A treatment of multi-scale hybrid systems involving deterministic and stochastic approaches, coarse graining and hierarchical closures

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Outline

• Motivation – climate modeling, catalysis, traffic flow

• The prototype hybrid system
  introduction and examples

• Part I. Deterministic closures:
  stochastic averaging, local mean field models

• Part II. Stochastic closures:
  coarse-graining in hybrid systems

• The role of rare events and phase transitions

• Intermittency and metastability phenomena.

• Conclusions

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Cell Biology: Epidermal Growth Factor binding/dimerization

Early events of EGF signaling

Spatial organization of EGF receptors can influence characteristics (dynamics) of
- EGF receptor dimerization
- EGF binding
- Intracellular activation and signaling

- “noisy” intercellular communication, synchronization
Surface processes: \{ \text{Catalysis, Chemical Vapor Deposition, Epitaxial growth, etc.} \}

[Vlachos, Schmidt, Aris, J. Chem. Phys 1990]
[Lam, Vlachos, Phys. Review B 2001]
Traffic Flow

We define a continuous time jump Markov process \( \{\sigma_t\}_{t \geq 0} \) on \( L^\infty(\Sigma, R) \) with generator

\[
L_N f(\sigma) = \sum_{x,y \in \mathcal{L}} c(x,y,\sigma)[f(\sigma^{x,y}) - f(\sigma)],
\]

and Arrhenius diffusion rate,

\[
c(x, y, \sigma) = \begin{cases} 
  c_0 e^{-U(x)}, & \sigma(x) = 1, \sigma(y) = 0 \\
  c_0 e^{-U(y)}, & \sigma(x) = 0, \sigma(y) = 1 \\
  0 & \text{otherwise}
\end{cases}
\]

where

\[
U(x) = \sum_{z \neq x} J(x, z) \sigma(z)
\]

such that for all test functions \( f \in L^\infty(\Sigma, R) \)

\[
\frac{d}{dt} E_\mu f(\sigma_t) = E_\mu L_N f(\sigma_t)
\]
We consider short vehicle potential interactions $J$,

$$J(x, y) = \gamma V (\gamma(x - y)), \quad x, y \in \mathcal{L}$$

where $\gamma$ is a parameter prescribing the range of microscopic interactions and $V : R \to R$ via,

$$V(r) = \begin{cases} 
J_0 & \text{if } 0 < r < 1 \\
0 & \text{otherwise}
\end{cases}$$

which enforces both:

- vehicles do not go backward in traffic

- local effect of the interactions (thus, once again, more realistic traffic conditions).
Vehicle histories in space and time. Parameters used: $c_0 = 2$, nearest neighbors used for potential is $L = 4$, and $J_0 = 1$. 
Vehicle histories in space and time. Parameters used: $c_0 = 2$, total lattice nodes = 500, nearest neighbors used for potential is $L = 4$, and $J_0 = 1$. Total number of vehicles 256.
Epidemiology

We develop an SIR model (epidemics with removal) for plant spread of disease based on stochastic dynamics.

We apply a contact process with generator,

\[ Lg(\sigma) = \sum_{x \in \mathcal{L}} c(x, \sigma)[g(\sigma^x) - g(\sigma)], \]

for \( g \in L^\infty(\Sigma; R) \) where \( \Sigma = \{0, 1\}^\mathcal{L} \). The microscopic rate for the contact process is given by,

\[ c(x, \sigma) = (1 - \sigma(x))B[\sigma(x)] + \sigma(x)R \]

where \( R \) is the rate of recovery and

\[ B[\sigma(x)] = J_1 + J_2 \sum_{y \neq x} f(x - y)\sigma(y) \]

denotes the infectivity. \( f \) is a given contact kernel.
Catalytic Reactors

- Microscopic descriptions of surface mechanisms on catalytic reactors, involve processes which undergo
  
  adsorption, desorption, reaction and surface diffusion

- On the other hand, the gas-phase modeling is based on continuum PDEs

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The microscopic stochastic surface processes are coupled to the continuum PDEs via boundary conditions and adsorption/desorption rates to and from the surface.

\[
\frac{dP}{dt} = \frac{P_0 - P}{\tau} + P^*(\bar{c}_d - \bar{c}_a).
\]

Here \(P_0\) is the pressure at the reactor’s inlet and \(P^*\) expresses surface capacity,
Climate Modeling

At the “microscopic” scale (1 – 10km)

- a fictional particle inhibits deep convection (called a CIN site), while

- an empty site corresponds to a spatial location with potential for deep convection (a PAC site).

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The prognostic variables solve a system of PDEs in the GCM mesh for the fluid and thermodynamic variables. The prognostic variables supply an external field for the microscopic rates of the PAC and CIN sites, while on the other hand the area fraction $\bar{\sigma}$ for deep convection which is specified by the microscopic stochastic model enters as a parameter in the PDEs.

The significance of this stochastic/deterministic coupling is underscored by the sensitivity of the PDE systems on the area fraction $\tilde{\sigma}$, even as a deterministic parameter.
Atmosphere/Ocean applications: Tropical convection.

- High precipitation
- Hot tower cumulus cloud with anvil top
- 16 km
- < 10 km

Planetary Boundary Layer

SEA SURFACE

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“Particles” and sub-grid scale effects: [Majda, Khouider, PNAS 2001]
The vertical velocity contours and $u$-$v$ flows.
$\epsilon = .1$ and $C_0 = 0$. 
The surface pressure contours and u-v flows.
$\epsilon = .1$ and $C_0 = 0$. 
The streamlines. $\epsilon = 0.1$ and $C_0 = 0$. 
Some challenges and questions:

- Disparity in scales and models;
  DNS require ensemble averages for large systems

- Model reduction, however no clear scale separation;
  need hierarchical coarse-graining

- Deterministic vs stochastic closures;
  when is stochasticity important?

- Error control, stability of the hybrid algorithm;
  efficient allocation of computational resources
  adaptivity, model and mesh refinement

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A mathematical prototype hybrid model

- We introduce the microscopic spin flip stochastic Ising process \( \{\sigma_t\}_{t=0} \).

- Coupled to a PDE/ODE that serves as a caricature of an overlying gas phase dynamics.

\[
\frac{d}{dt} Ef(\sigma) = \frac{1}{\tau_I} ELf(\sigma)
\]

\[
\frac{d}{dt} \vec{X} = \frac{1}{\tau_c} g(\vec{X}, \sigma)
\]

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The Stochastic Component: \[ \frac{d}{dt} Ef(\sigma) = \frac{1}{\tau_i} ELf(\sigma) \]

- We assume a lattice \( \Lambda \) and denote by \( \sigma(x) \) the value of the spin at location \( x \)

- A spin configuration \( \sigma \) is an element of the configuration space \( \Sigma = \{0,1\}^\Lambda \) and we write

\[ \sigma = \{\sigma(x) : x \in \Lambda\} \]

- The stochastic process \( \{\sigma_t\}_{t \geq 0} \) is a continuous time jump Markov process on \( L^\infty(\Sigma, R) \) with generator \( L \)

\[ Lf(\sigma) = \sum_{x \in \Lambda} c(x, \sigma)[f(\sigma^x) - f(\sigma)] \]
The Arrhenius spin-flip rate $c(x,s)$ at lattice site $x$ and spin configuration $s$ is given by

$$c(x,\sigma) = \begin{cases} c_d e^{-\beta U(x)} & \text{when } \sigma(x) = 0 \\ c_a & \text{when } \sigma(x) = 1 \end{cases}$$

with interaction potential $U(x) = \sum_{z \neq x}^{z \in \Lambda} J(x, z)\sigma(z) - h(\bar{X})$

and local interaction via $J(x, y) = \frac{1}{2L + 1} V\left(\frac{|x - y|}{2L + 1}\right)$

Parameters/Constants:

- $c_a = c_d = \frac{1}{\tau_I}$ where $\tau_I$ is the characteristic time of the stochastic process
- $L$ denotes the interaction radius
- $V$ is usual taken to be some uniform constant
Equilibrium states of the stochastic model are described by the Gibbs measure at the prescribed temperature $T$.

\[
\mu_{\beta,N}(d\sigma) = \frac{1}{Z} e^{-\beta H(\sigma)} P_N(d\sigma)
\]

where $H(\sigma) = -\frac{1}{2} \sum_{x \in \Lambda} U(x)\sigma(x)$ is the energy Hamiltonian for $\beta = \frac{1}{kT}$.

And $P_N(d\sigma) = \prod_{x \in \Lambda} \rho(d\sigma(x))$ with $\rho(\sigma(x) = 0) = \frac{1}{2}$, $\rho(\sigma(x) = 1) = \frac{1}{2}$.
The Stochastic Component: $\frac{d}{dt} Ef(\sigma) = \frac{1}{\tau_t} E L f(\sigma)$

The probability of a spin-flip at $x$ during time $[t, t+\Delta t]$ is

$$c(x, \sigma) \Delta t + O(\Delta t^2)$$

The dynamics as described here leave the Gibbs measure invariant since they satisfy detailed balance,

$$c(x, \sigma) = c(x, \sigma^x) \exp(-\beta \Delta_x H(\sigma))$$

where $\Delta_x H(\sigma) = H(\sigma^x) - H(\sigma)$
The Stochastic Component

In the case of a surface diffusion process we implement spin-exchange Arrhenius dynamics

\[ c(x, y, \sigma) = \begin{cases} 
    c_{\text{dif}} e^{-\beta[U_0 + U(x)]} & \sigma(x) = 1, \sigma(y) = 0 \\
    c_{\text{dif}} e^{-\beta[U_0 + U(y)]} & \sigma(x) = 0, \sigma(y) = 1 \\
    0 & \text{otherwise}
\end{cases} \]

where \( c_{\text{dif}} = 1/\tau_{\text{dif}} \)

We can mix spin-flip and spin-exchange dynamics based on the requirements/physics of the model.

In this case the corresponding generator of the combined mechanism for the dynamics comprised of spin-flip and spin exchange is given via,

\[ L = L_{\text{dif}} + L_{\text{ad}} \]
The Deterministic Component: \( \tau_c \frac{d\tilde{X}}{dt} = g(\tilde{X}, \overline{\sigma}) \)

We consider the following type of Complex Ginzburg Landau ODE

\[
\tau_c \frac{d\tilde{X}}{dt} = g(\tilde{X}, \overline{\sigma}) \equiv (a(\overline{\sigma}) + i\omega)\tilde{X} - \gamma \lvert \tilde{X} \rvert^2 \tilde{X} + \gamma \tilde{X}^*
\]

where \( \tilde{X} = X + iY \)

The Jacobian of the linearized system has eigenvalues

\[
\lambda = a(\overline{\sigma}) \pm i\sqrt{\omega^2 - \gamma^2}
\]
The Deterministic Component:  \( \tau_c \frac{d\tilde{X}}{dt} = g(\tilde{X}, \tilde{\sigma}) \)

Some examples for the ODE

**CGL:**  \( g(\tilde{X}, \sigma) = (a(\tilde{\sigma}) + i\omega)\tilde{X} - \gamma |\tilde{X}|^2 \tilde{X} + \gamma \tilde{X}^* \)

**Bistable:**  \( g(X, \sigma) = a(\tilde{\sigma})X + \gamma X^3 \)

**Saddle:**  \( g(X, \sigma) = a(\tilde{\sigma}) + \gamma X^2 \)

**Linear:**  \( g(X, \sigma) = a(\tilde{\sigma}) + b - cX \)

where \( a(\tilde{\sigma}) \) depends linearly on \( \tilde{\sigma} \)

Some examples for the PDE

\[
\partial_t Y = \frac{1}{\tau_c} \left( D \partial_x^2 Y + A \partial_x Y + RY + M \tilde{\sigma} + C \right)
\]

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The stochastic system and the ODE are coupled via, respectively:

- The **external field**, \( h \equiv h(\vec{X}) \)

- The **area fraction** \( \bar{\sigma} \) (or total coverage) defined as the spatial average of the stochastic process \( s \),

\[
\bar{\sigma} = \frac{1}{N} \sum_{x \in \Lambda} \sigma(x)
\]
Part I. Deterministic Closure

The main requirement is the ergodicity property of the stochastic process

\[ \lim_{T \to \infty} \frac{1}{T} \int_0^T g(\tilde{X}, \tilde{\sigma}_t) \, dt = \bar{g}(\tilde{X}) \]

where \( \bar{g}(\tilde{X}) = E_{\mu_{\beta,N}} g(\tilde{X}, \tilde{\sigma}) = \sum g(\tilde{X}, \tilde{\sigma}) \mu(d\sigma) \)

Due to special structure of \( g \) (depends linearly on \( S \)) we have

\[ \bar{g}(\tilde{X}) = E_{\mu_{\beta,N}} g(\tilde{X}, \tilde{\sigma}) = \bar{g}(\tilde{X}, E_{\mu_{\beta,N}} \tilde{\sigma}) = \bar{g}(\tilde{X}, u_{\beta,N}(h(\tilde{X}))) \]

Where \( u_{\beta,N}(h) \) can be found from the known Gibbs equilibrium measure

\[ u_{\beta,N}(h) = \frac{1}{Z} \sum_{\sigma} \sum_{x \in \Lambda} \sigma(x) e^{-\beta H(\sigma)} P_N(\sigma) \]

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Part I. Deterministic Closure

The main requirement is the **ergodicity property** of the stochastic process

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T g(\tilde{X}, \tilde{\sigma}_t) \, dt = \bar{g}(\tilde{X})$$

Due to special structure of $g$ (depends linearly on $\tilde{\sigma}$) we have

$$\bar{g}(\tilde{X}) = E_{\mu_{\beta,N}} g(\tilde{X}, \tilde{\sigma}) = \bar{g}(\tilde{X}, E_{\mu_{\beta,N}} \tilde{\sigma}) = \bar{g}(\tilde{X}, u_{\beta,N}(h(\tilde{X})))$$

Where $u_{\beta,N}(h)$ can be found from the known Gibbs equilibrium measure

$$u_{\beta,N}(h) = \frac{1}{Z} \sum_{\sigma} \sum_{x \in \Lambda} \sigma(x) e^{-\beta H(\sigma)} P_N(\sigma)$$

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Part I. Deterministic Closure

Suppose $\bar{X} = \bar{X}(t)$ is the solution of the hybrid system:

$$\begin{cases}
    \frac{d}{dt} f(\sigma) = \frac{1}{\tau_i} E L f(\sigma) \\
    \frac{d}{dt} \bar{X} = \frac{1}{\tau_c} g(\bar{X}, \sigma_t), \quad \text{for} \quad t \in [0, T] \\
    \bar{X}_0 = x
\end{cases}$$

And $\bar{x} = \bar{x}(t)$ is the solution of the (reduced) averaged system:

$$\begin{cases}
    \frac{d}{dt} \bar{x}_t = \frac{1}{\tau_c} g(\bar{x}_t, u_{\beta,N}(h(\bar{x}_t))) \quad \text{for} \quad t \in [0, T] \\
    \bar{x}_0 = x
\end{cases}$$

- On an arbitrary bounded time interval $[0, T]$ with fixed $N$ and $t_c$ we have:

$$\lim_{\tau_i \to 0} \mathbb{P}(\sup_{0 \leq t \leq T} |\bar{X}(t) - \bar{x}(t)| > \delta) = 0 \quad \text{for any} \quad \delta > 0$$

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Part I. Deterministic Closure

Calculate $u_{\beta,N}(h)$ Numerically

For a given external potential $h$ we calculate by Monte Carlo

$$E_{\mu_{\beta,N} \sigma} \rightarrow u_{\beta,N}(h) \quad \text{as} \quad t \rightarrow \infty$$

In fact in the nearest neighbor case

$$\lim_{N \rightarrow \infty} u_{\beta,N}(h) = u_{\beta}(h)$$

can be calculated explicitly

$$u_{\beta}(h) = \frac{1}{2} \frac{\sinh(\beta h)}{2\sqrt{\sinh^2(\beta h) + \exp(-4\beta J_0)}}$$

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Part I. Deterministic Closure

Calculate $u_{\beta,N}(h)$ analytically

In the long range interaction limit, $N = 2L + 1$ as $L,N \to \infty$

we obtain the usual mean-field formula where $u_\beta(h) = \lim_{N \to \infty} u_{\beta,N}(h)$

is the unique minimizer $(h \neq 0)$ of the free energy functional

$I[c] = \beta hc + r(c) - \beta \frac{J_0}{2} c^2$

where $r(c) = c \log c + (1 - c) \log(1 - c)$

We therefore solve the following nonlinear equation for $u_\beta(h)$

$$h = J_0 u_\beta - \frac{1}{\beta} \log \frac{u_\beta}{1 - u_\beta}$$
Stability and Potential Wells

Stability Profile, \( b=1, \gamma = 0.06, \beta J_0 = 2 \)

Energy Profile and Wells, \( b=1, \gamma = 0.06, \beta J_0 = 2 \)

Space X (Ext. Pot = 5X-1)
Solutions of the coupled system
Direct Numerical Simulation vs Deterministic Closure
A Rare Event

Direct Numerical Simulation vs Deterministic Closure

Deterministic closures can fail in extended time simulations.

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Another example: Coupled system with Hopf ODE
Direct Numerical Simulation vs Deterministic Closure

Fast Stochastic Case

Equivalent Characteristic Times

Slow Stochastic Case

Deterministic closures can fail if $\tau \gg 1$
Part II. Stochastic Closures

We define the coarse random process, \( \eta(k) = \sum_{x \in D_k} \sigma(x) \) for \( k=1, \ldots, m \)

and \( \eta = \{ \eta(k) : k \in \Lambda_c \} \) where \( \eta(k) \in \{0,1,\ldots,q\} \) and \( N = mq \)

where \( \Lambda_c = \frac{1}{m} Z \cap [0,1] \) (naturally \( \Lambda_c \subset \Lambda \))

Fine Lattice \( \Lambda \)

Coarse Lattice \( \Lambda_c \)

Total number of micro cells: \( N \)

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Part II. Stochastic Closures

The coarse grained generator for the Markovian process \( h \) is defined to be,

\[
L_c f(\eta) = \sum_{k \in \Lambda_c} c_a(k, \eta) [f(\eta + \delta_k) - f(\eta)] \\
+ c_d(k, \eta) [f(\eta - \delta_k) - f(\eta)]
\]

For any test function \( f \in L^\infty(H_{n,q}; R) \) where the coarse level adsorption/desorption rates are,

\[
c_a(k, \eta) = d_0[q - \eta(k)] \\
c_d(k, \eta) = d_0 \eta(k) e^{-\beta(U_0 + \overline{U}(k))}
\]

With a corresponding coarse potential

\[
\overline{U}(k) = \sum_{\substack{l \in \Lambda_c \\ l \neq k}} \overline{J}(k,l)\eta(l) + \overline{J}(0,0)(\eta(k) - 1) - h(\overline{X})
\]

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Note that these rates depend on the microscopic configuration $\sigma$ and not on the coarse random variable $T(\sigma)$. In order to derive a Markov process for the coarse variable $\eta$ we need to express these rates in terms of $\eta$. Indeed for the adsorption we readily have,

$$c_\text{a}(k) = \sum_{x \in D_u} c(x, \sigma)(1 - \sigma(x)) = \sum_{x \in D_u} d_0(1 - \sigma(x)) = d_0[q - \eta(k)]$$  \hspace{1cm} (21)

where $d_0 = 1/\tau_I$ and $U_0 = 0$ as before. Based on relation (21) we can therefore define the coarse grained adsorption rate

$$c_\text{a}^c(k, \eta) = d_0[q - \eta(k)]$$  \hspace{1cm} (22)

and expresses the rate by which $\eta(k)$ is increased by 1. We wish to obtain a similar such relation for the desorption,

$$c_\text{d}(k) = \sum_{x \in D_u} c(x, \sigma)\sigma(x) = d_0 \sum_{x \in D_u} \sigma(x)e^{-\beta(U_0 + U(x))}$$  

$$= d_0 \sum_{x \in D_u} \sigma(x)e^{-\beta(U_0 + \tilde{U}(\eta))} = e^{-\beta(U_0 + \tilde{U}(\eta)) + O\left(\frac{q}{2L+1}\right)} \sum_{x \in D_u} \sigma(x)$$  \hspace{1cm} (23)

where we used the approximation $U(x) = \tilde{U}(k) + O(q/(2L + 1))$ \cite{8} where

$$\tilde{U}(k) = \sum_{\substack{l \in \mathcal{L}_u \setminus \{\text{loc}\}}} \tilde{J}(k, l)\eta(l) + \tilde{J}(0, 0)(\eta(k) - 1) - h(X)$$  \hspace{1cm} (24)
Compare Stochastic Transient and Equilibrium Dynamics.

Microscopic \[ \frac{d}{dt} E \sigma f(\sigma) = \frac{1}{\tau_i} ELf(\sigma) \] vs Coarse Grained \[ \frac{d}{dt} E \eta f'(\eta) = \frac{1}{\tau_i} EL_{c}f'(\eta) \]
Compare Stochastic Transient and Equilibrium Dynamics.

Microscopic $\frac{d}{dt}Ef(\sigma) = \frac{1}{\tau_I}ELf(\sigma)$ vs Coarse Grained $\frac{d}{dt}Ef'(\eta) = \frac{1}{\tau_I}EL_c f'(\eta)$
Our Coarse Grained system therefore becomes,

\[
\begin{align*}
\frac{d}{dt} \bar{X} &= \frac{1}{\tau_c} g(\bar{X}, \bar{\eta}) \\
\frac{d}{dt} Ef'(\eta) &= \frac{1}{\tau_f} ELc f'(\eta)
\end{align*}
\]

and gives a stochastic closure at this level.

- This stochastic closure is expected to be valid for all time since no linearization arguments or use of expected values are involved.
- This stochastic closure is an approximation to the original hybrid system.

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Direct Numerical Simulation vs Stochastic Coarse Grained Closure (q=20).

Fast Stochastic Case

Equivalent Characteristic Times

Slow Stochastic Case

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Hopf Bifurcation
Direct Numerical Simulation vs Stochastic Coarse Grained Closure ($q=20$)

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Hopf Bifurcation
Microscopic System vs CGMC Closure
Hopf Bifurcation
Microscopic System vs CGMC Closure

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Rare events
and
Phase Transitions

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Revisit the rare event: Direct Numerical Simulation vs Stochastic Coarse Grained Closure

We can capture the rare event
In the case of phase transitions the Coarse Grained closure still agrees with the DNS solution.
Externally Driven Phase Transitions
Direct Numerical Simulation vs Coarse Grained Closure (for $q = 10$)
Externally Driven Phase Transitions
Microscopic Hybrid System vs CGMC (for $q = 20$) Closure
Externally Driven Phase Transitions
Direct Numerical Simulation vs Coarse Grained Closure ($q=50, 100$)
\[ \mathcal{R}(\pi_1|\pi_2) = \sum_{\sigma \in S} \pi_1(\sigma) \log \frac{\pi_1(\sigma)}{\pi_2(\sigma)}. \]

Using Jensen’s inequality we can show that the relative entropy can be thought of as a distance between two measures \( \pi_1 \) and \( \pi_2 \) since the following is true,

\[
\begin{align*}
\mathcal{R}(\pi_1|\pi_2) &\geq 0 \quad \text{and} \\
\mathcal{R}(\pi_1|\pi_2) &= 0 \quad \text{if and only if} \quad \pi_1(\sigma) = \pi_2(\sigma) \quad \text{for all} \quad \sigma \in S
\end{align*}
\]

Note that the relative entropy is not a true metric since \( \mathcal{R}(\pi_1|\pi_2) \neq \mathcal{R}(\pi_2|\pi_1) \) for all possible measures \( \pi_1, \pi_2 \). Nevertheless there is an important inequality which allows us to use the relative entropy as a tool for estimating distance between two measures \([23]\),

\[
\mathcal{R}(\pi_1|\pi_2) \geq \frac{1}{2} \left( \sum_{\sigma \in S} |\pi_1(\sigma) - \pi_2(\sigma)| \right)^2 \equiv \frac{1}{2} \| \pi_1 - \pi_2 \|_1^2
\]
Theorem 4.1 Suppose the process $\{\eta_t\}_{t \in [0,T]}$ defined by the coarse generator $L_c$ is the coarse approximation of the microscopic process $\{\sigma_t\}_{t \in [0,T]}$ then for any $q < L$ and $N$ where $mq = N$ the information loss as $q/L \to 0$ is

$$\frac{1}{N} R(T_* Q^c_{[0,T]} | Q^{c}_{\eta_0,[0,T]}) = TO\left(\frac{q}{2L + 1}\right)$$

(28)

$$\frac{1}{N} R((T_* \mu^N) | \mu^N_{\eta_0,q}) = O\left(\frac{q}{2L + 1}\right)$$

(29)

**Theorem:** Suppose the process $\{\eta_t\}_{t \in [0,T]}$ defined by the coarse generator $L_c$ is the coarse approximation of the microscopic process $\{\sigma_t\}_{t \in [0,T]}$ then for any $q < L$ and $N$ where $mq = N$ the information loss as $q/L \to 0$ is

$$\frac{1}{N} R(T_* Q^c_{[0,T]} | Q^{c}_{\eta_0,[0,T]}) = TO\left(\frac{q}{2L + 1}\right)$$

**Theorem:** Let $\psi$ be a test function on the coarse level s.t there exist a test function with property $\mu$ Given the initial configuration we define the coarse configuration Assume the microscopic process with the initial condition and the approximating coarse process with the initial condition then the weak error satisfies for

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Error Estimates

**Theorem:** Suppose the process \( \{ \eta_t \}_{t \in [0, T]} \) defined by the coarse generator \( L_c \) is the coarse approximation of the microscopic process \( \{ \sigma_t \}_{t \in [0, T]} \) then for any \( q < L \) and \( N \) where \( mq=N \) The information loss as \( q/L \to 0 \) is

\[
\frac{1}{N} R(TQ_{T \sigma_0, [0,T]} | Q_{T \eta_0, [0,T]}^c) = T \mathcal{O}\left( \frac{q}{L} \right)
\]

**Theorem:** Let \( \psi \in L^\infty(\Sigma_c) \) be a test function on the coarse level s.t there exist a test function \( \varphi \in L^\infty(\Sigma) \) with property \( \psi(T\sigma) = \varphi(\sigma) \). Given the initial configuration \( \sigma_0 \) we define the coarse configuration \( \eta_0 = T\sigma_0 \). Assume the microscopic process \( \{ \sigma_t \}_{t \in [0,T]} \) with the initial condition \( \sigma_0 \) and the approximating coarse process \( \{ \eta_t \}_{t \in [0,T]} \) with the initial condition \( \eta_0 = T\sigma_0 \) then the weak error satisfies for final time \( T \),

\[
| E[\psi(T\sigma_T)] - E[\psi(\eta_T)] | = C_T \left( \frac{q}{L} \right)^2
\]

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1. Details of the numerical calculation. We calculate $\text{err}(c)$ in two different ways. One is the so called "weak" $\text{err}(c)$ and the other is the equivalent "strong" form which are given as follows:

\[
\begin{align*}
\text{weak:} & \quad \text{err}(c) = \int_0^T |E[c^a(t,x) - c^f(t,x)]| \, dt \\
\text{strong:} & \quad \text{err}(c) = \int_0^T E[|c^a(t,x) - c^f(t,x)|] \, dt
\end{align*}
\]

where $x$ here denotes a realization and $t$ a time instance. This is implemented numerically as follows:

\[
\begin{align*}
\text{weak:} & \quad \text{err}(c) \approx \frac{1}{MN} \sum_{n=1}^M |\sum_{r=1}^N [c^a(n,r) - c^f(n,r)]| \\
\text{strong:} & \quad \text{err}(c) \approx \frac{1}{MN} \sum_{n=1}^M \sum_{r=1}^N |c^a(n,r) - c^f(n,r)|
\end{align*}
\]

where $n$ here is the discretization index in time and $r$ denotes the realization index. We assume $M$ total time discretizations and $N$ total realizations.

All the simulations are performed for the phase transition regime $\beta J_0 = 6$ and the following set of parameters: $N = 1000$, $L = 100$, $c_a = .07$ and $c_d = 1.$
Weak estimate. Linear best fit for err(c)

"Weak" Log. Slope Estimate
Noise driven behavior attributed to stochastic look-ahead organization

The PDE/stochastic model

We consider the following general system:

\[
\begin{align*}
\partial_t Y &= \frac{1}{\tau_c} \left( D \partial_x^2 Y + A \partial_x Y + RY + M \bar{\sigma} + C \right) \\
\mathbb{E} \partial_t f(\sigma) &= \mathbb{E} L f(\sigma)
\end{align*}
\]
Altering the solution profile: traveling waves

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Synchronization in time and space produces intermittent traveling waves

Without look-ahead

With look-ahead

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Noise driven behavior attributed to stochastic look-ahead organization

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Convective Instability

Mean Field

Stochastic

A=20

A=.2

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Intermittency and Metastability Phenomena

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Phase transitions II **Strong particle/particle interactions** (FhN equation)

\[
\frac{d}{dt} X = a \overline{\sigma} + b - cX \\
\frac{d}{dt} Ef(\sigma) = ELf(\sigma),
\]

**Step 1:** **Mean field approximations** (ODEs):

\[
\frac{d}{dt} x = au + b - cx \\
\frac{d}{dt} Ef(\sigma) = 1 - u - u e^{-\beta J_0 u + h(x(t))}
\]

**Bistable, excitable, oscillatory regimes** (strong interactions)

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Phase diagram and Stability for FhN System

Phase diagram

Streamlines

$u$ (Parameters: $J_0 = 6$, $c_a = 10$, $c_d = 10$)

$\beta J_0 = 2$, $c_a = 100$, $c_d = 100$

$\beta J_0 = 6$, $c_a = 10$, $c_d = 10$

$\beta J_0 = 6$, $c_a = 1$, $c_d = 1$
Step 2: For the full hybrid stochastic system the mean field approx. suggests:

- Bistability $\rightarrow$ random switching.
- Oscillatory regime $\rightarrow$ random oscillations
- Excitability $\rightarrow$ strong intermittency regime

![Graph showing oscillatory behavior](image)

a. Need model reduction through suitable closure.

b. Deterministic vs. stochastic closures; stochasticity can be important.

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3. Phase transitions in hybrid systems: strong particle/particle interactions:

Fitzhugh-Nagumo type system; comparison of

DNS of the hybrid system, $q = 1$

vs.

Coarse-Grainings $q = 10$, $q = 50$

Space/Time time series analysis:
Auto-correlations

We calculate the mean-removed auto-correlation for a signal $y(t)$ as follows,

$$
g_{yy}(m) = \begin{cases} 
    \sum_{n=0}^{N-|m|-1} \left( y(n+m) - \frac{1}{N} \sum_{i=0}^{N-1} y(i) \right) \left( y(n) - \frac{1}{N} \sum_{i=0}^{N-1} y(i) \right) & \text{for } m \geq 0 \\
    g_{yy}(-m) & \text{for } m < 0 
\end{cases}
$$
Analysis of CG signal for $X$, $q=1$ and $q=10$
Conclusions

✓ Presented a coupled Prototype Hybrid System consisting of:

\[
\begin{cases}
\text{Stochastic Noise Model} \\
\text{ODE/PDE}
\end{cases}
\]

capable of describing the behavior of several different physical systems

✓ Studied two types of closures for this system:
  a) Deterministic (averaging principle, mean field)
  b) Stochastic (coarse grained Monte Carlo)

✓ Examined solutions under extreme phenomena exhibiting
  • rare events,
  • phase transitions and
  • intermittency/metastability effects.

✓ Deterministic type closures (averaging principle / mean field) are valid for finite time intervals \( T \ll \infty \) and for the case of fast stochastic dynamics \( \tau \rightarrow \infty \) relative to the ODE

✓ The (stochastic) Coarse Grained Monte Carlo closure seems to be always valid under certain conditions: \( q \leq L \)

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•Last but not least the CGMC method offers much more than just agreement in average quantities.

There is spatial agreement as well

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Microscopic System vs Coarse Grained Closure
Spatial Lattice Simulations (non-averaged)
through a phase transition!
Related Publications

Stochastic Models


Hybrid Deterministic/Stochastic Systems


Coarse-Grained Models


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We compute the fast Fourier transform of our discrete signal for a number of frequency bins \( \omega \) which matches the size of the signal and are defined as follows,

\[
\omega_j = \frac{2\pi(j - 1)}{N_k} \quad \text{for} \quad j = 1, \ldots, N_k \quad \text{and} \quad k = 1, \ldots, m
\]

We define \( y_k(t) \) to be the \( k \)th piece of our stationary signal,

\[
y_k(t) = y(kN_k + t) \quad \text{for} \quad t = 1, \ldots, N_k
\]

The Fourier transform therefore for each of the \( m = 40 \) signal pieces is found from,

\[
I^k(\omega_j) = \frac{1}{N_k} \sum_{j=1}^{N_k} y_k(l)e^{-i\omega_j} \quad \text{for} \quad k = 1, \ldots, m
\]

for each \( \omega_j \). Note that \( I^k(\omega_j) \) is complex. We then calculate the square of the amplitude of the transform

\[
\text{Sample Periodogram:} \quad I_r^k = |I^k|^2.
\]

This is the power spectrum over each frequency \( \omega_j \). A smoothed version of the above is presented in our figures by averaging all such contributed \( I_r \) from each piece of the signal via,

\[
\text{Ensemble Periodogram:} \quad I = EI_r^k = \frac{1}{m} \sum_{k=1}^{m} I_r^k
\]
Cross-Corr

Cross-corr for q = 0

Cross-corr for q = 50

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The Free Energy Minimizer $u_\beta(h)$

Magnetization vs. External Potential $h$

- $\beta J_0 = 6$
- $\beta J_0 = 4$
- $\beta J_0 = 2$

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