PennState

Mori-Zwanzig reduction methods with applications to transport problems

Xiantao Li

Penn State University

April 2, 2019

Motivation

- **Comprehensive mathematical models**
  - Complex dynamical system
  - Microscopic mechanism, detailed interactions, many variables, etc.
  - Applications: growing interest in nanoscale devices and structures

- **Challenges**
  - Large number of degrees of freedom
  - multiple time scales
  - overwhelming computational cost

- Question: how to find alternative reduced models with fewer variables?

Large dimensional system (full dynamics) → Reduced model for certain quantities of interest

Outline

I. Projection formalism

1. Conventional projection formalism
2. Systematic approximations and parameter estimation

II. Connection to Galerkin projections

1. Reduced-order techniques
2. Subspace projections.

III. Applications to heat conduction models in molecular dynamics

1. Energy transport example
2. A new projection formalism – oblique projection
3. Connections to stochastic PDEs

IV. Summary

Part I. Projection Formalism

NAKAJIMA 1958, MORI 1965, ZWANZIG 1973, CHORIN 1998, …

Time evolution of observables

Nonlinear dynamical system: $x' = f(x),\ x(0) = x_0.$

Observable $a(t, x_0) \coloneqq \varphi\big(x(t)\big),\ \dim(a) \ll \dim(x)$

Time derivative $\partial_t a(t, x_0) = \frac{\partial\varphi\big(x(t)\big)}{\partial x} f\big(x(t)\big) = \frac{\partial\varphi\big(x(t)\big)}{\partial x}\frac{\partial x(t)}{\partial x_0} f(x_0) = \frac{\partial\varphi\big(x(t)\big)}{\partial x_0} f(x_0)$

Notation $a(t) \coloneqq a(t, x_0),\qquad a \coloneqq a(0, x_0) = \varphi(x_0)$

Liouville operator $L \coloneqq f(x_0)\cdot\nabla_{x_0}$ (independent of time)

Dynamics of $a(t)$ $\partial_t a(t) = La(t)$

Time evolution $a(t) = e^{tL}a(0)$

The equations are not closed. We will use projections.

Choices of coarse-grain variables

Coarse-grain variables $a = \varphi(x)$:

- $\dim(a) \ll \dim(x)$.
- representative of the overall dynamics.

Specific choices:

- $x = (x_1, x_2, \cdots, x_n, x_{n+1}, \cdots x_N) = (\bar{x}, \tilde{x})$. $a = \bar{x}$. (Chorin et al. 2002)
- Fourier or generalized Fourier modes $x = \sum_i q_i \phi_i + \sum_i \xi_i \psi_i$. $a = q$. (Chorin et al. 1998)
- center of mass. $M_\alpha = \sum_{i \in S_\alpha} m_i x_i$. S_α is a subset of atoms.
- reaction coordinates (collective variables, such as dihedral angles).
- local energy (Chu and Li 2018) $E_\alpha = \sum_{i \in S_\alpha} \frac{1}{2} m_i \dot{x}_i^2 + V_i(x)$.
- Local density, $\sum_i \delta\big(x - q_i(t)\big)\delta\big(p - p_i(t)\big)$ or correlation (Akcasu&Duderstadt 1969, Boley 1974)
- A self-adjoint operator A.
- Density matrix: $\rho_A = tr_B \rho$.

PennState

Choices of projection operators

- Neglecting fine-scale components: $Pg(x) = Pg(\bar{x}, \tilde{x}) = g(\bar{x}\,, 0)$. (Chorin et al. 2002)
- Conditional expectation: $Pg(x) = E[g(x)|a(x) = A] = \frac{\int g(x)\delta(a(x)-A)\rho(x)dx}{\int \delta(a(x)-A)\rho(x)dx}$. (Zwanzig 1961)
- $PX = tr_B(X) \otimes \rho_B$. Lindblad formalism.
- Orthogonal projection: $Pg(x) = \langle g, a^T\rangle\langle a, a^T\rangle^{-1}a$. (Mori 1965)
  - Correlation: $\langle g, f^T\rangle_{ij} = \int g_i(x)f_j(x)\rho(x)\,dx$, or $\beta^{-1}\int_0^\beta tr\left(\rho_{eq}g(i\lambda)f(0)\right)d\lambda$.
- Oblique projection: $Pg(x) = \langle g, b^T\rangle\langle b, b^T\rangle^{-1}b$. (Chu & Li 2018, Lei & Li 2019)
  - $\dim(b) = \dim(a)$
  - $b = -\nabla S(a)$
- Projection of the flux (Chu & Li 2018)
  - Conservation law $\partial_t a + \nabla \cdot q(x) = 0$
  - Apply projection to $q(t)$ → Generalized constitutive relation

The general Mori-Zwanzig equation

- Define $Q = I - P$.
- Dyson's formula $e^{tL} = \int_0^t e^{(t-s)L} PLe^{sQL} ds + e^{tQL}$.
- We start with $\partial_t a(t) = La(t) = e^{tL}La = e^{tL}PLa + e^{tL}QLa$.
- Orthogonal dynamics equation:

$$\partial_t a(t) = e^{tL}PLa + \int_0^t e^{(t-s)L} PLe^{sQL} QLa \, ds + e^{tQL}QLa$$

- The first two terms are in principle functions of $a(s), 0 \leq s \leq t$.
- The last term $F(t) = e^{tQL}QLa$ is often regarded as random noise.
- The actual form will depend on the specific choice of the projection operator.

Zwanzig's projection (Zwanzig 1961, 1973)

Projection $Pg(x) = E[g(x)|\varphi(x) = a] = \frac{1}{\Omega(a)} \int g(x)\rho(x)\delta(\varphi(x) - a)\, dx\,.$

The Generalized Langevin Equation (for Hamiltonian systems, Hijon et al 2009):

$$\partial_t a(t) = v\big(a(t)\big) - \int_0^t \theta(a(t-s), s)\partial_a S\big(a(t-s)\big)ds + k_B \int_0^t \partial_a \theta(a(t-s), s)\, ds + F(t)$$

Markovian term $v\big(a(t)\big) := e^{tL} PLa = E[L\varphi(x)|\varphi(x) = a(t)].$

Entropy $S(a) = k_B \ln \Omega(a)$

Noise $F(t) = e^{tQL} QLa$

Kernel function $\theta(a,t) = \frac{1}{k_B} E[F(t) F^T(0)|\varphi(x) = a]$

Implementation difficulties (Chorin & Stinis 2007, Español et al. 2010)

- conditional expectations $v(\cdot)$ and $\partial S(\cdot)$ -- constrained MD
- Markovian approximation $\theta(a,t) \approx \theta_T(a)\delta(t)$
- Higher order approximations are non-trivial

Mori's projection (Mori. 1965)

Projection operator: $Pg(x) = \langle g, a^T \rangle \langle a, a^T \rangle^{-1} a.$

The Generalized Langevin Equation (GLE): $a'(t) = \Omega a(t) - \int_0^t \theta(s) a(t-s) ds + F(t).$

Markovian term: $e^{tL} PLa = \langle La, a^T \rangle \langle a, a^T \rangle^{-1} a(t) =: \Omega a(t).$

The memory term: a convolution

$$\int_0^t e^{(t-s)L} PLF(s) ds = \int_0^t e^{(t-s)L} \langle LF(s), a \rangle \langle a, a^T \rangle^{-1} a \, ds =: -\int_0^t \theta(s) a(t-s) ds \, .$$

The memory term becomes a linear convolution, with memory kernel,

$$\theta(t) = -\langle LF(t), a^T \rangle \langle a, a^T \rangle^{-1} = \langle F(t), QLa \rangle \langle a, a^T \rangle^{-1} = \langle F(t), F(0)^T \rangle \langle a, a^T \rangle^{-1}$$

The **second fluctuation-dissipation theorem (Kubo 1966):** $\langle F(t), F(0)^T \rangle = \theta(t) \langle a, a^T \rangle$

Zwanzig's example

A particle connected to harmonic springs

$$H = \frac{1}{2}mv^2 + U(x) + \sum_j \frac{1}{2}p_j^2 + \frac{1}{2}\omega_j^2\left(q_j - \gamma_j x\right)^2$$

The generalized Langevin equation

$$mx'' = -U'(x) - \int_0^t \theta(t-\tau)x'(\tau)d\tau + F(t).$$

The kernel function

$$\theta(t) = \sum_j \frac{\gamma_j^2}{\omega_j^2}\cos\omega_j t.$$

$F(t)$ is a stationary Gaussian process. $\langle F(t+s), F(s)^T\rangle = k_B T\theta(t)$

Extension to crystalline solids: (Li and E, 2007, Li 2010).

Example: 1D chain (Li 2010, Chu and Li 2018).

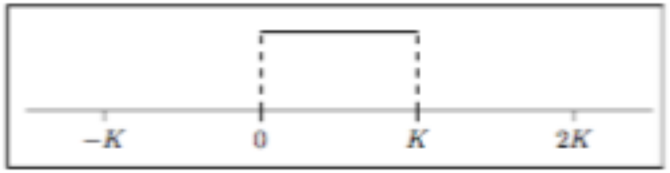
Consider a linear ODE system $x'' = -Ax, \quad x \in \mathbb{R}^N$.

Define the CG variable $a = \Phi^T x$ (linear displacements)

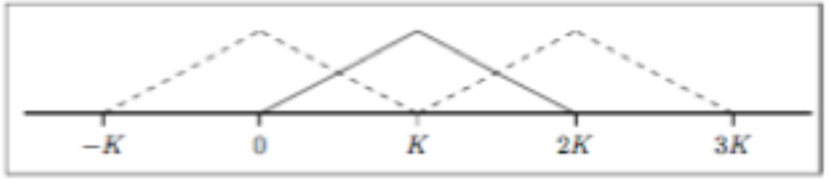
Projection operator as matrix projection, i.e. $Pg(x) = g(\Phi\Phi^T x)$.

Let $\Sigma = [\Phi, \Psi]$ be an orthonormal matrix where $\Phi \in \mathbb{R}^{N\times n}$, $\Psi \in \mathbb{R}^{N\times(N-n)}$, $m \ll N = nK$.

Piecewise constant averaging



Piecewise linear averaging



GLE $\partial_{tt} a(t) = -\mathcal{K} a(t) - \int_0^t \theta(t-s) a(s)\, ds + F(t)$

Kernel function $\theta(t) = \Phi^T A \Psi \cos(\Omega t) \Omega^{-2} \Psi^T A \Phi, \Omega^2 = \Psi^T A \Psi$.

Second fluctuation–dissipation theorem $\langle F(t) F^T(t') \rangle = k_B T \theta(t - t')$.

Approximation of the memory term

Averaged equation $\dot{a}(t) = \Omega a(t) - \theta(t) \star a(t) + noise$

Extended dynamics of the memory $z = \theta \star a$

Laplace transform of the kernel function $\Theta(\lambda) = \int_0^{+\infty} \theta(t) e^{-t/\lambda} dt$

Rational approximation $R_{k,k}(\lambda) = \left(I - \lambda B_1 - \cdots - \lambda^k B_k\right)^{-1}\left(A_0 + \lambda A_1 + \cdots + \lambda^k A_k\right)$

Approximation: $\tilde{z}(\lambda) \approx R_{k,k}(\lambda)\tilde{a}(\lambda)$

Extended dynamics of auxiliary variables

$$\begin{cases} \dot{a} = \Omega a - z_1 \\ \dot{z}_1 = A_1 a + B_1 z_1 + z_2 \\ \dot{z}_2 = A_2 a + B_2 z_1 + z_3 \\ \quad \cdots\cdots \\ \dot{z}_k = A_2 a + B_k z_1 \end{cases} \longrightarrow \text{Approximate GLEs} \begin{cases} \dot{a} = \Omega a - e^{\mathrm{T}} z \\ \dot{z} = \boldsymbol{A} a + \boldsymbol{B} z \end{cases}$$

Examples of low order approximations

- Zeroth order model

$$\dot{a}(t) = \Gamma a(t) + F(t)$$

- Equivalent approximation $\theta(t) \approx \Gamma\delta(t)$

- How to determine Γ?
  - Standard maximum likelihood function from Girsanov theorem gives $\Gamma = 0$
  - Green-Kubo type formula (Hijon et al 2006)

$$\Gamma = \langle a, a^T \rangle \left[\int_0^{+\infty} \langle a(t), a \rangle dt \right]^{-1}$$

- First order model

$$\dot{a}(t) = \Omega a(t) - z(t)$$
$$\dot{z}(t) = Aa(t) + Bz(t) + F(t)$$

- Equivalent approximation $\theta(t) \approx e^{Bt}A$

Sum of exponentials (including cosine and sine)

- How to determine A, B?
  - Green-Kubo type formula
  - Matching $\langle \dot{a}, \dot{a} \rangle$ and $\langle a, a \rangle$
  - $A = \langle \dot{a}, \dot{a} \rangle \langle a, a \rangle^{-1}$
  - $B = -A\Gamma^{-1}$

Questions:

- How to generalize the parameter estimation approach to higher order models?
- How to relate these parameters to the time series of a?

Parameter Estimation

Existing methods

- Kalman filter (Fricks et al 2009, Harlim and Li 2015)
- NARMAX (Chorin and Lu, 2015)
- Linear response (Zhang, Harlim and Li 2019)
- Machine learning?

Two-point Padé approximation

- Long-time statistics

$$\lim_{\lambda\to\infty} R_{k,k}(\lambda) = \lim_{\lambda\to\infty} \Theta(\lambda)$$

- Short-time statistics

$$R_{k,k}(0) = \Theta(0)$$

$$R'_{k,k}(0) = \Theta'(0)$$

$$R''_{k,k}(0) = \Theta''(0)$$

$$\cdots\cdots$$

- As λ goes to infinity,

$$\Theta(+\infty) = \lim_{s\to 0_+} \int_0^{+\infty} \theta(t) e^{-st} dt$$

- As $\lambda \approx 0_+$, $\Theta(\lambda) = \lambda\theta(0) + \lambda^2\theta'(0) + \lambda^3\theta'(0) + \cdots$

$$\Theta(0) = 0$$

$$\Theta'(0) = \theta(0) = \langle \dot{a}, \dot{a} \rangle \langle a, a \rangle^{-1}$$

$$\Theta''(0) = 2\theta'^{(0)} = \cdots\cdots$$

Approximation with Gaussian additive noise

Markovian embedding of the GLE

$$\begin{cases} \partial_t a = \Omega a - e^{\mathrm{T}} z \\ \partial_t z = A a + B z + \sigma \xi \end{cases}$$

$\xi(t)$ is the standard Gaussian white noise

Stability condition -- Lyapunov equation

Zeroth order approximation:

$$\partial_t a(t) = \Gamma a(t) + \sigma \xi(t),$$

Covariance of a is M

$$\Gamma = \langle a, a^T \rangle \left[\int_0^{+\infty} \langle a(t), a \rangle dt \right]^{-1} \approx \gamma \nabla_h^2$$

$$\Gamma M + M \Gamma + \sigma^T \sigma = 0$$

First order approximation:

$$\partial_t a(t) = \Omega a(t) - z(t)$$

$$\partial_t z(t) = A_1 a(t) + B_1 z(t) + \sigma \xi(t)$$

Parameters from Padé approximation

- $A_1 = \langle \dot{a}, \dot{a} \rangle \langle a, a \rangle^{-1}$
- $B_1 = -A_1 \Gamma^{-1}$
- $B_1 A_1 + A_1 B_1^T + \sigma^T \sigma = 0$

Part II. Connections to Galerkin-Petrov projection

A reduced-order viewpoint

The full dynamics (Langevin):

$$x' = v, v' = Ax - \gamma v + \sigma W'(t)$$

A partition of the degrees of freedom: $x = \Phi q + \Psi \xi, v = \Phi p + \Psi \eta$

- Φ and Ψ: orthogonal matrices
- q and p: Linear CG variables
- A GLE can also be derived (Ma, Li and Liu 2017).

The partitioned Langevin dynamics (Sweet et al 2008)

$$\xi' = \eta, \eta' = -A_{22}\xi - A_{21}q - \Gamma_{21}p + \zeta_2'(t)$$

We write it as $y' = Ay + Ru(t) + g(t)$.

- Low dimensional input: $u = (q, p)$
- Low dimensional output: $f_{12} = -A_{12}\xi$
- Reduced-order methods?

Subspace projections (Ma, Li and Liu, 2019).

Stochastic reduced-order problem: $y' = Ay - Rp + \zeta(t), w(t) = L^T y, \boldsymbol{FDT}$.

Galerkin projection: $y \in Range(V)$, s.t., $y' - Ay + Rp - \zeta(t) \perp Range(W)$.

The projection yields an approximate kernel function and an approximate noise.

Question: *Would the second fluctuation-dissipation theorem be satisfied automatically?*

Yes, if $V = \left[R, AR, A^2R, \cdots, A^\ell R\right]$ and $W = \left[A^{-T}L, L, A^T L, \cdots, {A^{\ell-1}}^T L\right]$.

Computationally, the block Lanczos algorithm provides biorthogonal basis.

PennState

Galerkin and Mori's projection of nonlinear dynamics

A Hamiltonian system of ODEs: $y' = J\nabla H(y), y = (q,p)$

Project $\mathbf{a}(t)$ onto a set of projection bases $\{\boldsymbol{\psi}_i\}_{i=1}^{M}$ by:

$$\mathbf{a}(t) \approx \tilde{\mathbf{a}}(t) := \sum_{i=1}^{M} \boldsymbol{c}_i(t)\boldsymbol{\psi}_i(\mathbf{x}_0)$$

Determine $\{\boldsymbol{c}_i\}_{i=1}^{M}$ by a set of test bases $\{\boldsymbol{\phi}_i\}_{i=1}^{M}$

$$\langle \dot{\tilde{\mathbf{a}}}, \boldsymbol{\phi}_i \rangle = \langle L\tilde{\mathbf{a}}, \boldsymbol{\phi}_i \rangle, \qquad i = 1, \dots, M$$

$$\dot{\hat{\mathbf{C}}}\,\hat{\mathbf{M}} = \hat{\mathbf{C}}\hat{\mathbf{K}}, \quad \hat{\mathbf{C}} := [\boldsymbol{c}_1, \boldsymbol{c}_2, \dots, \boldsymbol{c}_M] \quad [\hat{\mathbf{M}}]_{ij} = \langle \boldsymbol{\psi}_i, \boldsymbol{\phi}_j \rangle, [\hat{\mathbf{K}}]_{ij} = \langle L\boldsymbol{\psi}_i, \boldsymbol{\phi}_j \rangle$$

Theorem (H Lei and X. Li). *By choosing projection bases* $\{\boldsymbol{\psi}_i\}_{i=1}^{2} = \{\mathbf{a}, L\mathbf{a}\}$ *and test bases* $\{\boldsymbol{\phi}_i\}_{i=1}^{2} = \{L^{-1}\mathbf{a}, \mathbf{a}\}$, the Galerkin projection yields the same approximation of the memory function as the two-point Pade approximation.

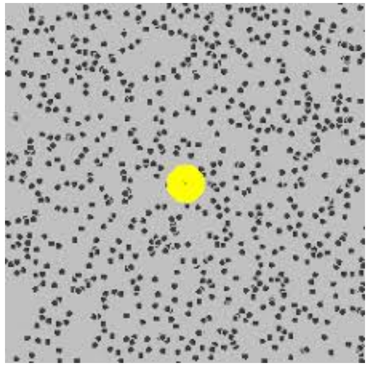
The noise has to be introduced separately.

In practice, the algorithms are more robust if the basis functions are orthogonalized, e.g., by the Lanczos method.

PennState

Numerical example: diffusion process

(Lei and Li, 2019, Lei, Baker and Li, 2017)



- A tagged particle interacts with solvent particles

$$\boldsymbol{F}_{ij} = \begin{cases} a(1.0 - r_{ij}/r_c)\boldsymbol{e}_{ij}, & r_{ij} < r_c, \\ 0, & r_{ij} > r_c, \end{cases}$$

where $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$, $r_{ij} = |\boldsymbol{r}_{ij}|$ and $\boldsymbol{e}_{ij} = \boldsymbol{r}_{ij}/r_{ij}$.

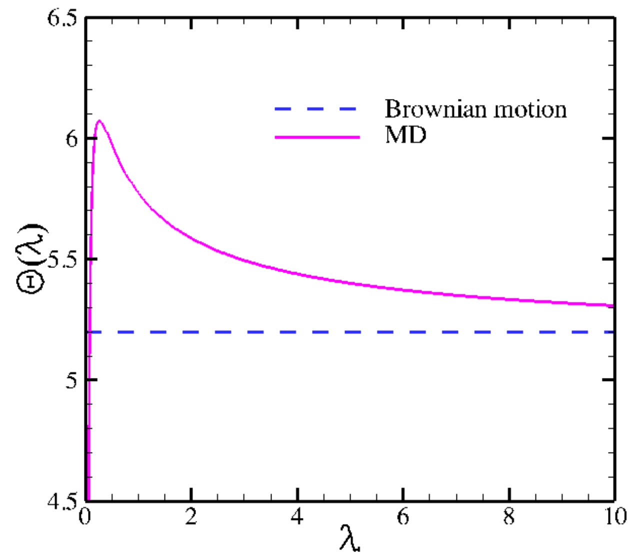
- Governed generalized Langevin equation

$$\mathbf{v} := \dot{\mathbf{q}} = \mathbf{p}/m,$$

$$\dot{\mathbf{p}} = -\beta \int_0^t \boldsymbol{\theta}(t-s)\mathbf{v}(s)ds + \mathbf{R}(t).$$

- Markovian approximation (Einstein's theory)

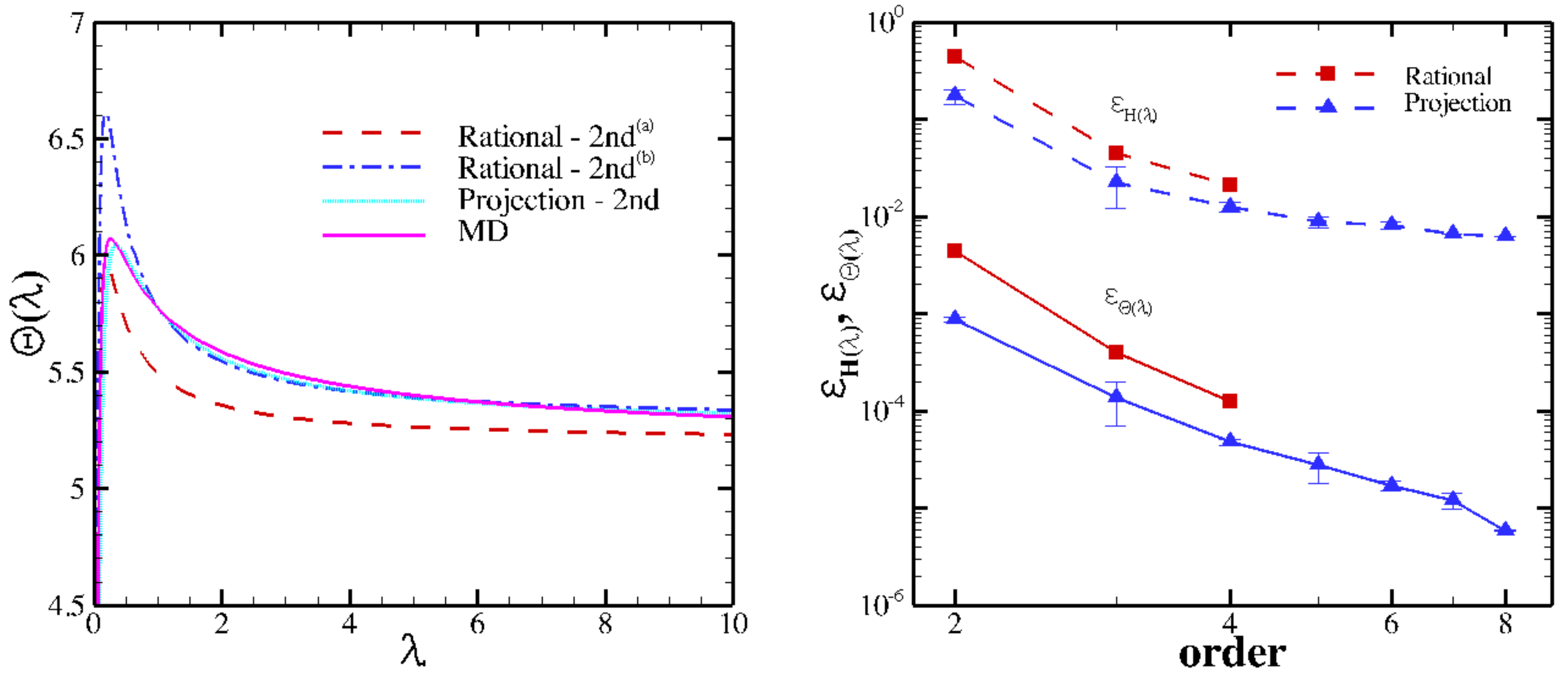
$$\int_0^t \boldsymbol{\theta}(t-s)\mathbf{v}(s)ds \approx \left[\int_0^\infty \boldsymbol{\theta}(s)ds\right]\mathbf{v}(t).$$



$\boldsymbol{\Theta}(\lambda)$ obtained from MD data

PennState

Construction of memory kernel

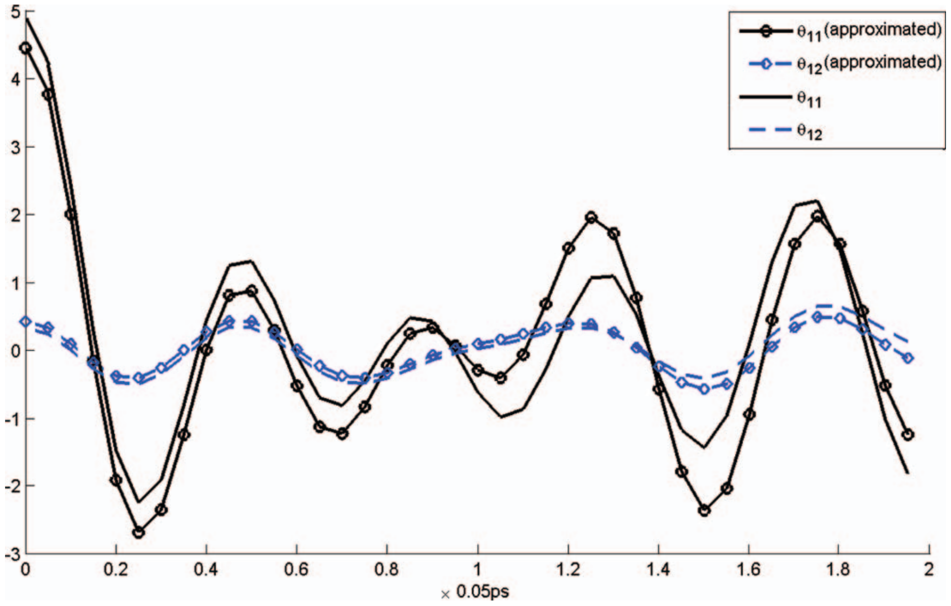


PennState

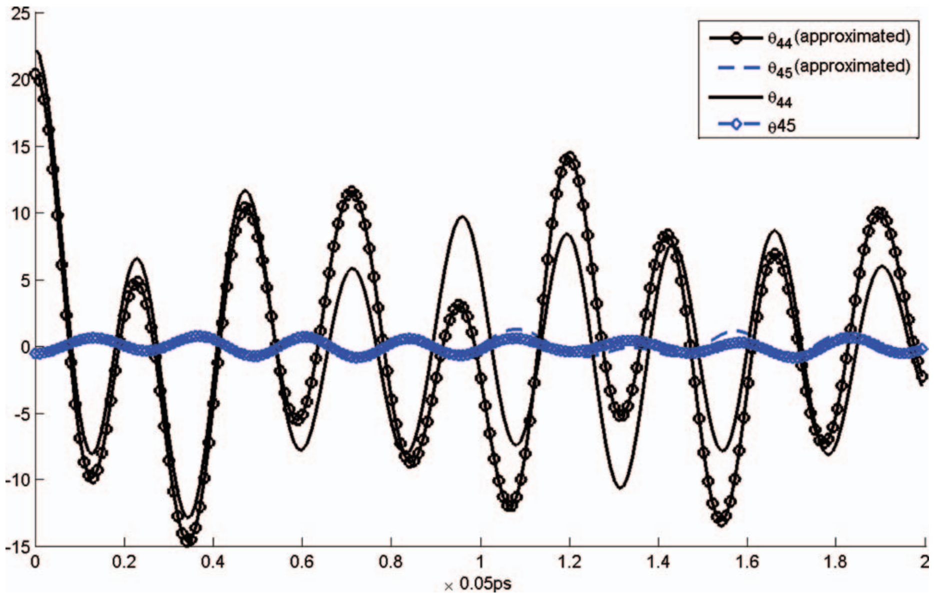
Prediction of time-correlation function for protein dynamics

(Chen, Li and Liu, J Chem Phys. 2014))

RTB basis: each residue of the protein is represented by a rigid body



Translational modes



Rotational modes

Part IV. Applications to transport problems

Motivation

- Fourier's Law $q = -k\nabla T$ breaks down at small scales $10^{-6} \sim 10^{-9}$m
- Observations of heat pulses -- heat can travel like waves (*Both, et al. 2015*)
- Thermal conductivity depends on the system size (*Győry & Márkus, 2014*)
- Thermal fluctuation effects become important at small scales

PennState

Coarse-grain variables for heat conduction

Let x and v be the position and velocity of atoms, $(x, v) \in \Gamma = \mathbb{R}^{2N}$.
Full dynamics: molecular dynamics (Newton's 2nd Law)

$$\begin{cases} x' = v, & x(0) = x^0, \\ mv' = -\frac{\partial V(x)}{\partial x}, & v(0) = v^0, \end{cases} \quad (x^0, v^0) \sim \rho_0.$$

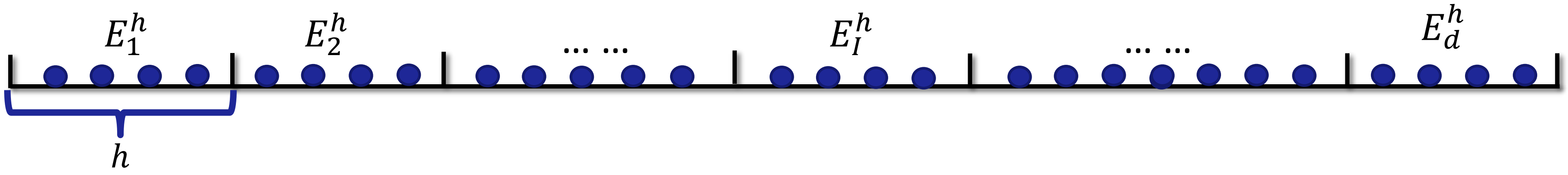
Nearest neighbor interaction $V(x) = \sum_{i=1}^{nd} \frac{1}{2}\phi(x_{i-1} - x_i) + \frac{1}{2}\phi(x_{i+1} - x_i)$.

Local energy (pairwise. Multi-body interactions: Wu and Li 2015)

$$E_I^h(t) = \sum_{i \in S_I} \frac{1}{2} m v_i^2 + \frac{1}{2}\varphi(x_{i-1} - x_i) + \frac{1}{2}\varphi(x_{i+1} - x_i).$$

Let the coarse-grain variable be shifted local energy:

$$a(t) = E^h(t) - \langle E^h \rangle$$



Approximation with Gaussian additive noise

In zeroth order approximation: $\partial_t a(t) = -\Gamma a(t) + \sigma\xi(t)$,

$$\Gamma \approx -\kappa\nabla_h^2 + \mu\nabla_h^4 + \cdots$$

Conventional Mori's projection with Gaussian additive noise

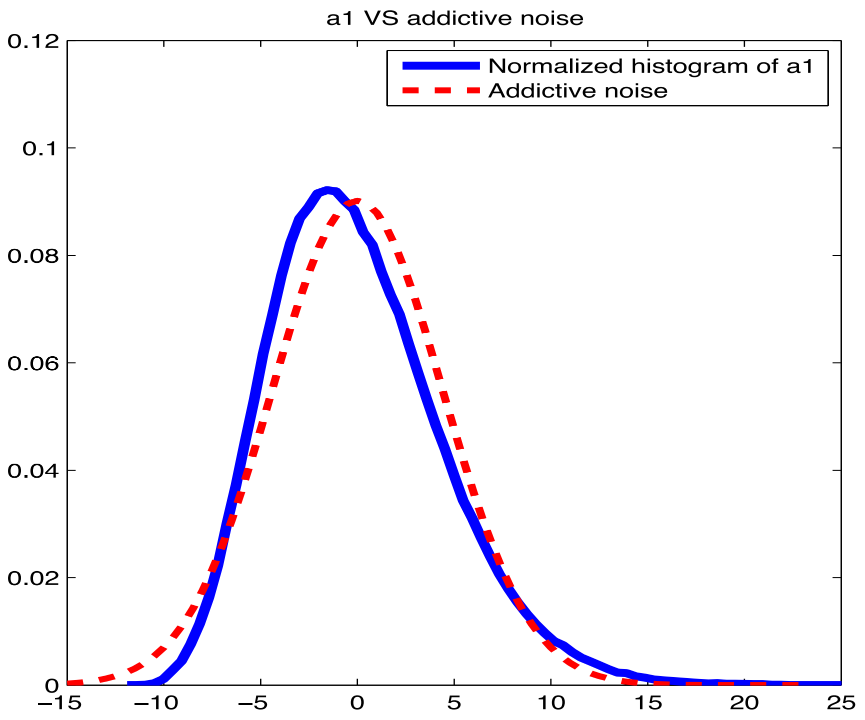
- Zeroth order $\partial_t a(t) = \kappa\nabla_h^2 a(t) + \sigma\xi(t)$

  convergence $\partial_t a(t) = \kappa\nabla^2 a(t) + \nabla\cdot\xi(t)$ (Du & Zhang 2002, Gyöngy 1999)
- First order $\partial_{tt} a(t) + \gamma\partial_t a(t) = c^2\nabla_h^2 a(t) + \sigma\xi(t)$
- Second order $\partial_{ttt} a(t) + \gamma_1\partial_{tt} a(t) + \gamma_2\partial_t a(t) = c_1^2\nabla_h^2 a(t) + c_2^2\nabla_h^2\partial_t a(t) + \sigma\xi(t)$
- Higher order models ……

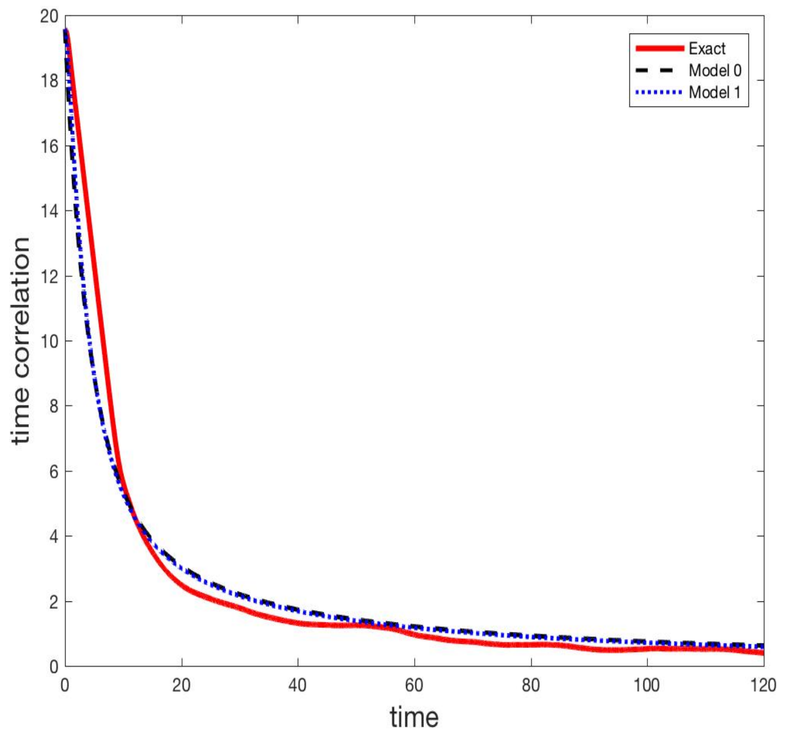
By additive noise approximation, $a(t)$ is expected to be Gaussian.

Experiments of local energy transport in nanotube

True distribution and numerical results from additive noise



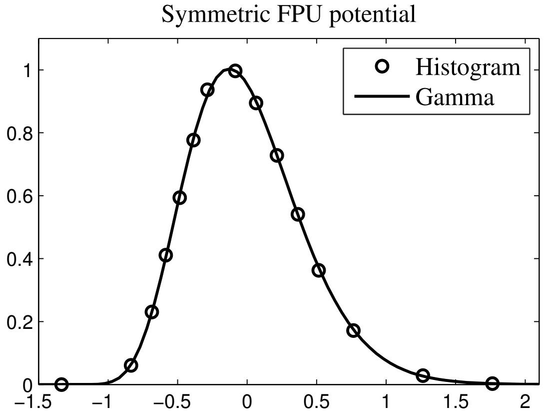
True correlation and numerical results by additive noise

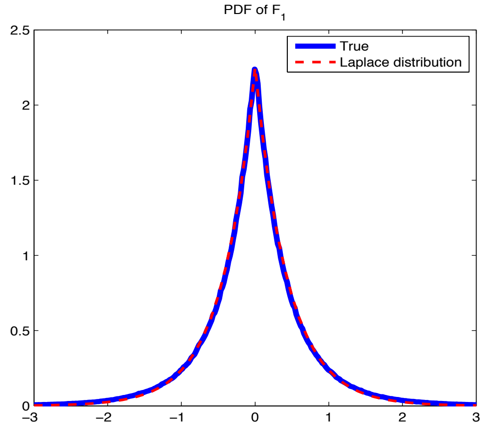


Correlation is well-captured but the PDF is not!

Experiments of local energy in nanotube system

1d chain example PDF of local energy





Equilibrium density in the form of Gamma distribution

$$\rho(a) = \frac{1}{Z}\prod_{i=1}^{n}(a_i - \mu_i)^{\alpha_i} e^{-\beta_i(a_i-\mu_i)}.$$

Parameters can be determined from data

- Maximum likelihood
- Fitting statistics

Question

- How to construct reduced models that are able to recover the non-Gaussian PDF?
- Multiplicative noise (Chu and Li, 2018).

Oblique projection (Chu and Li, preprint, 2019)

Oblique projection: $P\cdot=\langle\cdot,b^T\rangle\langle b,b^T\rangle^{-1}b.$

GLE: $\partial_t a(t)=\Omega b(t)-\int_0^t\theta(t-s)b(s)ds+F(t).$

Choices of b

1. Conventional Mori's projection $b=a$ $\quad\partial_t a(t)=\Omega a(t)-\int_0^t\theta(t-s)a(s)ds+F(t).$
2. Driving force $b=-\frac{\delta S(a)}{\delta a}$ potential of mean force (PMF)
   - Given data $a\sim\rho_{eq}(a)$, $S(a)=-\ln\rho_{eq}(a).$
   - Recover the PDF $\rho_{eq}(a)=\Xi_0^{-1}exp\big(-S(a)\big).$

Oblique projection (Cont'd)

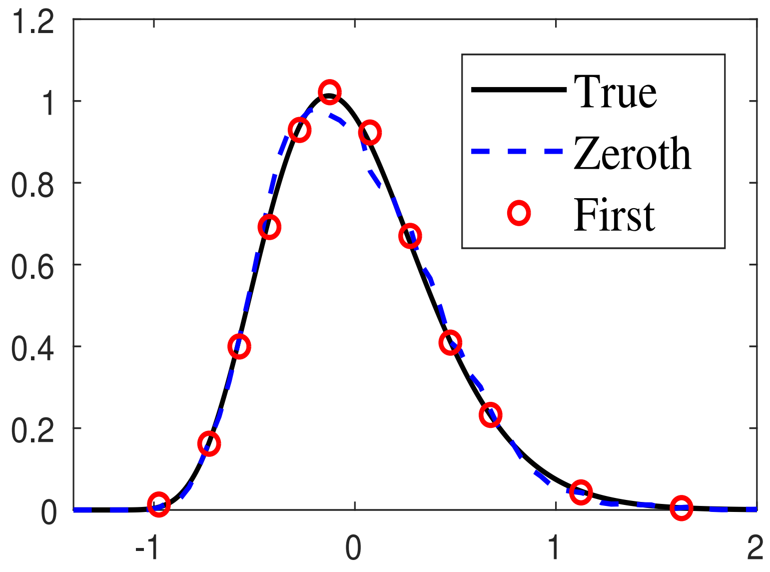
- $\rho_{eq}(a) = \Xi_0^{-1}\, exp\big(-S(a)\big)$ is known (from the data or empirical experiments)
- Define $b = -\dfrac{\delta S(a)}{\delta a}$.
- $\rho_{eq}(a)$ is the stationary solution of the Fokker-Planck equations of the following reduced models.

Zeroth order approximation	First order approximation
$\partial_t a(t) = -\Gamma \frac{\delta S(a)}{\delta a} + \sigma\xi(t)$ Stochastic phase-field crystal model (Elder & Grant 2004) $\sigma\sigma^T = \Gamma + \Gamma^T$ $\rho_{eq}(a) = \frac{1}{\Xi_0} exp[-S(a)]$	$\begin{cases} \partial_t a(t) = z \\ \partial_t z(t) = -A\frac{\delta S(a)}{\delta a} + Bz + \sigma\xi(t) \end{cases}$ $\sigma\sigma^T = BA + AB^T$ $\rho_{eq}(a,z) = \frac{1}{\Xi_1} exp\left[-S(a) - \frac{1}{2} z^T A^{-1} z\right]$

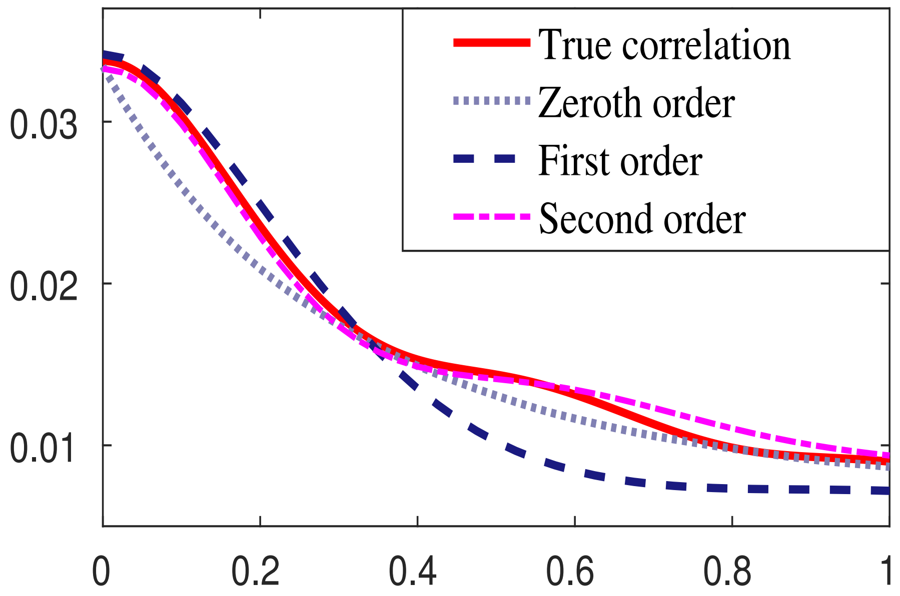
Numerical results of oblique projection

Energy transport in Carbon nanotube, a – local energy

The recovery of the non-Gaussian statistics



The prediction of auto-correlation



PennState

Summary

- A projection formalism to derive reduced models from a complex dynamical system.
- An oblique projection to obtain nonlinear dynamics and non-Gaussian PDF
- A Markovian embedding scheme to approximate the memory function.
- The connections to Galerkin projection.
- Application to dynamics of bio-molecules and generalized diffusion processes.

Open issues

- Selection of reduced variables
- State-dependent kernel functions
- More general approximation of the random noise