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

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CSCAMM

$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + \frac{F}{m}\frac{\partial f}{\partial v} =$

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Overview

1. Moment Models for Radiative Transfer
2. Optimal Prediction
3. A New Perspective on Moment Closure in Radiative Transfer

Overview

Radiative transfer equation

Boltzmann equation (no frequency dependence, isotropic scattering)

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

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

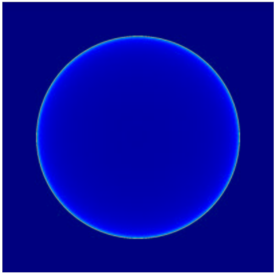
Key challenge

High dimensional phase space.

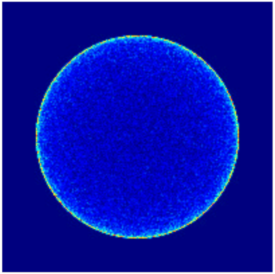
Popular numerical approaches

- **Monte-Carlo methods:** Solve particle transport directly
- **Discrete ordinates:** Discretize x and Ω by grid
- **Moment methods:** Fourier expansion in Ω (spherical Harmonics)

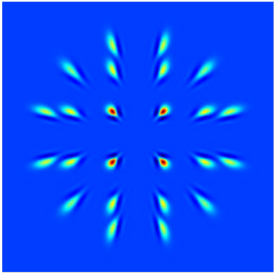
True solution



Monte Carlo



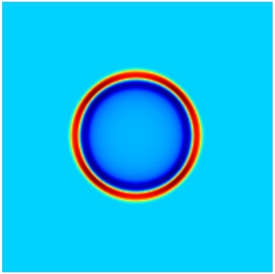
Discrete ordinates S_6



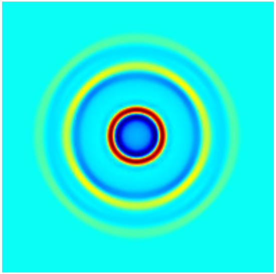
Figures from

T. A. Brunner, *Forms of approximate radiation transport*, Sandia Report, 2002

Moment model P_1



Moment model P_5



1D slab geometry

Plate (infinite in y and z). Intensity $u(x,\mu,t)$ depends only on x, the azimuthal flight angle $\theta = \arccos(\mu)$, and time.

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

Moment expansion

Infinite sequence of moments $\vec{u} = (u_0, u_1, \dots)$

$$u_k(x,t) = \int_{-1}^{1} u(x,\mu,t) P_k(\mu) \, \mathrm{d}\mu \ ,$$

where P_k Legendre polynomials.

Three term recursion for P_k yields

$$\partial_t u_k + b_{k,k-1}\partial_x u_{k-1} + b_{k,k+1}\partial_x u_{k+1} = -c_k u_k + q_k \ .$$

Moment system

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

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

Linear infinite "hyperbolic" system, equivalent to original equation.

Moment closure problem

Truncate system after N-th moment.

- P_N closure: $u_{N+1} = 0$
- Diffusion correction to P_N: $u_{N+1} = -\frac{1}{\kappa+\sigma}\frac{N+1}{2N+3}\partial_x u_N$ [Levermore 2005]
- Other linear closures: simplified P_N (parabolic system)
- Nonlinear closures: minimum entropy, flux-limited diffusion

Examples of linear closures

- P_1 system:
$$\begin{cases}\partial_t u_0 + \partial_x u_1 &= -\kappa u_0 + q_0 \\ \partial_t u_1 + \tfrac{1}{3}\partial_x u_0 &= -(\kappa+\sigma) u_1\end{cases}$$
- Diffusion approximation:
$$\partial_t u_0 = -\kappa u_0 + q_0 + \partial_x \tfrac{1}{3(\kappa+\sigma)} \partial_x u_0$$
- Diffusion correction to P_2 (from P_3):
Consider $\partial_t u_3 = 0$. Thus $u_3 = -\frac{1}{\kappa+\sigma}\frac{3}{7}\partial_x u_2$.
$$\begin{cases}\partial_t u_0 + \qquad\qquad \partial_x u_1 &= -\kappa u_0 + q_0 \\ \partial_t u_1 + \tfrac{1}{3}\partial_x u_0 + \tfrac{2}{3}\partial_x u_2 &= -(\kappa+\sigma) u_1 \\ \partial_t u_2 + \tfrac{2}{5}\partial_x u_1 &= -(\kappa+\sigma) u_2 + \partial_x \tfrac{1}{\kappa+\sigma}\tfrac{9}{35}\partial_x u_2\end{cases}$$
- Simplified (simplified) P_3 (SSP_3): [Frank, Klar, Larsen, Yasuda, JCP 2007]
$$\partial_t \begin{pmatrix} u_0 \\ u_2 \end{pmatrix} = \frac{1}{3(\kappa+\sigma)} \begin{pmatrix} 1 & 2 \\ \frac{2}{5} & \frac{11}{7} \end{pmatrix} \cdot \partial_{xx} \begin{pmatrix} u_0 \\ u_2 \end{pmatrix} - \begin{pmatrix} \kappa & 0 \\ 0 & \kappa+\sigma \end{pmatrix} \cdot \begin{pmatrix} u_0 \\ u_2 \end{pmatrix} + \begin{pmatrix} q_0 \\ 0 \end{pmatrix}$$

Moment closure

- Approximate infinite moment system by finitely many moments.
- Closure problem: Model truncated moments.

Classical approach

- Assume truncated moments close to 0 or quasi-stationary.
- Manipulate moment equations.
- Foundations by asymptotic analysis and (formal) series expansions.

A new perspective

- Approximate average solution w.r.t. a measure.
- Mori-Zwanzig formalism yields exact evolution of truncated system by memory term.
- Approximations to memory term yield existing and new systems.

Overview

Optimal Prediction

Introduced by Chorin, Kast, Kupferman, Levy, Hald, et al.

- Underresolved computation (reduce computational effort by using prior statistical information).
- Sought is average solution of a system, where part of initial data is known and the rest is sampled from an underlying measure.
- Optimal Prediction approximates average solution by a system smaller than the full system.

A. Chorin, R. Kupferman, D. Levy, *Optimal prediction for Hamiltonian partial differential equations*, J. Comp. Phys., 162, pp. 267–297, 2000.
A. Chorin, O. Hald, R. Kupferman, *Optimal prediction with memory*, Physica D 166, 3–4, pp. 239–257, 2002.

A. Chorin, O. Hald, *Stochastic tools in mathematics and science*, Springer, 2006.

Evolution equation

$$\tfrac{d}{dt}x = R(x)\ ,\ \ x(0) = \mathring{x}\ .$$

Assume measure on phase space $f(x)$.
Example: Hamiltonian system $f(x) = Z^{-1}e^{-\beta H(x)}$, where $\beta = 1/(k_B T)$.

Splitting the variables

Split $x = (\hat{x}, \tilde{x})$ into resolved variables $\hat{x}$, and unresolved variables $\tilde{x}$.
Block system

$$\frac{d}{dt}\begin{bmatrix}\hat{x}\\ \tilde{x}\end{bmatrix} = \begin{bmatrix}\hat{R}(\hat{x},\tilde{x})\\ \tilde{R}(\hat{x},\tilde{x})\end{bmatrix}\ ,\ \begin{bmatrix}\hat{x}(0)\\ \tilde{x}(0)\end{bmatrix} = \begin{bmatrix}\mathring{\hat{x}}\\ \mathring{\tilde{x}}\end{bmatrix}\ .$$

Averaging unresolved variables

Resolved initial conditions $\mathring{\hat{x}}$ are known. Yields conditioned measure for $\tilde{x}$

$$f_{\mathring{\hat{x}}}(\tilde{x}) = \tilde{Z}^{-1}f(\mathring{\hat{x}},\tilde{x})$$

Average of function $u(\hat{x},\tilde{x})$ w.r.t. $f_{\hat{x}}(\tilde{x})$ is conditional expectation

$$Pu = \mathbb{E}[u|\hat{x}] = \frac{\int u(\hat{x},\tilde{x})f(\hat{x},\tilde{x})\,\mathrm{d}\tilde{x}}{\int f(\hat{x},\tilde{x})\,\mathrm{d}\tilde{x}}\ .$$

Orthogonal projection w.r.t. $(u,v) = \mathbb{E}[uv]$. Hence optimal prediction.

Example: Weather forecast

Computational weather models (Navier-Stokes + X).

- **Goal:** Predict temperature in Washington D.C. tomorrow 3pm.
- **Available:** Temperature right now at few positions on the map.
- **Problem:** Temperature in most places unknown.
- **Classical approach:** Interpolate unknown initial conditions from known initial conditions. Run one simulation.

Average solution

- **New paradigm:** Find average solution, where known initial conditions are fixed, and unknown initial conditions are sampled from a distribution.
- **Current approach:** Monte-Carlo. Run many simulations. Costly!

Ensemble averages on television weather forecast

- **Optimal prediction:** Obtain average solution by a single simulation.

Average solution

Nonlinear system of ODE

$$\tfrac{d}{dt}x = R(x)\ .$$

Ensemble of solutions $\varphi(x,t)$ by phase flow

$$\begin{cases}\partial_t\varphi(x,t) = R(\varphi(x,t)) \\ \varphi(x,0) = x\end{cases}$$

Average solution

$$P\varphi(x,t) = \mathbb{E}[\varphi(x,t)|\hat{x}] = \frac{\int \varphi((\hat{x},\tilde{x}),t) f(\hat{x},\tilde{x})\,\mathrm{d}\tilde{x}}{\int f(\hat{x},\tilde{x})\,\mathrm{d}\tilde{x}}\ .$$

Smaller system for resolved variables

Mori-Zwanzig formalism [H. Mori 1965, R. Zwanzig 1980] yields approximate evolution for $\widehat{P\varphi}(t)$

$$\partial_t\widehat{P\varphi}(t) = PR\,\widehat{P\varphi}(t) + \int_0^t K(t-s)\widehat{P\varphi}(s)\,\mathrm{d}s\ .$$

Optimal prediction

Nonlinear system of ODE: $\frac{d}{dt}x = R(x)$.

Conditional expectation projection: $Pu = \mathbb{E}[u|\hat{x}]$.

Average solution is approximated by

- **First order OP:**

$$\frac{d}{dt}\hat{x} = \mathcal{R}(\hat{x}) \ ,$$

  where $\mathcal{R}(\hat{x}) = PR = \mathbb{E}[R(\hat{x}, \tilde{x})|\hat{x}]$.

- **OP with memory:**

$$\frac{d}{dt}\hat{x}(t) = \mathcal{R}(\hat{x}(t)) + \int_0^t K(t-s)\hat{x}(s)\,\mathrm{d}s \ ,$$

  where memory kernel $K(t)$ involves orthogonal dynamics ODE

$$\frac{d}{dt}x = (I - P)R(x) \ .$$

  In general as costly to solve as full ODE.
  But: Independent of initial conditions $\mathring{\hat{x}}$. Can be pre-computed.

Overview

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 q for now).

Solution $\vec{u}(t) = e^{tR}\mathring{\vec{u}}$.

Linear ensemble average solution

- Consider Gaussian measure $f(\vec{u}) = \frac{1}{\sqrt{(2\pi)^n \det(A)}} \exp\left(-\frac{1}{2}\vec{u}^T A^{-1}\vec{u}\right)$.
- 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)
- Conditional expectation projection is matrix multiplication $P\vec{u} = E\vec{u}$

  $E = \begin{bmatrix} I & 0 \\ \tilde{\hat{A}}\hat{\hat{A}}^{-1} & 0 \end{bmatrix}$. Meaning: Given $\hat{\vec{u}}$, $\tilde{\vec{u}}$ is centered around $\tilde{\hat{A}}\hat{\hat{A}}^{-1}\hat{\vec{u}}$.
- Average solution $P\vec{u}(t) = e^{tR}E\mathring{\vec{u}}$ is particular solution (linearity).

Linear optimal prediction

- 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)

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

Proof: $M(t) = e^{tR} - \int_0^t e^{(t-s)RF} REe^{sR}\,ds - e^{tRF}$.
$\partial_t M(t) = RF\,M(t)\,,\ M(0) = 0$. Hence $M(t) = 0$.

- Differentiating Dyson's formula:

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

- Adding E from right yields evolution for average solution operator

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

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

Evolution for average solution

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

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

Approximations

- **First order OP:** $\partial_t \vec{u}(t) = \mathcal{R}\vec{u}(t)$
- **Piecewise constant quadrature for memory:**

  $$\partial_t \vec{u}(t) = \mathcal{R}\vec{u}(t) + \tau K(0)\vec{u}(t)\ ,$$

  where τ characteristic time scale.
- **Better approximation for short times:**

  $$\partial_t \vec{u}(t) = \mathcal{R}\vec{u}(t) + \min\{\tau, t\}K(0)\vec{u}(t)\ .$$

  Crescendo memory
  (Explicit time dependence models loss of information.)

Linear optimal prediction for the radiative transfer equations

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

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

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

Approximations

- **First order OP:** $\partial_t \hat{\vec{u}}(t) = \hat{\hat{R}}\hat{\vec{u}}(t)$ yields P_N closure.
- **Piecewise constant quadratures for memory** (with $\tau = \frac{1}{\kappa+\sigma}$)

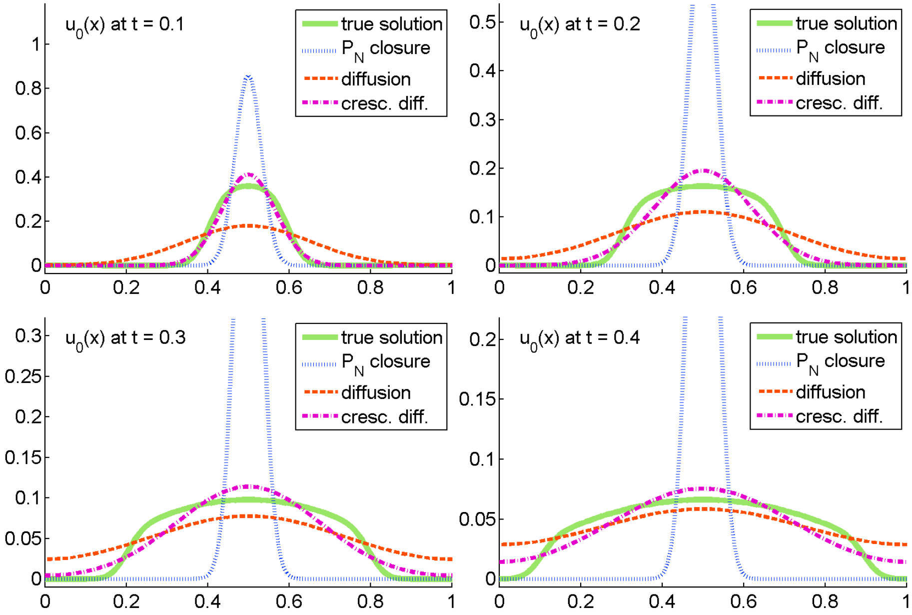
$$\partial_t \hat{\vec{u}}(t) = \hat{\hat{R}}\hat{\vec{u}}(t) + \tau \hat{\tilde{B}}\tilde{\hat{B}}\partial_{xx}\hat{\vec{u}}(t)$$

yields classical diffusion correction closure, and

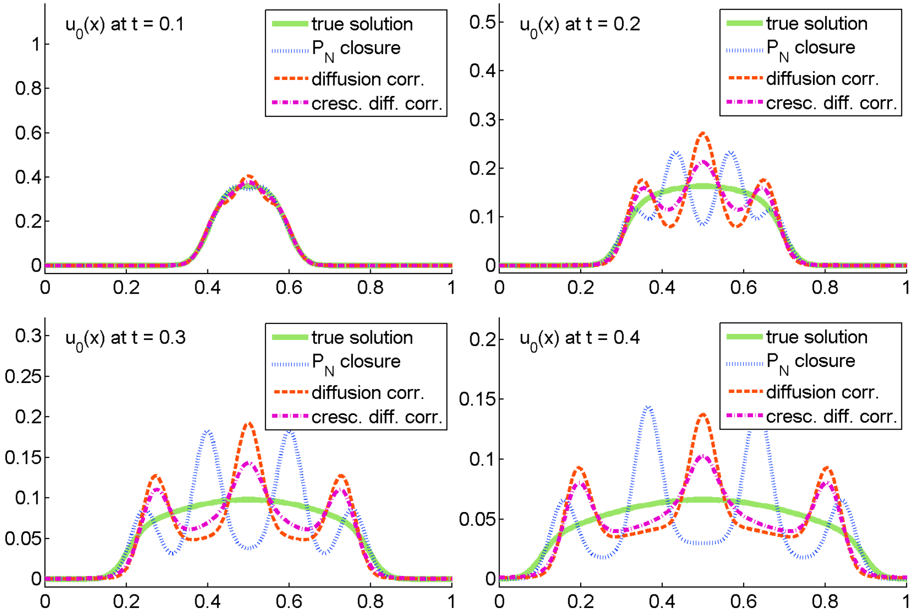
$$\partial_t \hat{\vec{u}}(t) = \hat{\hat{R}}\hat{\vec{u}}(t) + \min\{\tau, t\}\hat{\tilde{B}}\tilde{\hat{B}}\partial_{xx}\hat{\vec{u}}(t)$$

yields new crescendo diffusion correction closure (no extra cost!).

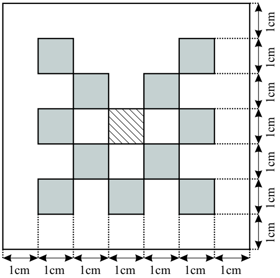
Various P_0 moment closures



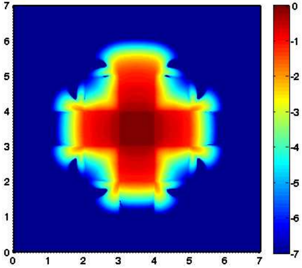
Various P_3 moment closures



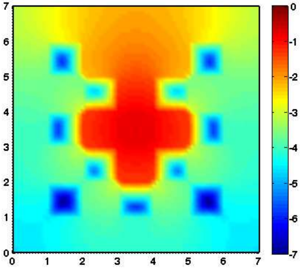
Geometry



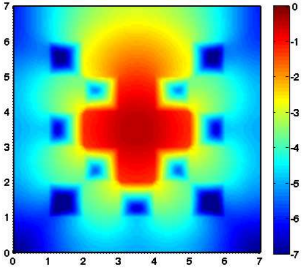
P_7 solution



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 $N = 2$):

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

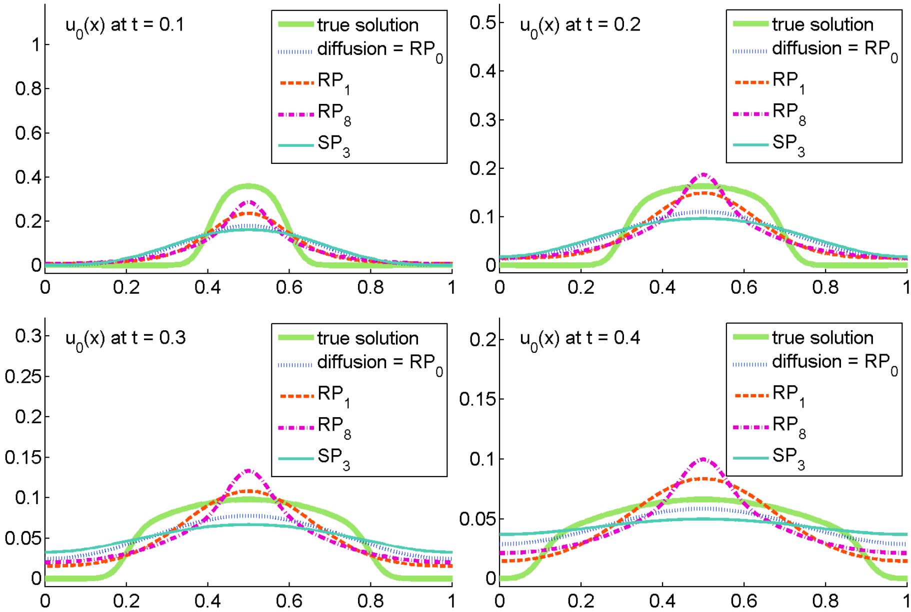
Optimal prediction approximation

Parabolic system

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

Diffusion matrix $D = \hat{\tilde{B}}\tilde{\hat{B}}$ is positive definite.

Various parabolic moment closures



Conclusions

- Optimal Prediction yields a new perspective on moment closure.
- A wide variety of new closures can be derived by different approximations of the memory convolution.
- Crescendo diffusion is a very simple modification to diffusion, that increases accuracy.

Future research directions

- Solution and storage of the orthogonal dynamics.
- Nonlinear measures ⇒ nonlinear closures?
- More complex applications, application to kinetic gas dynamics.

M. Frank, B. S., *Optimal prediction for radiative transfer: A new perspective on moment closure*, arXiv:0806.4707 [math-ph]
B. S., M. Frank, *Optimal prediction for moment models: Crescendo diffusion and reordered equations*, arXiv:0902.0076

`http://www-math.mit.edu/~seibold/research/truncation`

Thank you.