Quantum and Kinetic Transport: Analysis, Computations, and New Applications

Workshop I: Computational Kinetic Transport and Hybrid Methods

Optimal Prediction for Radiative Transfer: A New Perspective on Moment Closure

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Radiative transfer equation

Boltzmann equation (frequency-independent, isotropic scattering)

$$\underbrace{\tfrac{1}{c}\partial_t u + \Omega\cdot\nabla_x u}_{\text{advection}} = \underbrace{\sigma\left(\frac{1}{4\pi}\int_{4\pi} u \,\mathrm{d}\Omega' - u\right)}_{\text{scattering}} + \underbrace{\kappa\,(B(T)-u)}_{\text{absorption \& emission}}$$

for radiative intensity $u(x,\Omega,t)$.

1D slab geometry: Intensity $u(x,\mu,t)$ depends only on x, the azimuthal flight angle $\theta = \arccos(\mu)$, and time.

$$\partial_t u + \mu\partial_x u = -(\kappa+\sigma)u + \tfrac{\sigma}{2}\int_{-1}^{1} u \,\mathrm{d}\mu' + q\;.$$

Key challenge: High dimensional phase space.

Moment methods

Fourier expansion in Ω yields infinite sequence of moments $\vec{u} = (u_0, u_1, \dots)$ by

$$u_k(x,t) = \int_{4\pi} u(x,\Omega,t)\,Y_k(\Omega)\,\mathrm{d}\Omega\;,$$

where Y_k spherical Harmonics. The arising infinite "hyperbolic" moment system

$$\partial_t\vec{u} + B\cdot\nabla\vec{u} = -C\cdot\vec{u} + \vec{q}$$

is equivalent to the original equation.

1D slab geometry: Use Legendre polynomials for Y_k. Three term recursion yields

$$B = \begin{pmatrix} 0 & 1 & & & \\ \frac{1}{3} & 0 & \frac{2}{3} & & \\ & \frac{2}{5} & 0 & \frac{3}{5} & \\ & & \frac{3}{7} & 0 & \ddots \\ & & & \ddots & \ddots \end{pmatrix},\; C = \begin{pmatrix} \kappa & & & \\ & \kappa+\sigma & & \\ & & \ddots & \\ & & & \ddots \end{pmatrix},\; \vec{q} = \begin{pmatrix} 2\kappa q \\ 0 \\ \vdots \\ \vdots \end{pmatrix}\;.$$

Moment closure problem

Truncate system after N-th moment, i.e. consider resolved moments $\hat{\vec{u}} = (u_0, u_1, \dots, u_N)$, and model influence of unresolved moments $\tilde{\vec{u}} = (u_{N+1}, u_{N+2}, \dots)$ on resolved moments.

Examples of moment closures:

- P_N closure: $u_{N+1} = 0$
- Diffusion correction to P_N: $u_{N+1} = -\frac{1}{\kappa+\sigma}\frac{N+1}{2N+3}\partial_x u_N$ [4]
- Other linear closures: simplified P_N (parabolic system) [3]
- Nonlinear closures: minimum entropy, flux-limited diffusion

Classical approach:

- Assume unresolved moments close to zero or quasi-stationary.
- Manipulate moment equations.
- Foundations by asymptotic analysis and (formal) series expansions.

A new perspective:

- Consider average solution w.r.t. a measure [1].
- Mori-Zwanzig formalism [5, 7] yields its exact evolution by a memory term.
- Approximations to memory term recover existing and yield new closures.

References

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Linear optimal prediction

- Moment system:

$$\partial_t\vec{u} = R\vec{u}\;,\quad \vec{u}(0) = \mathring{\vec{u}}\;.$$

Differential operator $R\vec{u} = -B\cdot\partial_x\vec{u} - C\cdot\vec{u}$ (omit source).
Solution $\vec{u}(t) = e^{tR}\mathring{\vec{u}}$.

- Consider Gaussian measure $f(\vec{u}) = \frac{1}{\sqrt{\det(2\pi A)}}\exp\left(-\frac{1}{2}\vec{u}^T A^{-1}\vec{u}\right)$ [2].
- Decomposition $\vec{u} = \begin{bmatrix}\hat{\vec{u}}\\ \tilde{\vec{u}}\end{bmatrix}$ and $A = \begin{bmatrix}\hat{\hat{A}} & \hat{\tilde{A}}\\ \tilde{\hat{A}} & \tilde{\tilde{A}}\end{bmatrix} = A^T$ (covariance matrix)
- Given $\hat{\vec{u}}$, an average with respect to the conditioned measure $f_{\hat{\vec{u}}}(\tilde{\vec{u}}) = \tilde{Z}^{-1}f(\hat{\vec{u}},\tilde{\vec{u}})$ is the conditional expectation projection (orthogonal w.r.t. $(u,v) = \mathbb{E}[uv]$ [1])

$$P\vec{u} = \mathbb{E}[\vec{u}|\hat{\vec{u}}] = E\cdot\vec{u}\;,\quad\text{where}\quad E = \begin{bmatrix} I & 0\\ \tilde{\hat{A}}\hat{\hat{A}}^{-1} & 0\end{bmatrix}\;.$$

Meaning: Given $\hat{\vec{u}}$, then $\tilde{\vec{u}}$ is centered around $\tilde{\hat{A}}\hat{\hat{A}}^{-1}\hat{\vec{u}}$. Measure allows to prescribe correlation between resolved and unresolved moments.

- Ensemble average solution $P\vec{u}(t) = e^{tR}E\mathring{\vec{u}}$ is a particular solution with averaged initial conditions (linearity).

Mori-Zwanzig formalism

- Conditional expectation E and orthogonal projection $F = I - E$.
- Solution operator e^{tR} and orthogonal dynamics solution operator e^{tRF} satisfy Duhamel's principle (Dyson's formula)

$$e^{tR} = \int_0^t e^{(t-s)RF}REe^{sR}\,\mathrm{d}s + e^{tRF}\;.$$

- Differentiating Dyson's formula:

$$\partial_t e^{tR} = REe^{tR} + \int_0^t e^{(t-s)RF}RFREe^{sR}\,\mathrm{d}s + e^{tRF}RF\;.$$

- Adding E from right yields evolution for average solution operator

$$\partial_t e^{tR}E = \mathcal{R}e^{tR}E + \int_0^t K(t-s)e^{sR}E\,\mathrm{d}s\;,$$

where $\mathcal{R} = RE$ and $K(t) = e^{tRF}RFRE$ memory kernel.
Evolution for average solution:

$$\partial_t\bar{u}(t) = \mathcal{R}\bar{u}(t) + \int_0^t K(t-s)\bar{u}(s)\,\mathrm{d}s\;,$$

where $\mathcal{R} = RE$ and $K(t) = e^{tRF}RFRE$.

Approximations for radiative transfer

Here consider uncorrelated measure, i.e. covariance matrix A diagonal.

$$\hat{\hat{\mathcal{R}}} = \widehat{\widehat{RE}} = \hat{\hat{R}} = -\hat{\hat{B}}\partial_x - \hat{\hat{C}}\quad,\quad \hat{\hat{K}}(0) = \widehat{\widehat{RFRE}} = \hat{\tilde{R}}\tilde{\hat{R}} = \hat{\tilde{B}}\tilde{\hat{B}}\partial_{xx}$$

$$\hat{\tilde{B}}\tilde{\hat{B}} = \begin{pmatrix} 0 & \cdots & 0\\ \vdots & \ddots & \vdots\\ 0 & \cdots & \frac{(N+1)^2}{(2N+1)(2N+3)}\end{pmatrix}$$

Approximations:

- **Omitting the memory term:** $\partial_t\hat{\vec{u}}(t) = \hat{\hat{R}}\hat{\vec{u}}(t)$ yields classical P_N closure.
- **Piecewise constant quadrature for memory:**

$$\int_0^t K(t-s)\bar{u}(s)E\,\mathrm{d}s \approx \tau K(0)\bar{u}(t)$$

with characteristic time scale $\tau = \frac{1}{\kappa+\sigma}$, yields classical diffusion correction closure [4]

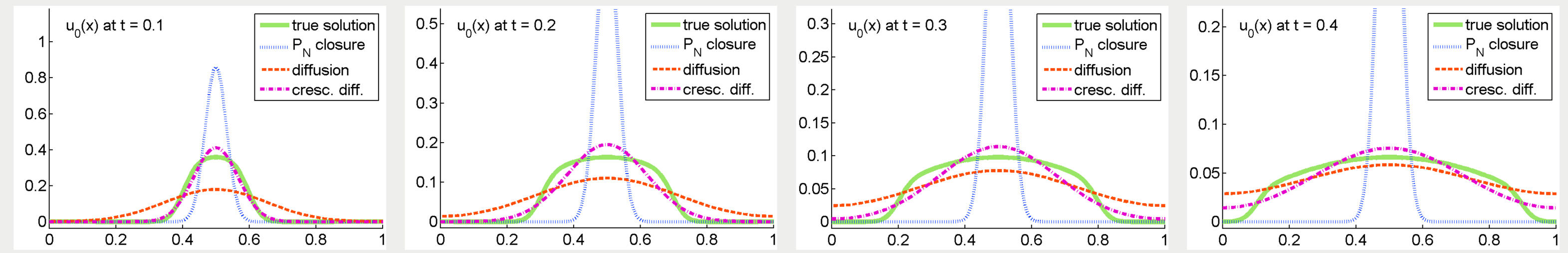
$$\partial_t\hat{\vec{u}}(t) = \hat{\hat{R}}\hat{\vec{u}}(t) + \tau\hat{\tilde{B}}\tilde{\hat{B}}\partial_{xx}\hat{\vec{u}}(t)\;.$$

- **Better approximation for short times:**

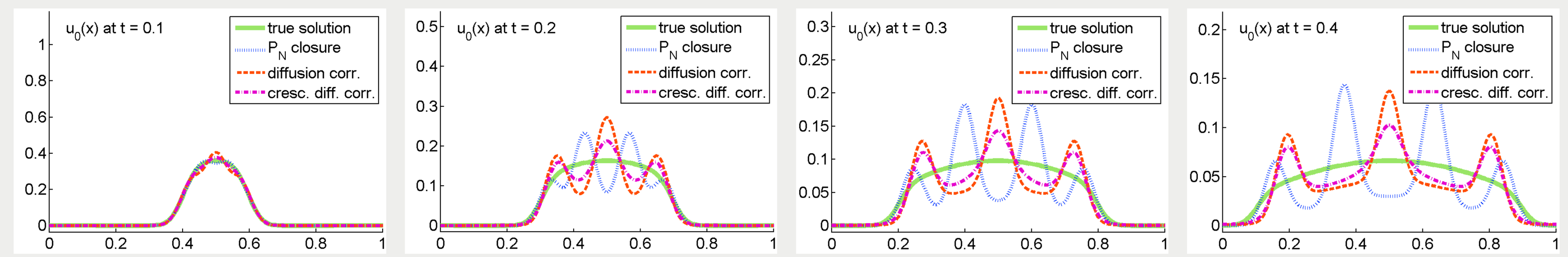
$$\partial_t\hat{\vec{u}}(t) = \hat{\hat{R}}\hat{\vec{u}}(t) + \min\{\tau,t\}\hat{\tilde{B}}\tilde{\hat{B}}\partial_{xx}\hat{\vec{u}}(t)\;.$$

Yields new crescendo diffusion correction closure (no extra cost!).
(Explicit time dependence models loss of information.)

1D slab geometry: Various P_0 moment closures

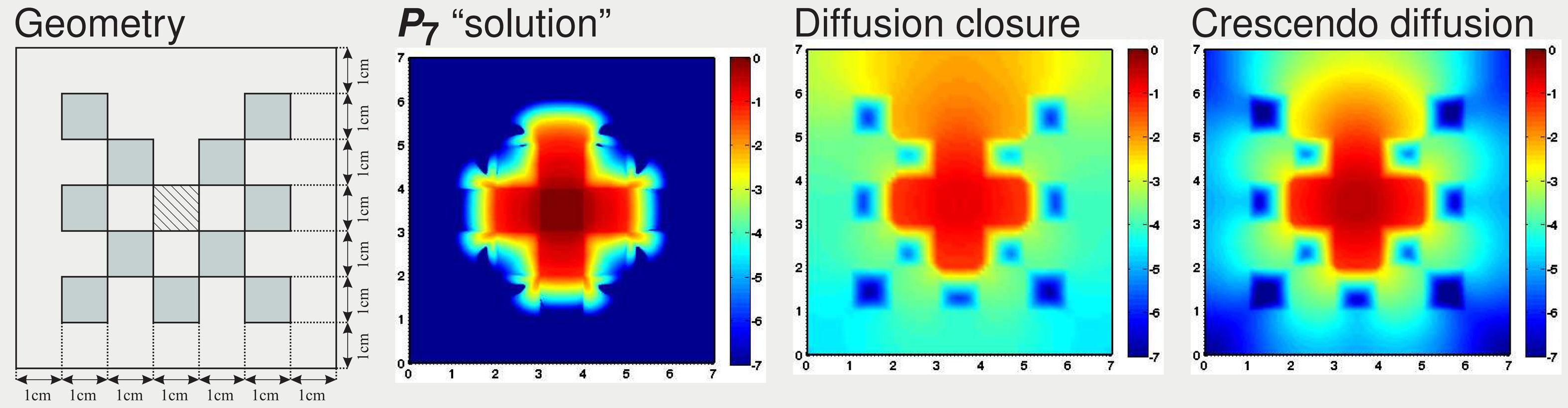


1D slab geometry: Various P_3 moment closures



2D slab geometry: Improvement by crescendo diffusion

Geometry | P_7 "solution" | Diffusion closure | Crescendo diffusion



Reordered P_N equations

Even-odd ordering of moments:
$\hat{\vec{u}} = (u_0, u_2, \dots, u_{2N})^T$ and $\tilde{\vec{u}} = (u_1, u_3, \dots, u_{2N+1}, u_{2N+2}, \dots)^T$.
Reordered advection matrix (here 1D with $N = 2$):

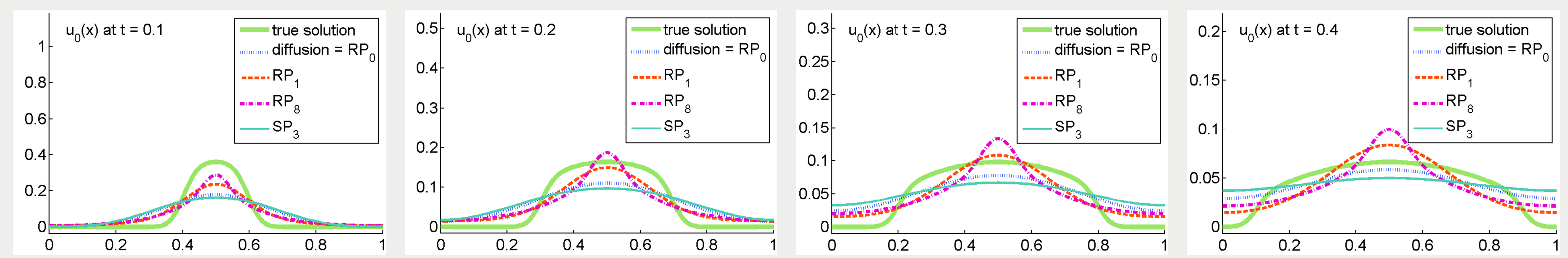
$$\begin{bmatrix}\hat{\hat{B}} & \hat{\tilde{B}}\\ \tilde{\hat{B}} & \tilde{\tilde{B}}\end{bmatrix} = \left[\begin{array}{ccc|cccc} & & & 1 & & & \\ & & & 2/5 & 3/5 & & \\ & & & & 4/9 & 5/9 & \\ \hline 1/3 & 2/3 & & & & & \\ & 3/7 & 4/7 & & & & \\ & & 5/11 & & & 6/11 & \\ & & & & 6/13 & & \ddots \\ & & & & & \ddots & \end{array}\right]$$

Mori-Zwanzig formalism yields parabolic system

$$\partial_t\hat{\vec{u}}(t) = -\hat{\hat{C}}\hat{\vec{u}}(t) + \frac{1}{\kappa+\sigma}D\partial_{xx}\hat{\vec{u}}(t)\;,$$

which we call reordered P_N equations (RP_N) [6].
Diffusion matrix $D = \hat{\tilde{B}}\tilde{\hat{B}}$ is positive definite.
(RP_1 system is equivalent to SSP_3 system [3].)

1D slab geometry: Various parabolic moment closures



Messages

- The Mori-Zwanzig formalism yields an integro-differential equations that is equivalent to the original radiative transfer equation.
- Various approximations to the memory term recover existing and yield new closures.
- Crescendo diffusion is a simple modification to existing diffusion closures that comes at no extra cost, and improves results.
- The reordered P_N equations are a new family of parabolic approximations.

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