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

Benjamin Seibold
MIT Applied Mathematics

Collaborator
Martin Frank (TU Kaiserslautern)

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Overview

1. Moment Models for Radiative Transfer
2. Optimal Prediction
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1. Moment Models for Radiative Transfer

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Radiative transfer equation

Boltzmann equation (no frequency dependence, isotropic scattering)

\[
\frac{1}{c} \partial_t u + \Omega \cdot \nabla_x u = \sigma \left( \frac{1}{4\pi} \int_{4\pi} u \, d\Omega' - u \right) + \kappa (B(T) - u)
\]

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 \( \Omega \) by grid
- **Moment methods**: Fourier expansion in \( \Omega \) (spherical Harmonics)
Moment Models for Radiative Transfer

Equations and approaches

True solution

Monte Carlo

Discrete ordinates $S_6$

Moment model $P_1$

Moment model $P_5$

Figures from
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.

\[
\partial_t u + \mu \partial_x u = -(\kappa + \sigma) u + \frac{\sigma}{2} \int_{-1}^{1} u \, d\mu' + q
\]

Moment expansion

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

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

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

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

\[ B = \begin{pmatrix}
0 & 1 & 2/3 & 3/5 & 3/7 & \cdots \\
\frac{2}{3} & 0 & \frac{2}{5} & \cdots & & \\
\frac{3}{5} & \frac{2}{3} & 0 & \cdots & & \\
\frac{3}{7} & \frac{3}{5} & \frac{2}{3} & 0 & \cdots & \\
\cdots & \cdots & \cdots & \cdots & \cdots & \\
\end{pmatrix}, \quad C = \begin{pmatrix}
\kappa & \kappa + \sigma & \cdots \\
\kappa + \sigma & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \\
\cdots & \cdots & \cdots & \cdots & \cdots & \\
\end{pmatrix}, \quad \vec{q} = \begin{pmatrix}
2\kappa \sigma \\
2\kappa \sigma & \cdots \\
0 & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \\
\end{pmatrix} \]

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

- $P_1$ system:

$$\begin{align*}
\partial_t u_0 + \partial_x u_1 &= -\kappa u_0 + q_0 \\
\partial_t u_1 + \frac{1}{3} \partial_x u_0 &= -(\kappa + \sigma) u_1
\end{align*}$$

- Diffusion approximation:

$$\partial_t u_0 = -\kappa u_0 + q_0 + \partial_x \frac{1}{3(\kappa + \sigma)} \partial_x u_0$$

- Diffusion correction to $P_2$ (from $P_3$):

  Consider $\partial_t u_3 = 0$. Thus $u_3 = -\frac{1}{\kappa + \sigma} \frac{3}{7} \partial_x u_2$.

$$\begin{align*}
\partial_t u_0 + \partial_x u_1 &= -\kappa u_0 + q_0 \\
\partial_t u_1 + \frac{1}{3} \partial_x u_0 + \frac{2}{3} \partial_x u_2 &= -(\kappa + \sigma) u_1 \\
\partial_t u_2 + \frac{2}{5} \partial_x u_1 &= -(\kappa + \sigma) u_2 + \partial_x \frac{1}{\kappa + \sigma} \frac{9}{35} \partial_x u_2
\end{align*}$$

- Simplified (simplified) $P_3$ (SSP$_3$): [Frank, Klar, Larsen, Yasuda, JCP 2007]

$$\partial_t \begin{pmatrix} u_0 \\ u_2 \end{pmatrix} = \frac{1}{3(\kappa + \sigma)} \begin{pmatrix} \frac{2}{5} & \frac{11}{7} \end{pmatrix} \cdot \partial_{xx} \begin{pmatrix} u_0 \\ u_2 \end{pmatrix} - \begin{pmatrix} \kappa & 0 \\ 0 & \kappa + \sigma \end{pmatrix} \cdot \begin{pmatrix} u_0 \\ u_2 \end{pmatrix} + \begin{pmatrix} q_0 \\ 0 \end{pmatrix}$$
Moment models

- 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.
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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.

Evolution equation
\[ \frac{d}{dt} x = R(x), \quad x(0) = \tilde{x}. \]

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
\[
\frac{d}{dt} \begin{bmatrix} \hat{x} \\ \tilde{x} \end{bmatrix} = \begin{bmatrix} \hat{R}(\hat{x}, \tilde{x}) \\ \tilde{R}(\hat{x}, \tilde{x}) \end{bmatrix}, \quad \begin{bmatrix} \hat{x}(0) \\ \tilde{x}(0) \end{bmatrix} = \begin{bmatrix} \hat{x} \\ \tilde{x} \end{bmatrix}.
\]

Averaging unresolved variables
Resolved initial conditions \( \hat{x} \) are known. Yields conditioned measure for \( \tilde{x} \)
\[
f_{\hat{x}}(\tilde{x}) = Z^{-1} f(\hat{x}, \tilde{x})
\]
Average of function \( u(\hat{x}, \tilde{x}) \) w.r.t. \( f_{\hat{x}}(\tilde{x}) \) is conditional expectation
\[
Pu = \mathbb{E}[u|\hat{x}] = \frac{\int u(\hat{x}, \tilde{x}) f(\hat{x}, \tilde{x}) d\tilde{x}}{\int f(\hat{x}, \tilde{x}) d\tilde{x}}.
\]
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!
- **Optimal prediction**: Obtain average solution by a single simulation.
Average solution
Nonlinear system of ODE
\[ \frac{d}{dt} x = R(x) . \]

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

Smaller system for resolved variables
Mori-Zwanzig formalism [H. Mori 1965, R. Zwanzig 1980] yields approximate evolution for \( \hat{P}\varphi(t) \)
\[
\partial_t \hat{P}\varphi(t) = PR \hat{P}\varphi(t) + \int_0^t K(t - s)\hat{P}\varphi(s) ds .
\]
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:**
  \[ \frac{d}{dt} \hat{x} = R(\hat{x}), \]
  where \( R(\hat{x}) = PR = \mathbb{E}[R(\hat{x}, \tilde{x})|\hat{x}] \).

- **OP with memory:**
  \[ \frac{d}{dt} \hat{x}(t) = R(\hat{x}(t)) + \int_{0}^{t} K(t-s)\hat{x}(s) \, ds, \]
  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 \( \hat{x} \). Can be pre-computed.
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Moment system

\[ \partial_t \bar{u} = R \bar{u} , \quad \bar{u}(0) = \hat{\bar{u}} \]

Differential operator \( R \bar{u} = -B \cdot \partial_x \bar{u} - C \cdot \bar{u} \) (omit source \( q \) for now).

Solution \( \bar{u}(t) = e^{tR} \hat{\bar{u}}. \)

Linear ensemble average solution

- Consider Gaussian measure \( f(\bar{u}) = \frac{1}{\sqrt{(2\pi)^n \det(A)}} \exp \left( -\frac{1}{2} \bar{u}^T A^{-1} \bar{u} \right). \)

- Decomposition \( \bar{u} = \begin{bmatrix} \hat{\bar{u}} \\ \tilde{\bar{u}} \end{bmatrix} \) and \( A = \begin{bmatrix} \hat{A} & \hat{\tilde{A}} \\ \tilde{\hat{A}} & \tilde{\tilde{A}} \end{bmatrix} = A^T \) (covariance matrix)

- Conditional expectation projection is matrix multiplication \( P \bar{u} = E \bar{u} \)

\[
E = \begin{bmatrix} I & 0 \\ \tilde{\hat{A}} \hat{A}^{-1} & 0 \end{bmatrix}. \] Meaning: Given \( \hat{\bar{u}}, \tilde{\bar{u}} \) is centered around \( \tilde{\hat{\bar{u}}} \hat{A}^{-1} \hat{\bar{u}}. \)

- Average solution \( P \bar{u}(t) = e^{tR} E \hat{\bar{u}} \) 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)

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

Proof: $M(t) = e^{tR} - \int_0^t e^{(t-s)RF} RE e^{sR} ds - e^{tRF}$.  

$$\frac{\partial_t M(t) = RF M(t), M(0) = 0. \text{ Hence } M(t) = 0.$$  

- Differentiating Dyson’s formula:

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

- Adding $E$ from right yields evolution for average solution operator

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

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

\[ \partial_t \bar{u}^m(t) = \mathcal{R} \bar{u}^m(t) + \int_0^t K(t - s) \bar{u}^m(s) \, ds , \]

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

Approximations

**First order OP:** \( \partial_t \bar{u}(t) = \mathcal{R} \bar{u}(t) \)

**Piecewise constant quadrature for memory:**

\[ \partial_t \bar{u}(t) = \mathcal{R} \bar{u}(t) + \tau K(0) \bar{u}(t) , \]

where \( \tau \) characteristic time scale.

**Better approximation for short times:**

\[ \partial_t \bar{u}(t) = \mathcal{R} \bar{u}(t) + \min\{\tau, t\} K(0) \bar{u}(t) . \]

**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.

\[
\begin{align*}
\hat{\mathbb{R}} &= \hat{\mathbb{R}} E = \hat{\mathbb{R}} = -\hat{B} \partial_x - \hat{C} ,
\hat{K}(0) &= \hat{R} \hat{F} \hat{R} \mathbb{E} = \hat{R} \hat{R} = \hat{B} \hat{B} \partial_{xx} \\
\hat{B} \hat{B} &= \begin{pmatrix}
0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & \frac{(N+1)^2}{(2N+1)(2N+3)}
\end{pmatrix}
\end{align*}
\]

Approximations

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

\[
\partial_t \hat{\mathbb{u}}(t) = \hat{\mathbb{R}} \hat{\mathbb{u}}(t) + \tau \hat{B} \hat{B} \partial_{xx} \hat{\mathbb{u}}(t)
\]

yields classical diffusion correction closure, and

\[
\partial_t \hat{\mathbb{u}}(t) = \hat{\mathbb{R}} \hat{\mathbb{u}}(t) + \min\{\tau, t\} \hat{B} \hat{B} \partial_{xx} \hat{\mathbb{u}}(t)
\]

yields new **crescendo diffusion** correction closure (no extra cost!).
Various $P_0$ moment closures

- $u_0(x)$ at $t = 0.1$
- $u_0(x)$ at $t = 0.2$
- $u_0(x)$ at $t = 0.3$
- $u_0(x)$ at $t = 0.4$

Legend:
- **true solution**
- $P_N$ closure
- diffusion
- cresc. diff.
Various $P_3$ moment closures

- $u_0(x)$ at $t = 0.1$
- $u_0(x)$ at $t = 0.2$
- $u_0(x)$ at $t = 0.3$
- $u_0(x)$ at $t = 0.4$
A New Perspective on Moment Closure

Geometry

$P_7$ solution

Diffusion closure

Crescendo diffusion
Reordered $P_N$ equations

Even-odd ordering of moments:
$\hat{u} = (u_0, u_2, \ldots, u_{2N})^T$ and $\tilde{u} = (u_1, u_3, \ldots, u_{2N+1}, u_{2N+2}, \ldots)^T$.

Reordered advection matrix (here $N = 2$):

$$
\begin{bmatrix}
\hat{B} & \hat{\tilde{B}} \\
\tilde{\hat{B}} & \tilde{\tilde{B}}
\end{bmatrix} =
\begin{bmatrix}
1/3 & 2/3 & 1 \\
1/3 & 2/3 & 3/7 & 4/7 & 5/9 \\
& 4/9 & 5/9 \\
& & & & & & & 6/11 \\
& & & & & & & & & & 6/13 \\
& & & & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots
\end{bmatrix}
$$

Optimal prediction approximation

Parabolic system

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

Diffusion matrix $D = \hat{B} \tilde{B}$ is positive definite.
Various parabolic moment closures

$u_0(x)$ at $t = 0.1$

- True solution
- Diffusion = $RP_0$
- $RP_1$
- $RP_8$
- $SP_3$

$u_0(x)$ at $t = 0.2$

$u_0(x)$ at $t = 0.3$

$u_0(x)$ at $t = 0.4$
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 $\Rightarrow$ nonlinear closures?
- More complex applications, application to kinetic gas dynamics.


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

Thank you.