Uncertainty Quantification for multiscale kinetic equations with uncertainties

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outline

I. Basics of Kinetic equations, asymptotic limits, and Asymptotic-Preserving (AP) schemes

II. kinetic equations with random uncertainties and stochastic-AP schemes

III. Hypocoercivity theory based regularity, local sensitivity and numerical analysis for random kinetic equations

IV. Numerical strategies for high-dimensional random space

I. Basics of kinetic equations

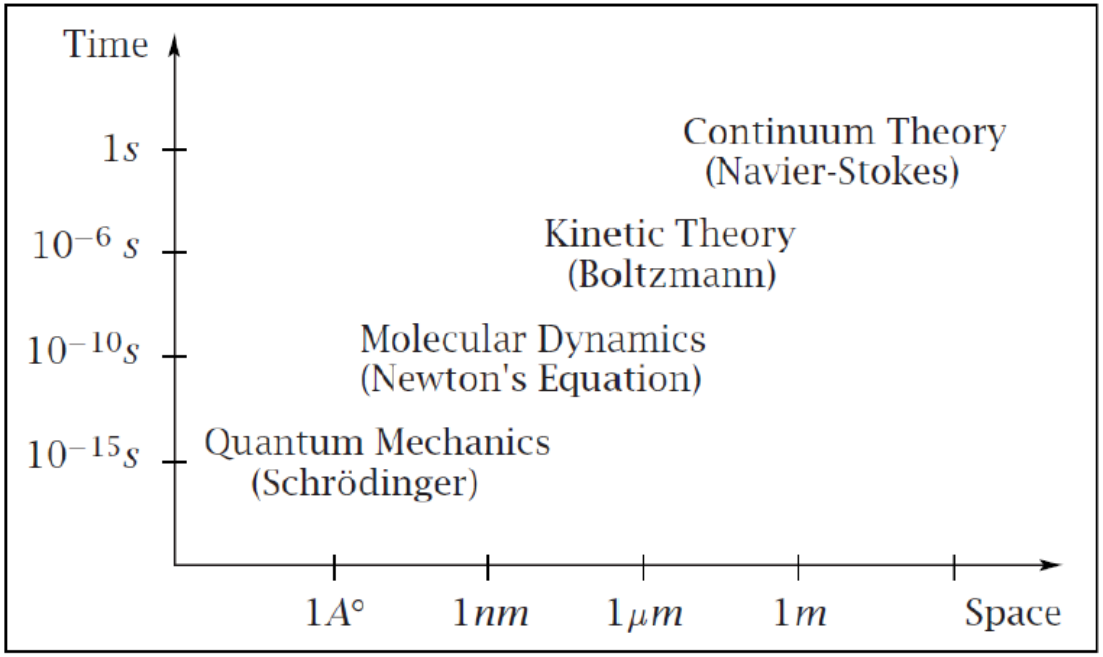


Figure 1. Different laws of physics are required to describe properties and processes of fluids at different scales.

- E & Engquist, AMS Notice (2003)

Kinetic equations

$$f_t + k \cdot \nabla_x f - \nabla_x V \cdot \nabla_k f = 1/\varepsilon\, B(f)$$

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

Applications

- Rarefied gas (astronautics)
- Plasma (Vlasov-Poisson, Vlasov-Maxwell, Landau-Fokker-Planck,…)
- Semiconductor device modeling
- Microfluidics
- Nuclear reactor
- Astrophysics
- Multiphase flows
- Environmental science, energy, social science, neuronal networks, biology, …

Examples of kinetic equations

Linear transport equation (neutron transport, radiative transfer, etc.)

$$\varepsilon\,\partial_t f + v\cdot\nabla_x f = \frac{1}{\varepsilon}\mathcal{L}(f) + \varepsilon G\,. \tag{4.1}$$

In (4.1), $G = G(t,x)$ is the source term, ε is the mean free path, $\mathcal{L}(f)$ is the anisotropic collision term defined by

$$\mathcal{L}(f) = \int \sigma(v,w)\{M(v)f(w) - \mathcal{M}(w)f(v)\}dw\,,$$

with the normalized Maxwellian M defined by

$$M(v) = \frac{1}{(\pi)^{d/2}}\exp(-|v|^2)\,.$$

The anisotropic scattering kernel σ is rotationally invariant and satisfies

$$\sigma(v,w) = \sigma(w,v) > 0\,.$$

Fokker-Planck equation

- Diffusion due to Brownian motion

$$\partial_t f + \frac{1}{\delta}\mathbf{v}\cdot\nabla_{\mathbf{x}} f - \frac{1}{\epsilon}\nabla_{\mathbf{x}}\phi\cdot\nabla_{\mathbf{v}} f = \frac{1}{\delta\epsilon}\mathcal{F}f$$

$$\mathcal{F}f = \nabla\cdot\left(M\nabla\left(\frac{f}{M}\right)\right)$$

where M is the *global equilibrium* or *global Maxwellian*,

$$M = \frac{1}{(2\pi)^{\frac{N}{2}}} e^{-\frac{|\mathbf{v}|^2}{2}}$$

ϕ potential

The Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\varepsilon} \mathcal{Q}(f, f)(\mathbf{v}), \quad \mathbf{x} \in \Omega \subset \mathbb{R}^d, \ \mathbf{v} \in \mathbb{R}^d$$

- $f(t, \mathbf{x}, \mathbf{v})$ is the **phase space distribution function** of time t, position $\mathbf{x}$, and velocity $\mathbf{v}$
- ε is the **Knudsen number**, ratio of the mean free path and the characteristic length scale: $\varepsilon \sim O(1)$ kinetic regime; $\varepsilon \ll O(1)$ fluid regime
- $\mathcal{Q}(f, f)$ is the **collision operator**, a quadratic integral operator modeling the interaction of particles

Collision operator

$$\mathcal{Q}(f,f)(\mathbf{v}) = \int_{\mathbb{R}^d}\int_{S^{d-1}} B(\mathbf{v}-\mathbf{v}_*,\sigma)[f(\mathbf{v}')f(\mathbf{v}'_*) - f(\mathbf{v})f(\mathbf{v}_*)]\,\mathrm{d}\sigma\mathrm{d}\mathbf{v}_*$$

$(\mathbf{v},\mathbf{v}_*)$ and $(\mathbf{v}',\mathbf{v}'_*)$ are the velocity pairs before and after collision:

$$\begin{cases} \mathbf{v}' = \dfrac{\mathbf{v}+\mathbf{v}_*}{2} + \dfrac{|\mathbf{v}-\mathbf{v}_*|}{2}\sigma \\ \mathbf{v}'_* = \dfrac{\mathbf{v}+\mathbf{v}_*}{2} - \dfrac{|\mathbf{v}-\mathbf{v}_*|}{2}\sigma \end{cases}$$

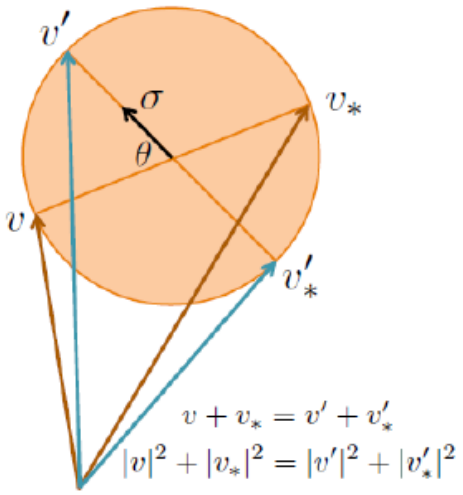
$$B(\mathbf{v}-\mathbf{v}_*,\sigma) = B(|\mathbf{v}-\mathbf{v}_*|, \tfrac{\sigma\cdot(\mathbf{v}-\mathbf{v}_*)}{|\mathbf{v}-\mathbf{v}_*|})$$

Variable hard sphere (VHS) model

$B = b_\lambda|\mathbf{v}-\mathbf{v}_*|^\lambda,\ -d < \lambda \le 1$

$\lambda = 1$: hard sphere molecule

$\lambda = 0$: Maxwell molecule



Challenges in kinetic computation

- High dimension (phase space, 6d for Boltzmann)
- Multiple scales
- uncertainty

uncertainties

- Derivation of kinetic equations for hard spheres: from Newton's second law for N-body particles, by taking mean field limit (let N go to infinity)— model uncertainty
- Except for special molecules (e.g. hard spheres), the collision kernel is empirical— coefficient uncertainty
- Initial and boundary data, forcing, boundary, etc. also contain measurement errors/uncertainties– data uncertainty

Geometry and Experience

by

Albert Einstein

- 27 January 1921 address at the Prussian Academy of Sciences in Berlin

One reason why mathematics enjoys special esteem, above all other sciences, is that its laws are absolutely certain and indisputable, while those of all other sciences are to some extent debatable and in constant danger of being overthrown by newly discovered facts……. As far as the laws of mathematics refer to reality, they are not certain; and as far as they are certain, they do not refer to reality.

I. Multiscales

- Kinetic equations usually have macroscopic limits, governed by the moments of the density distribution, as the small parameter (Knudsen number) goes to zero

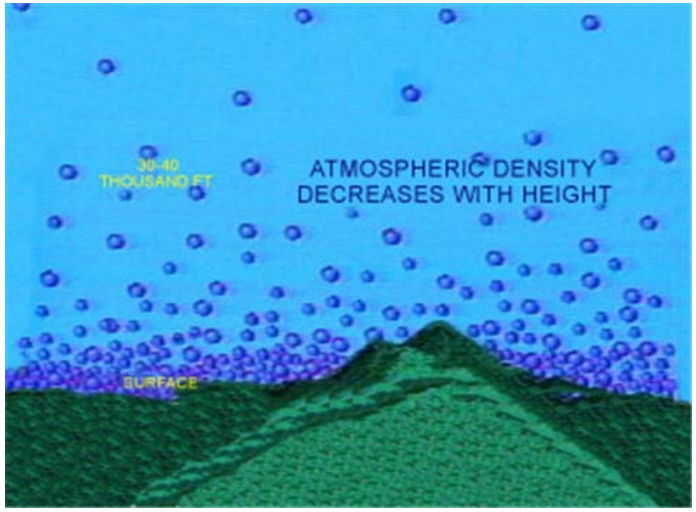
Multiscale problems

- Space shuttle reentry

  $\varepsilon : 10^{-8} \sim 1$ meters

- Fluid equations not adequate in boundary layers shock layers,…
- Military jets and supersonic flights: F1x, F2x, F3x:

  Mach number 1.8—2.5
- Different properties of materials require different physical laws at different scales



Scales in Boltzmann equation

- When ε is small ($kn \leq 0.01$), 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

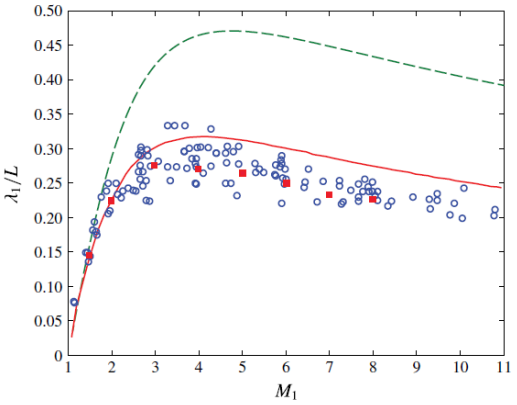


FIGURE 1. (Colour online) Inverse shock thickness, λ_1/L, as a function of upstream Mach number, M_1, for argon gas: ○, experimental results of Linzer & Hornig (1963), Camac (1965), Russell (1965), Schultz-Grunow & Frohn (1965), Robben & Talbot (1966), Schmidt (1969), Rieutord (1970), Garen *et al.* (1974) and Alsmeyer (1976); – – –, NSF theory; ■, direct simulation Monte Carlo results of Bird (1970); ——, theoretical results of Lumpkin & Chapman (1992), Woods (1993) and Reese *et al.* (1995).

（from S. Paolucci & C. Paolucci JFM ’18)

Some Space Shuttle Data (NASA TR/2006-213486 T. Rivell)

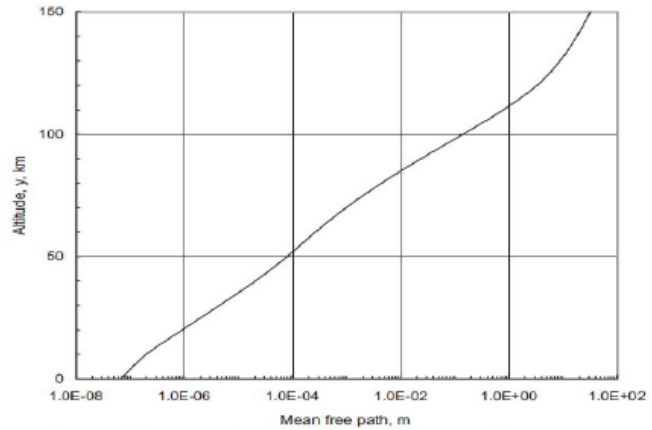


Figure 11. Mean free path vs. altitude, 1976 U.S. Standard Atmosphere.

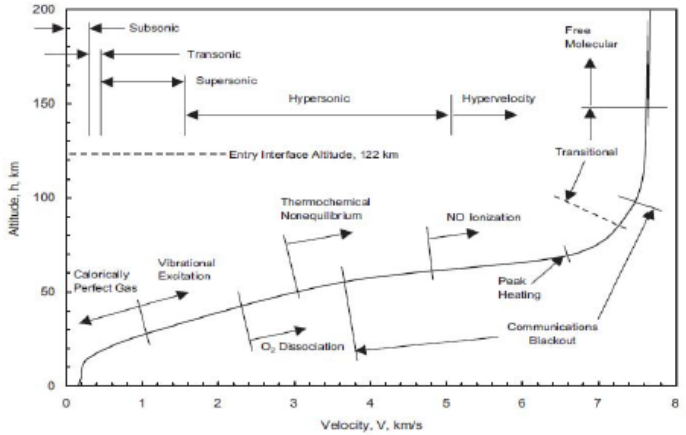


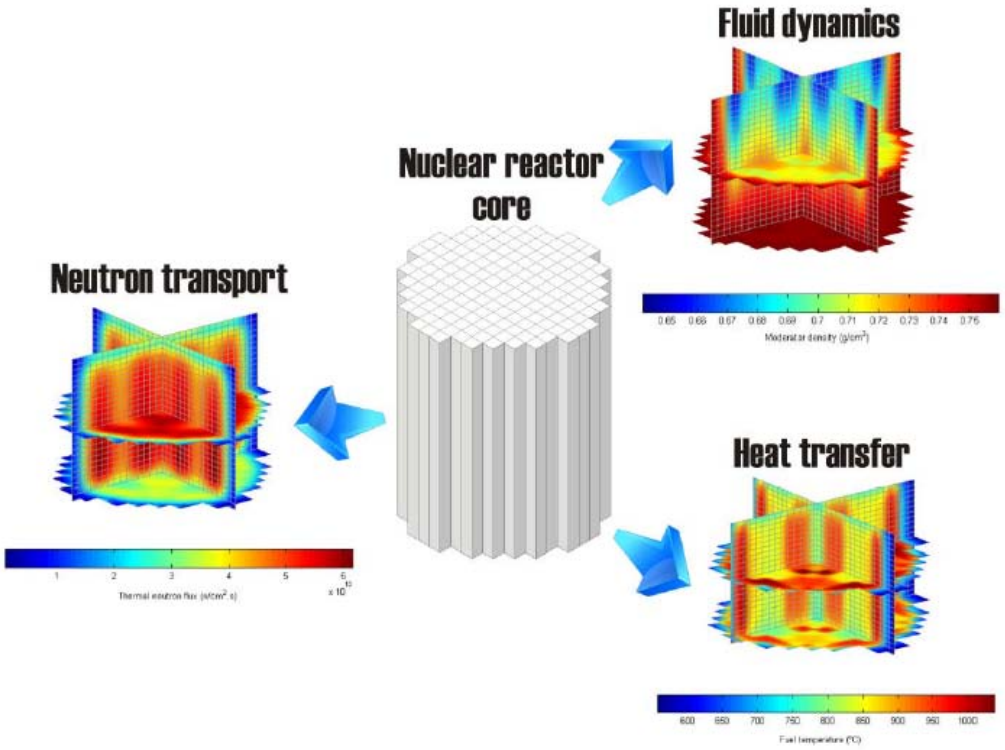
Figure 19. Space Shuttle Orbiter re-entry trajectory.

TABLE 1. FLOW REGIME BOUNDARIES

Flow Regime	Anderson (1989)[a]	Regan and Anandakrishnan (1993)
Free molecular	$Kn >> 1$	$Re < M/3$
Near free molecular	$Kn > 1.0$	—
Transitional	$1.0 > Kn > 0.03$	$M/3 < Re < 10{,}000\ M^2$
Continuum	$Kn < 0.2$	$Re > 10{,}000\ M^2$

[a] Note the overlap of the continuum and transitional flow regimes. Anderson (1989) notes that in this region ($0.03 < Kn < 0.2$) temperature and velocity slip effects (discontinuities) are present at the body surface.

Multiscale simulation of a nuclear reactor



Diffusion limit of linear transport equation

$$\varepsilon\,\partial_t f + v\cdot\nabla_x f = \frac{1}{\varepsilon}\mathcal{L}(f) + \varepsilon G\,. \tag{4.1}$$

In (4.1), $G = G(t,x)$ is the source term, ε is the mean free path, $\mathcal{L}(f)$ is the anisotropic collision term defined by

$$\mathcal{L}(f) = \int \sigma(v,w)\{M(v)f(w) - \mathcal{M}(w)f(v)\}dw\,,$$

with the normalized Maxwellian M defined by

$$M(v) = \frac{1}{(\pi)^{d/2}}\exp(-|v|^2)\,.$$

The anisotropic scattering kernel σ is rotationally invariant and satisfies

$$\sigma(v,w) = \sigma(w,v) > 0\,.$$

The collision operator $\mathcal{L}$ has the following properties:

$$\mathcal{L}(f) = 0 \Longrightarrow f(t,x,v) = \rho(x,t)\, M(v)\,,$$

with

$$\rho(t,x) = \int f(v)\, dv := \langle\, f\,\rangle\,.$$

We also assume that the collision frequency λ satisfies the following bound for some positive constant μ,

$$\lambda(v) = \int \sigma(v,w)\, \mathcal{M}(w)\, dw \leq \mu\,.$$

As $\varepsilon \to 0$, one can show that $f(x,v,t)$ is approximated by

$$f \approx \rho(x,t)\, M(v)$$

where ρ satisfies the diffusion equation [**108, 99**]

$$\partial_t \rho = \nabla_x \cdot (D \nabla_x \rho) + G \tag{4.2}$$

with the diffusion coefficient matrix

$$D = \int \frac{M(v)}{\lambda(v)} v \otimes v\, dv\,.$$

Scaling limit of Fokker-Planck equation

$$\partial_t f + \tfrac{1}{\delta}\mathbf{v}\cdot\nabla_{\mathbf{x}} f - \tfrac{1}{\epsilon}\nabla_{\mathbf{x}}\phi\cdot\nabla_{\mathbf{v}} f = \tfrac{1}{\delta\epsilon}\mathcal{F} f$$

$$\mathcal{F} f = \nabla\cdot\left(M\nabla\left(\frac{f}{M}\right)\right)$$

where M is the *global equilibrium* or *global Maxwellian*,

$$M = \frac{1}{(2\pi)^{\frac{N}{2}}} e^{-\frac{|\mathbf{v}|^2}{2}}$$

ϕ potential

- High field limit $\delta = 1$

$$\partial_t \rho + \nabla \cdot (\rho \nabla_{\mathbf{x}} \phi) = 0,$$

- Parabolic limit $\delta = \epsilon$

$$\partial_t \rho - \nabla \cdot (\nabla_{\mathbf{x}} \rho - \rho \nabla_{\mathbf{x}} \phi) = 0,$$

Fluid approximations of the Boltzmann equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f = \frac{1}{\varepsilon} \mathcal{Q}(f)$$

- Conservations of mass, momentum and total energy $\int_{\mathbb{R}^{d_v}} \mathcal{Q}(f)\phi(v)dv = 0, \quad \text{for } \phi(v) = 1, v, |v|^2$
- H-Theorem (entropy condition) $-\frac{d}{dt}\int_{\mathbb{R}^{d_v}} f \log f dv = -\int_{\mathbb{R}^{d_v}} \mathcal{Q}(f)\log(f)dv \geqslant 0.$
- Moments $\rho = \int_{\mathbb{R}^{d_v}} f(v)dv = \int_{\mathbb{R}^{d_v}} \mathcal{M}_{\rho,u,T}(v), \quad u = \frac{1}{\rho}\int_{\mathbb{R}^{d_v}} vf(v)dv = \frac{1}{\rho}\int_{\mathbb{R}^{d_v}} v\mathcal{M}_{\rho,u,T}(v)dv,$
  $T = \frac{1}{d_v\rho}\int_{\mathbb{R}^{d_v}} |u-v|^2 f(v)dv = \frac{1}{d_v\rho}\int_{\mathbb{R}^{d_v}} |u-v|^2 \mathcal{M}_{\rho,u,T}(v)dv.$
- Local Maxwellian (equilibrium) $\mathcal{M}_{\rho,u,T}(v) = \frac{\rho}{(2\pi T)^{d_v/2}} \exp\left(-\frac{|u-v|^2}{2T}\right)$

when $\varepsilon \to 0$, $Q(f) \to 0$ $\qquad f(t,x,v) = \mathcal{M}$

the moments converge to the compressible Euler equations

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \nabla_x \cdot \rho u = 0, \\ \dfrac{\partial \rho u}{\partial t} + \nabla_x \cdot (\rho u \otimes u + p\,\mathrm{I}) = 0, \\ \dfrac{\partial E}{\partial t} + \nabla_x \cdot ((E+p)u) = 0, \end{cases}$$

$$p = (\gamma - 1)\left(E - \frac{1}{2}\rho |u|^2\right)$$

$$\gamma = (d_v + 2)/d_v$$

If one expands to the next order (the Chapman-Enskog expansion) then one gets the compressible Navier-Stokes equations

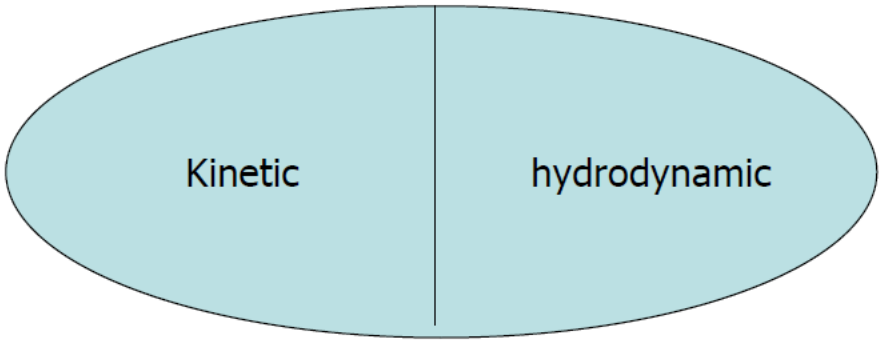
Kinetic and hydrodynamic equations

- 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

Multi-physics 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 schemes

- 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
- No coupling with macroscopic equations, thus avoid the difficulty of interface condition/treatment as in other multiscale methods

Numerical issues when ε is small

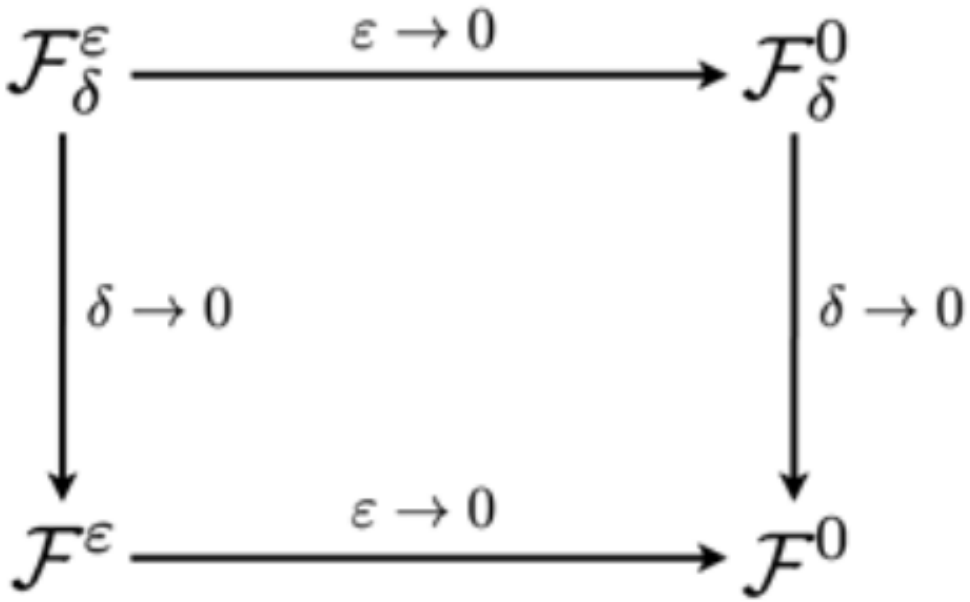
- Numerical stiffness: an explicit collision term would require $\Delta t = O(\varepsilon)$
- Implicit collision allows Δt to be independent of ε, but inverting the non-local collision term is numerically difficult and expensive
- Does the underresolved computation gives the correct macroscopic solutions?

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



AP→ Uniform convergence (Golse-J-Levermore '99)

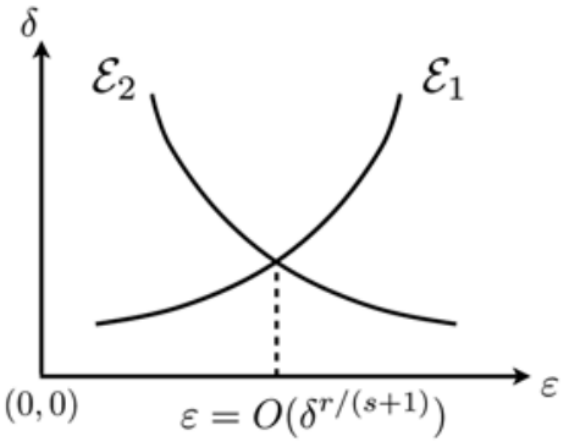
- Classical estimate

$$\mathcal{E}_1 = \|\mathcal{F}^\varepsilon_\delta - \mathcal{F}^\varepsilon\| = O(\delta^r/\varepsilon^s)\,, \quad 1 \le s \le r$$

- AP: $\mathcal{E}_2 = \|\mathcal{F}^\varepsilon_\delta - \mathcal{F}^\varepsilon\| = O(\varepsilon + \delta^r)$

- Uniform error estimate:

$$\|\mathcal{F}^\varepsilon_\delta - \mathcal{F}^\varepsilon\| = \min(\mathcal{E}_1, \mathcal{E}_2)$$



which has an upper bound around $\varepsilon = O(\delta^{r/(s+1)})$. This gives

$$\|\mathcal{F}^\varepsilon_\delta - \mathcal{F}^\varepsilon\| = O(\delta^{r/(s+1)})\,, \qquad \text{uniformly in} \quad \varepsilon\,. \tag{1.6}$$

- Review articles: Jin 2010 (general);
  Degond-Dulezet 2017 (plasma)

Examples of AP schemes

- Linear transport equation

Method 1: parity formulation (Jin-Pareschi-Toscani '99)

Split (4.1) into two equations, one for v and one for $-v$:

$$\varepsilon\,\partial_t f(v) + v\cdot\nabla_x f(v) = \frac{1}{\varepsilon}\mathcal{L}(f)(v) + \varepsilon G, \tag{4.3}$$

$$\varepsilon\,\partial_t f(-v) - v\cdot\nabla_x f(-v) = \frac{1}{\varepsilon}\mathcal{L}(f)(-v) + \varepsilon G, \tag{4.4}$$

Define the even- and odd-parities [94] as

$$r(t,x,v) = \frac{1}{2}\,[f(t,x,v) + f(t,x,-v)], \tag{4.5}$$

$$j(t,x,v) = \frac{1}{2\varepsilon}\,[f(t,x,v) - f(t,x,-v)]. \tag{4.6}$$

Adding and subtracting the two equations in (4.4) lead to

$$\partial_t r + v\cdot\nabla_x j = \frac{1}{\varepsilon^2}\mathcal{L}(r) + G, \tag{4.7}$$

$$\partial_t j + \frac{1}{\varepsilon^2} v\cdot\nabla_x r = -\frac{1}{\varepsilon^2}\,\lambda j\,; \tag{4.8}$$

The idea of [**70**] was to rewrite (4.7) and (4.8) into the following form

$$\partial_t r + v \cdot \nabla_x j = \frac{1}{\varepsilon^2}\mathcal{L}(r) + G, \tag{4.9}$$

$$\partial_t j + v \cdot \nabla_x r = -\frac{1}{\varepsilon^2}\left[\lambda j + (1-\varepsilon^2\psi) v \cdot \nabla_x r\right], \tag{4.10}$$

where $\psi = \psi(\varepsilon)$ is a free parameter satisfying $0 \le \psi \le 1/\varepsilon^2$. The simplest choice of ψ is

$$\psi(\varepsilon) = \min\left\{1, \frac{1}{\varepsilon}\right\}.$$

$$\partial_t r = \frac{1}{\varepsilon^2}\mathcal{L}(r) + G,$$

$$\partial_t j = \frac{1}{\varepsilon^2}\left[-\lambda j - (1-\varepsilon^2\phi)(v \cdot \nabla_x r)\right],$$

$$\partial_t r + v \cdot \nabla_x j = 0,$$

$$\partial_t j + v \cdot \nabla_x r = 0.$$

Method 2: Micro-macro decomposition

- Klar-Schmeiser (‘01), Bennoune-Lemou-Mieusseun (‘08)

$$f = \rho M + \varepsilon g$$

$$\Pi : \Pi(\,\cdot\,)(v) := M\langle\,\cdot\,\rangle,$$

$$\partial_t \rho + \nabla_x \cdot \langle vg \rangle = G$$

$$\varepsilon^2 \partial_t g + \varepsilon(I - \Pi)(v \cdot \nabla_x g) + v \cdot M \nabla_x \rho = \mathcal{L} g + (I - \Pi)\varepsilon G$$

$$\frac{g^{n+1} - g^n}{\Delta t} + \frac{1}{\varepsilon}(I - \Pi)(v \cdot \nabla_x g^n) = \frac{1}{\varepsilon^2}\mathcal{L} g^{n+1} - \frac{1}{\varepsilon^2} v \cdot M \nabla_x \rho^n$$

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} + \nabla_x \cdot \langle v g^{n+1} \rangle = G$$

AP property

One-dimensional Spatial discretization

In one space dimension, a staggered grid can be used by also defining $x_{i+1/2} = (i + 1/2)\Delta x$. Now the macroscopic density ρ will be defined at gridpoint x_i, while g is defined at $x_{i+1/2}$. Using upwind discretization for the space derivative, one arrives at

$$\frac{\rho_i^{n+1} - \rho_i^n}{\delta t} + \left\langle v \frac{g_{i+1/2}^{n+1} - g_{i-1/2}^{n+1}}{\Delta x} \right\rangle = G\,, \tag{4.25}$$

$$\begin{aligned} &\frac{g_{i+1/2}^{n+1} - g_{i+1/2}^n}{\Delta x} + \frac{1}{\varepsilon \Delta x}(I - \Pi)\Big(v^+(g_{i+1/2}^n - g_{i-1/2}^n) + v^-(g_{i+3/2}^n - g_{i+1/2}^n)\Big) \\ &\qquad = \frac{1}{\varepsilon^2}\mathcal{L} g_{i+1/2}^{n+1} - \frac{1}{\varepsilon^2} v M \frac{\rho_{i+1}^n - \rho_i^n}{\Delta x}\,, \end{aligned} \tag{4.26}$$

where $v^{\pm} = (v \pm |v|)/2$.

As $\varepsilon \to 0$, (4.26) gives

$$g_{i+1/2}^{n+1} = \mathcal{L}^{-1}(vM)\frac{\rho_{i+1}^n - \rho_i^n}{\delta x}$$

which when applied to (4.25) gives the following scheme

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} + D\,\frac{\rho_{i+1}^n - 2\rho_i^n + \rho_{i-1}^n}{(\Delta x)^2} = G\,.$$

- Uniform stability (J.G. Liu and Mieusseun)

$$\Delta t \le \frac{\Delta x^2 \sigma_{\min}}{3} + \frac{2}{3}\varepsilon \Delta x$$

Some other issues

- Higher (2 or higher) order in time: Implicit-Explicit (IMEX) Runge-Kutta: Caflisch-Jin-Russo ('95), Pareschi-Russo ('05), …
- How to deal with implicit nonlinear collision operators: BGK-penalty (Filbet-Jin)

  (related idea: exponential integrator: Dimarco-Paraschi-Li, etc.)

avoiding inverting nonlinear collision operator yet still uniformly stable in terms ε

An efficient AP scheme for Boltzmann (Filbet-J)

- A major challenge for AP-Boltzmann is that the implicit collision—which is inevitable—is daunting to solve
- We introduced a BGK penalization method:

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

explicit implicit

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

An explicit-implicit time discretization

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

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

stability requires: $\beta > 1/2 \sup|\beta_A|$; best choice: $\beta \sim \sup|\beta_A|$;

can be made time-dependent

Explicit Implementation:
Taking the moments:
$\langle f^{n+1}-f^n \rangle/\Delta t + \nabla_x \cdot \langle k\ f^n \rangle = 0$ ($\langle B \rangle = \langle M-f \rangle = 0$)
This defines $(\rho, u, T)^{n+1}$, thus M^{n+1}. The rest is explicit!

Can still use legacy code to obtain $B(f^n)$!

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!

Properties

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

classical AP scheme requires that

$$\text{For any } f^0, f^n - M^n = O(\epsilon) \text{ for any } n \geq 1$$

namely any data will be projected to the local Maxwellian in one time step (strongly AP)

This scheme does NOT have this property: it takes several steps (after initial layer) (relaxed AP)

If $\Delta t >> \epsilon$, then for any f_0, there exsits an $N(\epsilon)$, such that

$f^n - M^n = O(\epsilon)$ for $n > N(\epsilon)$

Can prove this for hyperbolic relaxation problem

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

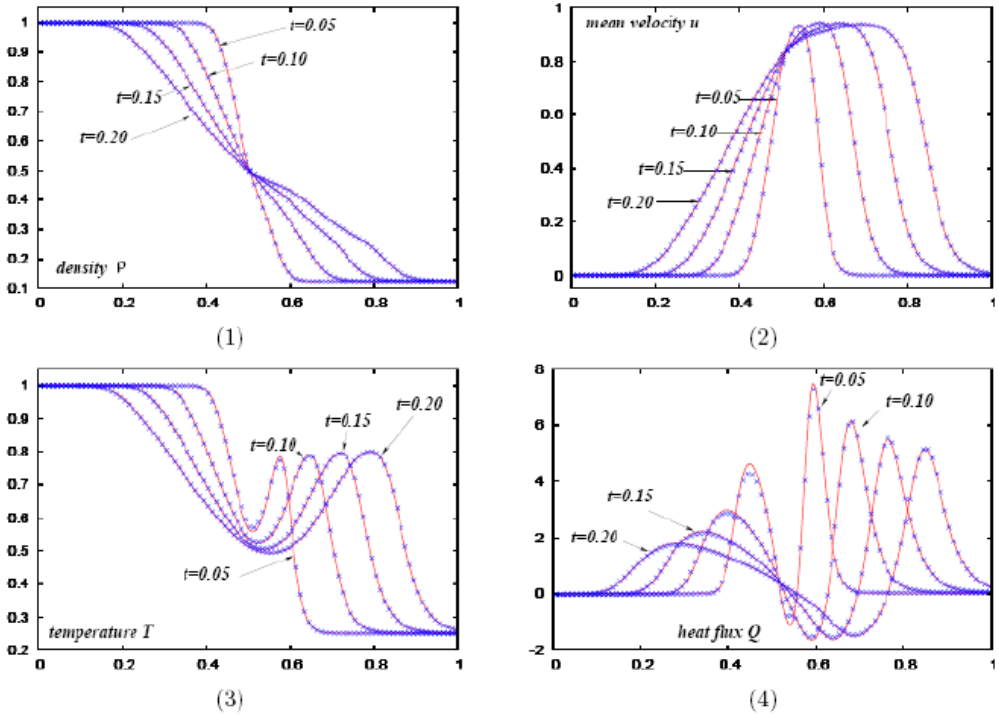


FIGURE 3. Sod tube problem ($\varepsilon = 10^{-2}$), dots (x) represent the numerical solution obtained with our second order method (2.3) and lines with the Runge-Kutta method: evolution of (1) the density ρ, (2) mean velocity u, (3) temperature T and (4) heat flux $\mathbb{Q}$ at time $t = 0.05, 0.1,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

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

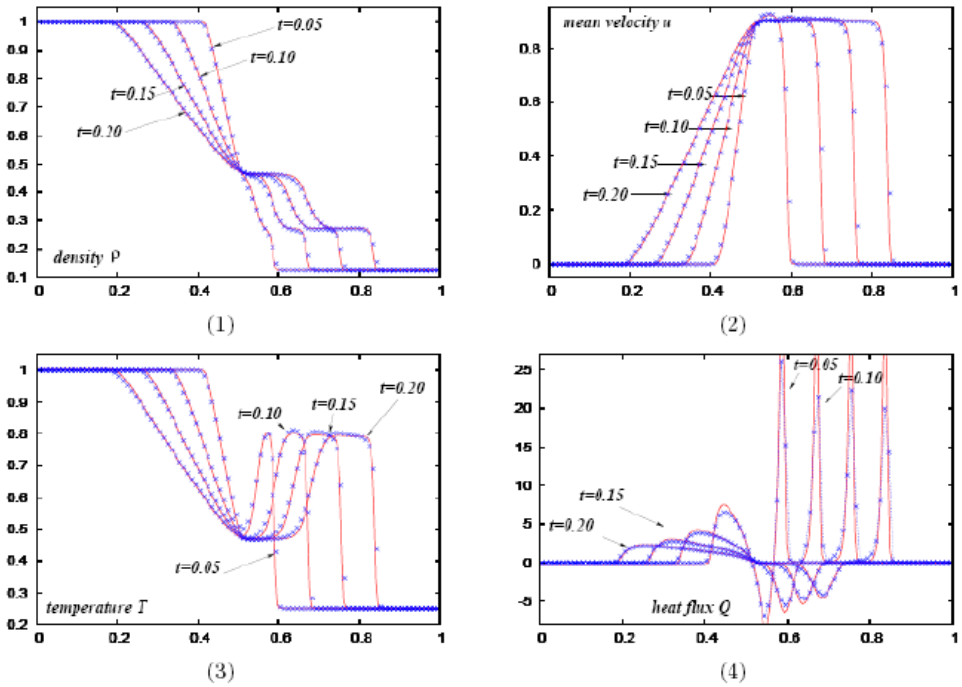
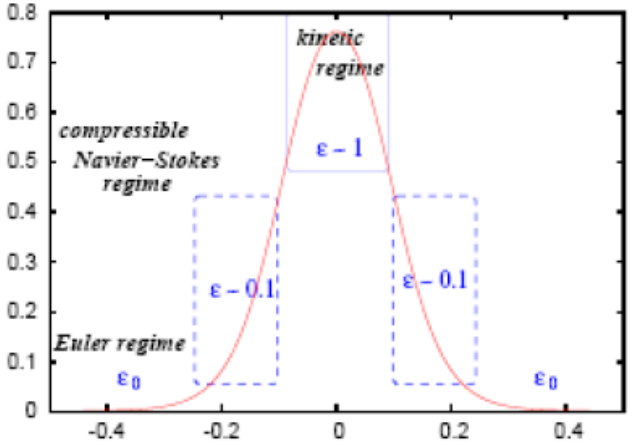


FIGURE 4. Sod tube problem ($\varepsilon = 10^{-3}$), dots (x) represent the numerical solution obtained with our second order method (2.3) and lines with the Runge-Kutta method: evolution of (1) the density ρ, (2) mean velocity u, (3) temperature T and (4) heat flux $\mathbb{Q}$ at time $t = 0.05$,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

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



- Initial data not in local Maxwellian:

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

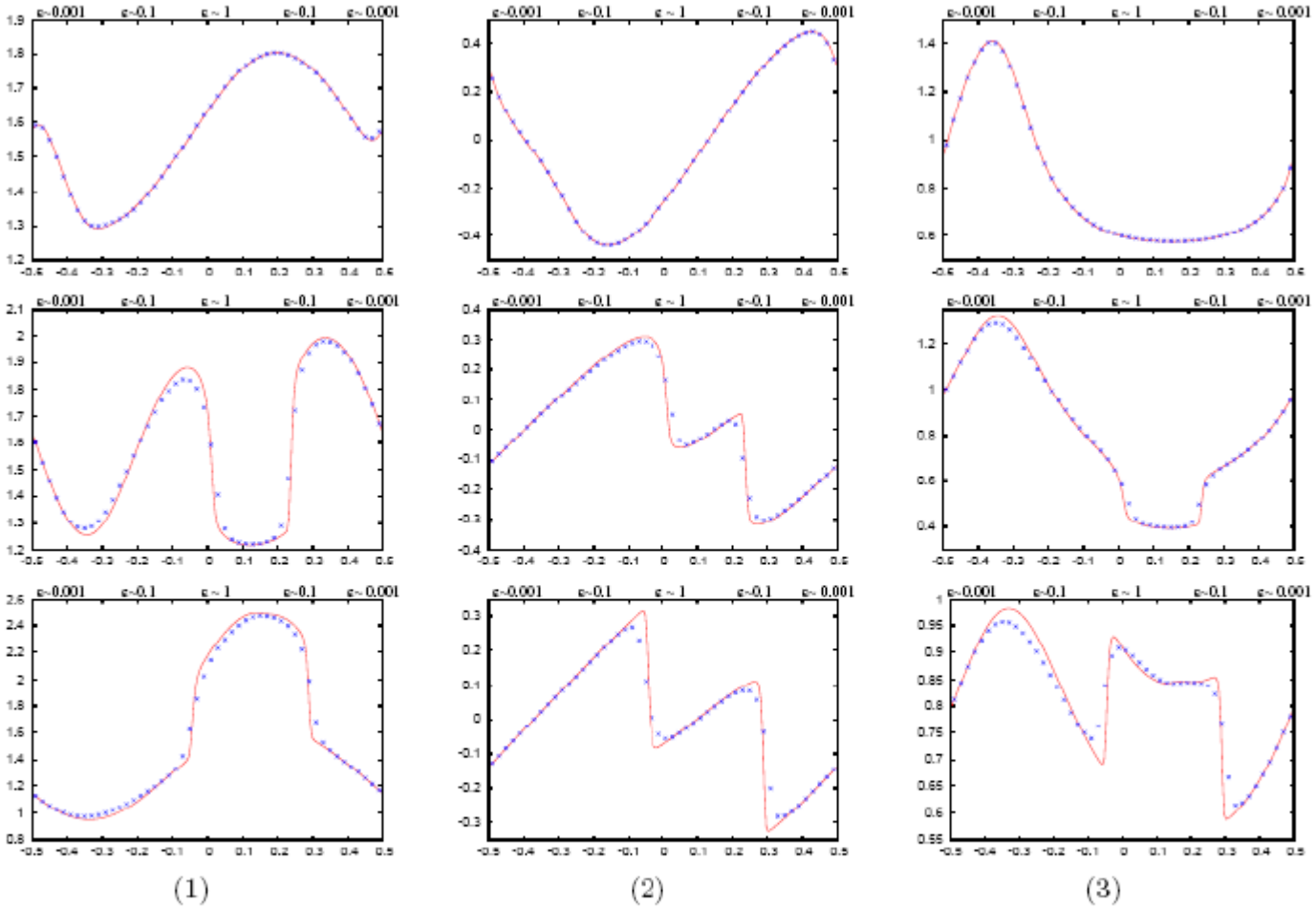


FIGURE 7. Mixing regime problem ($\varepsilon_0 = 10^{-3}$), comparison of the numerical solution to the Boltzmann equation obtained with the AP scheme (2.3) using $n_x = 50$ (dots x) and $n_x = 200$ points (line): evolution of (1) the density ρ, (2) mean velocity u, (3) temperature T at time $t = 0.25$,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

The exponential integrator method
(Gabetta-Pareschi-Toscani, Giacomo-Pareschi, Li-Pareschi)

One can write (3.22) as

$$\partial_t f + v \cdot \nabla_x f = \frac{\beta}{\varepsilon}\left(\frac{\mathcal{Q}^+(f)}{\beta} - \mathcal{M}\right) + \frac{\beta}{\varepsilon}(\mathcal{M} - f)\,, \tag{3.26}$$

with

$$\mathcal{Q}^+(f) = \mathcal{Q}(f) + \beta f\,.$$

$$\partial_t[(f - \mathcal{M})\, e^{\beta t/\varepsilon}] = \frac{1}{\varepsilon}[\mathcal{Q}^+(f) - \beta\mathcal{M}]\, e^{\beta t/\varepsilon}\,. \tag{3.27}$$

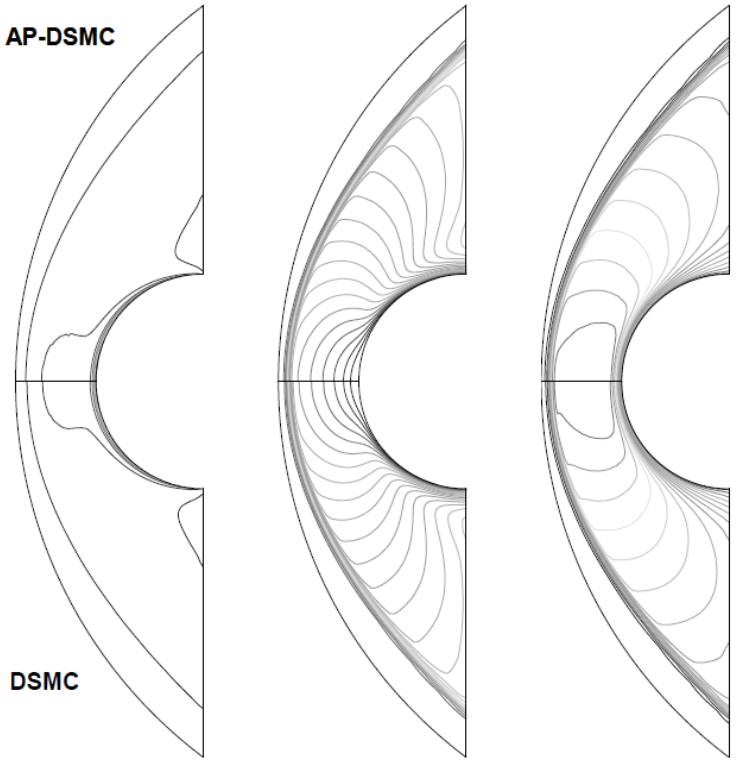
If one discretizes the above equation by the forward Euler method one arrives at

$$f^* = e^{-\beta\Delta t/\varepsilon} f^n + \left[1 - e^{-\beta\Delta t/\varepsilon} - \frac{\beta}{\varepsilon} e^{-\beta\Delta t/\varepsilon}\right]\mathcal{M}^n + \frac{\beta}{\varepsilon}\, e^{-\beta\Delta t/\varepsilon}\, \frac{\mathcal{Q}^+(f^n)}{\beta}\,. \tag{3.28}$$

for $\varepsilon \ll 1$, (3.28) gives $f^* = M^n + o(\varepsilon)$

A Mach 10 problem (AP-DSMC, Ren-Liu-Jin, JCP '14)

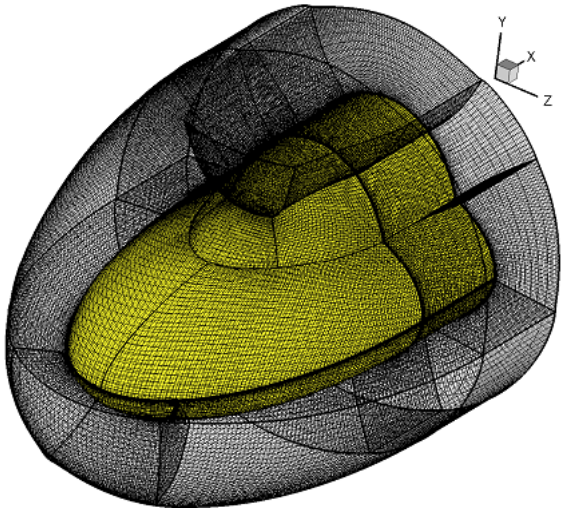
$\varepsilon = 10^{-3}$

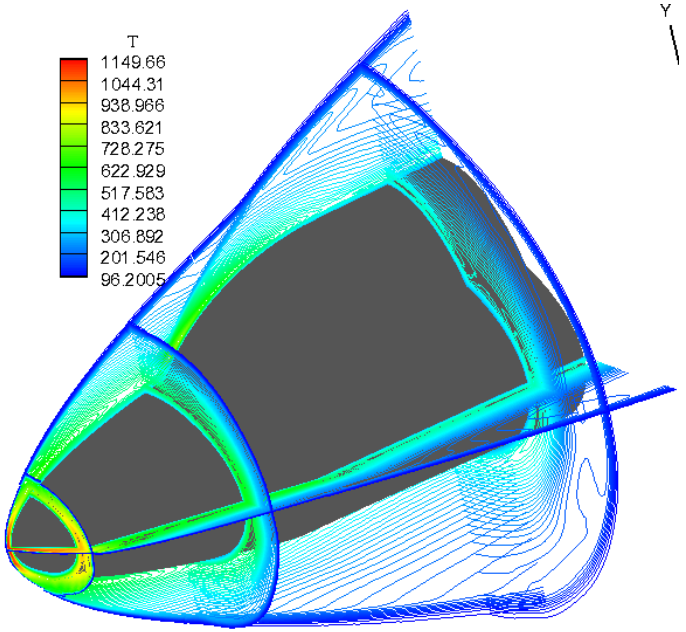


- Time step of AP-DSMC is 10 times larger than DSMC
- CPU time for AP-DSMC is 5 times smaller

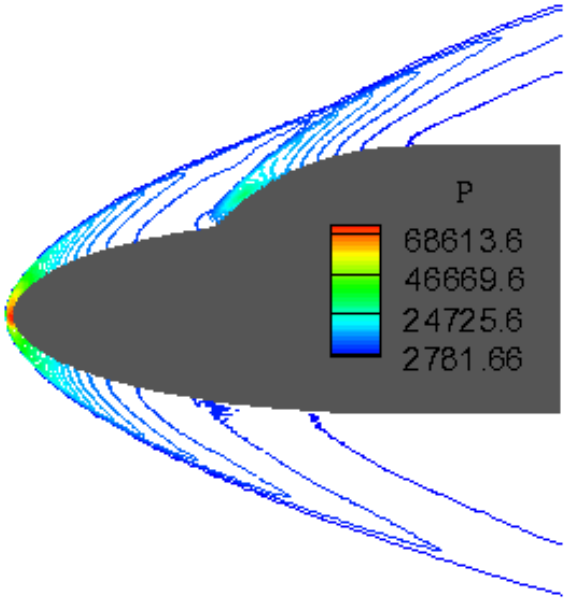
- Contour of density, velocity and temperature

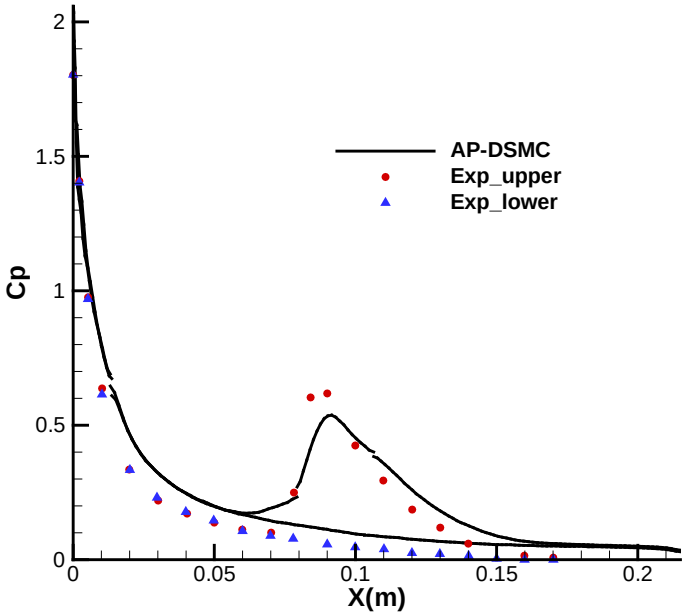
Flows around 3d double-ellipsoid (left: computational geometry; right: temperature Ma=7.8, Kn=1.93e-5)





Pressure distribution





Landau-Fokker-Planck operator (for plasma)
(Jin-Yan, JCP 2011)

$$Q(f) = \nabla_v \cdot \int_{\mathbb{R}^{N_v}} A(v - v_*)(f(v_*)\nabla_v f(v) - f(v)\nabla_{v_*} f(v_*))dv_*,$$

$$A(z) = \Psi(z)\left(I - \frac{z \otimes z}{|z|^2}\right), \qquad \Psi(z) = |z|^{\gamma+2}$$

Explicit collision term requires Δ t=O(ϵ (Δ v)^2)

Use the Fokker-Planck operator

$$P_{FP}(f) = P_{FP}^M f = \nabla_v \cdot \left(M \nabla_v \left(\frac{f}{M}\right)\right)$$

as the penalty (we use a symmetirc discretization so the Conjugate-Gradient method to can be used to invert the symmetric matrix)