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

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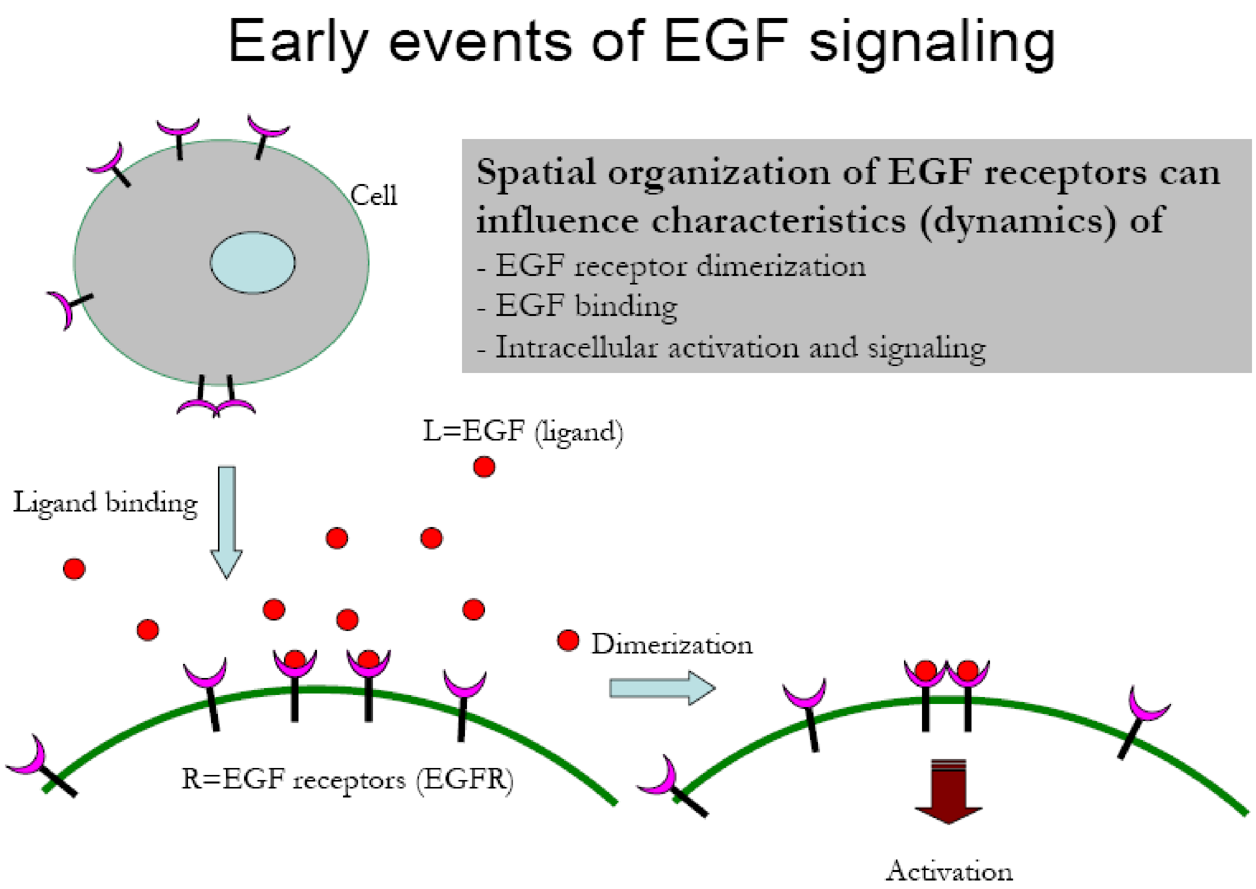
Work partially supported by NSF-DMS-0606807 and DOE-FG02-05ER25702

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

Cell Biology: Epidermal Growth Factor binding/dimerization



- "noisy" intercellular communication; synchronization

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 algrithm;
  efficient allocation of computational resources
  adaptivity, model and mesh refinement

A mathematical prototype hybrid model

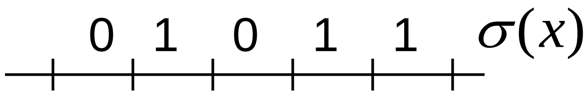
- We introduce the microscopic spin flip stochastic Ising process $\{\sigma_t\}_{t \geq o}$
- Coupled to a PDE/ODE that serves as a caricature of an overlying gas phase dynamics.

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

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

The Stochastic Component: $\frac{d}{dt} Ef(\sigma) = \frac{1}{\tau_I} ELf(\sigma)$

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



- A spin configuration σ 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 Stochastic Component: Arrhenius Spin-Flip Dynamics

The Arrhenius spin-flip rate c(x,s) at lattice site x and spin configuration σ 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 $U(x) = \sum_{\substack{z \neq x \\ z \in \Lambda}} J(x,z)\sigma(z) - h(\vec{X})$

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 τ_I is the characteristic time of the stochastic process
- L denotes the interaction radius
- V is usual taken to be some uniform constant

The Stochastic Component: $\frac{d}{dt} Ef(\sigma) = \frac{1}{\tau_I} ELf(\sigma)$

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 $\rho(\sigma(x)=0) = \frac{1}{2}, \quad \rho(\sigma(x)=1) = \frac{1}{2}$

The Stochastic Component: $\frac{d}{dt} Ef(\sigma) = \frac{1}{\tau_I} ELf(\sigma)$

The probability of a spin-flip at x during time [t, t+Δt] 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 Deterministic Component $\tau_c \frac{d\vec{X}}{dt} = g(\vec{X}, \overline{\sigma})$

Some examples for the ODE

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

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

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

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

where $a(\overline{\sigma})$ depends linearly on $\overline{\sigma}$

Hybrid System Coupling

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 σ,

$$\bar{\sigma} = \frac{1}{N} \sum_{x \in \Lambda} \sigma(x)$$

Part I. Deterministic Closure

The main requirement is the ergodicity property of the stochastic process

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

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

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

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

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

Part I. Deterministic Closure

Suppose $\vec{X} = \vec{X}(t)$ is the solution of the

hybrid system:

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

And $\bar{x} = \bar{x}(t)$ is the solution of the

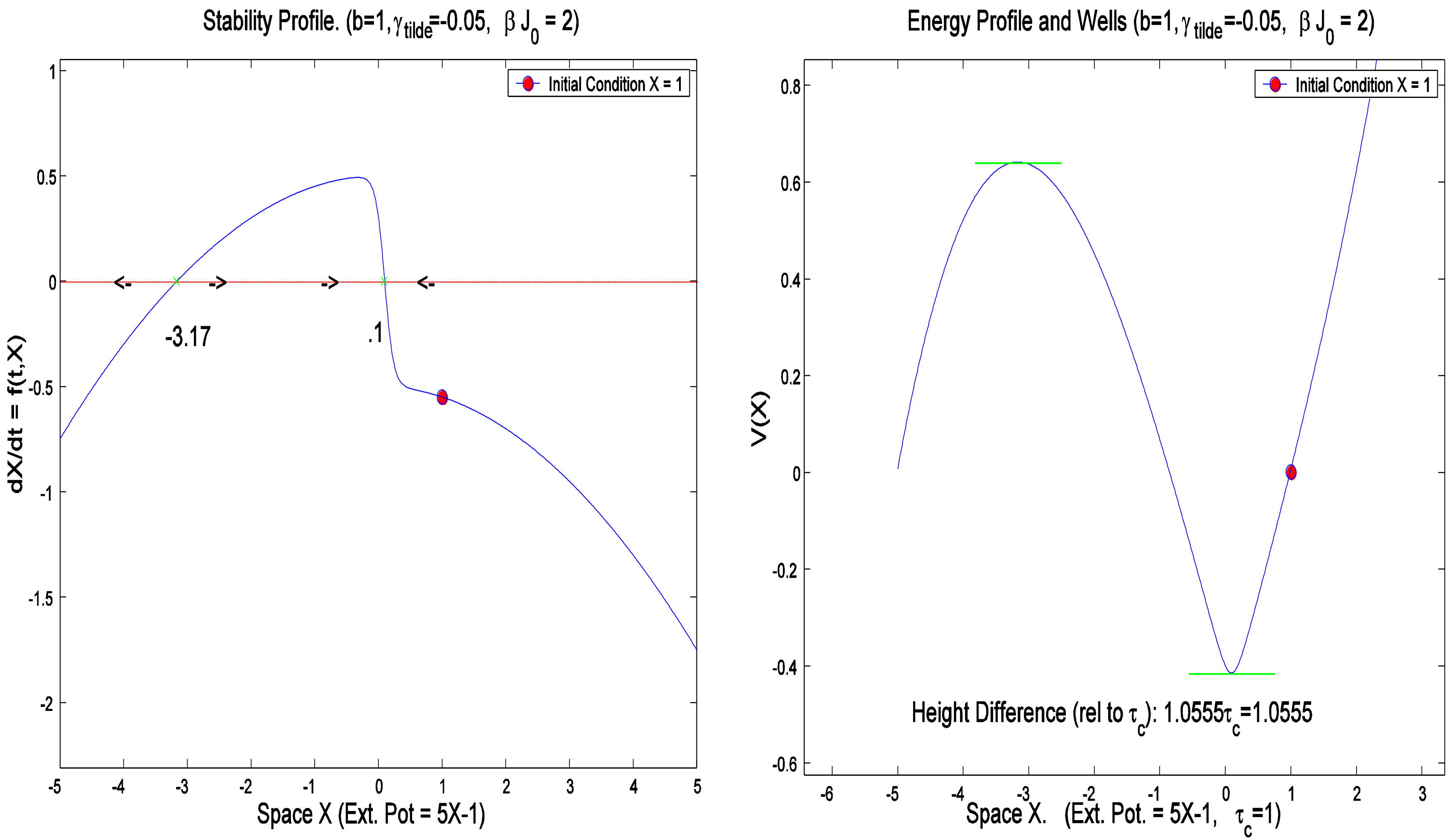
(reduced) averaged system:

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

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

$$\lim_{\tau_I \to 0} \mathrm{P}(\sup_{0 \le t \le T} | \overrightarrow{X}(t) - \bar{x}(t) | > \delta) = 0 \quad \text{for any } \delta > 0$$

Stability and Potential Wells



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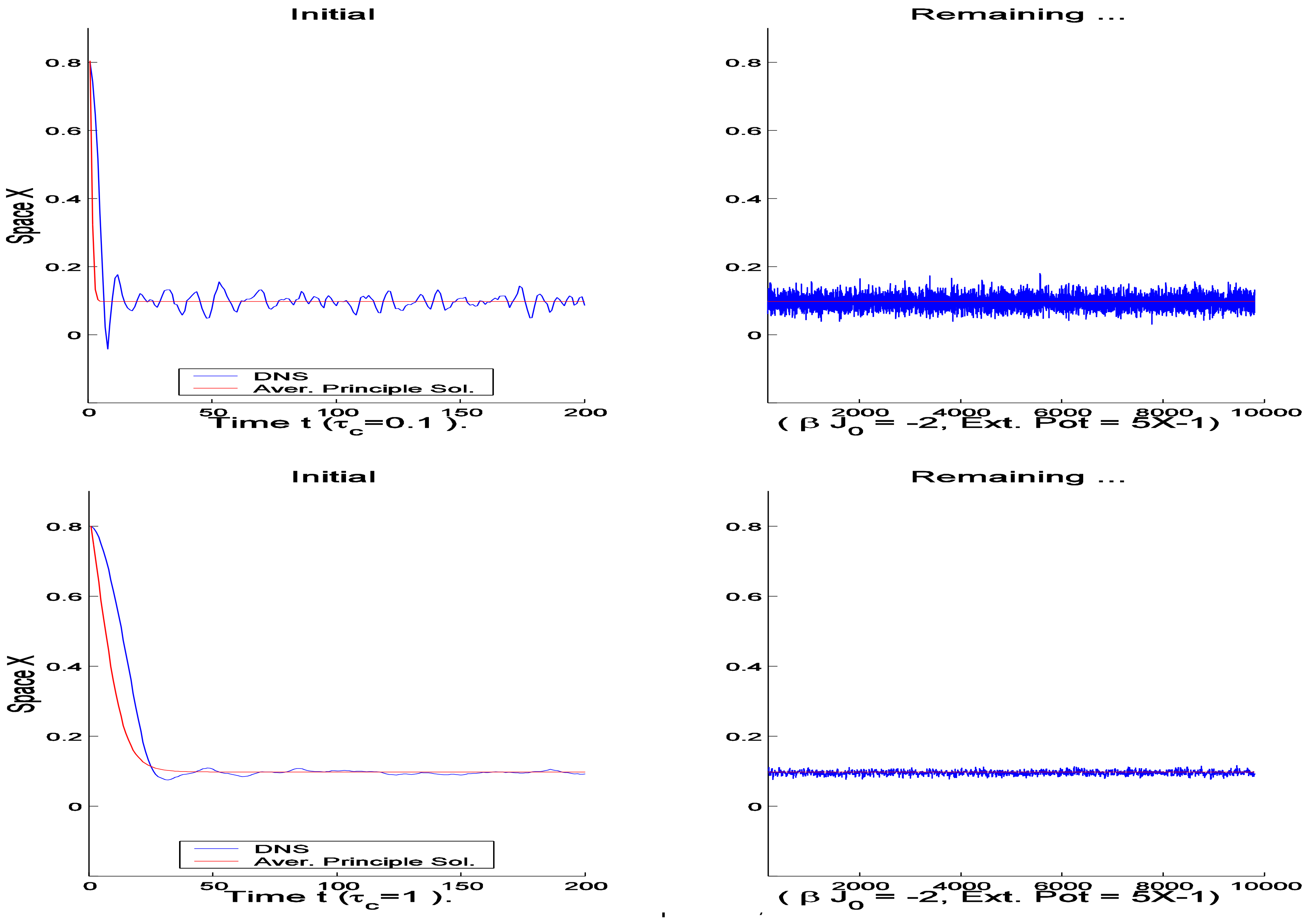
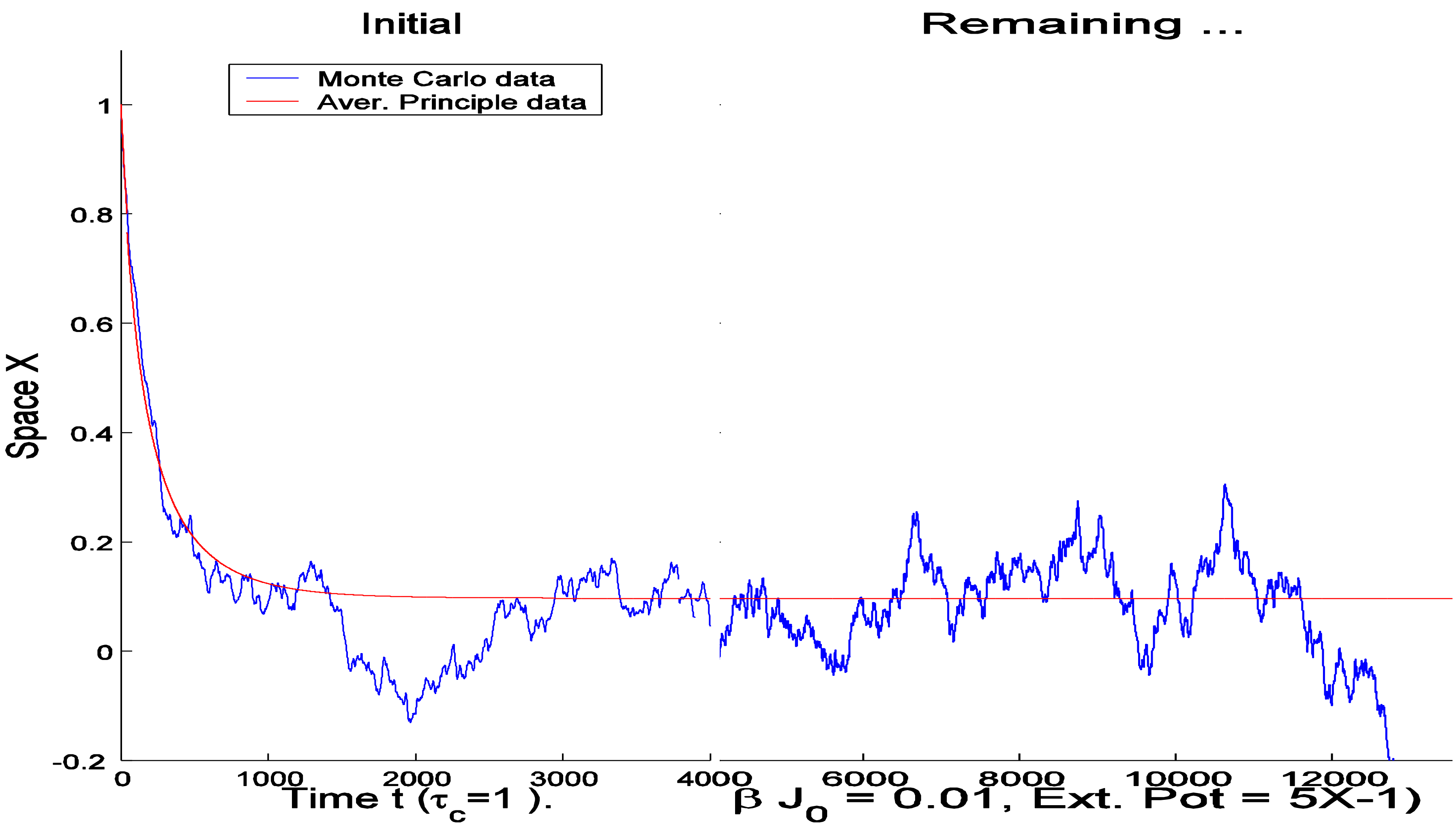
Solutions of the coupled system
Direct Numerical Simulation vs Deterministic Closure



A Rare Event

Direct Numerical Simulation vs Deterministic Closure



Deterministic closures can fail in extended time simulations.

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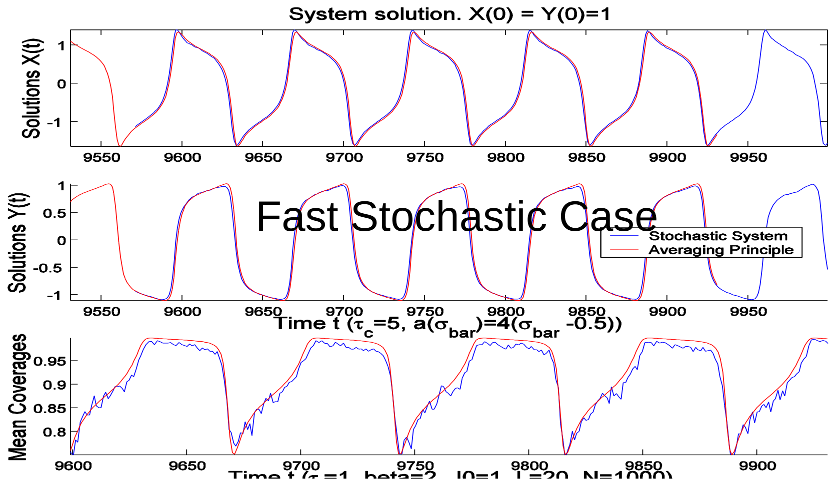
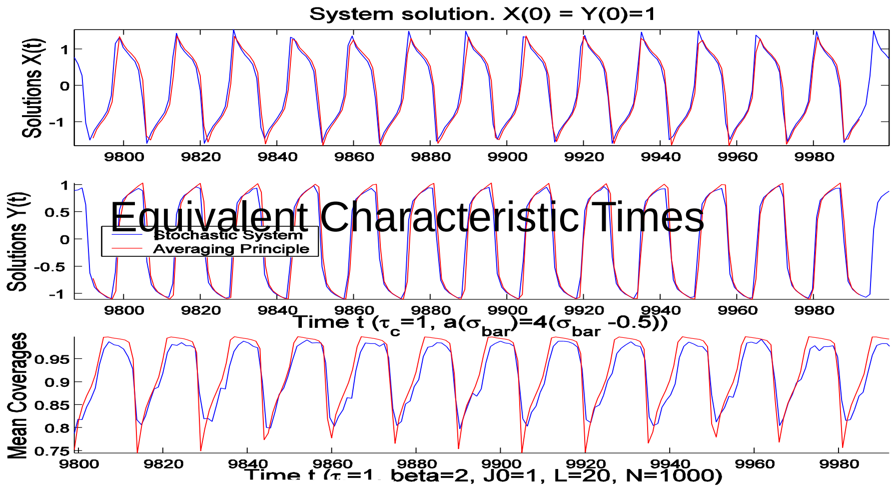
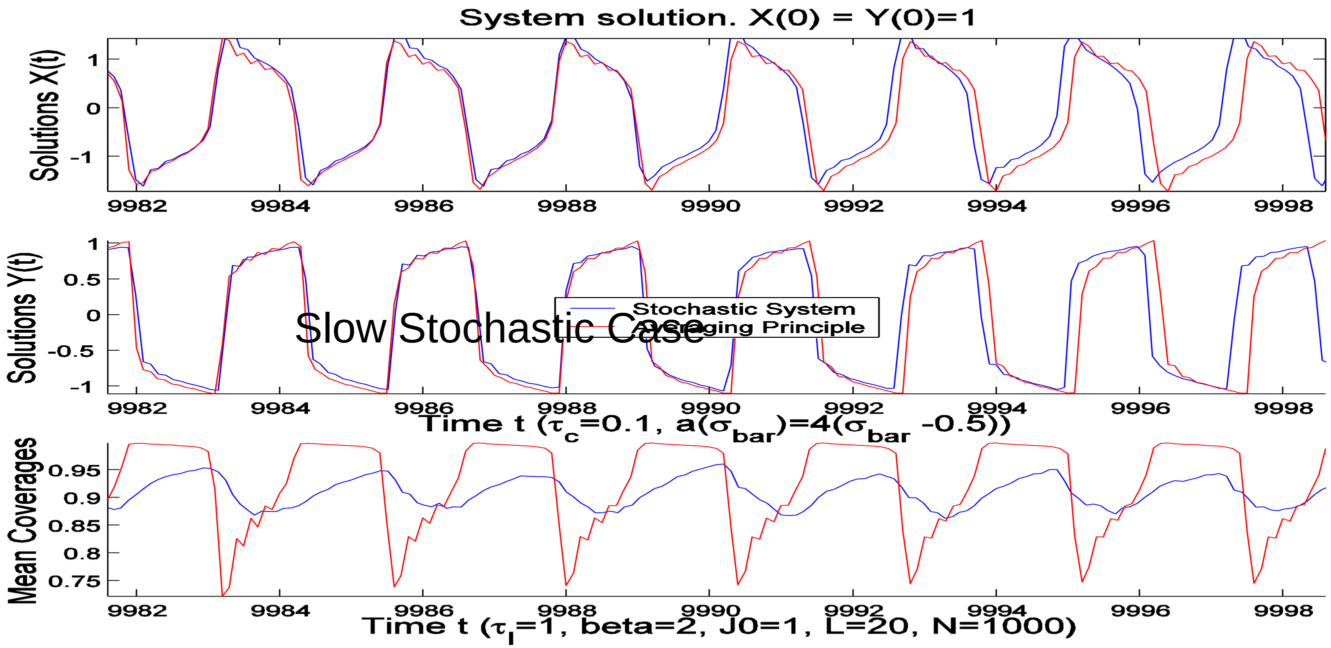
Another example: Coupled system with Hopf ODE

Direct Numerical Simulation vs Deterministic Closure







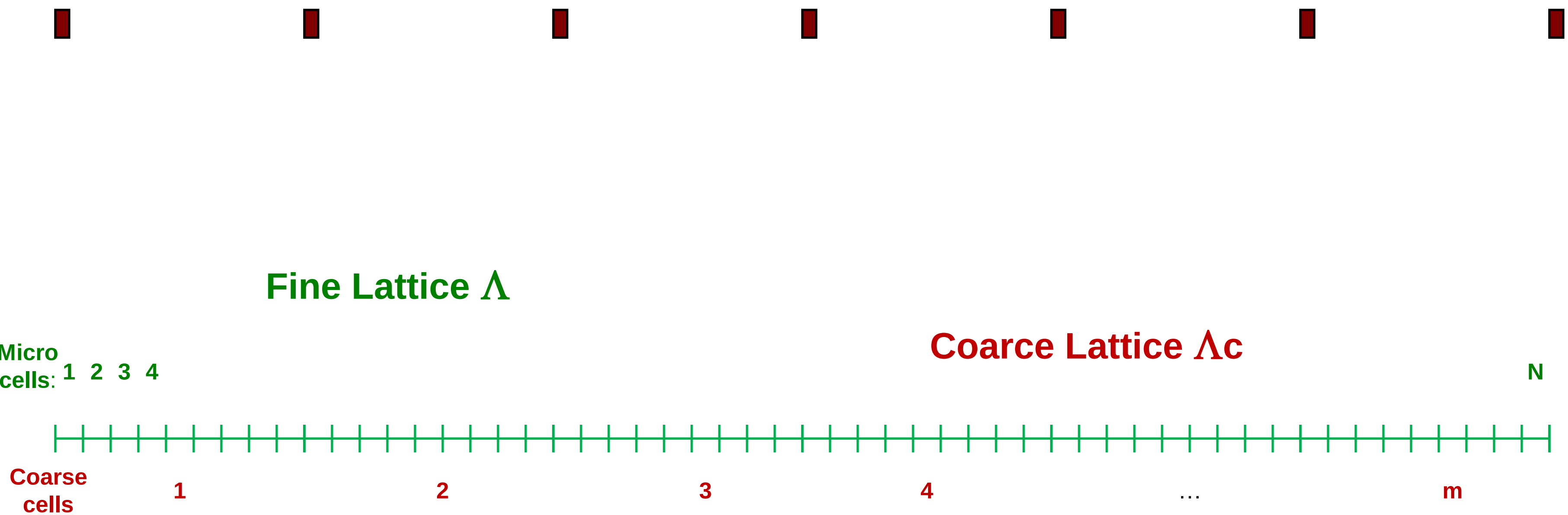
Deterministic closures can fail if $\tau >> 1$

Part II. Stochastic Closures

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

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

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



Total number of micro cells: N

Part II. Stochastic Closures

The coarse grained generator for the Markovian process $\boldsymbol{\eta}$ 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,

$$c_a(k,\eta) = d_0[q - \eta(k)]$$

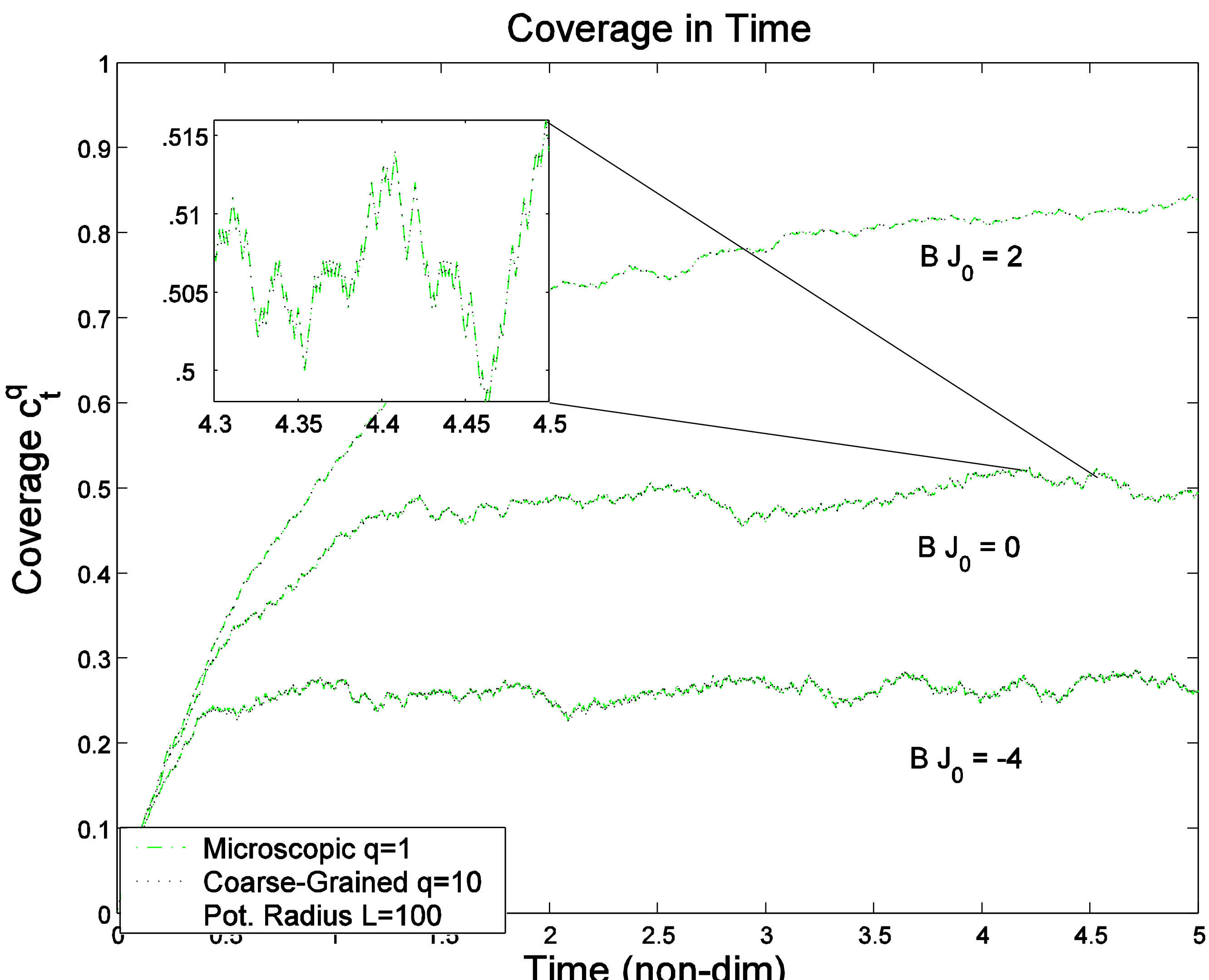
$$c_d(k,\eta) = d_0 \eta(k) e^{-\beta(U_0 + \bar{U}(k))}$$

With a corresponding coarse potential

$$\bar{U}(k) = \sum_{\substack{l \in \Lambda_c \\ l \neq k}} \bar{J}(k,l)\eta(l) + \bar{J}(0,0)(\eta(k)-1) - h(\vec{X})$$

Compare Stochastic Transient and Equilibrium Dynamics.

$$\text{Microscopic} \quad \frac{d}{dt}Ef(\sigma) = \frac{1}{\tau_I}ELf(\sigma) \quad \text{vs} \quad \text{Coarse Grained} \quad \frac{d}{dt}Ef'(\eta) = \frac{1}{\tau_I}EL_c f'(\eta)$$



Coarse Grained Stochastic Closure

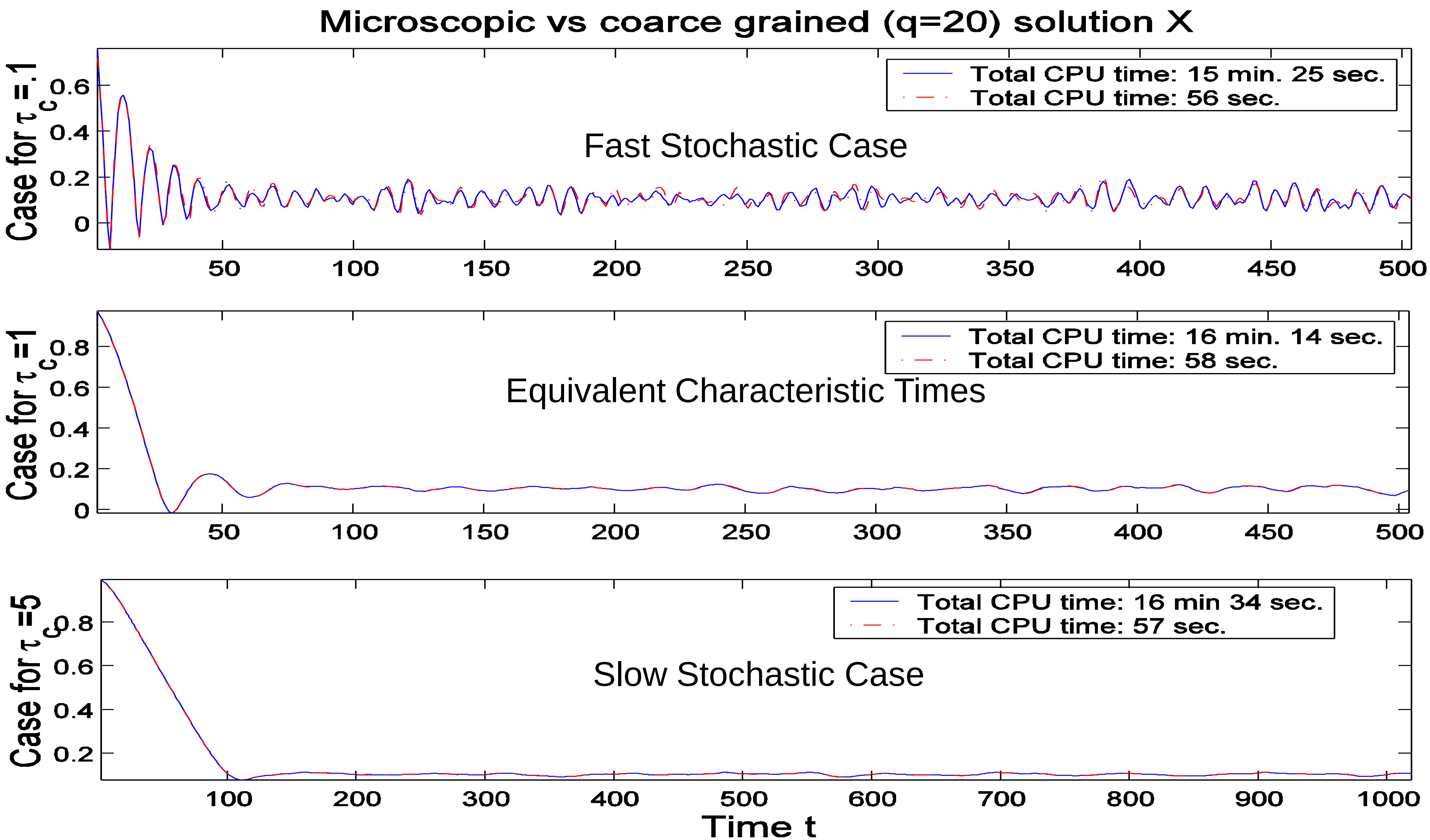
Our Coarse Grained system therefore becomes,

$$\begin{cases} \dfrac{d}{dt}\vec{X} = \dfrac{1}{\tau_c} g(\vec{X}, \overline{\eta}) \\ \dfrac{d}{dt} Ef'(\eta) = \dfrac{1}{\tau_I} EL_c f'(\eta) \end{cases}$$

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

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



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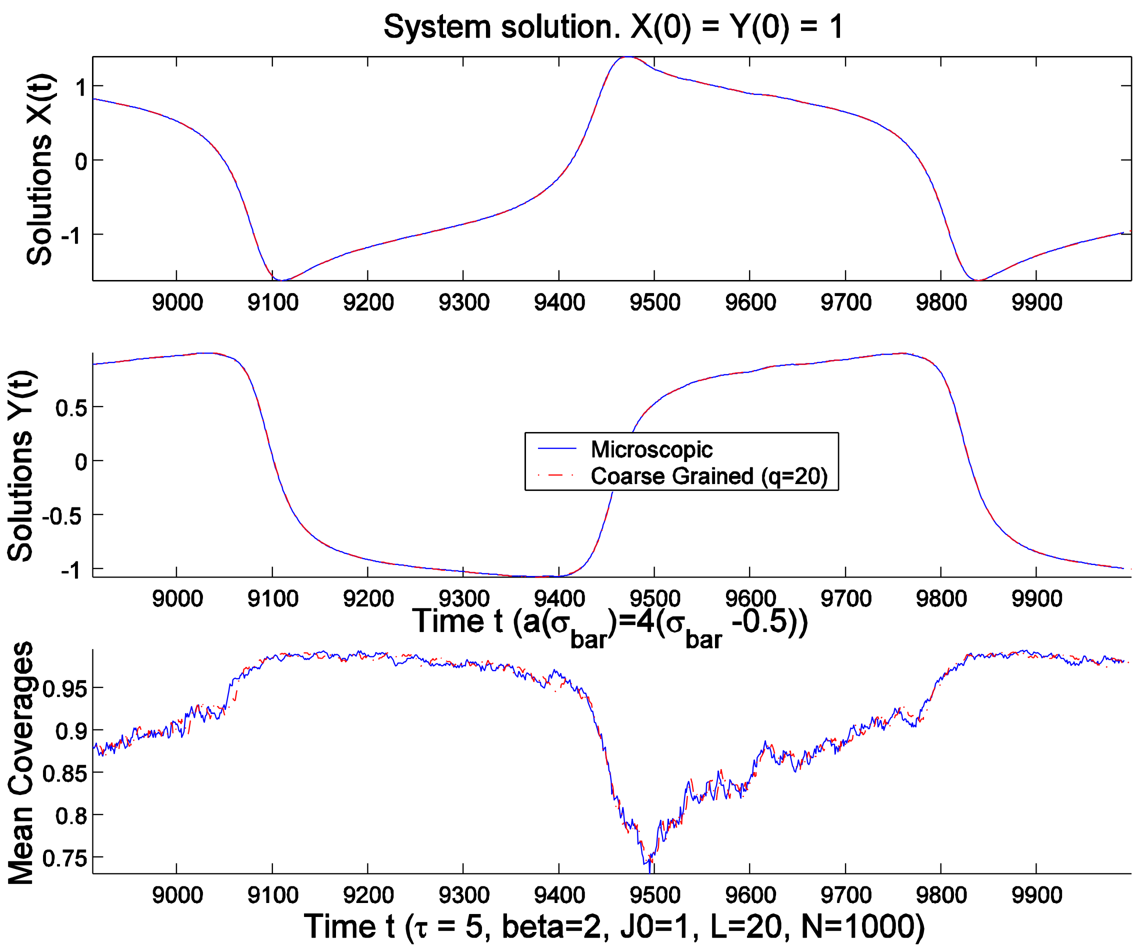
Hopf Bifurcation

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



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Rare events
and
Phase Transitions

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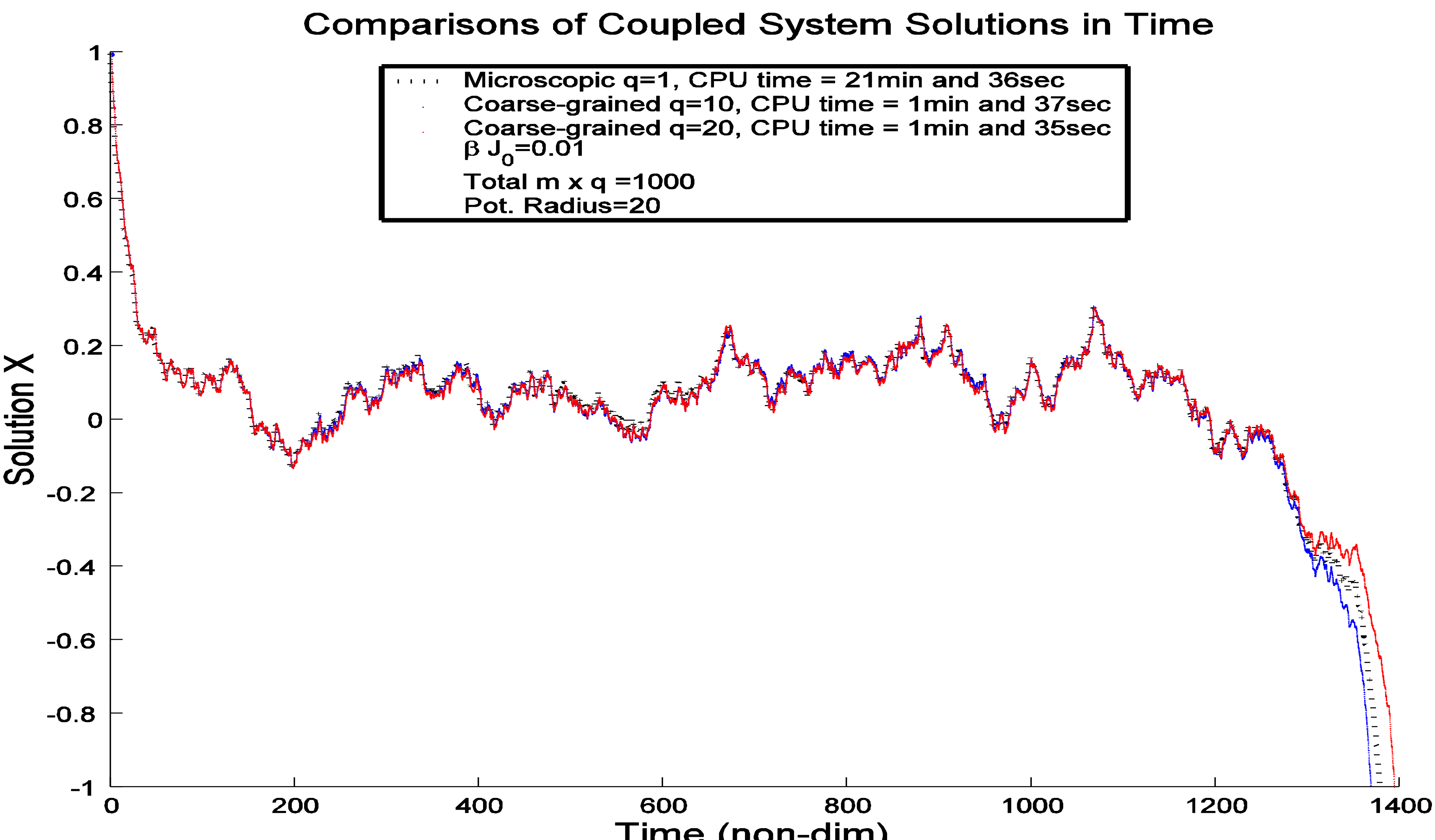
Revisit the rare event: Direct Numerical Simulation vs Stochastic Coarse Grained Closure

We can capture the rare event



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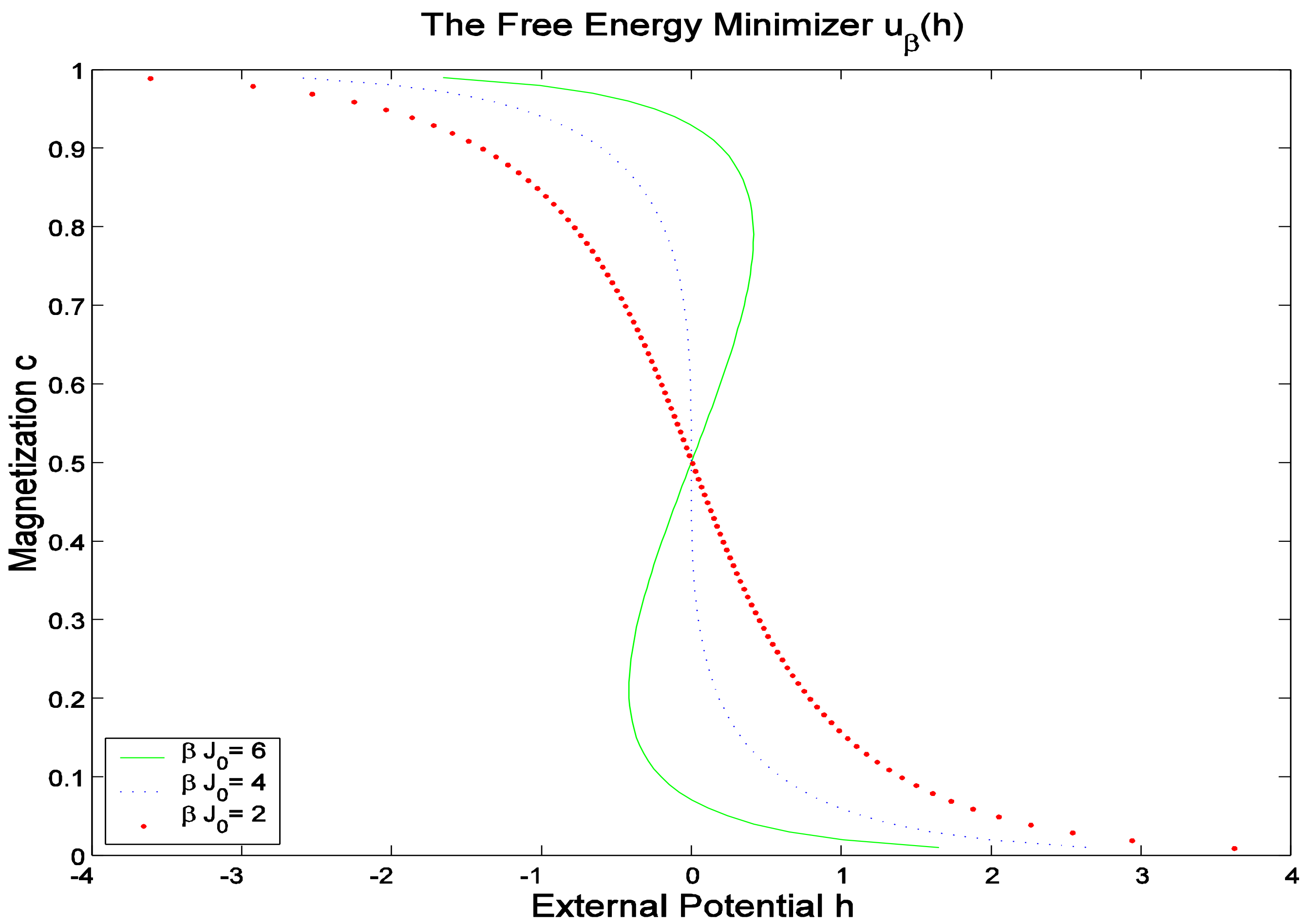
In the case of phase transitions the Coarse Grained closure still agrees with the DNS solution.



q	DNS	2	4	5	10	20	25	50	100
Rel Error %	*0*	*.01*	*.22*	*.38*	*.82*	*3.42*	*4.91*	*17.69*	*77.73*
CPU(sec)	*309647*	*132143*	*85449*	*58412*	*38344*	*16215*	*7574*	*4577*	*345*

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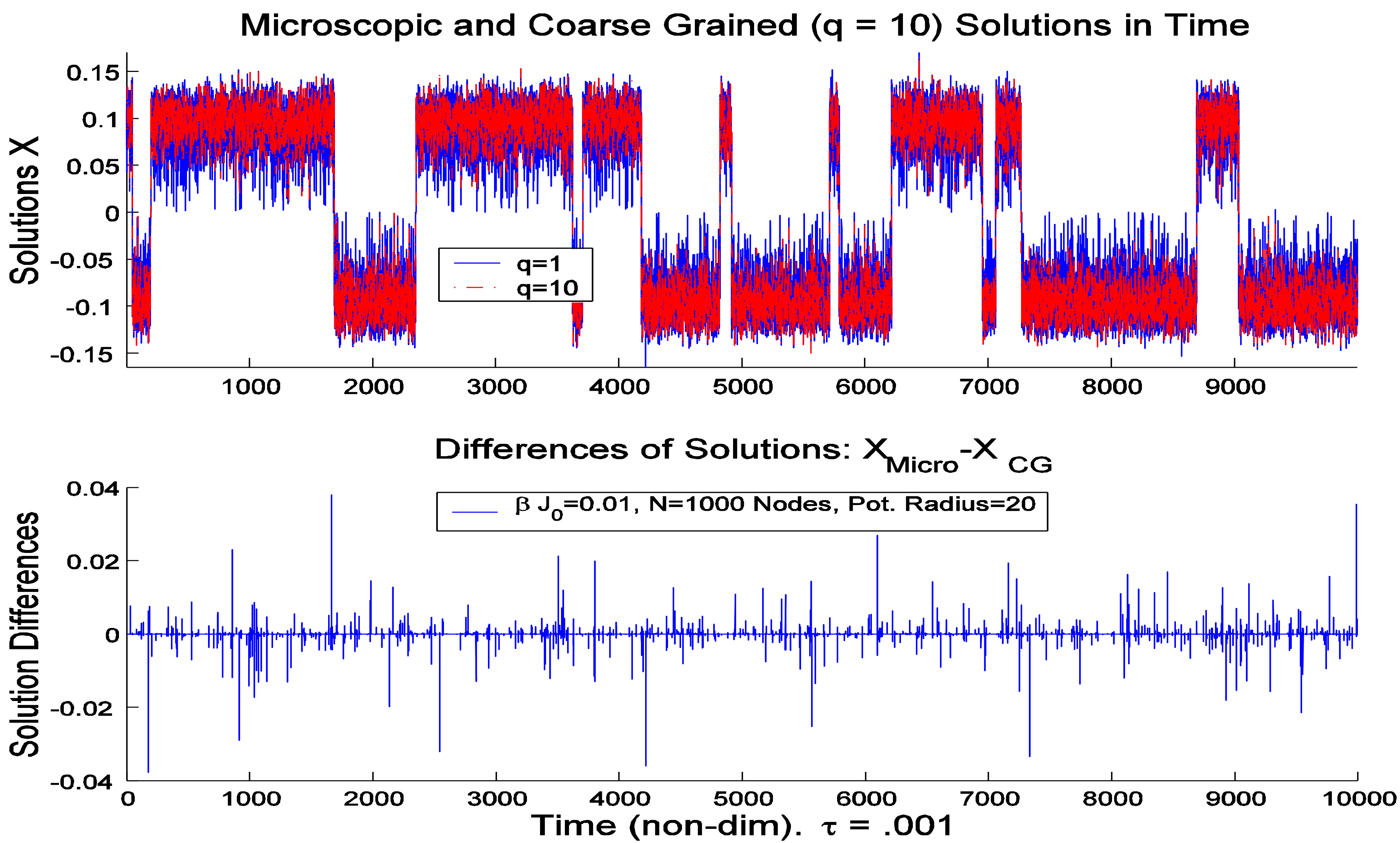
to error estimate

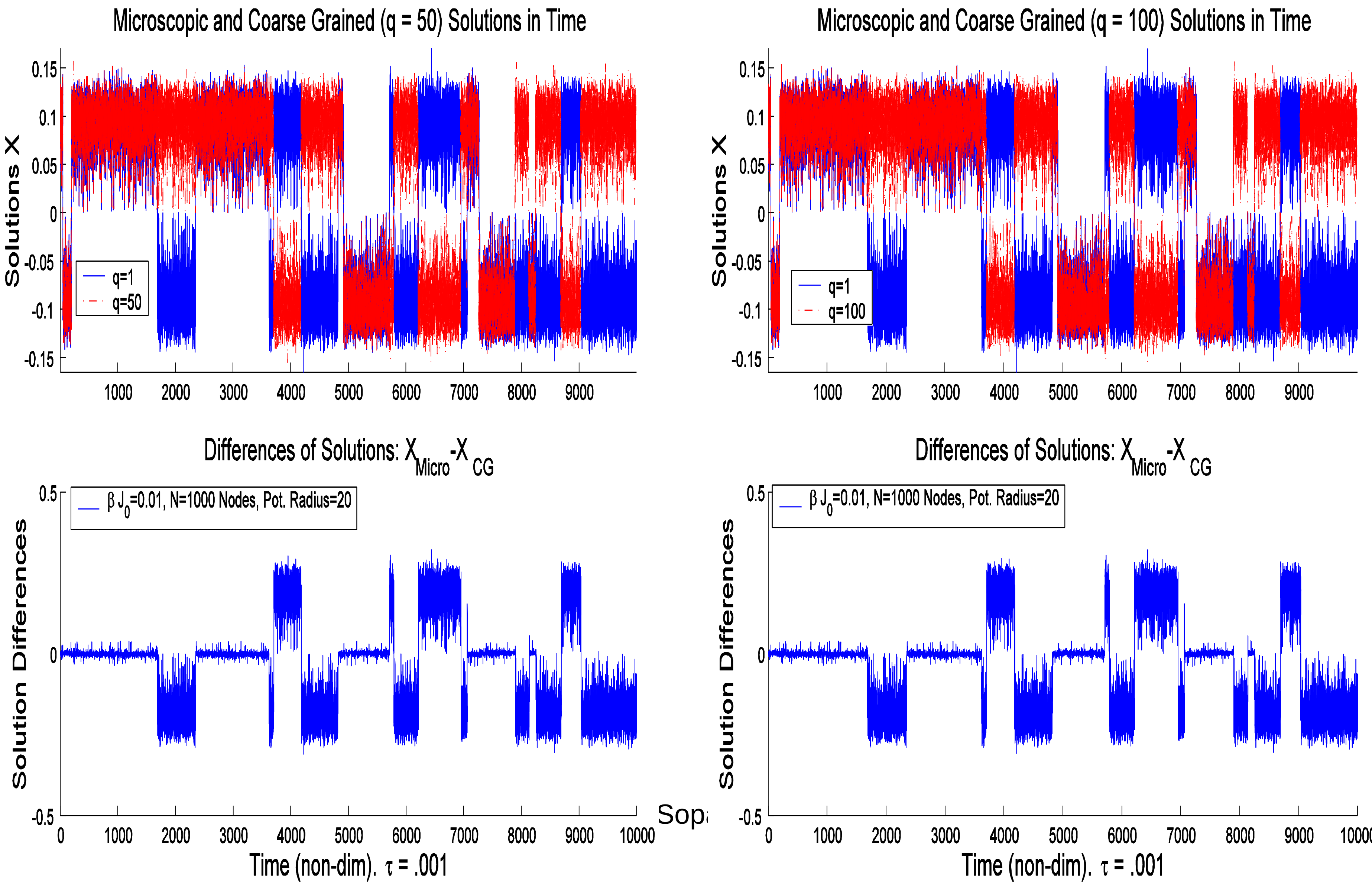
Externally Driven Phase Transitions

Direct Numerical Simulation vs Coarse Grained Closure (for q = 10)



Externally Driven Phase Transitions

Direct Numerical Simulation vs Coarse Grained Closure (q=50, 100)



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 -> 0 is

$$\frac{1}{N} R(TQ_{T\sigma_0,[0,T]} \mid Q^c_{\eta_0,[0,T]}) = T\, O\left(\frac{q}{L}\right)$$

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 σ_0 we define the coarse configuration $\eta_0 = T\sigma_0$ Assume the microscopic process $(\{\sigma_t\}_{t\geq 0}, \Lambda\}$ with the initial condition σ_0 and the approximating coarse process $(\{\eta_t\}_{t\geq 0}, \Lambda_c\}$ with the initial condition $\eta_0 = T\sigma_0$ then the weak error satisfies for final time T,

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

Intermittency and Metastability Phenomena

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

$$\frac{d}{dt}X = a\overline{\sigma} + b - cX$$

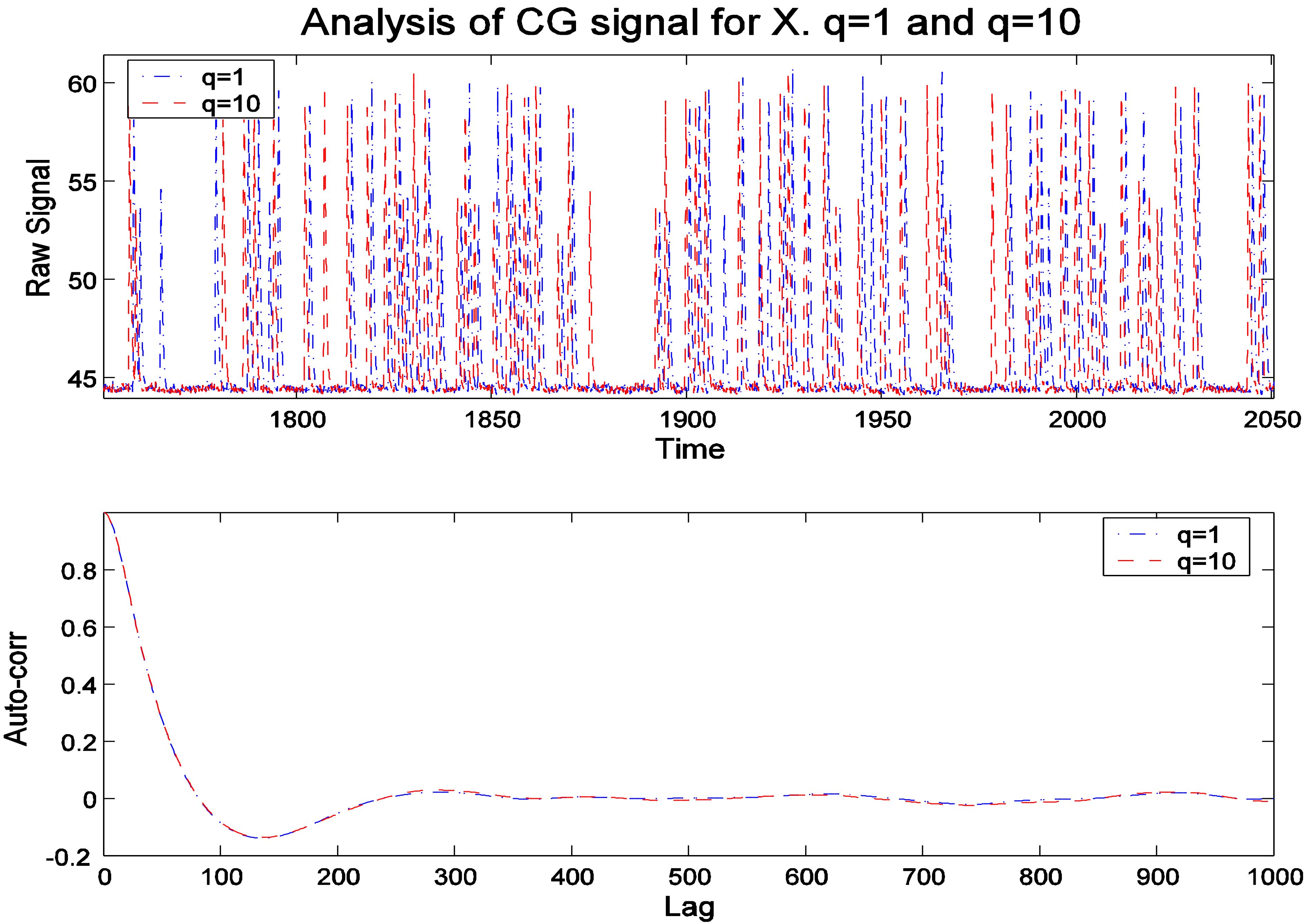
$$\frac{d}{dt}Ef(\sigma) = ELf(\sigma),$$

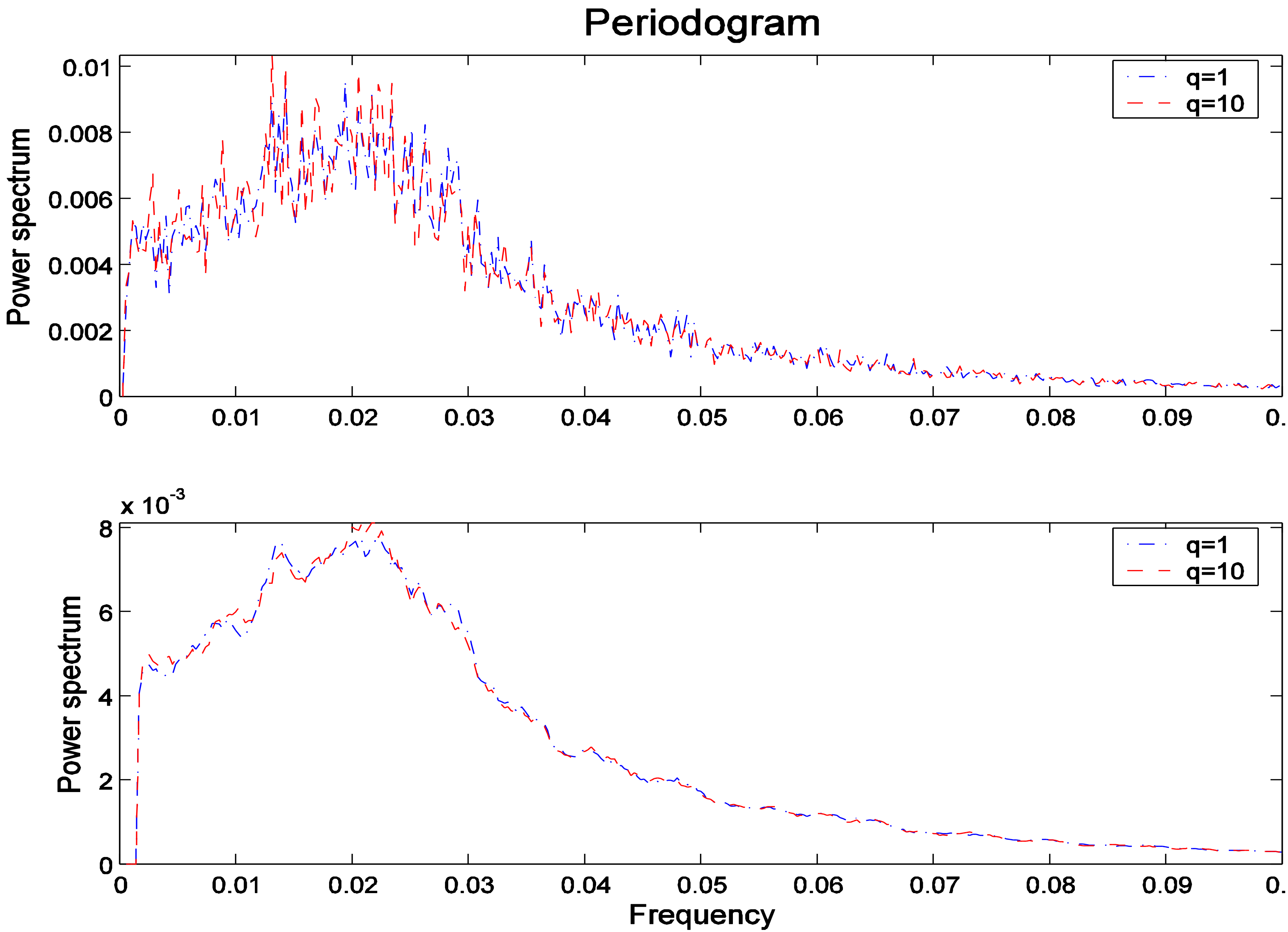
Step 1: Mean field approximations (ODEs):

$$\frac{d}{dt}x = au + b - cx$$

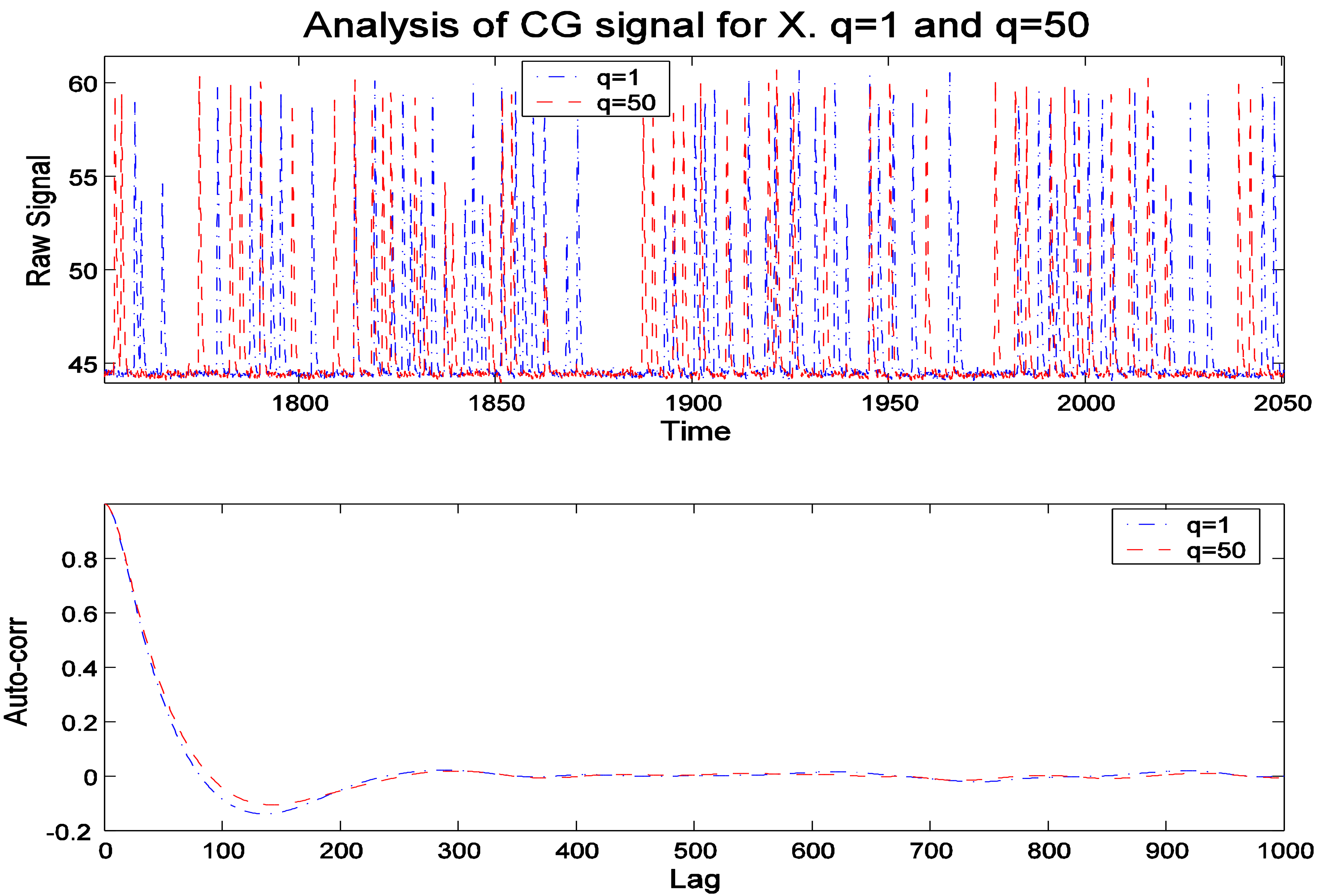
$$\frac{d}{dt}Ef(\sigma) = 1 - u - ue^{-\beta J_0 u + h(x(t))}$$

Bistable, excitable, oscillatory regimes (strong interactions)


Analysis of CG signal for X. q=1 and q=10
q=1
q=10
Raw Signal
60
55
50
45
1800
1850
1900
1950
2000
2050
Time
q=1
q=10
Auto-corr
0.8
0.6
0.4
0.2
0
-0.2
0
100
200
300
400
500
600
700
800
900
1000
Lag


Periodogram
Power spectrum
0.01
0.008
0.006
0.004
0.002
0
0 0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09 0.1
q=1
q=10
x 10-3
8
6
4
2
0
Frequency

to end



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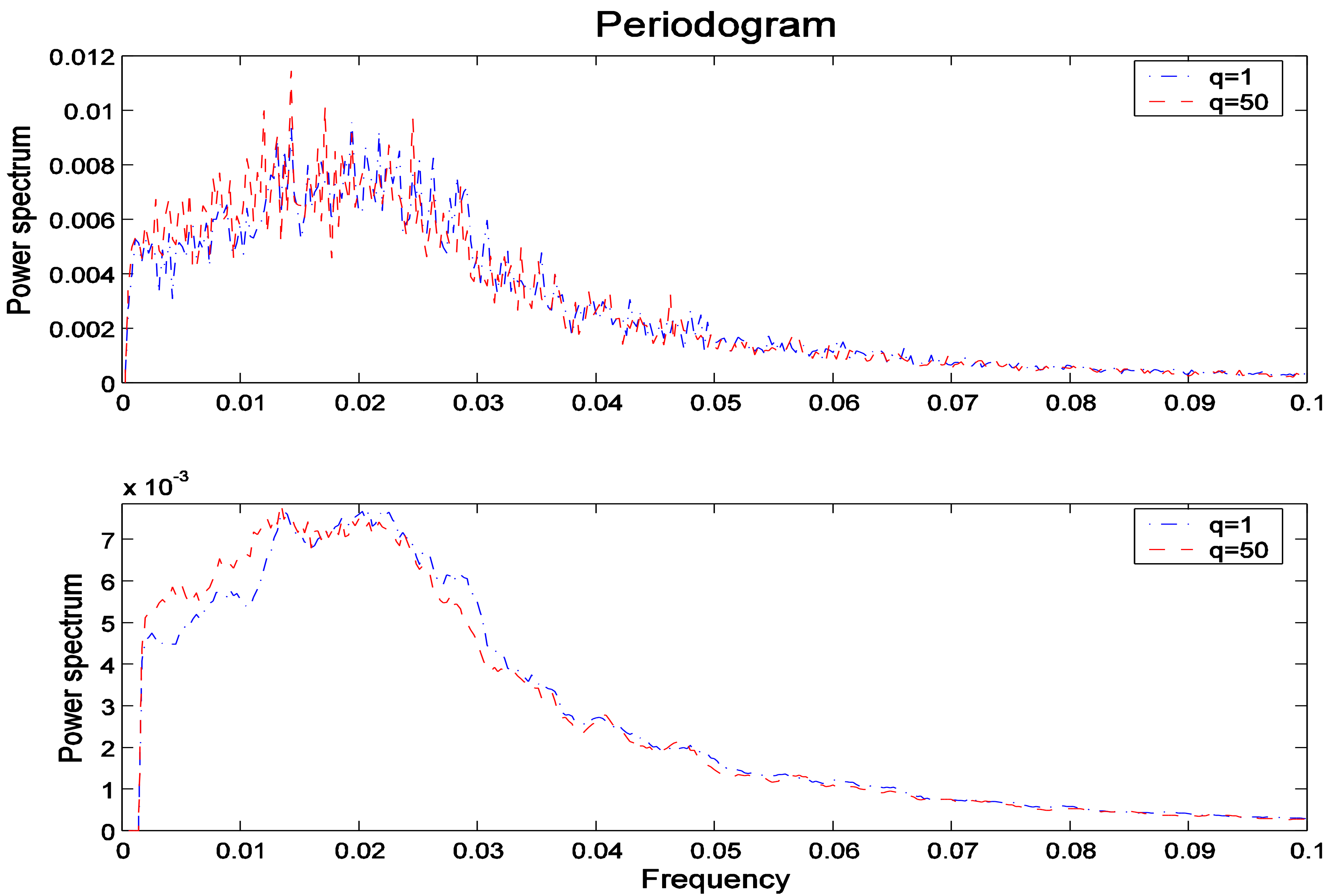

Periodogram
Power spectrum
0.012
0.01
0.008
0.006
0.004
0.002
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0.1
q=1
q=50
x 10^-3
7
6
5
4
3
2
1
Frequency

Conclusions

- ✓ Presented a coupled Prototype Hybrid System consisting of:

$$\begin{cases} \text{Stochastic Noise Model} \\ \text{CGL type} - \text{General Bifurcating ODE} \end{cases}$$

  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.

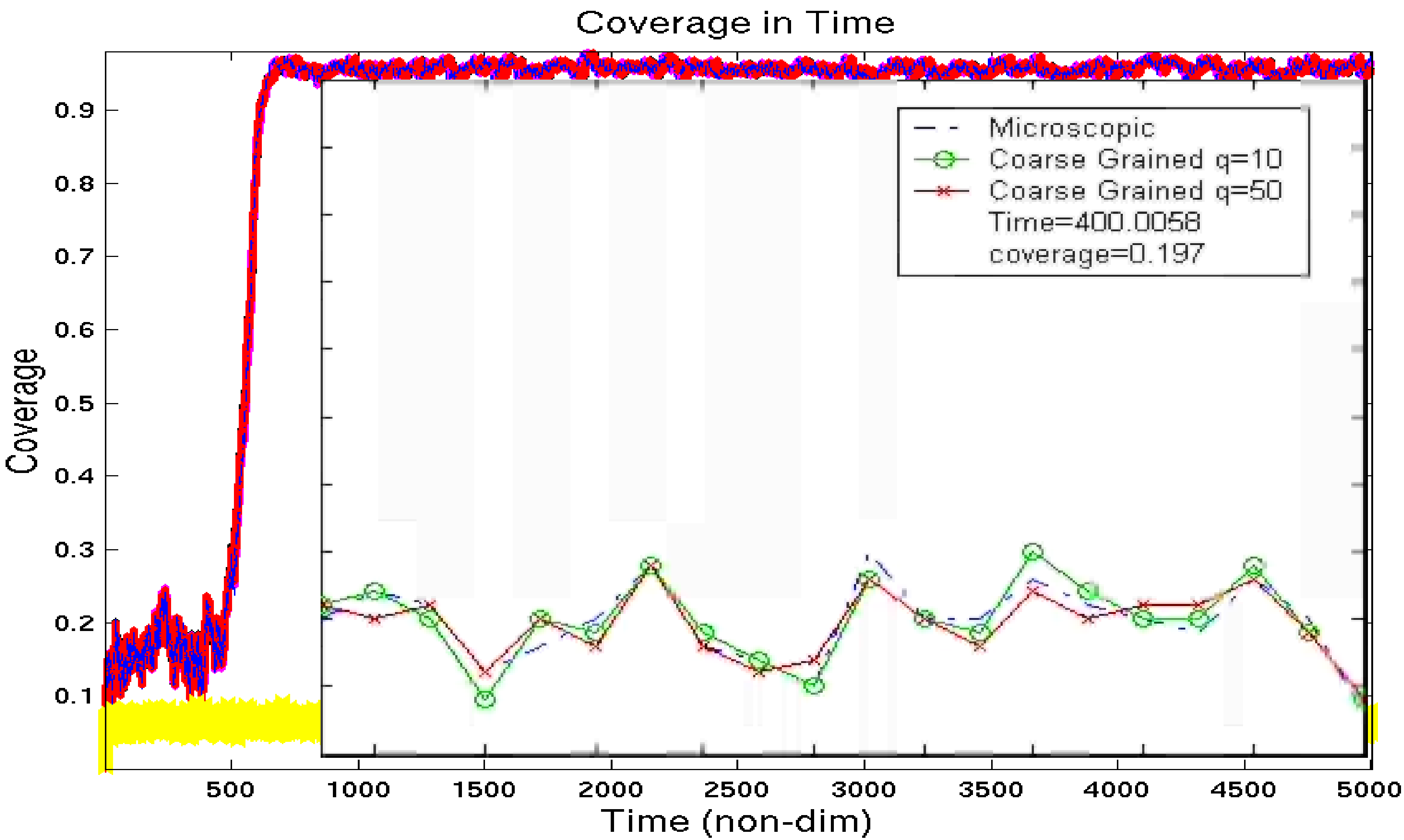
- ✓ Deterministic type closures (averaging principle / mean field) are valid for finite time intervals $(T << \infty)$ and for the case of fast stochastic dynamics $(\tau \to \infty)$ relative to the ODE

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

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

There is spatial agreement as well

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



Recent Relevant Publications

Stochastic Models

• Sopasakis, *Physica A*, (2003).
• Sopasakis and Katsoulakis, *SIAM J. Applied Math*. (2005).
• Alperovich and Sopasakis, *Physica Review E*, submitted, (2007).
• Dundon and Sopasakis, *Transportation and Traffic Theory*, to appear, (2007).

Hybrid Deterministic/Stochastic Systems

• Katsoulakis, Majda, Sopasakis, *Comm. Math. Sci*. (2004).
• Katsoulakis, Majda, Sopasakis, *Comm. Math. Sci*. (2005).
• Katsoulakis, Majda, Sopasakis, *Nonlinearity*, (2006).
• Katsoulakis, Majda, Sopasakis, *AMS Contemporary Math*. to appear, (2007).

Coarse-Grained Models

•Katsoulakis, Plechac, Sopasakis, *IMA* preprtint 2019, (2005)
•Katsoulakis, Plechac, Sopasakis, *SIAM J. Numerical Analysis*, (2006).

Partially Supported by:
• NSF-DMS-0606807
• DE-FG02-05ER25702