) realignement for several grids

Changing the order



MiMe, $\mathrm{Kn} = 10^{-5}$, density and temperature profiles with first order MiMe scheme (cyan), second order MiMe (magenta) and third order explicit (black)

Compressible Navier Stokes

To study the asymptotic properties of MiMe schemes, we consider the simple case of 1 degree of freedom, both in space and in velocity. We write $\varepsilon\tau$ instead of τ to emphasize the small parameter in the kinetic correction. The Compressible Navier Stokes equations in this case reduce to:

$$\partial_t \begin{pmatrix} \rho \\ m \\ E \end{pmatrix} + \partial_x \begin{pmatrix} m \\ 2E \\ \frac{m}{\rho}(E+\rho T) \end{pmatrix} = \varepsilon \partial_x \begin{pmatrix} 0 \\ 0 \\ \frac{3}{2}\tau\rho T \partial_x T \end{pmatrix}$$

so that the non-equilibrium correction occurs only in the energy equation.

Compressible Navier Stokes

Thus the equations we are solving with the BGK scheme in this case reduce to:

$$\partial_t \rho + \partial_x \cdot m = 0,$$
$$\partial_t m + \partial_x \cdot (2E) = 0,$$
$$\partial_t E + \partial_x \cdot \left\langle \frac{1}{2} \|v\|^2 v f \right\rangle = 0.$$

and we want to study the heat flux correction resulting from our schemes. For simplicity we consider only the first order semidiscrete in time scheme, with one degree of freedom both in space and in microscopic velocity.

Asymptotics for semidiscrete MiMe scheme

We consider the first order in time semidiscrete MiMe scheme. In the first time step, we set $U^0 = \langle \phi f^0 \rangle$. We write $M^n = M(\mathbf{U}^n)$, where $M(\mathbf{U})$ is the Maxwellian built with the moments $\mathbf{U}$. Then the semidiscrete in time first order scheme can be written as:

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} = -\partial_x \begin{pmatrix} m^n \\ 2E^n \\ \left\langle \frac{1}{2} v^3 f^n \right\rangle \end{pmatrix}$$

$$M^{n+1} = M(\mathbf{U}^{n+1})$$

$$\frac{f^{n+1} - f^n}{\Delta t} = -v\partial_x f^{n+1} + \frac{1}{\varepsilon\tau}\left(M^{n+1} - f^{n+1}\right).$$

Asymptotics for semidiscrete MiMe scheme

Here, M^n and f^n do not have exactly the same moments, but as $\varepsilon \to 0, f^n \to M^n$. Thus we decompose f in its equilibrium and kinetic part as: $f^n = M^n + \varepsilon g^n$, but recalling that $\langle \phi g \rangle \neq 0$. Still, we can compute the first order kinetic correction starting from the equation for f, finding:

$$g^n = -\frac{\tau}{\Delta t}\left(M^n - M^{n-1}\right) - \tau v \partial_x M^n + O(\varepsilon)$$

Asymptotics for semidiscrete MiMe scheme

Substituting the kinetic correction in the energy equation, we see that the flux becomes:

$$\left\langle \frac{1}{2} v^3 f^n \right\rangle = \left\langle \frac{1}{2} v^3 M^n \right\rangle - \varepsilon\tau \left[\left\langle \frac{1}{2} v^3 \frac{(M^n - M^{n-1})}{\Delta t} \right\rangle + \partial_x \left\langle \frac{1}{2} v^4 M^n \right\rangle \right] + O(\varepsilon^2)$$

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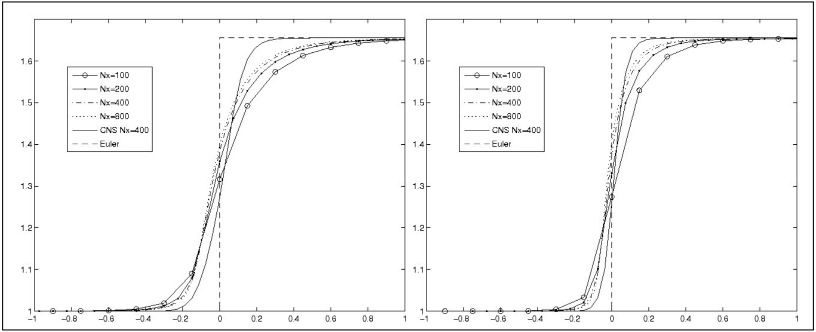
Asymptotics for semidiscrete MiMe scheme

Using the expressions $\langle v^3 M \rangle = \rho u^3 + 3\rho u T$, $\langle v^4 M \rangle = \rho u^4 + 6\rho u^2 T + 3\rho T^2$ and the conservation laws at order ε^0, we recover:

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} + \partial_x \begin{pmatrix} m \\ 2E \\ \frac{m}{\rho}(E + \rho T) \end{pmatrix} = \varepsilon \partial_x \begin{pmatrix} 0 \\ 0 \\ \frac{3}{2}\tau\rho T \partial_x T \end{pmatrix} + O(\varepsilon \Delta t + \varepsilon^2)$$

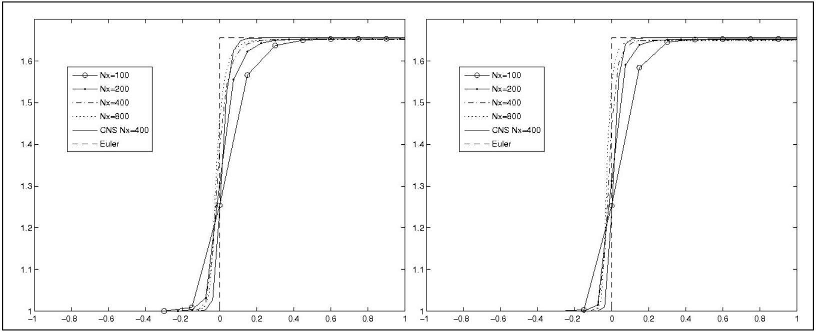
which is the Navier Stokes equation, corresponding to one degree of freedom in velocity space (which gives no shear viscosity).
Thus the semidiscrete first order MiMe scheme is consistent with the correct equation as $\Delta t \to 0$.

Convergence to CNS



MiMe2. Convergence to Compressible Navier-Stokes. Left to right: $\text{Kn} = 0.1$, $\text{Kn} = 0.05$

Convergence to CNS



MiMe2. Convergence to Compressible Navier-Stokes. Left to right, Kn $= 0.02$ and Kn $= 0.01$

Stabilization and realignement

The CNS solver is explicit and it uses a CFL:

$$\Delta t = 0.9 \min \left(\frac{h}{\alpha}, \frac{h^2}{3\mathrm{Kn}\, T_M \rho_M} \right)$$

where $\alpha = \max_x(|u| + \sqrt{3T})$ which can be quite penalising when Kn is relatively high, while MiMe scheme travels with a CFL:

$$\Delta t = 0.9 \frac{h}{\alpha}$$

The improved stability region is given by realignement. Let us see how it works...

Semidiscrete MiMe with realignement

The first order in time semidiscrete MiMe scheme with realignement can be written as follows. Given f^n:

$$\widetilde{\mathbf{U}}^n = \langle \phi f^n \rangle$$

$$\frac{\mathbf{U}^{n+1} - \widetilde{\mathbf{U}}^n}{\Delta t} = -\partial_x \begin{pmatrix} \widetilde{m}^n \\ 2\widetilde{E}^n \\ \langle \frac{1}{2} v^3 f^n \rangle \end{pmatrix}$$

$$M^{n+1} = M(\mathbf{U}^{n+1})$$

$$\frac{f^{n+1} - f^n}{\Delta t} = -v\partial_x f^{n+1} + \frac{1}{\varepsilon\tau}\left(M^{n+1} - f^{n+1}\right).$$

Semidiscrete MiMe with realignement

Again, M^n and f^n do not have exactly the same moments, but as $\varepsilon \to 0, f^n \to M^n$. Thus we decompose f as: $f^n = M^n + \varepsilon g^n$, but recalling that $\langle \phi g \rangle \neq 0$. Now the macroscopic equation can be written as:

$$\frac{\mathbf{U}^{n+1} - \mathbf{U}^n}{\Delta t} = -\langle v\phi\partial_x f^n \rangle + \frac{\widetilde{\mathbf{U}}^n - \mathbf{U}^n}{\Delta t}$$

which has the same asymptotics than the semidiscrete MiMe scheme, because the added term satisfies:

$$\frac{\mathbf{U}^{n+1} - \widetilde{\mathbf{U}}^{n+1}}{\Delta t} = \frac{\varepsilon\tau}{\varepsilon\tau + \Delta t}\partial_x \left\langle v\phi\left(f^{n+1} - f^n\right)\right\rangle = O\left(\frac{\varepsilon\Delta t}{\varepsilon\tau + \Delta t}\right).$$

Semidiscrete MiMe with realignement

On the other hand, if we consider the evolution equation for $\widetilde{\mathbf{U}}$, we have:

$$\frac{\widetilde{\mathbf{U}}^{n+1} - \widetilde{\mathbf{U}}^{n}}{\Delta t} = - \left[\frac{\varepsilon\tau}{\varepsilon\tau + \Delta t} \partial_x \left\langle v\phi f^{n+1} \right\rangle + \frac{\Delta t}{\varepsilon\tau + \Delta t} \partial_x \left\langle v\phi f^{n} \right\rangle \right].$$

In other words, if $\varepsilon \to 0$, we recover the evolution equation of MiMe scheme. If on the other hand ε is not too small, then the effect of realignement is to add an implicit term to the integration of the equation for macroscopic moments, thus increasing its stability region.

Conclusion

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Perspectives

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2. We think of using this BGK solver in domain decomposition strategies, where one could use the kinetic solver (here BGK) with the same time step of the Euler (hydrodynamic) solver. This approach has already been partially carried out in Alaia, Puppo, JCP 2012.

Thank you!