Projective integration for nonlinear collisional kinetic equations

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Université de Lille

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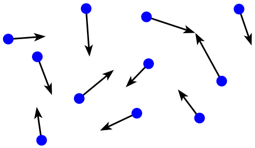
Purple SHARK-FV

Outline of the talk

A hierarchy of fluid models for modeling a rarefied gas

- Microscopic: Newton equations for N-particles systems;



$(x_i(t), v_i(t))_{1,\dots,N}$

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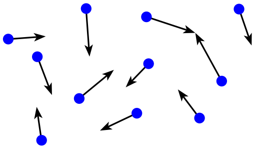

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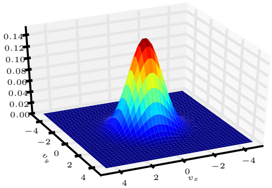

$f^\varepsilon(t, x, v)$

$N \to \infty$

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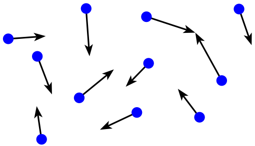

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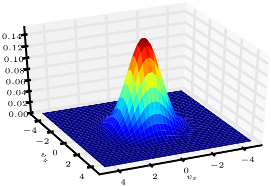

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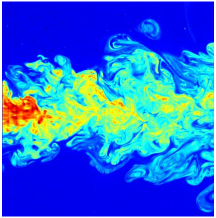

$\rho(t,x), \mathbf{u}(t,x), E(t,x)$

$N \to \infty$ $\varepsilon \to 0$

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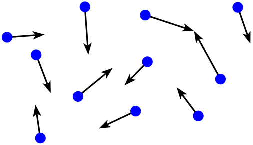

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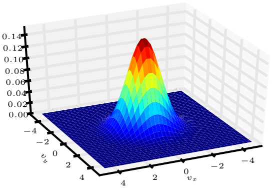

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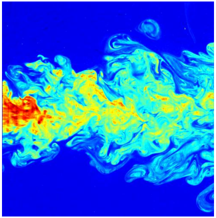

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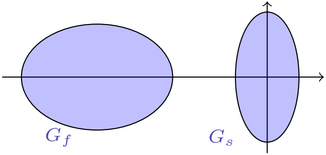
$N \to \infty$ $\qquad$ $\varepsilon \to 0$

- Theoretical works: C. Cercignani, C. Bardos, R. DiPerna, P.-L. Lions, D. Levermore, C. Villani, F. Golse, L. Saint-Raymond;
- Numerical simulations: E. Tadmor, B. Perthame, P. Degond, L. Pareschi, E. Sonnendrücker, S. Jin, F. Filbet.

Projective Integration "*à la* Gear and Kevrekidis"

Let us consider the system of ODEs

$$(1) \qquad \begin{cases} u'(t) = g(u(t)), & t > 0 \\ u(0) = u_0 \in \mathbb{R}^N, \end{cases}$$



where N is large and

- $\partial g / \partial u$ eigenvalues are clustered into two groups G_f, $G_s \subset \mathbb{C}$, separated by a large gap ($\sim$ stiffness): G_s is located in a neighborhood of the origin (slow components), and G_f lies far in the left-half plane (fast components).
- Because of the stiffness in g (through G_f), the solution u is projected on a low dimensional equilibrium manifold in a very short time.

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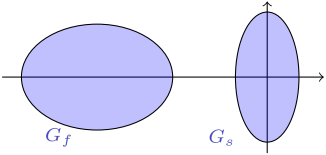

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- Because of the stiffness in g (through G_f), the solution u is projected on a low dimensional equilibrium manifold in a very short time.

Formal idea:

- Perform a number of small time steps of an inner integrator, corresponding to the fast rate of damping of u towards the equilibrium manifold.
- Extrapolate forward with a large time step, corresponding to the slow manifold.
- The inner integrator can be explicit because its time steps δt will be chosen very small, e.g.

$$\delta t \simeq \mathcal{O}\left(\min |\lambda| : \lambda \in G_f\right)$$

Projective Forward Euler (PFE) scheme

Gear, Kevrekidi, SINUM, 2003

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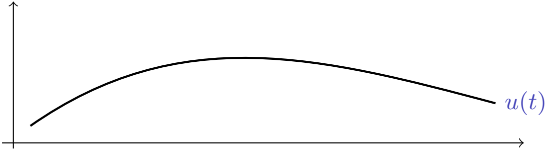

Inner integrator. Forward Euler method with small time step δt:

$$u^{k+1} = u^k + \delta t \, g(u^k), \qquad k = 0, 1, \ldots .$$

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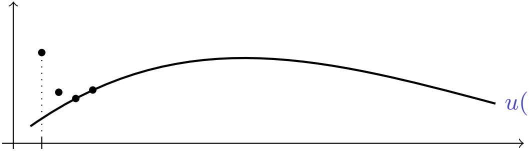

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Outer integrator. Let Δt be a regular time step, given say by a hyperbolic CFL, and u^n be an approximation of the solution at time $t^n = n\Delta t$

- First take $K+1$ inner steps of size δt using the inner integrator, and denote by $u^{n,k}$ the numerical solution at time $t^{n,k} = n\Delta t + k\delta t$.

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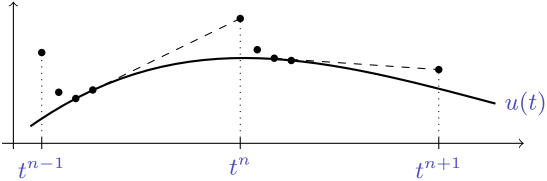

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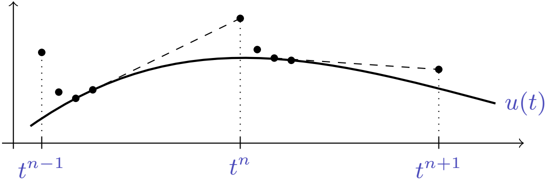
- First take $K+1$ inner steps of size δt using the inner integrator, and denote by $u^{n,k}$ the numerical solution at time $t^{n,k} = n\Delta t + k\delta t$.
- Extrapolate in time (projective Forward Euler, PFE) to compute $u^{n+1} := u^{n+1,0}$

$$u^{n+1} = u^{n,K+1} + (\Delta t - (K+1)\delta t)\frac{u^{n,K+1} - u^{n,K}}{\delta t}.$$

- Iterate

Linear stability

$$\begin{cases} u'(t) = \lambda u(t), & t > 0 \\ u(0) = u_0 \in \mathbb{R}, \end{cases}$$



Inner integrator. Forward Euler method with small time step δt:

$$u^{k+1} = (1 + \lambda\delta t)\, u^k = (1 + \lambda\delta t)^{k+1}\, u^0, \qquad k = 0, 1, \dots .$$

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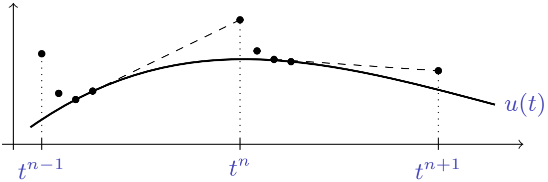

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Outer integrator. Δt is the regular time step, and $u^n \simeq u(t^n)$:

- After $K + 1$ inner steps of size δt using the inner integrator:

$$u^{n,k} = (1 + \lambda\delta t)^{K+1} u^n$$

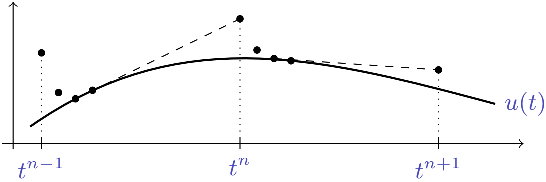
- Extrapolate in time (projective Forward Euler, PFE):

$$\begin{aligned} u^{n+1} &= u^{n,K+1} + M\delta t \frac{u^{n,K+1} - u^{n,K}}{\delta t}, \\ &= ((M+1)\tau - M)\, \tau^K u^n, \end{aligned}$$

where $\tau = 1 + \lambda\delta t$ and $M = \Delta t/\delta t - (K + 1)$.

Linear stability (cont'd)

$$\begin{cases} u'(t) = \lambda u(t), \quad t > 0 \\ u(0) = u_0 \in \mathbb{R}, \end{cases}$$



We have $u^{n+1} = \sigma(\tau) u^n$ where $\sigma(\tau) = ((M+1)\tau - M)\,\tau^K$ and $M = \Delta t/\delta t - (K+1)$.

Theorem (Gear, Kevrekidis, 2003, SINUM)

Let $\mathcal{D}(\lambda, r) = \{z \in \mathbb{C} : |z - \lambda| \le r\}$. Then

$$|\sigma(\tau)| \le 1 \Leftrightarrow \tau \in \mathcal{D}\left(1 - \frac{\delta t}{\Delta t}, \frac{\delta t}{\Delta t}\right) \cup \mathcal{D}\left(0, \left(\frac{\delta t}{\Delta t}\right)^{1/K}\right).$$

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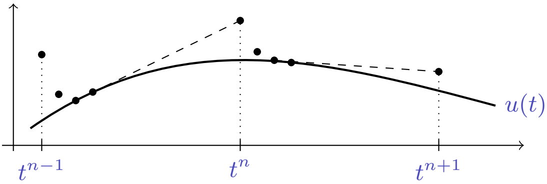

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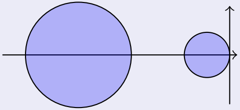
Corollary. The PFE method is linearly stable if, and only if

$$\lambda \in \mathcal{D}\left(-\frac{1}{\Delta t}, \frac{1}{\Delta t}\right) \cup \mathcal{D}\left(-\frac{1}{\delta t}, \frac{1}{\delta t}\left(\frac{\delta t}{\Delta t}\right)^{1/K}\right)$$



Projective Runge-Kutta method

Higher-order projective Runge-Kutta (PRK) methods can be constructed by replacing each time derivative evaluation k_s in a classical Runge-Kutta method by $K+1$ steps of an inner integrator as follows:

$$s = 1: \begin{cases} u^{n,k+1} &= u^{n,k} + \delta t g(u^{n,k}), \qquad 0 \leq k \leq K \\ k_1 &= \dfrac{u^{n,K+1} - u^{n,K}}{\delta t} \end{cases}$$

$$2 \leq s \leq S: \begin{cases} u_s^{n+c_s,0} &= u^{n,K+1} + (c_s \Delta t - (K+1)\delta t) \sum_{l=1}^{s-1} \dfrac{a_{s,l}}{c_s} k_l, \\ u_s^{n+c_s,k+1} &= u_s^{n+c_s,k} + \delta t g(u_s^{n+c_s,k}), \qquad 0 \leq k \leq K \\ k_s &= \dfrac{u_s^{n+c_s,K+1} - u_s^{n+c_s,K}}{\delta t} \end{cases}$$

$$u^{n+1} = u^{n,K+1} + (\Delta t - (K+1)\delta t) \sum_{s=1}^{S} b_s k_s.$$

To ensure consistency, the Runge-Kutta matrix $\mathbf{a} = (a_{s,i})_{s,i=1}^S$, weights $\mathbf{b} = (b_s)_{s=1}^S$, and nodes $\mathbf{c} = (c_s)_{s=1}^S$ satisfy the usual conditions $0 \leq b_s \leq 1$ and $0 \leq c_s \leq 1$, as well as:

$$\sum_{s=1}^{S} b_s = 1, \qquad \sum_{i=1}^{S-1} a_{s,i} = c_s, \quad 1 \leq s \leq S.$$

A general Boltzmann-like equation

Scaled form

Study of a particle distribution function $f^\varepsilon(t,x,v)$, depending on the time $t>0$, space position $x \in \Omega \subset \mathbb{R}^{d_x}$, $d_x \in \{1,2,3\}$ and particle velocity $v \in \mathbb{R}^{d_v}$, $d_v \geq d_x$, solution to

$$\left\{ \begin{aligned} & \frac{\partial f^\varepsilon}{\partial t} + v \cdot \nabla_x f^\varepsilon = \frac{1}{\varepsilon}\, \mathcal{Q}(f^\varepsilon), \\ & f^\varepsilon(0,x,v) = f_{in}(x,v), \end{aligned} \right. \tag{2}$$

where $\mathcal{Q}$ is the collision operator, describing the microscopic collision dynamics between particles and ε is the Knudsen number, ration between the mean free path between collisions and the typical length scale.

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- $\rightarrow$ Huge phase space (up to 7-D!) $\Rightarrow$ Deterministic numerical simulations very costly!
- $\rightarrow$ Stiff (possibly multi-scale), highly nonlinear problem $\Rightarrow$ Impliciting almost impossible!

Mathematical properties of the collision operator

- Conservation of mass, momentum and kinetic energy

$$\int_{\mathbb{R}^3} \mathcal{Q}(f)(v)\,dv = 0, \quad \int_{\mathbb{R}^3} \mathcal{Q}(f)(v)\,v\,dv = 0, \quad \int_{\mathbb{R}^3} \mathcal{Q}(f)(v)\,|v|^2\,dv = 0;$$

- Dissipation of Boltzmann entropy

$$\int_{\mathbb{R}^3} \mathcal{Q}(f)(v)\,\log(f)(v)\,dv \le 0;$$

- Explicit equilibria, known as Maxwellian distribution

$$\mathcal{Q}(f) = 0 \quad \Leftrightarrow \quad f = \mathcal{M}_{\rho,\boldsymbol{u},T} := \frac{\rho}{(2\pi T^{3/2})} \exp\left(-\frac{|v-\boldsymbol{u}|^2}{2T}\right);$$

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- 0^{th} order fluid limit $\varepsilon \to 0$ given by the compressible Euler system

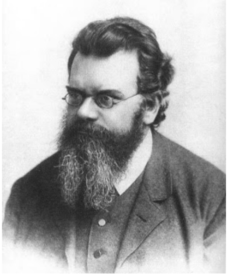
$$\begin{cases} \partial_t \rho + \mathrm{div}_x(\rho\, \boldsymbol{u}) \,=\, 0, \\ \partial_t(\rho\, \boldsymbol{u}) + \mathrm{div}_x\left(\rho\, \boldsymbol{u} \otimes \mathbf{u} \,+\, \rho T\, \mathbf{I}\right) \,=\, \mathbf{0}_{\mathbb{R}^3}, \\ \partial_t E + \mathrm{div}_x\left(\boldsymbol{u}\,(E \,+\, \rho T)\right) \,=\, 0. \end{cases}$$

The Boltzmann equation

It describes the non equilibrium behavior of a diluted gas of solid particles, interacting only via binary elastic collisions

Applications

Microscale flow in MEMS, space shuttle atmospheric re-entry, ...



Boltzmann collision operator

$$\mathcal{Q}_{\mathcal{B}}(f)(v) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left[f'_* f' - f_* f \right] B(|v - v_*|, \cos\theta) \, d\sigma \, dv_*,$$

where B is the collision kernel, $\cos\theta := (v - v_*) \cdot \sigma$ and

$$v' = \frac{v + v_*}{2} + \frac{|v - v_*|}{2} \sigma, \qquad v'_* = \frac{v + v^*}{2} - \frac{|v - v_*|}{2} \sigma.$$

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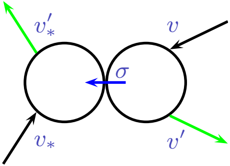

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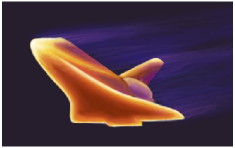
The BGK equation

The BGK[1] equation replaces the quadratic Boltzmann operator by a nonlinear relaxation operator which mimics its main features.

Applications

Same as before, but the simpler structure of the operator allows for easier computations (with a cost in accuracy)



BGK operator

$$\mathcal{Q}_{\mathcal{BGK}}(f)(v) = \nu(rho)\left[\mathcal{M}_{\rho_f,\boldsymbol{u}_f,T_f}(v) - f(v)\right],$$

where

$$(\rho_f, \boldsymbol{u}_f, T_f) = \int_{\mathbb{R}^d} f(t,x,v)\,\varphi(v)\,dv$$

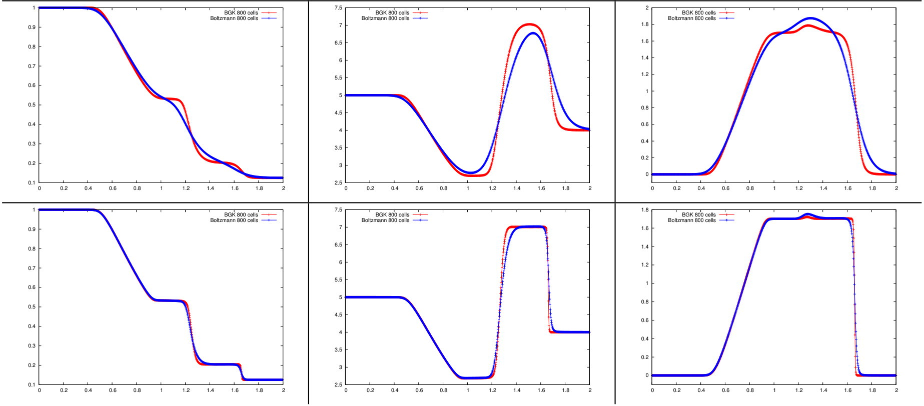
for $\varphi(v) = (1, v, |v - \boldsymbol{u}_f|^2)$ are the mass, velocity and local temperature of f and $\mathcal{M}_{\rho,\boldsymbol{u},T}$ the associated Maxwellian distribution.

[1] Bhatnagar, Gross, Krook, *Phys. Rev.* (1954)

Riemann problem (Sod's tube) $1D_x \times 2D_v$

BGK vs. Boltzmann

Density ρ	Temperature T	Velocity u_x



BGK (red) and Boltzmann (blue) solutions for $\varepsilon = 10^{-2}$ (top) and $\varepsilon = 10^{-4}$, at $t = 0.15$ with 800 spatial cells and 64^2 velocity cells

Kinetic approximation of conservation laws

Let $f^\varepsilon \in L^1_{x,v}\left((1+v)\,dv\right)$ solution to the kinetic equation

(3) $$\partial_t f^\varepsilon + v\partial_x f^\varepsilon = \frac{1}{\varepsilon}\left(R[u^\varepsilon] - f^\varepsilon\right)$$

where

$$\int_{\mathbb{R}} R[u^\varepsilon](v)(1,v)\,dv = \left(\int_{\mathbb{R}} f^\varepsilon(v)\,dv, g(u^\varepsilon)\right).$$

Then, when $\varepsilon \to 0$, u^ε converges toward u, solution to the scalar conservation law

(4) $$\partial_t u + \partial_x g(u) = 0$$

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Theorem (Lafitte, Leijon, Melis, Samaey, 2012-2014)

Choosing the parameters of the PFE scheme as $K = 2$, $\delta t = \varepsilon$ and Δt as the hyperbolic CFL coming from (4) provides a ε-uniformly stable time integrator for (3), whose limit is a stable approximation to (4). It is also consistent in the linear case.

Kinetic approximation of conservation laws

Let $f^\varepsilon \in L^1_{x,v}((1+v)\,dv)$ solution to the kinetic equation

(3) $$\partial_t f^\varepsilon + v\partial_x f^\varepsilon = \frac{1}{\varepsilon}\left(R[u^\varepsilon] - f^\varepsilon\right)$$

where

$$\int_{\mathbb{R}} R[u^\varepsilon](v)(1,v)\,dv = \left(\int_{\mathbb{R}} f^\varepsilon(v)\,dv, g(u^\varepsilon)\right).$$

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Proof. Compute the slow and fast eigenvalue branches:

$$\lambda^s = -\lambda_1^s\varepsilon + i\mu^s(1+\varepsilon^2) + \mathcal{O}(\varepsilon^3), \qquad \lambda^f = -\frac{1}{\varepsilon} - \lambda_1^f\varepsilon - i\mu^f(1+\varepsilon^2) + \mathcal{O}(\varepsilon^3)$$

then use the stability criterion of the PFE method.

Spectrum of the linearized BGK and Boltzmann operators

And now, for something (slightly) different

Denoting by $\mathcal{M}$ the global Maxwellian distribution $\mathcal{M}_{1,0,1}$, one can define the linearized BGK and Boltzmann operators as

$$\mathcal{L}_{\mathcal{M}}\, g := \mathcal{M}^{-1}\left(\mathcal{Q}(\mathcal{M}, g) + \mathcal{Q}(g, \mathcal{M})\right) = K_{\mathcal{M}} g - \nu(v)\, g$$

where $K_{\mathcal{M}}$ is a compact operator on $L^2_v\left(\mathcal{M}^{-1} dv\right)$ and ν is bounded by below.
Going to Fourier in space, one can then define the linearized Boltzmann equation by

$$\partial_t g = \frac{1}{\varepsilon} K_{\mathcal{M}} g - \left(\nu(v)/\varepsilon + i\,\varepsilon\gamma \cdot v\right) g. \tag{5}$$

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Theorem (Grad '56, McLennan '65, Nicolaenko '71, Ellis-Pinsky '75)

The spectrum of the RHS of (5) is composed of

- fast modes: Eigenvalues located at a distance at least $1/\varepsilon$ on the left of the imaginary axis;
- slow modes: if $|\varepsilon| \ll 1$, exactly $D_v + 2$ eigenvalues branches given by

$$\lambda^{(j)}(|\gamma|) := i\, \lambda_1^{(j)}\, \varepsilon|\gamma| - \lambda_2^{(j)}\, \varepsilon^2 |\gamma|^2 + \mathcal{O}\left(\varepsilon^3 |\gamma|^3\right),$$

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In the Boltzmann case, an essential spectrum also exists...

THE FIRST AND SECOND FLUID APPROXIMATIONS TO THE LINEARIZED BOLTZMANN EQUATION (*)

By **Richard S. ELLIS and Mark A. PINSKY**

1.A. Introduction

Let $p_\varepsilon(t, x, \xi)$ be the solution of the Boltzmann equation :

$$\frac{\partial p}{\partial t} + \xi . \operatorname{grad} p = \frac{1}{\varepsilon} \mathrm{Q}\, p, \tag{1.1}$$

$$\lim_{t \downarrow 0} p(t, x, \xi) = f(x, \xi),$$

in a Euclidean domain D, where boundary conditions are prescribed on ∂ D if D is finite. When $\varepsilon \to 0$, a great simplification occurs in the solution of (1.1), known as a "contraction of the description". This is formally treated by the Chapman-Enskog expansion at the physical level of rigor [17].

To make this precise, Grad [8] first considered (1.1) in a cube $\mathrm{D} \subset \mathrm{R}^3$ with periodic boundary conditions, where Q is the linearized collision operator corresponding to a spherically symmetric potential function with a hard core. Using a priori estimates for (1.1), he proved that for f suitably smooth

$$\mathrm{T}_\varepsilon(t) f - \mathrm{E}(t) f = 0(\varepsilon) \qquad (\varepsilon \downarrow 0), \tag{1.2}$$

$$\mathrm{T}_\varepsilon\left(\frac{t}{\varepsilon}\right) f - \mathrm{N}_\varepsilon\left(\frac{t}{\varepsilon}\right) f = 0(\varepsilon) \qquad (\varepsilon \downarrow 0), \tag{1.3}$$

where $\mathrm{T}_\varepsilon(t) f = p_\varepsilon$ is the solution of (1.1) and $\mathrm{E}(t), \mathrm{N}_\varepsilon(t)$ denote, respectively, the solution operators for the linear Euler and Navier-Stokes equations with viscosity and heat conduction coefficients proportional to ε. These systems of partial differential equations are derived by means of the classical Chapman-Ensokg-Hilbert expansion as applied to the linearized Boltzmann equation (1.1).

(*) Research supported in part by National Science Foundation Grant GP 28576.

PI for the BGK and Boltzmann equations

The spectrum of the linearized BGK operator is composed of

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$$\lambda^{(j)}(|\gamma|) := i\,\lambda_1^{(j)}\,\varepsilon|\gamma| - \lambda_2^{(j)}\,\varepsilon^2|\gamma|^2 + \mathcal{O}\left(\varepsilon^3|\gamma|^3\right),$$

- Fast (exponential?) rate of damping of the solution to the full BGK equation toward Maxwellian distribution $\Rightarrow$ Linear regime $\Rightarrow$ Taking the same parameters for the PFE scheme as before $K = 2$, $\delta t = \varepsilon$ and Δt as the hyperbolic CFL coming from the compressible Euler dynamics will give an ε-stable, uniformly accurate, explicit time integrator for the BGK equation!

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- In the Boltzmann case, an essential spectrum also exists... Need to use Telescopic Projective Integration[2], which brings a $\log(1/\varepsilon)$ dependency on δt. But this is another story ;-)

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Summary of the numerical solvers

Numerically solving the kinetic equation

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

- Introduce a Cartesian grid $\mathcal{V}$ of $\mathbb{R}^{D_v}$ by $\mathcal{V} = \{v_k = k\Delta v + a,\ k \in \mathcal{K}\}$ and denote the discrete collision invariants on $\mathcal{V}$ by $m_k = (1, v_k, \frac{1}{2}|v_k|^2)$.
- Replace the continuous distribution function f by a N-vector $f_{\mathcal{K}}(x,t)$, where each component is assumed to be an approximation of f at location v_k:

$$f_k(x,t) \approx f(x, v_k, t).$$

  The fluid quantities are then obtained from f_k :

$$U(x,t) = \sum_k m_k f_k(x,t)\, \Delta v.$$

- The discrete velocity model becomes a set of N equations for f_k

$$\partial_t f_k + v_k \cdot \nabla_x f_k = \mathcal{Q}(f_k),$$

  where the term $\mathcal{Q}(f_k)$ couples all the equations.
- Free transport term $\mathrm{div}_x(v_k f_k)$ computed with WENO reconstruction.
- PRK time stepping.

Spectral discretization of Boltzmann collision operator

Truncation of the Boltzmann operator (assume now that $f = f(v)$ only):

- If the distribution function f have compact support on $\mathcal{B}_0(R)$, then $\mathrm{supp}(Q(f,f)(v)) \subset \mathcal{B}_0(\sqrt{2}R)$.
- Thus, to write a spectral approximation which avoids aliasing, it is sufficient that $f(v)$ is restricted to $[-T,T]^{D_v}$ with $T \geq (2+\sqrt{2})R$.
- Assuming $f(v) = 0$ on $[-T,T]^{D_v} \setminus \mathcal{B}_0(R)$, we extend $f(v)$ to a periodic function on the set $[-T,T]^3$.
- The choice $T = (3+\sqrt{2})R/2$ guarantees the absence of intersection between periods where f is different from zero.

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Fourier representation of the collision operator:

- Let us take $T = \pi$ and hence $R = \lambda\pi$ with $\lambda = 2/(3+\sqrt{2})$.
- The distribution function is represented as the truncated Fourier series

$$f_N(v) = \sum_{k=-N}^{N} \hat{f}_k e^{ik\cdot v}, \qquad \hat{f}_k = \frac{1}{(2\pi)^{D_v}} \int_{[-\pi,\pi]^{D_v}} f(v) e^{-ik\cdot v}\, dv.$$

Spectral discretization of Boltzmann collision operator II

$$\mathcal{Q}_{\mathcal{B}}(f)(v) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left[f'_* f' - f_* f \right] B(|v - v_*|, \cos\theta)\, d\sigma\, dv_*,$$

- We then obtain a spectral quadrature by projecting the Boltzmann operator on the space of trigonometric polynomials of degree $\leq N$, i.e.

$$\hat{\mathcal{Q}}_k = \int_{[-\pi,\pi]^3} \mathcal{Q}(f_N) e^{-ik\cdot v}\, dv, \quad k = -N, \ldots, N.$$

- By substituting the truncated Fourier series f_N in $\hat{Q}$ one gets

$$\hat{\mathcal{Q}}_k = \sum_{\substack{l,m=-N \\ l+m=k}}^{N} \hat{f}_l\, \hat{f}_m \hat{\beta}(l,m), \quad k = -N, \ldots, N,$$

- $\hat{\beta}(l,m) = \mathcal{B}(l,m) - \mathcal{B}(m,m)$ are given by

$$\mathcal{B}(l,m) = \int_{\mathcal{B}_0(2\lambda\pi)} \int_{\mathbb{S}^2} |q| \sigma(|q|, \cos\theta) e^{-i(l\cdot q^+ + m\cdot q^-)}\, d\omega\, dq.$$

  with $q^+ = \frac{1}{2}(q + |q|\omega), \quad q^- = \frac{1}{2}(q - |q|\omega)$.

- The evaluation of $\mathcal{B}(l,m)$ requires $\mathcal{O}(N^2)$ operations.

Fast spectral discretization

In order to reduce the number of operations needed to evaluate the collision integral, the main idea is to use the so-called Carleman representation.

- This gives

$$\mathcal{Q}_B(f) = \int_{\mathcal{R}^3} \int_{\mathcal{R}^3} \tilde{B}(x,y)\delta(x \cdot y) \left[f(v+y)\, f(v+x) - f(v+x+y)\, f(v) \right] dx\, dy,$$

with

$$\tilde{B}(|x|,|y|) = 2^{d_v - 1}\, \sigma\left(\sqrt{|x|^2 + |y|^2}, \frac{|x|}{\sqrt{|x|^2+|y|^2}} \right) \left(|x|^2 + |y|^2\right)^{-\frac{d_v - 3}{2}}.$$

- This transformation permits to get to the following new spectral quadrature formula

$$\hat{\mathcal{Q}}_k = \sum_{\substack{l,m=-N \\ l+m=k}}^{N} \hat{\beta}_F(l,m)\, \hat{f}_l\, \hat{f}_m, \quad k = -N, ..., N$$

where $\hat{\beta}_F(l,m) = \mathcal{B}_F(l,m) - \mathcal{B}_F(m,m)$ are now given by

$$\mathcal{B}_F(l,m) = \int_{\mathcal{B}_0(R)} \int_{\mathcal{B}_0(R)} \tilde{B}(x,y)\, \delta(x \cdot y)\, e^{i(l \cdot x + m \cdot y)}\, dx\, dy.$$

Fast spectral discretization II

- Now, we look for a convolution structure. The aim is to approximate each $\hat{\beta}_F(l,m)$ by a sum

$$\hat{\beta}_F(l,m) \simeq \sum_{p=1}^{A} \alpha_p(l)\alpha'_p(m)$$

- This gives a sum of A discrete convolutions and so the algorithm can be computed in $O(A\,N\log_2 N)$ operations by means of standard FFT techniques.

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An example, the two dimensional case:

- Make the decoupling assumption

$$\tilde{B}(x,y) = a(|x|)\,b(|y|);$$

  satisfied if e.g. $\tilde{B}$ is constant (2D Maxwellian molecules, 3D hard spheres).
- This gives

$$\mathcal{B}_F(l,m) = \int_0^{\pi} \phi_R^2(l\cdot e_\theta)\,\phi_R^2(m\cdot e_{\theta+\pi/2})\,d\theta, \quad \phi_R^2(s) = 2\,R\,\mathrm{sinc}(Rs).$$

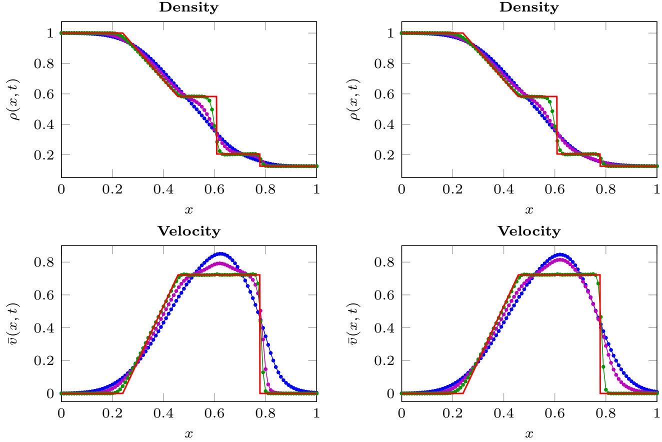
- A regular discretization of M equally spaced points gives

$$\mathcal{B}_F(l,m) = \frac{\pi}{M}\sum_{p=0}^{M-1} \alpha_p(l)\alpha'_p(m), \quad \alpha_p(l) = \phi_R^2(l\cdot e_{\theta_p}),\ \alpha'_p(m) = \phi_R^2(m\cdot e_{\theta_p+\pi/2})$$

$1D_x - 1D_v$ BGK

Sod shock tube problem, PRK4 time integrator, WENO 3 in x

First moments of the solution to the BGK equation with $\nu = 1$ (left) and $\nu = \rho$ (right)



$\Delta t = 0.4\Delta x$, $\Delta x = 0.01$, $N_v = 80$, $K = 2$ and $\delta t = \varepsilon$, for $\varepsilon = 10^{-1}$ (blue dots), 10^{-2} (purple dots), and 10^{-5} (green dots). Red line: hydrodynamic limit $\varepsilon \to 0$

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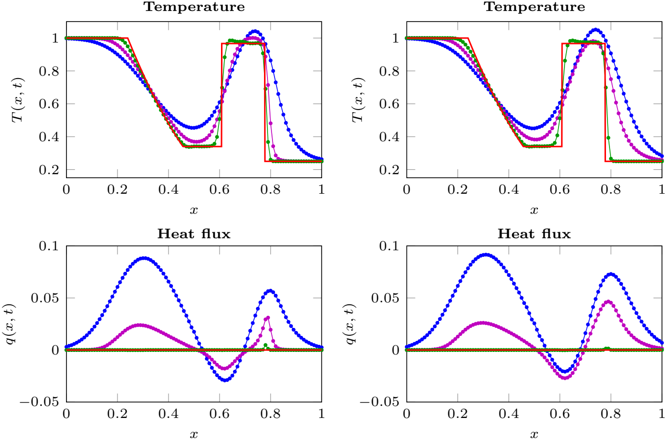

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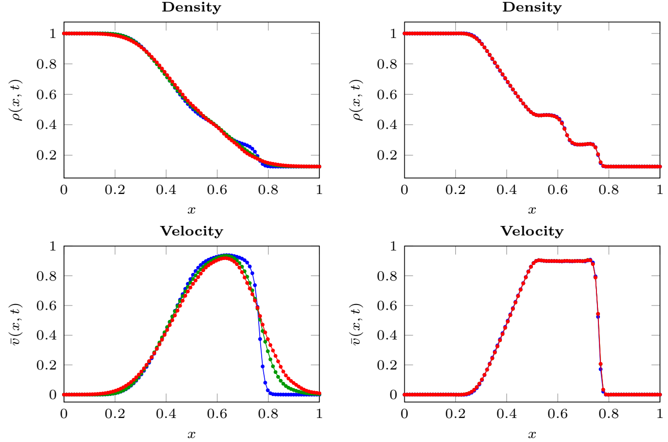
$1D_x - 2D_v$ BGK vs. Boltzmann

Sod shock tube problem, PRK4 time integrator, WENO 2 in x, fast spectral in v

First moments of BGK equation with $\nu = 1$ (blue), $\nu = \rho$ (green) and Boltzmann (red)



$\Delta t = 0.4\Delta x$, $\Delta x = 0.01$, $N_v = 32^2$, $K = 2$ and $\delta t = \varepsilon$, for $\varepsilon = 10^{-2}$ (left), and 10^{-5} (right).

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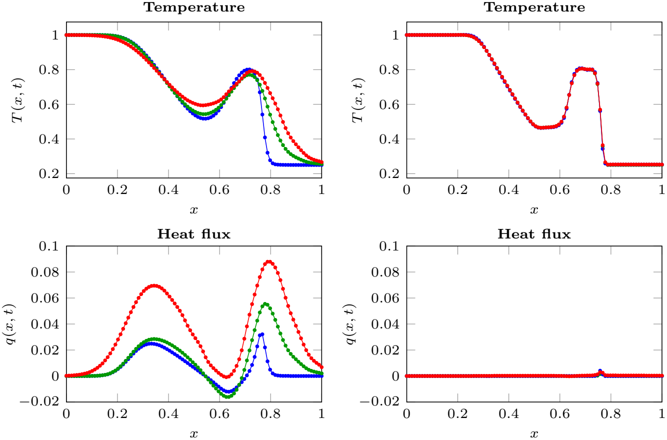

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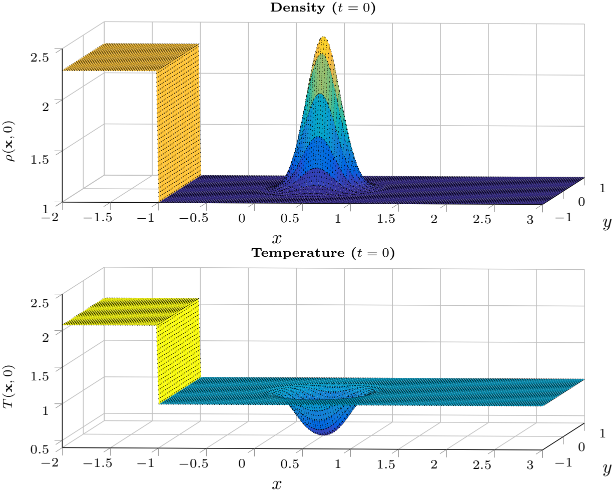
$2D_x - 2D_v$ BGK

Shock-Bubble interaction, PRK4 time integrator, WENO 2 in x, $\varepsilon = 10^{-5}$, $\nu = 1$



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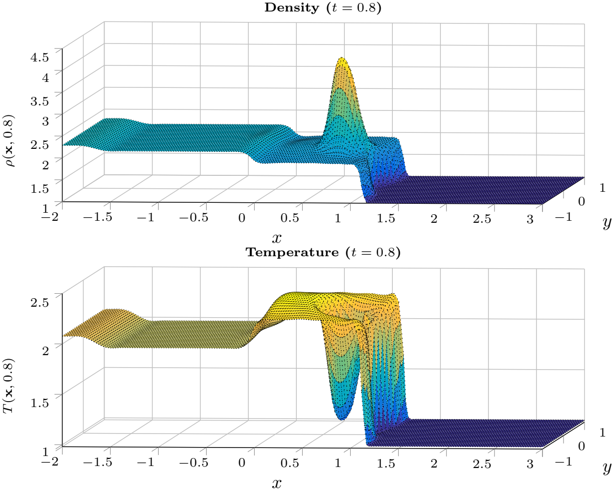

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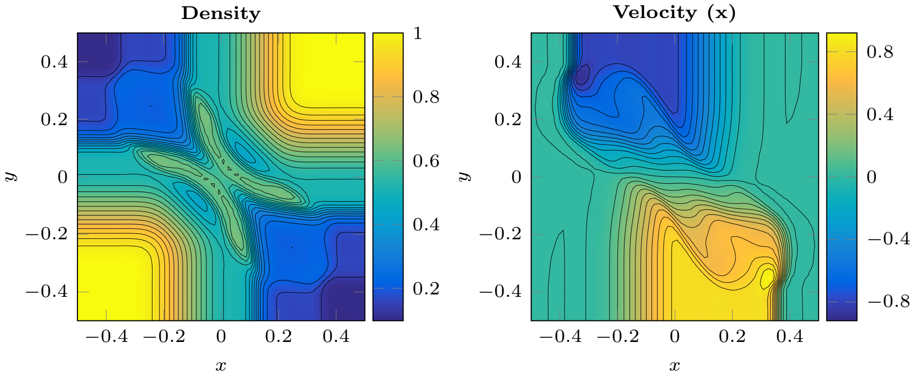
$2D_x - 2D_v$ Boltzmann

Double Sod shock, TPRK4 time integrator, WENO 2 in x, $\varepsilon = 5.10^{-5}$, $\nu = 1$



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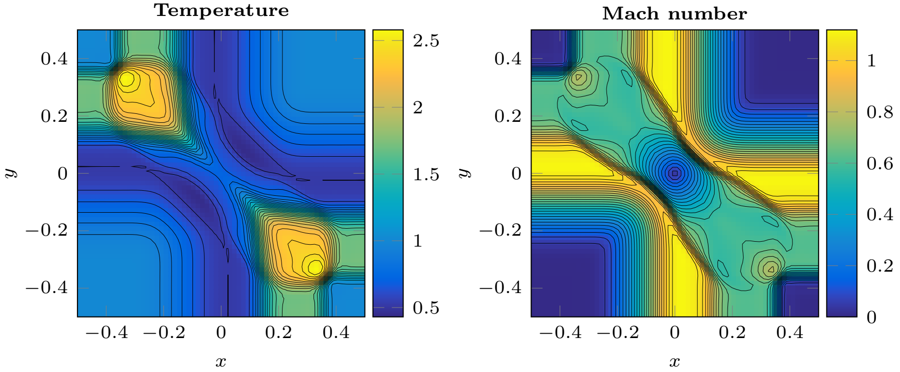

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Conclusion

- We have built and implemented a deterministic, high order, explicit and asymptotic preserving solvers for nonlinear kinetic equations;
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Thanks a lot for your attention!