High Fidelity, Moment-Based Methods for Particle Transport: The confluence of PDEs, Optimization, and HPC

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The equations that describe particle transport start off as an integro-differential equation

- We are interested in the phase-space density of particles, N, that travel in straight-lines between collisions. The equation that describes this is the linear-Boltzmann equation:

$$(\partial_t + v\Omega\cdot\nabla + v\sigma_{\mathrm{t}}(x,t))\,N(x,\Omega,v,t) =$$
$$\int_{\mathbb{S}_2} d\Omega' \int_0^\infty dv'\, v'\sigma_s(x,t,\Omega'\to\Omega, v'\to v)N(x,\Omega,v,t) + Q(x,\Omega,v,t)$$

- $\Omega \in \mathbb{S}_2$ is the direction of the particle's flight (angular variable), v is the particle speed.
- The interaction probabilities (cross-sections) are the total cross-section σ_{t} which is the average number of collisions a particle undergoes with the material medium per unit distance travelled, and
- The double-differential scattering cross-section, $\sigma_s(x,t,\Omega'\to\Omega,v'\to v)$ is the mean number of particles that scatter to direction Ω and speed v per particle traveling in the differential phase space element.

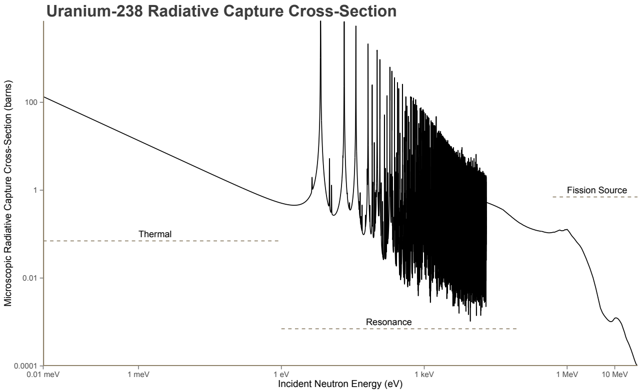
Applications

This equation very accurately describes the behavior of a variety of transport processes

- Neutrons in a nuclear reactor, oil well, imaging
- X-rays in high energy density situations: inertial confinement fusion, astrophysical radiating shocks
- Atmospheric radiative transfer
- Neutrinos in core-collapse supernovae
- Electron/ion transport in radiotherapy, space weather, electronics

Radical Simplifications

- For this talk we will make the assumption that the discretization in speed (energy) is a solved problem, and we only need to consider a single speed equation.
- Additionally, we will assume that the scattering is isotropic.
- Both of these are simplifications for real systems.



Simplified Equations

- After these simplifications we can write the resulting equation as

$$\left(v^{-1}\partial_t + \Omega \cdot \nabla + \sigma_{\mathrm{t}}(x,t)\right)\psi(x,\Omega,t) = \frac{\sigma_{\mathrm{s}}(x,t)}{4\pi}\phi(x,t) + Q(x,\Omega,t),$$

  where $\psi = vN$ and

$$\phi(x,t) = \int_{\mathbb{S}_2} d\Omega\, \psi(x,\Omega,t) = \langle \psi \rangle.$$

- We will also assume that $v = 1$. This is the same as scaling the time variable.
- Initial condition: $\psi(x,\Omega,0) = F(x,\Omega)$, and boundary conditions are inflow conditions:

$$\psi(x,\Omega,t) = \Gamma(x,\Omega,t) \quad \text{for } x \in \partial V,\ \hat{n}\cdot\Omega < 0.$$

Numerical Challenges

- Phase space complexity
  - Need for thousands of unknowns per spatial degree of freedom
- Multiscale phenomenon
  - In problems where the scattering is large, the transport equation asymptotically limits to a diffusion equation for the particles
  - Need numerical methods that preserve this fact when the mesh does not resolve the collision length scales.
- Coupling to other physics (fluid flow, etc.)

Discrete Ordinates (S_n) method

- The discrete ordinates method is a collocation method in angle that solves the transport equation along a particular directions (Ω_j) and uses a quadrature rule, $\{w_j, \Omega_j\}$ to estimate the collision terms. (Chandrasekhar)
- Leads to a simple, triangular system of discrete equations for each direction when the backward Euler method is used in time and a simple iteration strategy is used

$$(\Omega_j \cdot \nabla + \sigma_{\mathrm{t}}^*)\, \psi_j^{\ell+1}(x, t^{n+1}) = \frac{\sigma_{\mathrm{s}}(x,t)}{4\pi} \sum_{j'} w_{j'} \psi_{j'}^{\ell}(x, t^{n+1}) + Q_j^*,$$

  $\sigma_{\mathrm{t}}^* = \sigma_{\mathrm{t}} + \Delta t^{-1}$ and $Q_j^* = Q + \psi_j(x, t^n)$.
- As a result when, $\sigma_{\mathrm{s}}/\sigma_{\mathrm{t}}$ is small this iteration convergences quickly, otherwise need to include the solution of a diffusion equation in the iteration.
- This is the best understood method for deterministic particle transport.

Monte Carlo

- Rather than discretize phase space directly we sample particles and advect them based on stochastic collision processes.
- Can be very accurate and operate on general domains in space and energy.
- Slow convergence $N^{-1/2}$ typically limits applicability.
- For steady-state problems it is considered the gold standard, if you can afford the simulation.

Spherical Harmonic Functions

- Decompose the angle Ω into components

$$\Omega = (\Omega_1, \Omega_2, \Omega_3)^T = (\sin\vartheta\cos(\varphi), \sin\vartheta\sin(\varphi), \cos\vartheta)^T$$

- The normalized, complex spherical harmonic of degree ℓ and order k are

$$Y_\ell^k(\Omega) = \sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-k)!}{(\ell+k)!}}e^{ik\varphi}P_\ell^k(\cos\vartheta)\,,$$

where P_ℓ^k is an associated Legendre function.

- For convenience, we use normalized, real-valued spherical harmonics m_ℓ^k and for each degree ℓ. For given $N > 0$, set

$$\mathbf{m}_\ell = (m_\ell^{-\ell}, m_\ell^{-\ell+1}, \dots, , m_\ell^{\ell-1}, m_\ell^{\ell})^T \quad \text{and} \quad \mathbf{m} = (\mathbf{m}_0^T, \mathbf{m}_1^T, \dots, \mathbf{m}_N^T)^T$$

- The components of $\mathbf{m}$ form an orthonormal basis for the polynomial space

$$\mathbb{P}_N = \left\{\sum_{\ell=0}^{N}\sum_{k=-\ell}^{\ell} c_\ell^k m_\ell^k : c_\ell^k \in \mathbb{R} \text{ for } 0 \le \ell \le N,\ |k| \le \ell\right\}. \tag{1}$$

Spherical Harmonics (P_N) Equations

- Spectral approximation in Ω

$$\psi \approx \psi_{\mathrm{P}_N} \equiv \mathbf{m}^T \mathbf{u}_{\mathrm{P}_N}$$

where $\mathbf{u}_{\mathrm{P}_N} = \mathbf{u}_{\mathrm{P}_N}(t,x)$ solves the P_N equations

$$\begin{cases} \partial_t \mathbf{u}_{\mathrm{P}_N} + \mathbf{A}\cdot\nabla_x \mathbf{u}_{\mathrm{P}_N} + \sigma_{\mathrm{a}} \mathbf{u}_{\mathrm{P}_N} + \sigma_{\mathrm{s}} \mathbf{G} \mathbf{u}_{\mathrm{P}_N} = \mathbf{s}\,, & (t,x) \in (0,\infty)\times\mathbb{R}^3 \\ \mathbf{u}_{\mathrm{P}_N}(0,x) = \langle \mathbf{m}\psi_0(x,\cdot)\rangle\,, & x \in \mathbb{R}^3 \end{cases}$$

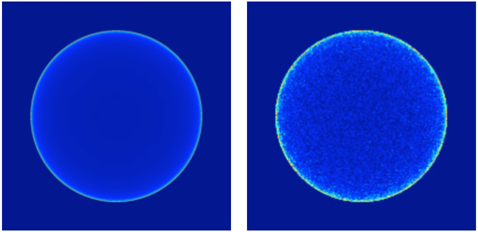
with
  - $\mathbf{s} := \langle \mathbf{m} S \rangle$
  - $\mathbf{A}\cdot\nabla_x \equiv \sum_{i=1}^3 \mathbf{A}_i \partial_{x_i}$ and each $\mathbf{A}_i = \langle \Omega_i \mathbf{m}\mathbf{m}^T \rangle$ is symmetric
  - $\mathbf{G} \geq 0$ is diagonal

- Angle brackets denote integration over $\mathbb{S}^2$: $\langle\cdot\rangle := \int_{\mathbb{S}^2} (\cdot)\, d\Omega$

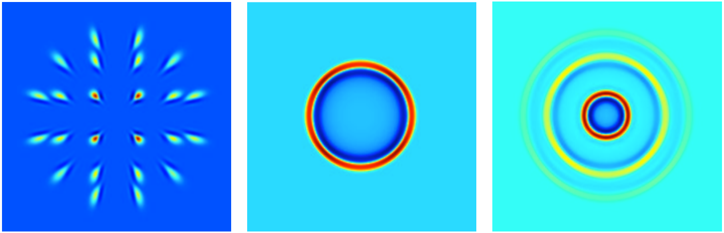
Properties of the P_N Equations

- Good Stuff
  - Fast convergence for smooth solutions
  - Preserve rotational invariance of the transport operator
  - Harmonics are eigenfunctions of the scattering operator
- Bad Stuff
  - Gibbs phenomena near wave fronts
  - Negative values for the concentration $\langle \psi \rangle$ in multi-D
  - May be ill-posed in steady-state (A_i can have zero eigenvalues)
  - Challenging boundary conditions

The Line Source Problem: All Methods have issues[1]



(a) analytic (b) Monte-Carlo



(c) S_6 (d) P_1 (e) P_5

[1] T. A. Brunner. "Forms of Approximate Radiation Transport", Tech. Rep. SAND2002-1778 Sandia National Laboratories, Jul 2002.

The issue is the closure

- The standard P_N closure simply truncates the expansion for $l > N$.
- The Gibbs oscillations are a result.
- The negative densities are problematic for coupled simulations: what does a negative absorption rate density mean?
- Other methods have been proposed to alleviate this issue
  - The M_N methods use the ansatz

$$\psi \approx e^{\mathbf{p}^T \mathbf{c}}$$

    to close the system.
  - Solve an optimization problem to assure that the ansatz is positive.
- Idea: Apply filters to the expansion to damp oscillations.

Filter functions

Filtering is commonly used to handle spatial gradients in linear and nonlinear advection. We use it here for the angular approximation.

Definition

A filter of order α is a real-valued function $f \in C^{\alpha}(\mathbb{R}^+)$ that satisfies

$$\text{(i) } f(0) = 1\,, \quad \text{(ii) } f^{(a)}(0) = 0, \text{ for } a = 1, \dots, \alpha - 1\,, \quad \text{(iii) } f^{(\alpha)}(0) \neq 0.$$

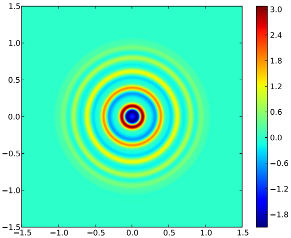
- Several variations in the definition, but (i) and (ii) are standard.
- Define $f_{\ell,N} := f(\frac{\ell}{N+1})$.
- To implement, apply the filter $\mathbf{u}_{\mathrm{P}_N} \to \mathbf{u}_{\mathrm{FP}_N}$ where

$$[\mathbf{u}_{\mathrm{FP}_N}]_\ell = f_{\ell,N}[\mathbf{u}_{\mathrm{P}_N}]_\ell$$

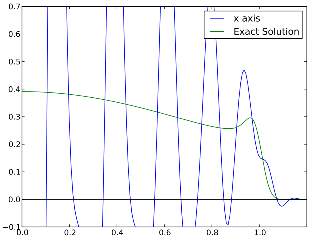
after each step of a time integration routine.[2]

[2] RGM, C.D Hauck, J. Comput. Phys., 229 (2010), pp. 5597–5614

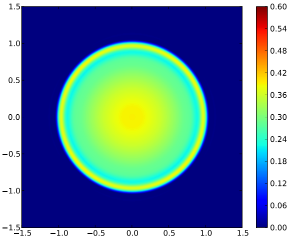
Back to the Linesource



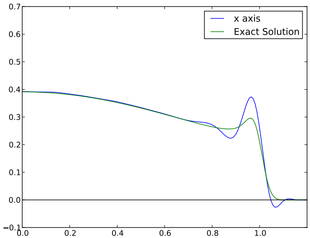
(a) P_{11}



(b) P_{11}-Lineout



(c) FP_{11}



(d) FP_{11}-Lineout

Filtered Spherical Harmonic Equations[3]

- The filtering procedure can be generalized to look like an anisotropic scattering operator.
- Let $\psi \approx \psi_{\mathrm{FP}_N} \equiv \mathbf{m}^T \mathbf{u}_{\mathrm{P}_N}$, where $\mathbf{u}_{\mathrm{FP}_N}$ satisfies

$$\partial_t \mathbf{u}_{\mathrm{FP}_N} + \mathbf{A} \cdot \nabla_x \mathbf{u}_{\mathrm{FP}_N} + \sigma_{\mathrm{a}} \mathbf{u}_{\mathrm{FP}_N} + \sigma_{\mathrm{s}} \mathbf{G} \mathbf{u}_{\mathrm{FP}_N} + \sigma_{\mathrm{f}} \mathbf{G}_{\mathrm{f}} \mathbf{u}_{\mathrm{FP}_N} = \mathbf{s}$$

- The matrix $\mathbf{G}_{\mathrm{f}} \geq 0$ is diagonal with components

$$(\mathbf{G}_{\mathrm{f}})_{(\ell,k),(\ell,k)} = -\log f_{\ell,N}$$

It can be interpreted as anisotropic scattering or angular diffusion.

- The issue of choosing the filter strength remains.

[3] D. Radice, E. Abdikamalov, L. Rezzola, and C. Ott, A new spherical harmonics scheme for multi-dimensional radiation transport I: static matter configurations, J. Comput. Phys., 242 (2013), pp. 648–669

Convergence of the Filtered Expansion

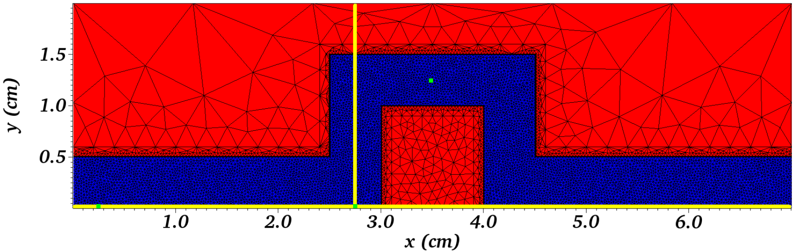
- Frank, Hauck and Kuepper give theorems for the convergence of filtered P_N.
- The error in the expansion

$$E_N = \|\psi_{\mathrm{FP}_N} - \psi\|_{L^2}$$

converges at a rate that is the smaller of the order of convergence of the unfiltered method, k, or the filter order, α:

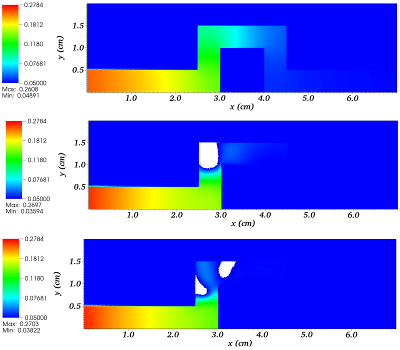
$$E_N = O(N^{-min(k,\alpha)}).$$

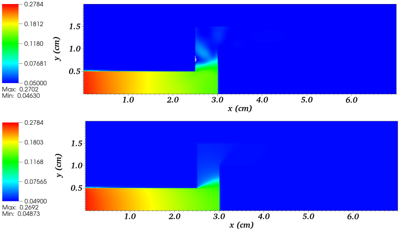
Test problem: Crooked Pipe



- This is a standard high energy density radiative transfer test problem.
- Blue region is optically thin (little interaction between radiation and material)
- Red regions are optically thick (strong collisions between radiation and material)
- Radiation source at left entrance.

Unfiltered calculation

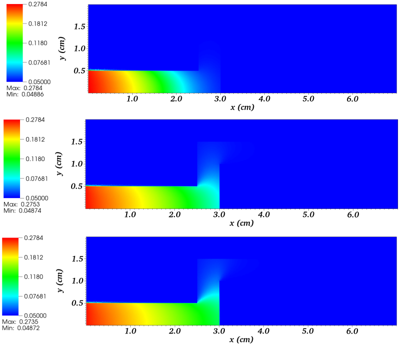


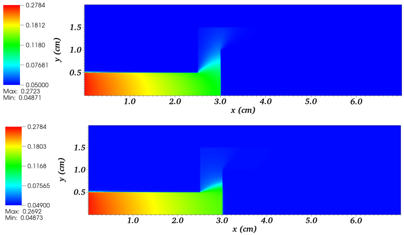


Material temperature (in keV) at $t = 3.5$ ns (from top to bottom)
left: P_1, P_3, P_5
right: P_7, P_{39}

The white regions show where the radiation density is negative.

Uniformly filtered calculation





Material temperature (in keV) at $t = 3.5$ ns (from top to bottom)
left: P_1, P_3, P_5
right: P_7, P_{39}

Filter strength value

With the Lanczos filter and $\sigma_\mathrm{f} = 5000\ \mathrm{m}^{-1}$:

$$\sigma_\mathrm{f}\, f(\ell = 1, N_0 = 7) \approx 13\,\mathrm{m}^{-1} \sim \sigma_\mathrm{t} = 20\,\mathrm{m}^{-1} \qquad (2)$$

Choosing the location of the filter

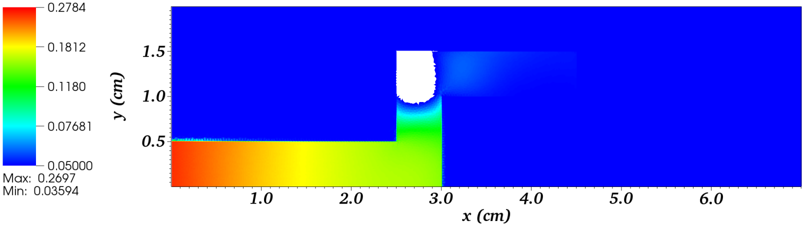


Figure: Material temperature T (in keV) at $t = 3.5$ ns for unfiltered P_3.

Choosing the location of the filter

- σ_f on the order of the cross-section (same units)
- activated where negativity arises and in an upstream region of a comparable size.

Local filter

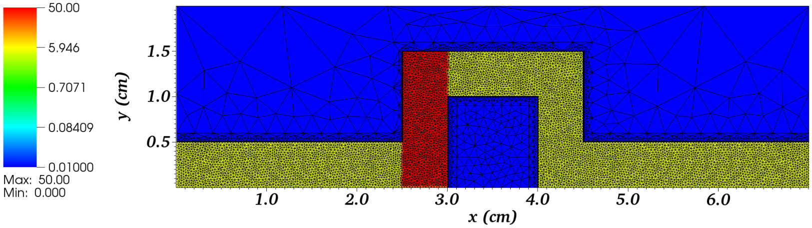
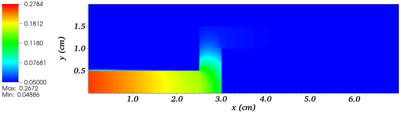
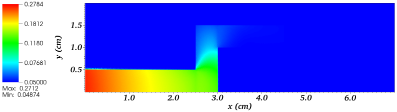
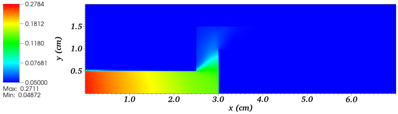


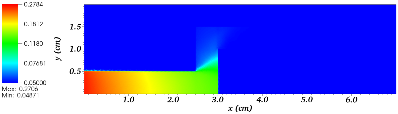
Figure: Value of σ_{f} (in cm^{-1}) for the locally filtered calculations.

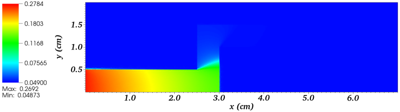
Locally filtered calculation







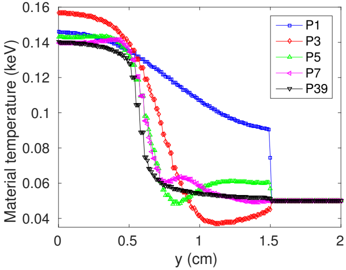


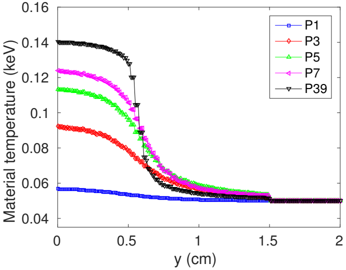


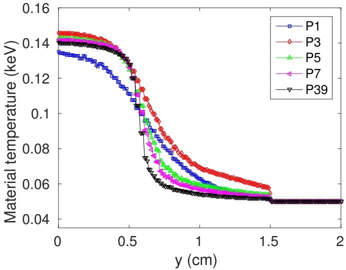
Material temperature (in keV) at $t = 3.5$ ns (from top to bottom)
left: P_1, P_3, P_5
right: P_7, P_{39}

T along $y = 0$ at $t = 3.5$ ns

T along $x = 2.75$ cm at $t = 3.5$ ns





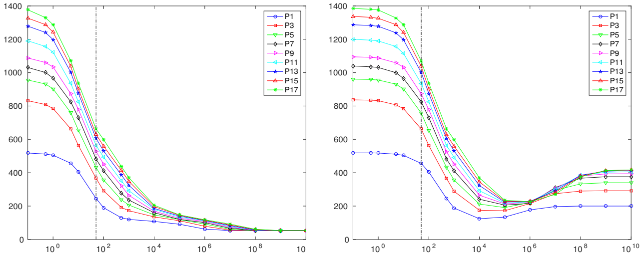


	Unfiltered	Uniformly	Locally
P_1	0.04946	0.06134	0.01489
P_3	0.02351	0.03715	0.01925
P_5	0.01008	0.02235	0.00887
P_7	0.00804	0.01499	0.00573

Figure: Clockwise from top left: Unfiltered, Uniformly filtered, L2 error, Locally Filtered

Computational Cost

- The solution for a given time step involves the solution of a linear system of size $N_x \times N_\Omega$.
- We have not been able to develop a good preconditioner yet.
  - The system has a non-trivial nullspace when there are no collisions.
- Increasing the filter strength does improve the convergence.
- Number of GMRES iterations for first timestep



(a) Uniform filtering

(b) Local filtering

Enforcing Positivity

- For nonlinear problems, positivity may be a strict requirement.
- Our goal is to modify the FP_N equations to enforce positivity.

Positive, Filtered Spherical Harmonics (FP_N^+)

We implement the filter in the context of a kinetic scheme:

1. Given a kinetic distribution ψ, compute

$$\boxed{\mathcal{E}_{\mathrm{FP}_N}[\psi] = \mathbf{m}^T \mathbf{u}_{\mathrm{FP}_N}[\psi] = \mathbf{m}^T \mathbf{F} \mathbf{u}_{\mathrm{P}_N}[\psi]}$$

   where $\mathbf{F}$ is a filtering matrix and $\mathbf{u}_{\mathrm{P}_N}[\psi] = \langle \mathbf{m}\psi \rangle$.[4]

2. Find $\mathbf{u}_{\mathrm{FP}_N^+}[\psi]$, which solves

$$\boxed{\begin{array}{ll} \underset{\mathbf{u}\in\mathbb{R}^n}{\text{minimize}} & \displaystyle\frac{1}{2}\int_{\mathbb{S}^2} \left| \mathcal{E}_{\mathrm{FP}_N}[\psi] - \mathbf{m}^T\mathbf{u} \right|^2 \, d\Omega \\ \text{subject to} & \displaystyle\int_{\mathbb{S}^2} \mathbf{m}^T\mathbf{u}\, d\Omega = \int_{\mathbb{S}^2} \mathbf{m}^T \mathbf{u}_{\mathrm{FP}_N}\, d\Omega \\ & (\mathbf{m}^T\mathbf{u})(\Omega_q) \geq 0\,, \ \forall\ \Omega_q \in Q \end{array}}$$

   where Q is a quadrature set.

3. Advance the kinetic equation with initial condition

$$\boxed{\mathcal{E}_{\mathrm{FP}_N^+}[\psi] = \mathbf{m}^T \mathbf{u}_{\mathrm{FP}_N^+}[\psi]}$$

[4] $\langle \cdot \rangle$ is integration over $[-1, 1]$ or $\mathbb{S}^2$.

Convergence results

Convergence of the Positive Filtered Expansion

- The error in the expansion

$$E_N = \|\psi_{FP_N^+} - \psi\|_{L^2}$$

  converges at a rate that is the smaller of the order of convergence of the unfiltered method, k, or the filter order, α:

$$E_N = O(N^{-min(k,\alpha)}).$$

- Same as the convergence for standard FP_N .

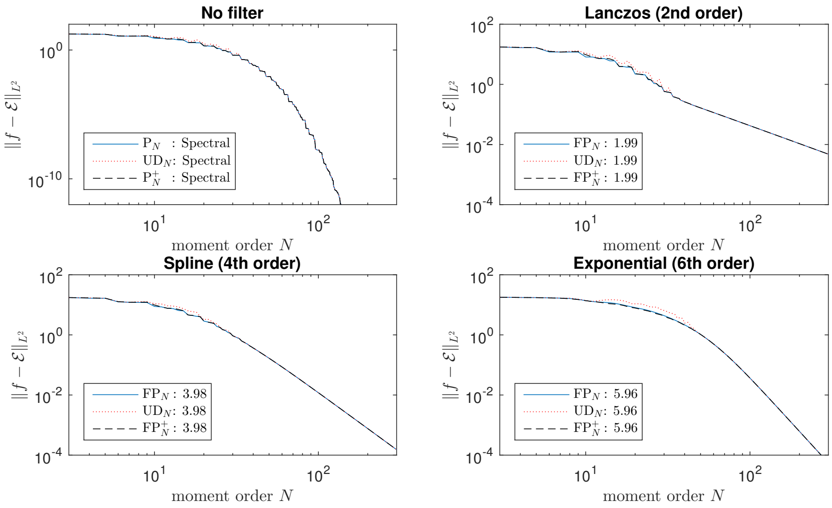


Figure: Smooth function on $[-1, 1]$ ($f \in C^\infty([-1, 1])$).

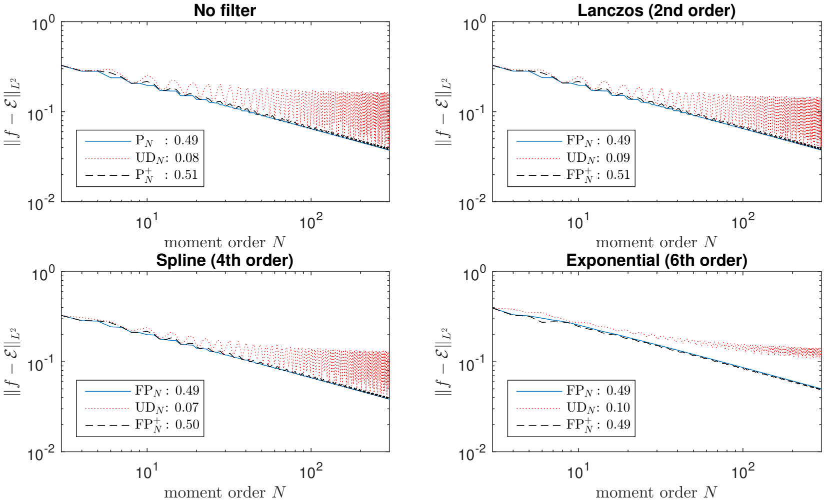


Figure: Step function on $[-1, 1]$ ($f \in H^q([-1, 1])$, $\forall q < 0.5$).

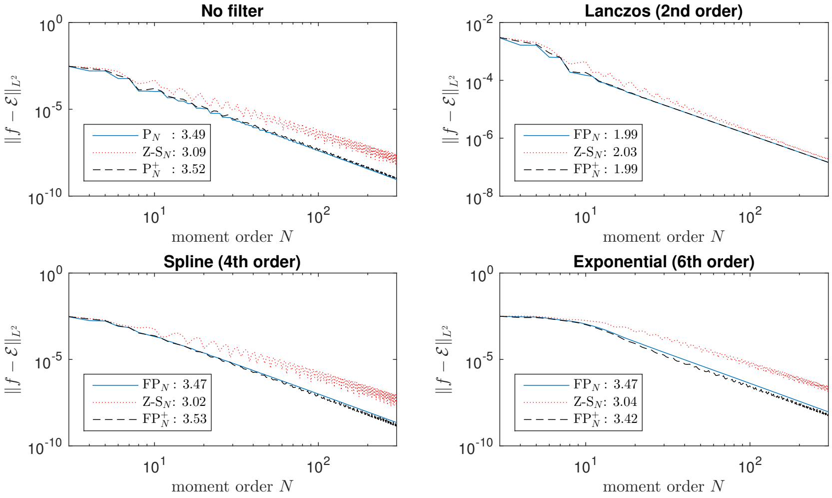


Figure: Sobolev function on $[-1, 1]$ ($f \in H^q([-1, 1])$, $\forall q < 3.5$.

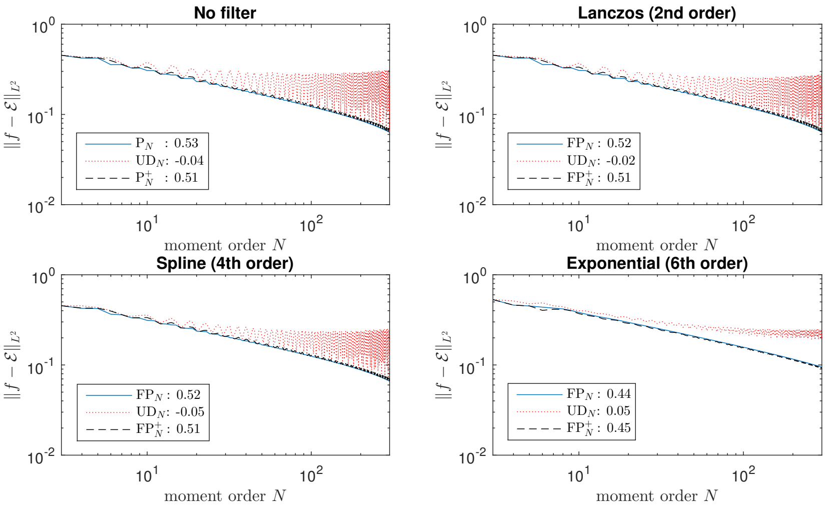


Figure: Singular function on $[-1, 1]$ ($f \in L^2([-1, 1])$).

Linesource results

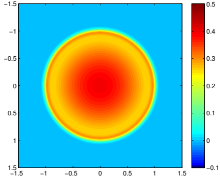


Figure: Exact solution

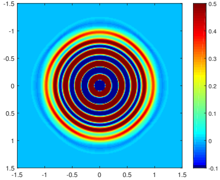


Figure: P_{11}

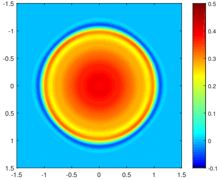


Figure: FP_{11}

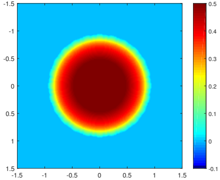


Figure: UD_{11}

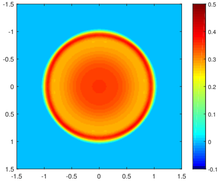


Figure: FP_{11}^{+}

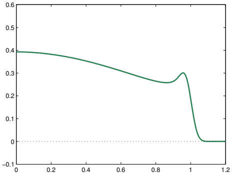


Figure: Exact solution

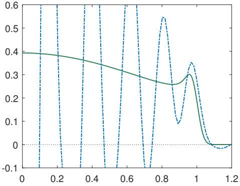


Figure: P_{11}

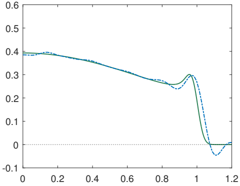


Figure: FP_{11}

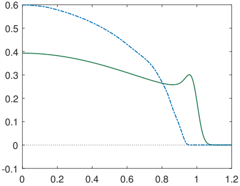


Figure: UD_{11}

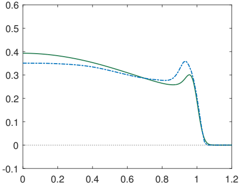


Figure: FP_{11}^{+}

Line Source Efficiency

Which is more efficient: a better, more expensive limiter or a cheaper limiter with more moments? The optimization is completely local, though so it should scale.

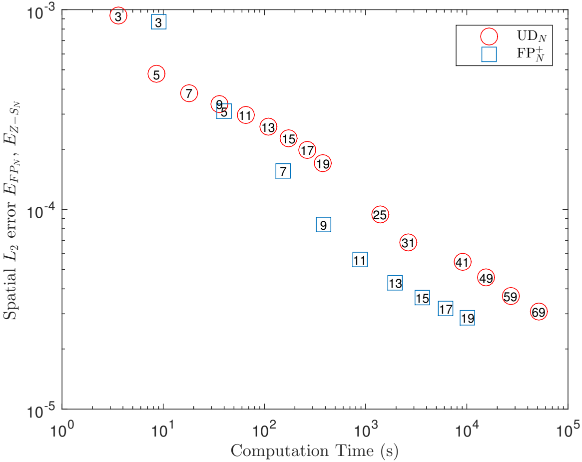


Figure: Serial Efficiency Comparison, based on L^2 error in concentration.

Conclusions

- Problems of particle transport are hard and there is no perfect method.
- Moment-based methods have some positive properties, but the also drawbacks.
- Spectral Convergence is possible, but leads to issues with positivity and oscillations.
- Filtering and optimization-based closures are promising, but still work to do.