Deterministic Methods for the Boltzmann Equation

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AM281.1 Convection-Dominated Problems
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Outline

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(Navier-Stokes Equations)

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Density function:

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} f(v, x, t) \mathrm{d}x \mathrm{d}v = n(t).$$

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Knudsen Number

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

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$k_n \rightarrow 0$: Continuum limit.

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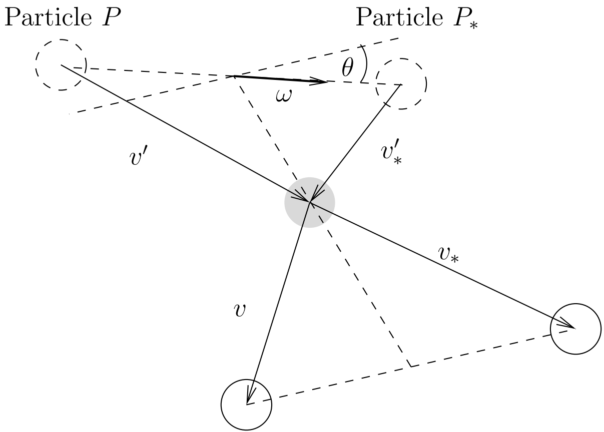
Binary Collisions



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Q is a spatially local operator!

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Of course, one can cook up many more complicated collision kernels.

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- Positivity (if there is time)

Questions?

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Outline

General Framework

- Semi-discrete form of Boltzmann equation

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f_1(y) + f_2(y)$$

- f_1 and f_2 may have significantly different properties
  - f_1 represents convection
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- f_1 and f_2 may have significantly different properties
  - f_1 represents convection
  - f_2 is usually a stiff discretization of collision
- Possible nonlinearity of f_1: high-order accurate explicit method
- Highly stiff f_2: implicit method
- Conservation? Positivity?

Splitting Methods

- Strategy 1: operator splitting
  - $S_1^{\Delta t}$ and $S_2^{\Delta t}$ are solution operators for

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f_1(y) \qquad \frac{\mathrm{d}y}{\mathrm{d}t} = f_2(y), \tag{1}$$

    respectively
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- Strategy 2: Runge-Kutta split methods
  - Create two separate Runge-Kutta methods for each of the ODE's in (1), but evolve them together
  - High-order accuracy requires coupling conditions between the two methods
  - Disadvantage: requires semi-discrete form of PDE

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- "Strang splitting"

$$S^{\Delta t} \approx S_1^{\Delta t/2} S_2^{\Delta t} S_1^{\Delta t/2}$$

  - Second-order in time
  - Not much more difficult than first-order splitting
  - Probably the most popular operator splitting algorithm used today

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  - Methods exist, but suffer from stability problems
  - Dia has developed 3rd, 4th order schemes
- Conservation?
  - Ohwada: second-order scheme

$$S^{\Delta t} \approx \frac{1}{2}\left(I + S_2^{\Delta t} S_2^{\Delta t}\right) S_1^{\Delta t}$$

  - Preserves mass, momemtum, energy (assuming the discrete collision operator does as well)
  - Slightly more work compared to Strang splitting

Runge-Kutta methods

- "Usual" s-stage Runge-Kutta methods have the form

$$y^{n+1} = y^n + \Delta t \sum_{j=1}^{s} b_j f(t^n + c_j \Delta t, Y_j)$$

$$Y_i = y^n + \Delta t \sum_{j=1}^{s} a_{ij} f(t^n + c_j \Delta t, Y_j)$$

where a_{ij} is an $s \times s$ matrix and b_j and c_j are $s \times 1$ matrices

- Can define explicit and implicit RK methods in this way

More Runge-Kutta

- Implicit-explicit (IMEX) RK idea: use different RK methods for each different term:

$$
\begin{aligned}
y^{n+1} =& y^n + \Delta t \sum_{j=1}^{s} \tilde{b}_j f_1(t^n + \tilde{c}_j \Delta t, Y_j) + \\
& \Delta t \sum_{j=1}^{s} b_j f_2(t^n + c_j \Delta t, Y_j), \\
Y_i =& y^n + \Delta t \sum_{j=1}^{s} \tilde{a}_{ij} f_1(t^n + \tilde{c}_j \Delta t, Y_j) + \\
& \Delta t \sum_{j=1}^{s} a_{ij} f_2(t^n + c_j \Delta t, Y_j)
\end{aligned}
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  - Second-order methods: 'midpoint' splitting, Strang splitting, Jin splitting, ...
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- Can’t have your cake and eat it, too

What do people actually do?

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- Mostly operator splitting (Strang)
- Splitting is, of course, not the only answer
- Could use just about any ODE discretization you want

Questions?

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1. Introduction
   - The Equation
   - Collisions
2. Time-Step Splitting
   - Operator splitting
   - Runge-Kutta
3. Transport
   - Flux-Balance Methods
   - Semi-Lagrangian Methods
4. Collision Operator
   - Discretization
   - Bobylev-Rjasanow's Integral Transform Method
   - Pareschi-Russo's Spectral Method
   - Mouhot-Pareschi's Sub-N^6 Method

The Vlasov Equation

- Recall that the transport part of the Boltzmann equation is the Vlasov equation:

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f + F \cdot \nabla_v f = 0.$$

  - Nonlinear: F depends on f
  - Conservation law: v is x-independent and F is v-independent

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  - Nonlinear: F depends on f
  - Conservation law: v is x-independent and F is v-independent
- Many methods exist to solve these types of equations
- What we'll talk about: methods designed specifically for the Vlasov/Boltzmann equation

Argh, More Splitting?

- Complexity: six-dimensional transport equation → two 3-dimensional systems is more tractable

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$$\frac{\partial f}{\partial t} = v \cdot \nabla_x f \qquad \frac{\partial f}{\partial t} = F \cdot \nabla_v f$$

- Go even farther: split three dimensional problems into three 1-dimensional problems?
- Consider simple 1D conservation law:

$$\frac{\partial f}{\partial t} + \frac{\partial (vf)}{\partial x} = 0$$

Flux-Balance Methods

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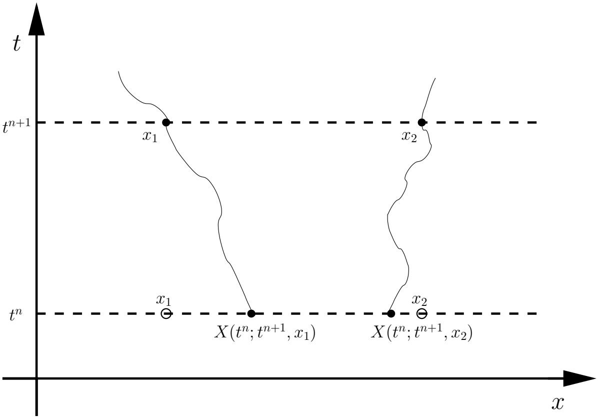
- Method of characteristics: f is constant along $x = X(t)$, where $X(t)$ solves the ODE

$$\frac{\mathrm{d}X(s)}{\mathrm{d}x} = v(s, X(s))$$
$$X(t^{n+1}) = x.$$

- $f(x, t^{n+1}) = f(X(t^n; t^{n+1}, x), t^n)$

Method of Characteristics



Flux-Balance Methods

- Use characteristics for finite-volume:

$$\int_{x_{i-1/2}}^{x_{i+1/2}} f(t^{n+1}, x)\mathrm{d}x = \int_{X(t^n;t^{n+1},x_{i-1/2})}^{X(t^n,t^{n+1},x_{i+1/2})} f(t^n, x)\mathrm{d}x$$

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- Define flux terms:

$$\Phi_{i+1/2}(t^n) = \int_{x_{i+1/2}-v\Delta t}^{x_{i+1/2}} f(t^n, x)\mathrm{d}x$$

Flux-Balance Methods

- Use characteristics for finite-volume:

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- Rewrite first equation as

$$\int_{x_{i-1/2}}^{x_{i+1/2}} f(t^{n+1},x)\mathrm{d}x = \int_{x_{i-1/2}}^{x_{i+1/2}} f(t^n,x)\mathrm{d}x + \frac{\Phi_{i-1/2}(t^n) - \Phi_{i+1/2}(t^n)}{\Delta x}$$

Flux-Balance Scheme

- Leads to the finite-volume fully-discrete scheme

$$f_i^{n+1} = f_i^n + \frac{\Phi_{i-1/2}(t^n) - \Phi_{i+1/2}(t^n)}{\Delta x}$$

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- How to evolve the scheme? Need to compute fluxes Φ.
  - No time-step restriction!
  - Explicitly compute integral definition (reconstruct f)
  - Compute pointwise primitive values (reconstruct primitive, F)

Flux-Balance – reconstructing f: PFC

- The ‘Positive and Flux-Conservative’ (PFC) method
- Third-order reconstruction using nonlinear slope limiters
- f is reconstructed as a quadratic polynomial

$$f_h(x) = f_i + \varepsilon^+ p_2^+(x)(f_{i+1} - f_i) + \varepsilon^- p_2^-(x)(f_i - f_{i-1})$$

- Preserves positivity of f
- Reconstruction preserves cell averages (mass)

Flux-Balance – reconstructing F: WENO

- ‘PWENO’: Pointwise WENO
  - Same principle as WENO
  - Reconstruction requires the primitive values inside cells (hence the ‘pointwise’ appellation)
  - More expensive than WENO: weights must be tailored depending on location $\rightarrow$ requires linear solve
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- Use PWENO to reconstruct $F(x_{j+1/2} - v\Delta t)$

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- Can't have your cake and eat it, too

Questions?

?

Outline

The Collision Operator

$$\frac{\partial f}{\partial t} = \frac{1}{k_n} Q(f,f)$$

$$Q(f,f) = \int_{\mathbb{R}^3} \int_{S^2} B \left[f(v')f(v'_*) - f(v)f(v_*) \right] \mathrm{d}\omega \mathrm{d}v_*$$

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- Conserves mass, momentum, energy:

$$\int_{\mathbb{R}^3} Q(f,f) \begin{cases} 1 \\ v \\ |v|^2 \end{cases} \mathrm{d}v = 0$$

The Collision Operator–Steady-State

Evolves towards ~~Gaussian in v~~ *Maxwellian*

$$f_\infty(v) := \frac{\rho}{(2\pi T)^{d/2}} \exp\left(-\frac{|V - v|^2}{2T}\right)$$

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- Does so even for *full* Boltzmann equation.

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$$Q^{\mathrm{lin}}(f,f) \approx \int_{\mathbb{R}^3}\int_{S^2} B[g(v')f_\infty(v'_*) + f_\infty(v')g(v'_*) - g(v)f_\infty(v_*) - f_\infty(v)g(v_*)]\mathrm{d}\omega \mathrm{d}v_*$$

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$\rightarrow$*Linear Vlasov-Boltzmann Equation*

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Still stronger than (i.e. implies) Navier-Stokes.

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v-space: infinite.

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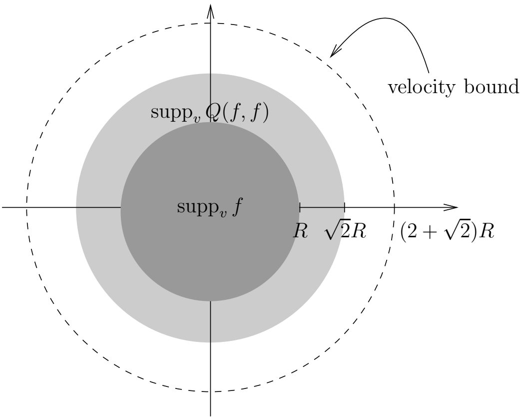
3. *With this limitation, we automatically also have* $v_* = v - g, v', v'_* \in \mathcal{B}(0,(2+\sqrt{2})R)$.

Compact support for Q



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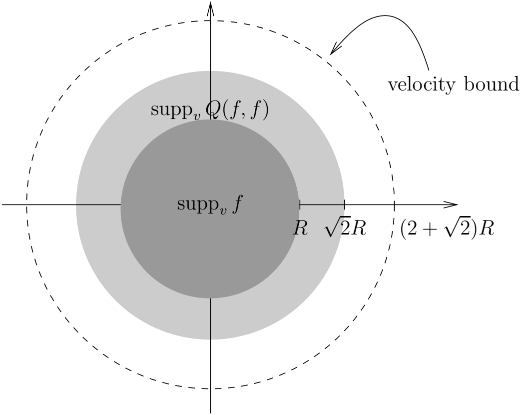

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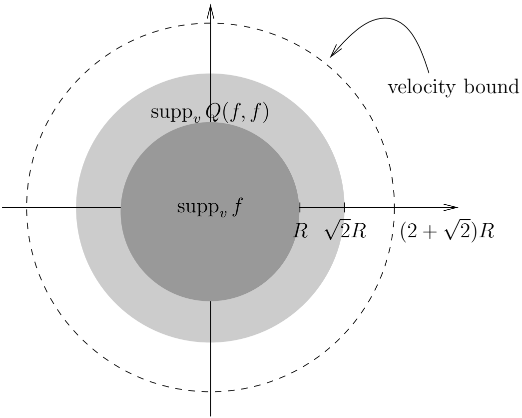

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using the midpoint rule

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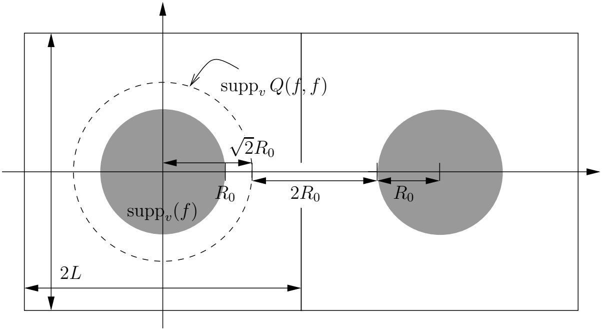

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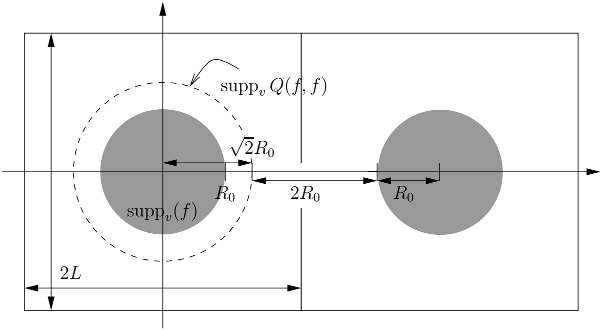
So v-space becomes (artificially) $2L$-periodic, with $L = nh_v/2$.



Avoid aliasing: choose $L \geqslant \frac{1}{2}(\sqrt{2}R_0 + 2R_0 + R_0) = \frac{3+\sqrt{2}}{2}R_0$.

Overview

	M	H	V	O	Order	Ops	Ms	Mm	En
DSMC	✓	✓	✓	✓	$N^{-1/2}$	N^3	✓	✓	✓
IbrR	✓	✓	✓	–	N^{-2}	N^6	✓	○	○
gen.	–	–	–	✓	N^{-2}	$N^6 \log N$	✓	○	○
BobR	–	3	–	–	N^{-2}	$N^6 \log N$	✓	○	○
ParRu	✓	✓	✓	–	$N^{-\infty}$	N^6	✓	○	○
MouP	2	3	–	–	$N^{-\infty}$	$N^5 \log N$	✓	○	○

Bobylev-Rjasanow's Integral Transform Method

Idea:

Rewrite $Q(f, f)$ into convolution integrals.
Exploit the Fast Fourier Transform to evaluate these integrals quickly.

skip the details

Bobylev-Rjasanow's Method

Lemma (Symmetric Representation)

The collision operator can be represented as

$$Q(f,f) = 4\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \tilde{B}(y,z)\delta(z\cdot y)[f(v+z)(f(v+y) - f(v)f(v+y+z)]\mathrm{d}y\mathrm{d}z,$$

with

$$\tilde{B}(y,z) := \frac{1}{|y+z|}B\left(|y+z|, \frac{y\cdot(y+z)}{|y||y+z|}\right).$$

skip the rest of this method

Bobylev-Rjasanow's Method

Theorem (Integral Transform Representation)

The collision operator for hard spheres *can also be represented as*

$$Q(f,f) = \int_{S^2}\int_{S^2} \delta(\omega_1 \cdot \omega_2)\left[\Phi(\omega_1)\Phi(\omega_2) - f\Psi(\omega_1,\omega_2)\right] \mathrm{d}\omega_1 \mathrm{d}\omega_2,$$

(note the implicit v-dependency)

Bobylev-Rjasanow's Method

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Remarks on Bobylev-Rjasanow

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- Integrating over all pairs of orthogonal unit vectors:
  Apply cleverness to exploit structure.
- Φ: "*Generalized X-ray Transform*"
- Ψ: "*Generalized Radon Transform*"
- Φ and Ψ of convolution type: good for FFT.

Rewriting X-Ray Transform→Fourier Transform

$$\Phi(v,\omega) = \mathcal{F}^{-1}[\mathcal{F}[\Phi](\xi,\omega)](v,\omega)$$

Rewriting X-Ray Transform→Fourier Transform

$$\begin{aligned}\Phi(v,\omega) &= \mathcal{F}^{-1}[\mathcal{F}[\Phi](\xi,\omega)](v,\omega)\\ &= \mathcal{F}^{-1}\left[\int_{\mathbb{R}^3}\Phi(v,\omega)e^{i(v\cdot\xi)}\mathrm{d}v\right](v,\omega)\end{aligned}$$

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(\tilde{v} := v+\rho\omega) &= \mathcal{F}^{-1}\left[\int_{\mathbb{R}^3} \int_{-\infty}^{\infty} |\rho| f(\tilde{v}) e^{i((\tilde{v}-\rho\omega)\cdot\xi)} \mathrm{d}\rho \mathrm{d}v\right](v,\omega)
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&= \mathcal{F}^{-1}\left[\varphi(\xi)d(\xi\cdot\omega)\right](v,\omega)
\end{aligned}$$

The Algorithm

$$Q(f,f) = \int_{S^2}\int_{S^2} \delta(\omega_1 \cdot \omega_2)\left[\Phi(\omega_1)\Phi(\omega_2) - f\Psi(\omega_1,\omega_2)\right] \mathrm{d}\omega_1 \mathrm{d}\omega_2$$

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Altogether: $N^6 \log N$.

Pareschi-Russo's Spectral Method

Idea:

Do Fourier-Galerkin on $\partial_t f = Q(f, f)$.
Demand that the residual of $\partial_t f_N = Q(f_N, f_N)$ is orthogonal to all trigonometric polynomials, where f_N is a Fourier expansion.

skip the details

Pareschi-Russo's Spectral Method

Expand

$$f_N(v) := \sum_{k \in K_N^3} \hat{f}_k e^{i(k \cdot v)}$$

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$$\text{Avoid aliasing:} \quad \pi = L \geqslant \frac{3+\sqrt{2}}{2} R_0.$$

Pareschi-Russo's Spectral Method

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Pareschi-Russo's Spectral Method

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$$\frac{\partial \hat{f}_k}{\partial t} = \sum_{m \in K_N^3} \hat{f}_{k-m} \hat{f}_m \hat{B}(k-m, m) - \sum_{m \in K_N^3} \hat{f}_{k-m} \hat{f}_m \hat{B}(m, m)$$

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with the *kernel modes*

$$\hat{B}(l, m) = \int_{\mathcal{B}(0,2R_0)} \int_{S^2} B(|g|, \cos\theta) e^{-ig\cdot\frac{(l+m)}{2} - i|g|\omega\cdot\frac{(m-l)}{2}} \mathrm{d}\omega \mathrm{d}g$$

Performance of the Pareschi-Russo Spectral Scheme

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  - Recall: naive method would take $O(N^6 N_a)$.
- Big plus: Rolled evaluation of problematic sphere integral into pre-computation.
- Loss term is sum of convolutions.
  $\rightarrow$ Can evaluate in $O(N^3 \log N)$.

Kernel modes of the Pareschi-Russo Spectral Scheme

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- The pre-evaluated $\hat{B}$ takes up only limited storage.

Kernel modes of the Pareschi-Russo Spectral Scheme

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- A far more explicit expression for $\hat{B}$ is available.

Analysis of the Pareschi-Russo Spectral Scheme

Theorem (Spectral Accuracy)

Let $f \in L^2([-\pi,\pi]^3)$. Then

$$\left\| Q^{\mathrm{tr}}(f,f) - \mathcal{P}_N Q^{\mathrm{tr}}(f,f) \right\|_2 \leqslant C \left(\|f - f_N\|_2 + \frac{\|Q^{\mathrm{tr}}(f_N,f_N)\|_{H^r_{\mathrm{per}}}}{N^r} \right)$$

for all $r \geqslant 0$.

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Can show stability after including some filtering in the scheme.

Mouhot-Pareschi's Spectral Method

Idea:

Combine the symmetric representation from Bobylev-Rjasanow with the Fourier-Galerkin approach from Pareschi-Russo.

skip the details

Symmetric Representation

Recall

Lemma (Symmetric Representation)

The collision operator can be represented as

$$Q(f,f) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \tilde{B}(y,z)\delta(z\cdot y)[f(v+z)f(v+y) - f(v)f(v+y+z)]\mathrm{d}y\mathrm{d}z,$$

with

$$\tilde{B}(y,z) := \frac{2^{d-1}}{|y+z|^{d-2}} B\left(|y+z|, \frac{y\cdot(y+z)}{|y||y+z|}\right).$$

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(slight generalization for multi-d)

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$$Q^R(f, f) := \int_{\mathcal{B}(0,R)} \int_{\mathcal{B}(0,R)} \tilde{B}(y, z) \delta(z \cdot y) [f(v+z) f(v+y) \\ - f(v) f(v+y+z)] \mathrm{d}y \mathrm{d}z$$

Fourier-Galerkin Derivation

▸ skip the details

$$0 \stackrel{!}{=} \int_{[-\pi,\pi]^d} \left(\frac{\partial f_N}{\partial t} - \left[Q^+(f_N, f_N) - L(f_N) f_N \right] \right) e^{-ik\cdot v} \mathrm{d}v$$

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Remarks on the Scheme

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- Discretize

$$\theta := p\pi/M, \quad \varphi := q\pi/M.$$

Fast Evaluation of the Scheme

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&= \frac{\pi^2}{M^2} \sum_{m \in K_N^3} \hat{f}_{k-m} \hat{f}_m \sum_{p,q=0}^{M} \alpha_{p,q}(k-m) \alpha'_{p,q}(m) \quad - \quad \text{loss} \\
&= \frac{\pi^2}{M^2} \sum_{p,q=0}^{M} \sum_{m \in K_N^3} \hat{f}_{k-m} \alpha_{p,q}(k-m) \hat{f}_m \alpha'_{p,q}(m) \quad - \quad \text{loss.}
\end{aligned}$$

Fast Evaluation of the Scheme

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$\rightarrow$ Sum of M^2 convolutions.

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\end{aligned}$$

$\rightarrow$ Sum of M^2 convolutions. Use FFT: $M^2 N^3 \log N$ operations.

Final Remarks on Mouhot-Pareschi

$$\frac{\partial \hat{f}_k}{\partial t} = \frac{\pi^2}{M^2} \sum_{p,q=0}^{M} \sum_{m \in K_N^3} \hat{f}_{k-m} \alpha_{p,q}(k-m) \hat{f}_m \alpha'_{p,q}(m) \quad - \quad \text{loss.}$$

- Fastest method around.

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- Spectrally accurate. (Similar result as for Pareschi-Russo)

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- Fastest method around.
- Spectrally accurate. (Similar result as for Pareschi-Russo)
- Only "sophisticated" numerical technique is FFT. Probably the easiest to implement of all three methods discussed.
- Some care needs to be taken to retain proper conservation.

Conclusion

	M	H	V	O	Order	Ops	Ms	Mm	En
DSMC	✓	✓	✓	✓	$N^{-1/2}$	N^3	✓	✓	✓
IbrR	✓	✓	✓	–	N^{-2}	N^6	✓	◦	◦
gen.	–	–	–	✓	N^{-2}	$N^6 \log N$	✓	◦	◦
BobR	–	3	–	–	N^{-2}	$N^6 \log N$	✓	◦	◦
ParRu	✓	✓	✓	–	$N^{-\infty}$	N^6	✓	◦	◦
MouP	2	3	–	–	$N^{-\infty}$	$N^5 \log N$	✓	◦	◦

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BobR	—	3	—	—	N^{-2}	$N^6 \log N$	✓	○	○
ParRu	✓	✓	✓	—	$N^{-\infty}$	N^6	✓	○	○
MouP	2	3	—	—	$N^{-\infty}$	$N^5 \log N$	✓	○	○

Additional topic: Wild expansion timestepping for the collision operator.

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Additional topic: Wild expansion timestepping for the collision operator.

- maintains positivity

Conclusion

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gen.	–	–	–	✓	N^{-2}	$N^6 \log N$	✓	∘	∘
BobR	–	3	–	–	N^{-2}	$N^6 \log N$	✓	∘	∘
ParRu	✓	✓	✓	–	$N^{-\infty}$	N^6	✓	∘	∘
MouP	2	3	–	–	$N^{-\infty}$	$N^5 \log N$	✓	∘	∘

Additional topic: Wild expansion timestepping for the collision operator.

- maintains positivity
- see notes

Questions?

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