III. Kinetic-Hydrodynamics Coupling

Kinetic Equations (of monatomic gases)

$$f_t + \; k \text{ ¢ } \nabla_x f - \nabla_x V \text{ ¢ } \nabla_k f = \; 1/\varepsilon \, B(f)$$

f(t,x,k): probability density distribution

t: time x: position k: particle velocity

V(x): potential Q(f): collision operator

ε: dimensionless mean free path or Knudsen number

Properties (for elastic collisions):

conservations of mass, moment and total energy;

H-theorem (entropy condition)

Kinetic and hydrodynamics equations

- Solving kinetic equations are much more expensive than solving hydrodynamic equations
- Defined in phase space (six dimension + time)
- More expensive when mean free path（Knudsen number=mfp/ typical domain length）is small

Scales in Kinetic (Boltzmann) Equations

- When ε is small (kn $\succeq$ 0.01), the moments of f solve the compressive Euler (to leading order) or Navier-Stokes equations (to $O(\varepsilon)$) of fluid dynamics, except at initial, boundary or shock layers
- When ε is not small the fluid equations are not valid, so one has to use the kinetic equations

Multiscale Problems

- Very often one needs to deal with multiscale phenomena:

² Space shuttle reentry

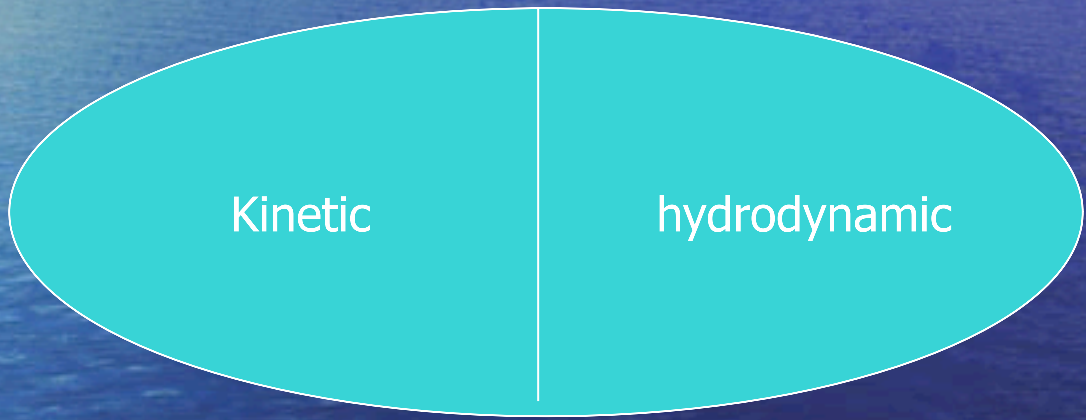
$\varepsilon : 10^{-8}$ » 1 meters

² fluid equations not accurate in boundary layers, shock layers, high Mach numbers (hypersonic flights)

² Different property of materials need different physical laws at different scales

Domain decomposition method

- Domain decomposition methods are useful in multiscale computation: coupling of microscopic and macroscopic models: multiphysics simulation



The difficulty is the interface condition: how to transfer data between different scales—often no unique solution; where to put the interface?

Asymptotic preserving methods

- Work in both kinetic and fluid regimes by solving only the kinetic equation
- When ε is small, and $\Delta x, \Delta t >> \varepsilon$ they automatically become a fluid dynamic solver

features

- No coupling with macroscopic equations, thus avoid the difficulty of interface condition/ treatment as in other multiscale methods
- AP schemes take macroscopic time steps and mesh sizes in the fluid regimes, thus are very efficient even for small Knudsen number

Fluid approximations of kinetic equations

- The Euler scaling

  moments:

  $\rho = \int f\, dk$ mass

  $\rho\, u = \int k f\, dk$ momentum

  $E = 1/2 \int |k|^2 f\, dk$ total energy

- when $\varepsilon \to 0$, $Q(f) \to 0$, then

  $f = \rho/(2\pi T)^{(d/2)} e^{-(k-u)^2/2T} = M$ local Maxwellian

- The moments ρ, $\rho\, u$, E solve the compressible Euler equations

- Chapman-Enskog expansion gives the compressible Navier-Stokes equations for $0 < \varepsilon << 1$

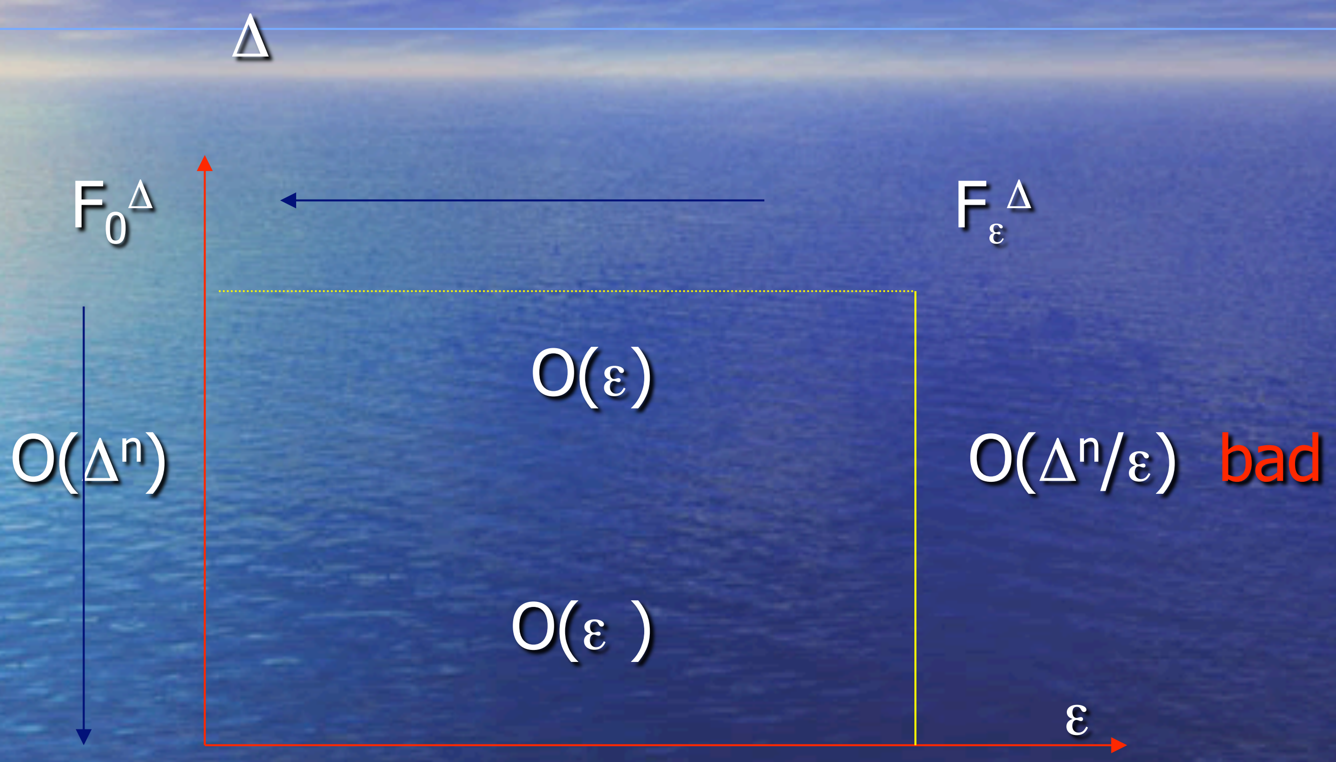
Numerical issues when ε is small

- Numerical stiffness: an explicit collision term would require $\Delta t=O(\varepsilon)$
- Implicit collision allows Δt to be independent of ε, but inverting the non-local collision term is numerically difficult and expensive
- Does the underresolved computation gives the correct macroscopic solutions?

Numerical goal

- Implicit collision that can be solved explicitly (or easily—no iterative Newton solvers): underresolved time step
- Schemes capture the macroscopic behavior without resolving the small Knudsen number
- Asymptotic-preserving:
  numerical scheme should preserve the discrete analog of the Chapman-Enskog expansion

Asymptotic preserving



limiting equation f_0 original equation f_ε

Error-estimates (*Golse-J-Levermore* SINUM '99)
for linear transport in diffusive regime

- Classical error analysis

  $|| F^{\Delta}_{\varepsilon} - f_{\varepsilon} || \succeq C\, \Delta^n/\varepsilon$

- if Asymptotic-preserving

  $|| F^{\Delta}_{\varepsilon} - f_{\varepsilon} || \succeq C\, (\Delta^n + \varepsilon)$

- This yields a uniform error estimate:

  $|| F^{\Delta}_{\varepsilon} - f_{\varepsilon} || \succeq C\, (\Delta)^{n/2}$

Development of AP schemes

- Transport and kinetic equations

  Larsen-Morel-Miller '89; Coron-Parthame '91; Jin-Levermore 93, Caflisch-Jin-Russo 95, Jin-Pareschi-Toscani '00, Klar 00, Lemou-Miusseun '08

- Hyperbolic systems with stiff relaxation

  Jin-Levermore '95

- Vlaosov-type equations in plasmas and quasineutral limit

  Crispel-Degond-Vignal '05 etc

- Fluid equations for uniform Mach number

  Haack-Jin-Liu '09 Degond-Tang '09

A simple example of AP scheme: hyperbolic system with relaxation (Jin-Xin '95)

$$u_t + v_x = 0 \quad (1)$$

$$v_t + a u_x = \frac{1}{\epsilon^2}[v - f(u)] \quad (2)$$

As $\epsilon^2 \to 0, v \to f(u)$, so the macroscopic equation is

$$u_t + f(u)_x = 0 \quad (3)$$

To solve (1) (2), use forward Euler for convection, fully implicit source term and upwind scheme for convection, then when $\epsilon^2 \to 0$, the limiting scheme is the Lax-Friedrichs scheme for (3)

This is an AP scheme for (3)

A typical numerical approach for the BGK model (Coron-Perthame SINUM '91)

$$f_t + k ¢ \nabla_x f = 1/\varepsilon (M - f)$$

Time splitting separates the two scales

- explicit scheme for (non-stiff) convection:
  $$f_t + k ¢ \nabla_x f = 0$$
- implicit scheme for stiff collision
  $$f_t = 1/\varepsilon (M\text{-}f)$$

Numerical approach

- use (non-oscillatory) shock capturing methods for convection
- Implicit collision treated explicitly

  $(f^{n+1}-f^{n})/\Delta t = 1/\varepsilon\ (M^{n+1}-f^{n+1})$

  note $M^{n+1}=M^{n}$

  due to conservation of mass, momentum and total energy

- Can be even solved exactly

  $f^{n+1}=(1-e^{-\Delta t/\varepsilon})M^{n}+ e^{-\Delta t/\varepsilon}\ f^{n}$

Asymptotic-preserving?

- For the implicit time discretization when $\varepsilon \to 0$, with Δt fixed, the collision leads to the correct local Maxwellian

  $f^{n+1} = M^{n+1}$

- also true for the exact solver

now plug into the convection step, and take moments
one gets the compressible Euler equation!

thus AP to the Euler limit (in time)

- In space, if one uses upwind for linear convection, then when $\varepsilon \to 0$, with Δx fixed, one gets the "kinetic scheme" for the Compressible Euler equations

thus AP in space

General collision operator

2 can't be explicitly solved !

- using the Wild sum

  (*Gabette,Pareschi, Toscani, '97*)

  what if the collision is not quadratic (quantum Boltzmann equation)?

Our aim is to find a simple way to integrate the nonlinear collision operator such that

1. Uniform stability in terms of ε
2. implicit collision can be handled as easily as the BGK operator
3. Asymptotic-preserving

A new idea:

- Penalize the nonlinear collision operator by the BGK operator

$$B(f, f) = [B(f,f) - \beta\,(M-f)] + \beta\,(M-f)$$

explicit ($[B(f,f) - \beta\,(M-f)]$) — implicit ($\beta\,(M-f)$)

For a suitably chosen constant β, this scheme will be uniformly stable in ε

Uniform and L-stability: an ODE example

Consider

$$f_t = [-\nu f + \beta \nu f] - \beta \nu f$$

Discretization:

$$(f^{n+1} - f^n)/\Delta t = [-\nu f^n + \beta \nu f^n] - \beta \nu f^{n+1}$$

For $\beta > ½$ the scheme is

1) Unconditionally stable
2) Converge to equilibrium: $|| f^{n+1} ||$ » $|1-1/\beta| \, ||f^n||$

(so f is driven quickly toward the local equilibrium f=0 for any initial data)

β » 1 is the best choice

An Explicit-Implicit scheme for Boltzmann

$(f^{n+1}-f^{n})/\Delta t + k$ ¢ $\nabla_x f^n$
$= 1/\varepsilon\, [B(f^n, f^n) + \beta\,(M^n - f^n] - \beta/\varepsilon\,(M^{n+1} - f^{n+1})$

Let $\beta_A = [B(f^n, f^n) - B(M^n, M^n)]/(f^n - M^n)$

stability requires: $\beta > 1/2 \sup |\beta_A|_{;}$ best choice: β » $\sup |\beta_A|_{;}$

can be made time-dependent

Explicit Implementation:
Taking the moments:
$\langle f^{n+1}-f^n \rangle/\Delta t + \nabla_x$ ¢ $\langle k\, f^n \rangle = 0$
This defines M^{n+1}. The rest is explicit!

properties

1) Stable if $\Delta t \gg \Delta x/c$ (no dependence on ε !)
2) If $\varepsilon \to 0$, then $f^{n+1} \to M^{n+1}$?

classical AP scheme requires that

$$\text{For any } f^0,\ f^n \ ¡\ M^n = O(^2) \text{ for any } n\ ,\ 1$$

namely any data will be projected to the local Maxwellian in one time step.

This scheme does NOT have this property

A related problem: Hyperbolic systems with Relaxation

$$\begin{cases} \dfrac{\partial u}{\partial t} + f_1(u,v)_x = 0\,, \\ \dfrac{\partial v}{\partial t} + f_2(u,v)_x = \dfrac{1}{\varepsilon} R(u,v)\,. \end{cases}$$

The relaxation term $R : \mathbb{R}^2 \mapsto \mathbb{R}$ is dissipative in the sense of [12]:

$$\partial_v R \leq 0\,. \tag{1.12}$$

It possesses a unique local equilibrium, namely, $R(u,v) = 0$ implies $v = g(u)$. At the local equilibrium, one has the macroscopic system

$$u_t + f_1(u, g(u))_x = 0\,.$$

This system can be derived by sending $\varepsilon \to 0$ in (1.11), the so-called zero relaxation limit ([12]).

An AP approximation

$$\frac{U^{n+1}-U^n}{\Delta t} + f_1(U^n,V^n)_x = 0, \tag{3.1}$$

$$\frac{V^{n+1}-V^n}{\Delta t} + f_2(U^n,V^n)_x = \frac{1}{\varepsilon}[R(U^n,V^n) + \beta(V^n - g(U^n))] - \frac{\beta}{\varepsilon}[V^{n+1} - g(U^{n+1})]. \tag{3.2}$$

thus if

$$\beta > \frac{1}{2}\sup|\partial_v R|,$$

there exists a constant C, and $0 < r < 1$ such that

$$|V^{n+1} - g(U^{n+1})| \le C\frac{\varepsilon\Delta t}{\varepsilon + \beta\Delta t} + r|V^n - g(U^n)|.$$

From here it is easy to see that

$$|V^n - g(U^n)| \le \frac{C}{1-r}\frac{\varepsilon\Delta t}{\varepsilon + \beta\Delta t} + r^n|V^0 - g(U^0)|$$

This clearly gives

$$|V^n - g(U^n)| \le \frac{C}{(1-r)\beta}\varepsilon + r^n|V^0 - g(U^0)| \tag{3.4}$$

If ¢ $t >>$ ², then for any V^0, there exists an $N($²$)$ such that
V^n ¡ $g(U^n) = O($²$)$ for any n , N

Some classical methods

- Linear penalty

$$[Q(f^n) - \mu f^n] + \mu f^{n+1}.$$

- Explicit Jacobian

$$Q(f^{n+1}) \approx Q(f^n) + \nabla Q(f^n)(f^{n+1} - f^n).$$

If ¢ $t >>$ ², then for any V^0, there exists an $N($²$)$ such that
V^n ¡ $g(U^n) = O($¢ $t)$ for any n ¸ N

No similar proof for Boltzmann

- But numerical results demonstrate a similar AP property

Spatial discretization

- If a high resolution upwind discretization is used for convection, then as $\varepsilon \to 0$,

one gets a high resolution kinetic scheme for Euler.

AP is space discretization!

Consistency to the Navier-Stokes equations

Chapman-Enskog expansion (fix Δt) ➔
compressible Navier-Stokes equations
$+O(\Delta t)$

Remarks:

- to capture the N-S solution one needs $\Delta t << \varepsilon$ (similar for Δx)
- Consistency error to Boltzmann: $O(\Delta t / \varepsilon)$

Higher order IMEX time descrization

- Second order Implicit-Explicit scheme

$$\begin{cases} 2\dfrac{f^* - f^n}{\Delta t} = \dfrac{Q(f^n) - P(f^n)}{\varepsilon} + \dfrac{P(f^*)}{\varepsilon}, \\[2ex] \dfrac{f^{n+1} - f^n}{\Delta t} = \dfrac{Q(f^*) - P(f^*)}{\varepsilon} + \dfrac{P(f^n) + P(f^{n+1})}{2\varepsilon}. \end{cases}$$

same AP property can be proved

Numerical examples: Sod shock tube, $\varepsilon=10^{-2}$

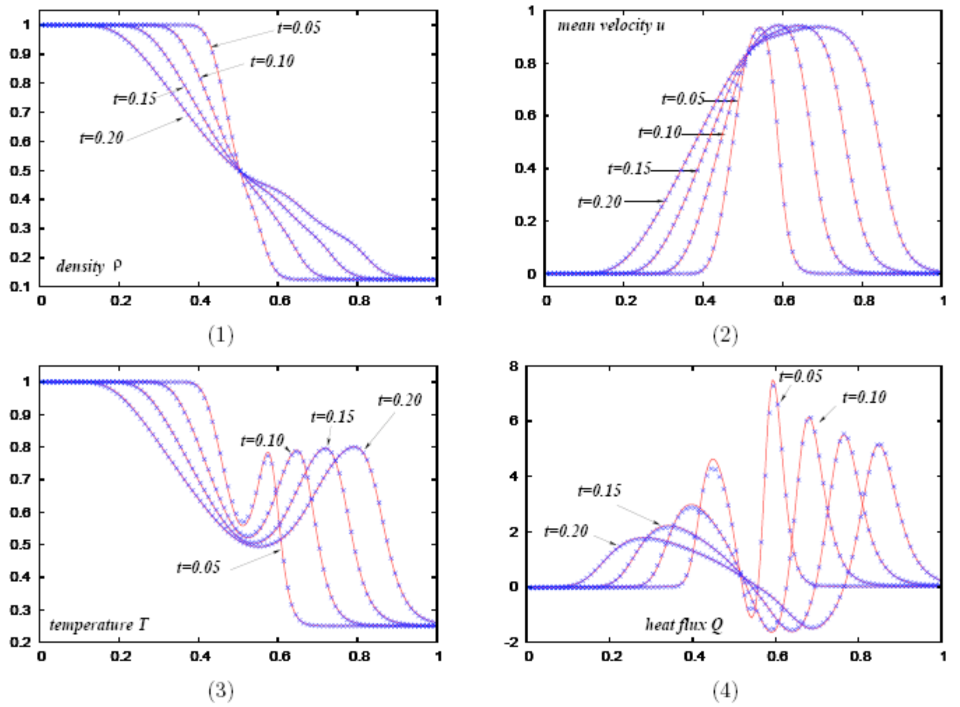


FIGURE 3. Sod tube problem ($\varepsilon = 10^{-2}$), dots (x) represent the numerical solution obtained with our second order method (2.3) and lines with the Runge-Kutta method: evolution of (1) the density ρ, (2) mean velocity u, (3) temperature T and (4) heat flux $\mathbb{Q}$ at time $t = 0.05, 0.1, 0.15$ and 0.2.

Sod shock tube: $\varepsilon=10^{-3}$

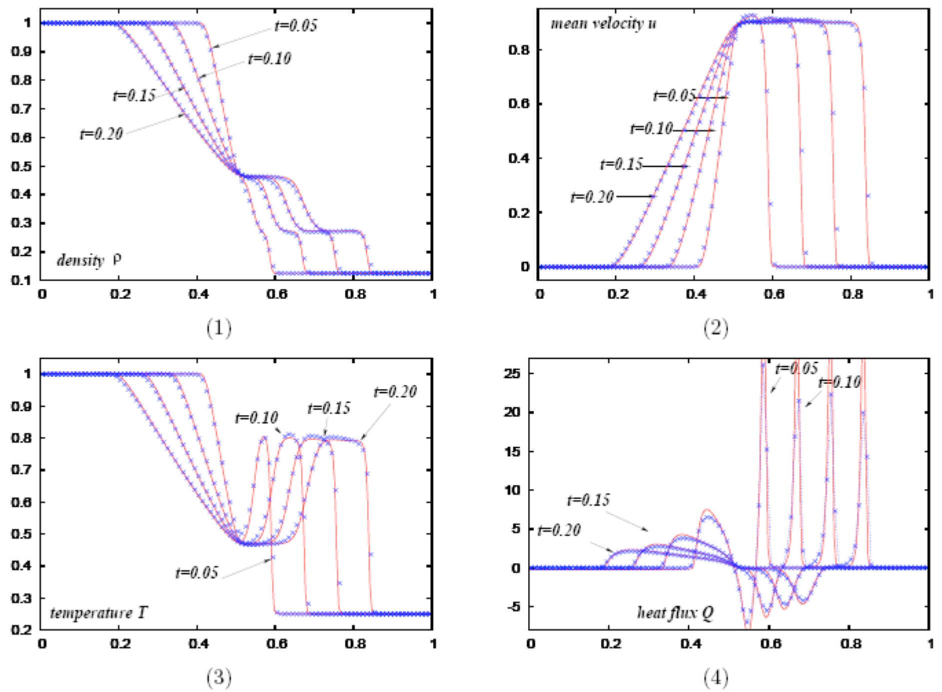
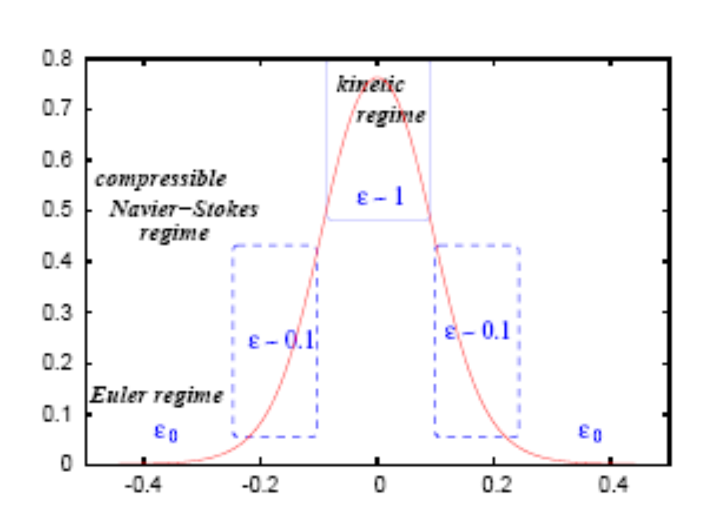


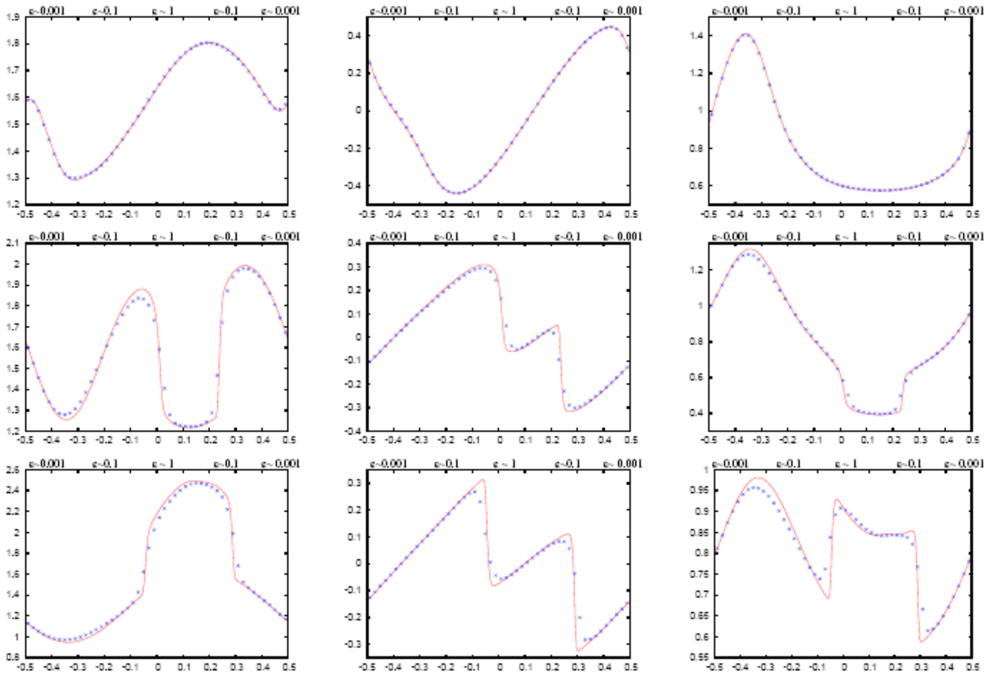
FIGURE 4. Sod tube problem ($\varepsilon = 10^{-3}$), dots (x) represent the numerical solution obtained with our second order method (2.3) and lines with the Runge-Kutta method: evolution of (1) the density ρ, (2) mean velocity u, (3) temperature T and (4) heat flux $\mathbb{Q}$ at time $t = 0.05$, 0.1, 0.15 and 0.2.

Variable ε: $\varepsilon \in [10^{-4}, 1]$



- Initial data not in local Maxwellian:

$$f_0(x,v) = \frac{\rho_0}{2}\left[\exp\left(-\frac{|v-u_0|^2}{T}\right) + \exp\left(-\frac{|v+u_0|^2}{T_0}\right)\right]$$



(1) (2) (3)

FIGURE 7. Mixing regime problem ($\varepsilon_0 = 10^{-3}$), comparison of the numerical solution to the Boltzmann equation obtained with the AP scheme (2.3) using $n_x = 50$ (dots x) and $n_x = 200$ points (line): evolution of (1) the density ρ, (2) mean velocity u, (3) temperature T at time $t = 0.25$, 0.5 and 0.75.

Other applications

- Stiff ODEs
- Hyperbolic systems with stiff relaxation

  $U_t + \nabla \text{¢} F(U) = 1/\varepsilon\ S(U)$
- High order parabolic equations
- Any dynamic system with one, stable local equalibirum

A nonlinear Fokker-Planck equation (*Carrillo-Toscani*)

- Describe a porous medium

$$\frac{\partial f}{\partial t} = \nabla_v \cdot (v f + \nabla_v f^m)$$

local Maxwellian:

$$\mathcal{M}(v) = \left(C - \frac{m-1}{2m} |v|^2 \right)_+^{1/(m-1)}$$

Entropy condition:

$$H(f) = \int_{\mathbb{R}^2} \left[|v|^2 f(t,v) + \frac{m}{m-1} f^m(t,v) \right] dv,$$

$$\frac{dH(f)}{dt} = -\int_{\mathbb{R}^2} f(t,v) \left| v + \frac{m}{m-1} \nabla f^{m-1} \right|^2 dv \le 0$$

Our Implicit-Explicit scheme

$$\frac{\partial f}{\partial t} = \underbrace{\Delta_v \left(f^m - m\,\mathcal{M}^{m-1} f\right)}_{\text{non stiff part}} + \underbrace{\nabla_v \cdot \left(v\,f + m\,\nabla_v \left(\mathcal{M}^{m-1} f\right)\right)}_{\text{stiff linear part}}$$

- Numerical example: m=3,

$$f_0(v) = \sum_{l\in\{1,2\}} \sum_{k\in\{0,\ldots,n-1\}} \frac{1}{10} 1_{\mathcal{B}(0,r_0)}(v - v_{k,l})$$

Convergence in time towards local Maxwellian

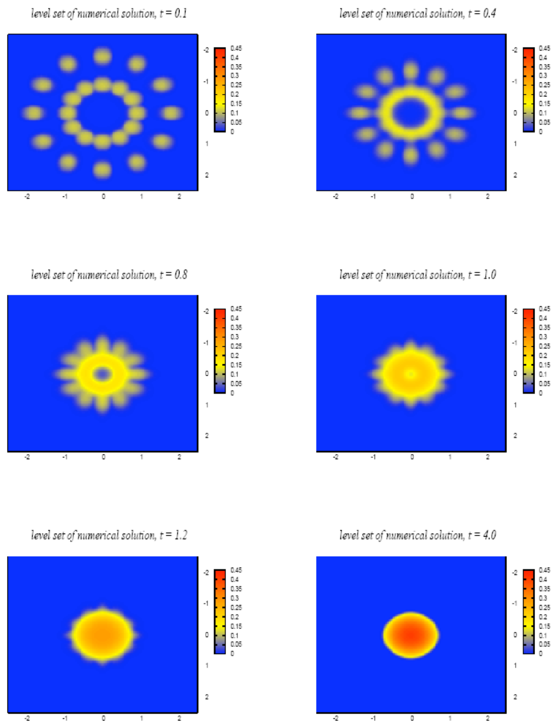


FIGURE 8. Nonlinear Fokker-Planck solution: convergence toward equilibrium (Barenblatt-Pattle distribution) obtained with the first order method (2.2) using $n_x = 100$ at time $t = 0.1, 0.4, 0.8, 1.0, 1.2$ and 4 with a large time step.

Convergence in time towards local Maxwellian

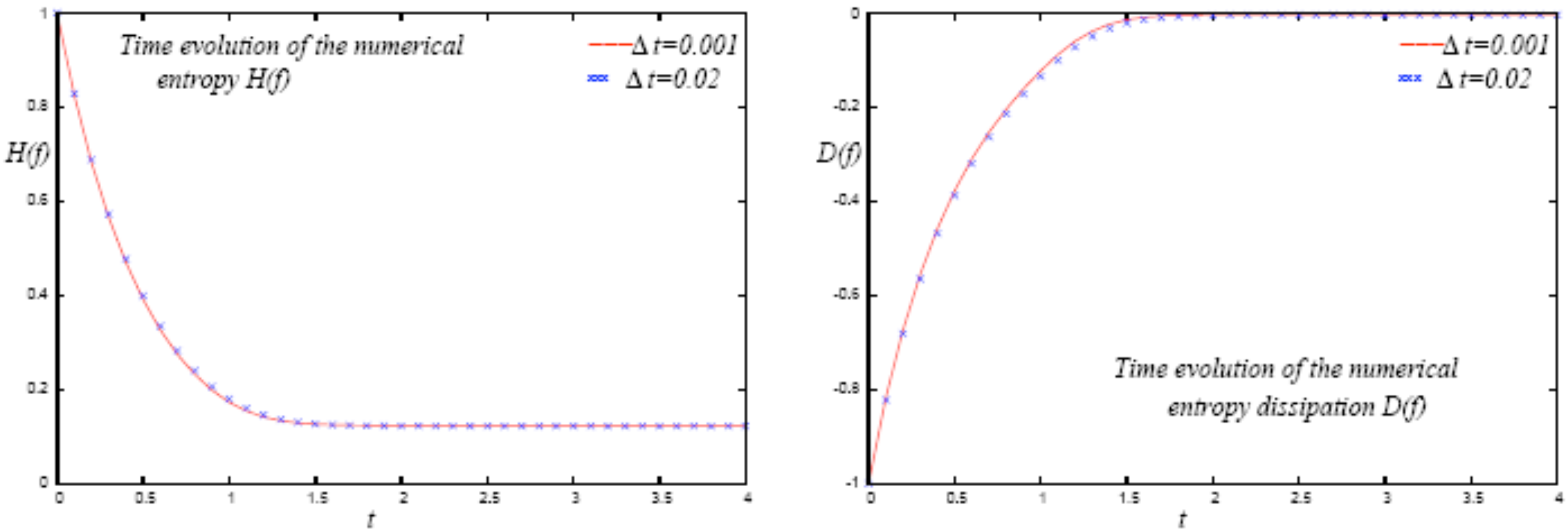


FIGURE 9. Nonlinear Fokker-Planck solution: convergence toward equilibrium (Barenblatt-Pattle distribution) obtained with the first order method (2.2) using $n_x = 100$ with $\Delta t = 0.02$ and 0.001.

Other applications and extensions

-- 4th order nonlinear parabolic equation:
Filbet-Shu

-- Monte-Carlo implementation
(operator splitting + exact BGK integrator):
Pareschi

-- quantum Boltzmann equation (Hu-J)

-- Landau-Fokker-Planck (J-Yan)

Conclusion

An asymptotic-preserving framework is presented for nonlinear kinetic equations and related problems with stiff sources:

In terms of implicit collisions, all one needs is to solve a BGK type collision operator (which can be implemented explicitly) : simple and general!