Mathematical and Computational challenges in Stochastic/Deterministic Hybrid Systems

Lecture 2

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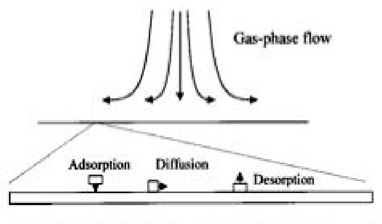
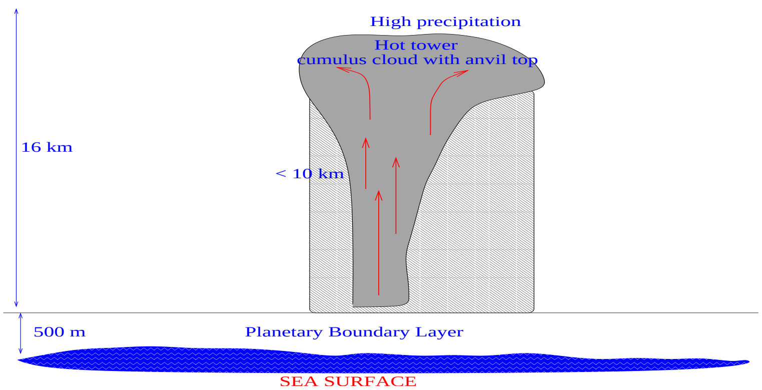
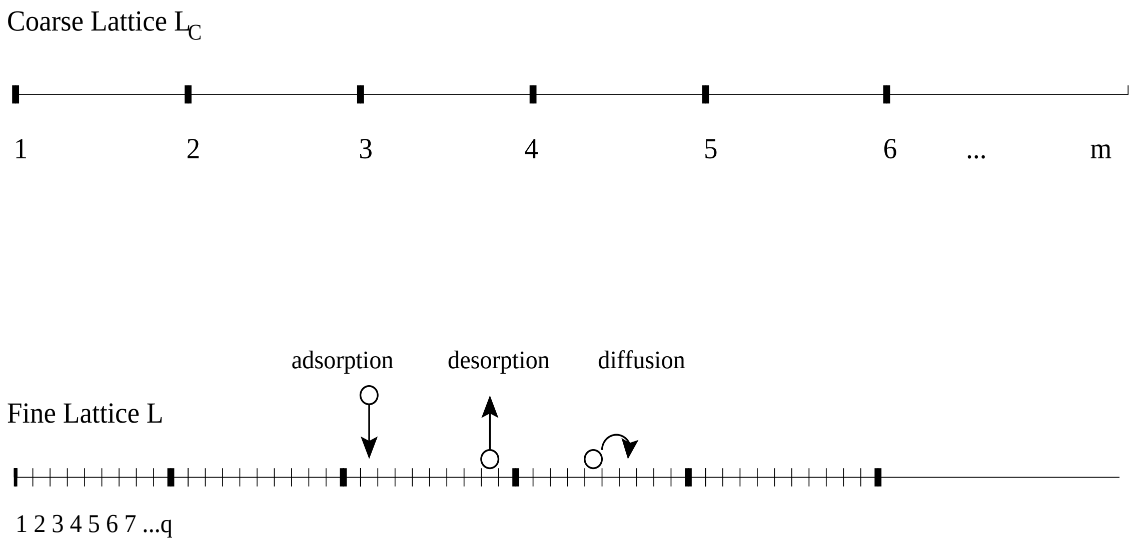
Surface processes: Catalysis, Chemical Vapor Deposition, epitaxial growth, etc.



Atmosphere/Ocean applications: Tropical convection.





$$\partial_t X = F[X, \sigma] \quad \text{(PDE/ODE system)}$$

$$\partial_t E f(\sigma) = E L_X f(\sigma) \quad \text{(stochastic model)}$$

X: Fluid/thermodynamic variables defined on top grid

L_X: generator of the subgrid stochastic process σ defined on the lower grid (subgrid)

Some challenges and questions:

- Disparity in scales and models; DNS require ensemble averages for a large system.
- 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.

MODEL SYSTEM

$$\begin{aligned} \partial_t X &= f(X, \bar{\sigma}) \quad \text{(ODE)} \\ \partial_t E f(\sigma) &= E L_X f(\sigma) \quad \text{(stochastic lattice model)} \end{aligned}$$

L_X: generator of a spatial stochastic process $\sigma_t(x)$.

$f(x) = f(x, \bar{\sigma})$: scalar bistable, saddle node, or spatially homogeneous complex Ginzburg-Landau equation (Hopf bifurcations), etc.

- $h = h(X)$: external field to the microscopic system.
- $\bar{\sigma} = \frac{1}{N} \sum_x \sigma_t(x)$: area fraction (spatial average).

Joint work with:

A. Majda (Courant), A. Sopasakis (UMass)

Related work:

B. Khouider(Victoria, Canada), P. Plecháč(Warwick, UK),

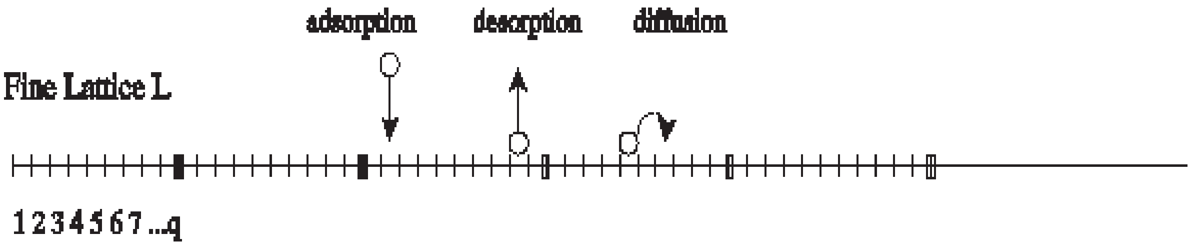
L. Rey-Bellet(UMass), A. Szepessy(KTH, Sweden),

J.Trashorras (Paris IX, France),

D.Tsagkarogiannis (Max Planck-Leipzig),

D.G. Vlachos(Chem. Eng. Delaware)

Stochastic lattice dynamics–Ising Systems



- *Spin:* $\sigma(x) \in \{0, 1\}$ at the lattice site $x \in \mathbf{Z}^d$ (vacant vs. occupied sites).
- *Spin configuration:* $\sigma = \{\sigma(x) \mid x \in \Lambda \subset \mathbf{Z}^d\}$, $|\Lambda| = N$: total number of lattice sites.

Hamiltonian: $H_N(\sigma) = -\frac{1}{2}\sum_{x \neq y} J(x, y)\sigma(x)\sigma(y) + h\sum_x \sigma(x)$

- h: external field
- J: potential with interaction range L.

Canonical Gibbs measure:

at the inverse temperature $\beta = \frac{1}{kT}$,

$$\mu_{\Lambda,\beta}(\sigma = \sigma_0) = \frac{1}{Z_{\Lambda,\beta}} \exp\Big\{ -\beta H_N(\sigma_0)\Big\} P_N(\sigma = \sigma_0)$$

[Probability of the configuration σ_0]

Partition function: $Z_{\Lambda,\beta} = \sum_{\sigma_0} \exp\Big\{ -\beta H_N(\sigma_0)\Big\} P_N(\sigma = \sigma_0)$

Prior distribution (no interactions, hight temp.):

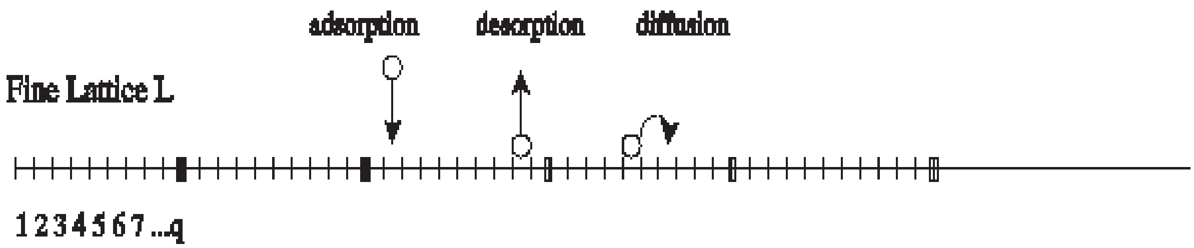
$$P_N(\sigma = \sigma_0) = \Pi_{x\in\Lambda} P(\sigma(x) = \sigma_0(x))$$

where

$$P(\sigma(x) = 1) = \frac{1}{2} \quad \text{and} \quad P(\sigma(x) = 0) = \frac{1}{2}.$$

i.e. the prior distribution is a product measure of Bernoulli distributions with parameter a.

Arrhenius adsoprtion/desorption dynamics:



$\sigma(x) = 0$ or 1: site x is resp. empty or occupied.

Generator: $L_X f(\sigma) = \sum_x c(x, \sigma, X)[f(\sigma^x) - f(\sigma)]$

Transition rate: $c(x, \sigma, X) = c_0 \exp\Big[- \beta U(x) \Big]$

$U(x)$: Energy barrier a particle has to overcome in jumping from a lattice site to the gas phase.

- Detailed Balance
- $U(x) = U(x, \sigma, X) = \sum_{z \neq x} J(x - z)\sigma(z) - h(X)$.
- strong interactions/low temperature $\rightarrow$ clustering/phase transitions

ODE for the large scales:

CGL: $f(\vec{X},\sigma) = (a(\bar{\sigma}) + i\omega)\vec{X} - \gamma|\vec{X}|^2\vec{X} + \widehat{\gamma}\vec{X}^*$

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

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

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

Coupling of the two systems: $h = h(X), f = f(x,\bar{\sigma})$.

- $h(X) = cX + h_0$, or $h(X) = c|X|^2 + h_0$
- $\bar{\sigma}$: affects the bifurcation diagram of the ODE

I. Deterministic closures

- Mean field models (uniform interactions in the micro-model)
- Local mean field models (weak interactions)
- Stochastic averaging (time scale separation)

$$\partial_t X^\epsilon = f(X^\epsilon, \bar{\sigma})$$

$$\partial_t E f(\sigma) = \frac{1}{\epsilon} E L_X f(\sigma)$$

Then, [Khasminskii, Kurtz, Papanicolaou, ... etc.]

$$\lim_{\epsilon \to 0} X^\epsilon = X$$

$$\partial_t X = \bar{f}(X)\,, \quad \bar{f}(x) = \int_\Sigma f(x, \bar{\sigma})\, {\mu^x}_{\text{equil}}(d\sigma)\,,$$

${\mu^x}_{\text{equil}}$ canonical Gibbs measure.

Remarks

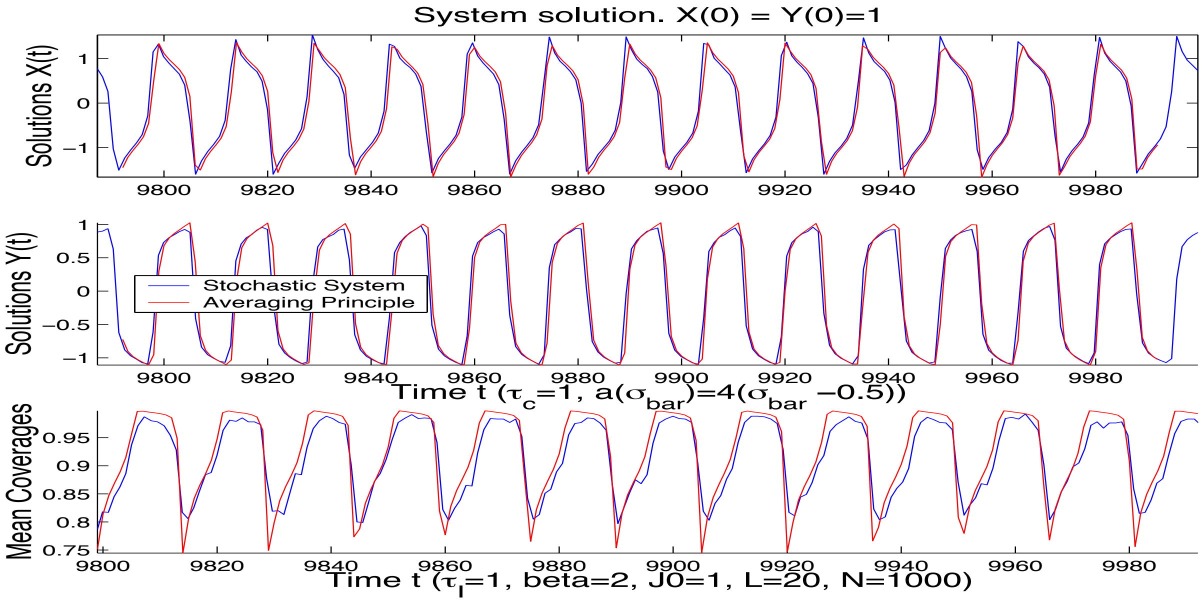
1. Evaluation of $\bar{f}(x) = \int_\Sigma f(x, \bar{\sigma})\, \mu^x{}_{\text{equil}}(d\sigma)$?

2. Theorem $\rightarrow \epsilon \ll 1$; how big can we take ϵ?

3. Need ergodicity for the micro process: no phase transitions in the microscopic model, i.e. only when we have weak interactions/high temperature

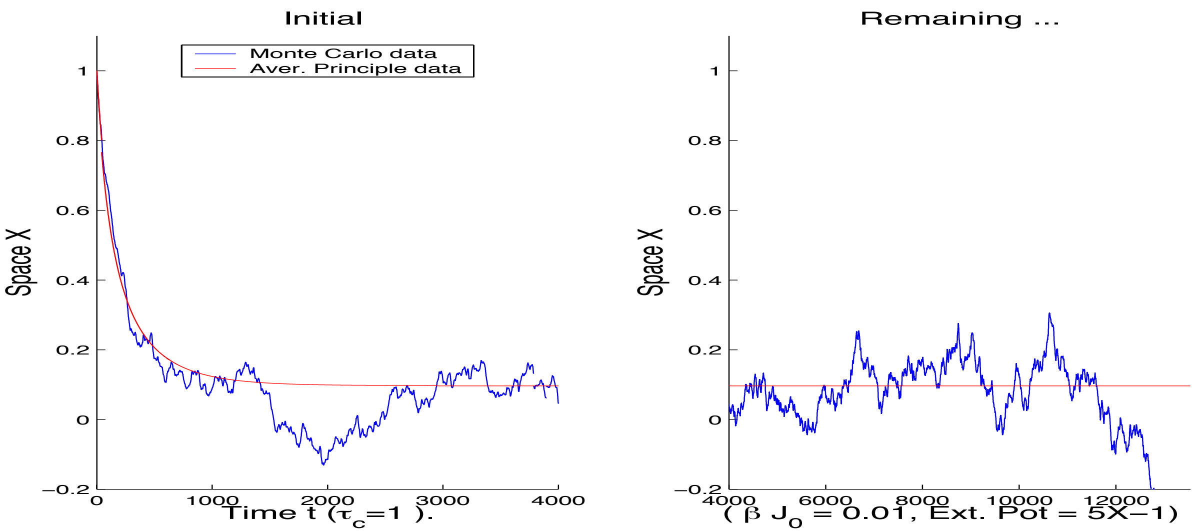
4. Finite time interval derivation [0, T]; large deviations from the averaged equation [Freidlin-Wentzell for SDE].

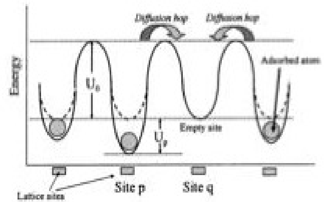
External ODE: $f(\vec{X},\sigma) = (a(\bar{\sigma}) + i\omega)\vec{X} - \gamma|\vec{X}|^2\vec{X} + \widehat{\gamma}\vec{X}^*$ (CGL)



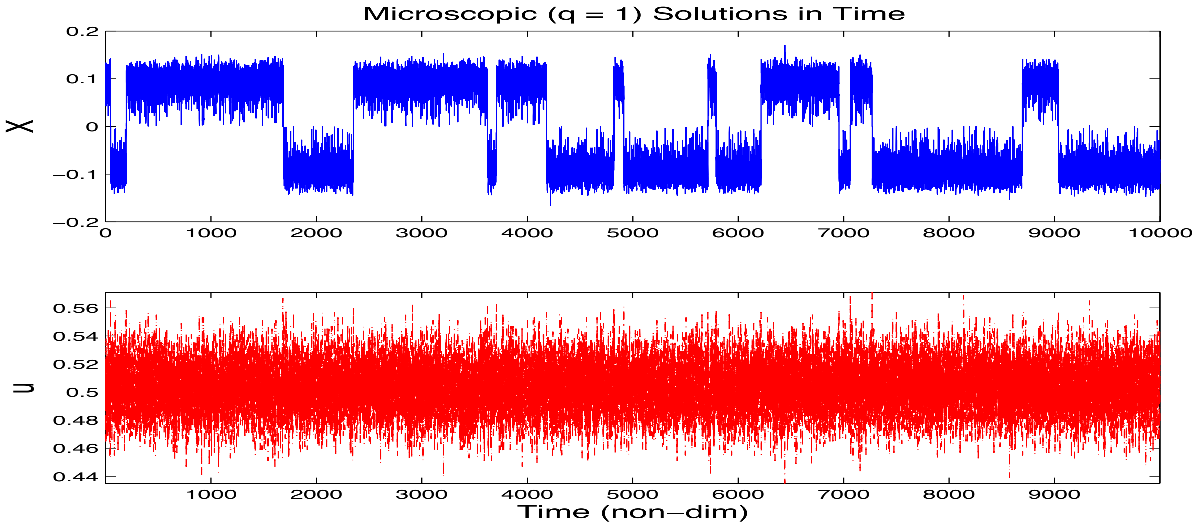
When stochastic fluctuations become important?

<u>External ODE</u>: $f(X,\sigma) = a(\bar{\sigma}) + \gamma X^2$, (saddle node bifurcation)





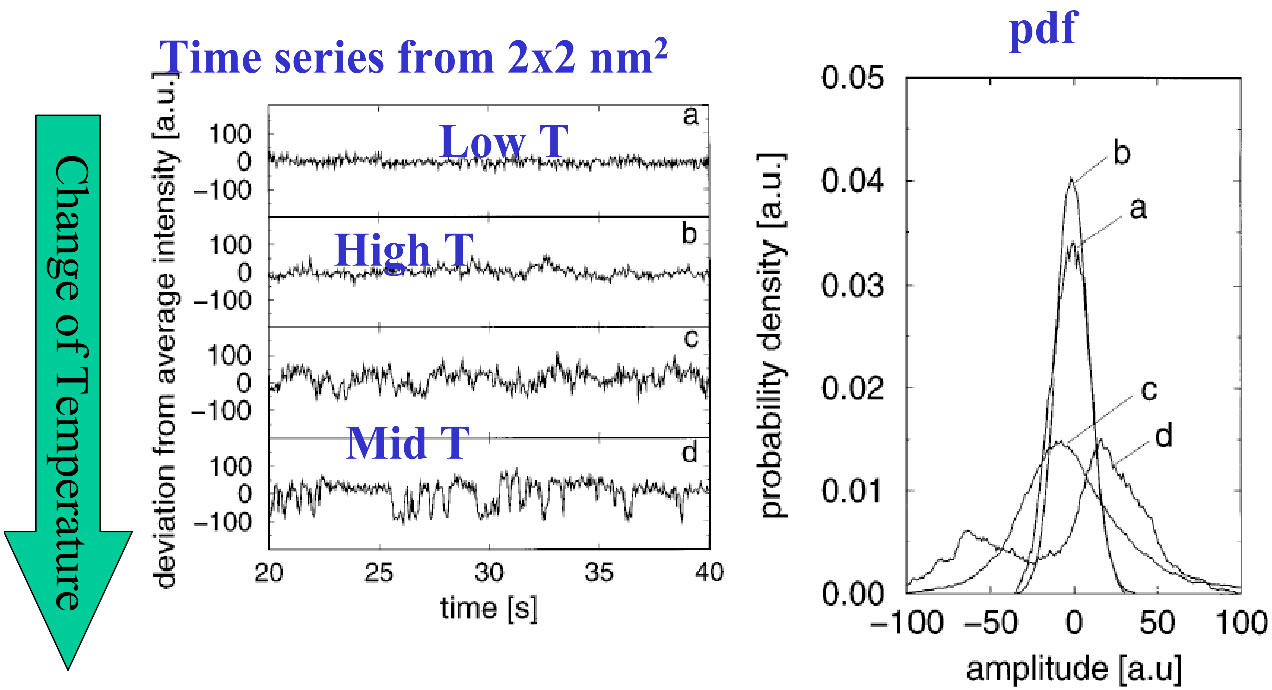
<u>External ODE</u>: $f(X,\sigma) = a(\bar{\sigma})X + \gamma X^3$, (Bistable)



- Deterministic closures capture correctly large scale features but miss the stochastically-driven transient dynamics.

Phase transitions in hybrid systems: How do we observe them in experiments?

Catalysis: CO on Pt oxidation example:



Suchorski, Evans, Imbihl et al., *Phys. Rev. Lett.* **89**, 1907 (1999)

Phase transitions in hybrid systems: strong particle/particle interactions

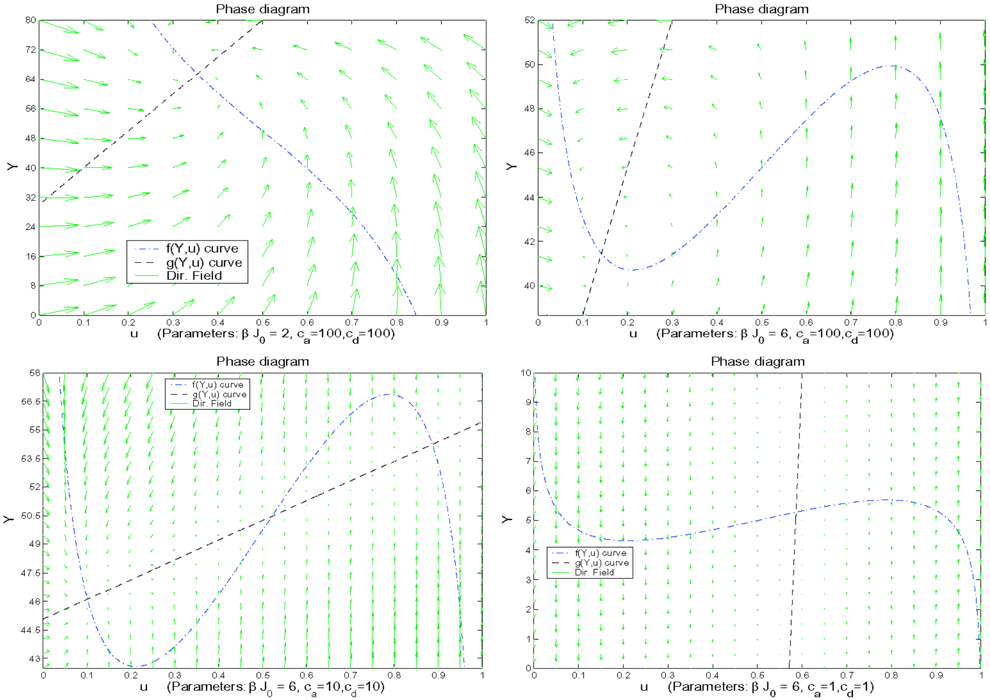
$$\frac{d}{dt}X = f(X,\overline{\sigma}) = a\bar{\sigma} + b - cX$$
$$\frac{d}{dt}Ef(\sigma) = E\mathcal{L}_X f(\sigma)\,, \quad h = h(X)$$

Step 1: mean field approximation (ODEs):

$$\frac{d}{dt}x = au + b - cx \equiv f(x,u)$$
$$\frac{d}{dt}u = (1-u) - u\,\mathrm{exp}[-\beta J_0 u + h(x(t))]$$

- one stable state (weak interactions J_0); stochasticity is not important
- bistable, excitable, oscillatory regimes (strong interactions)

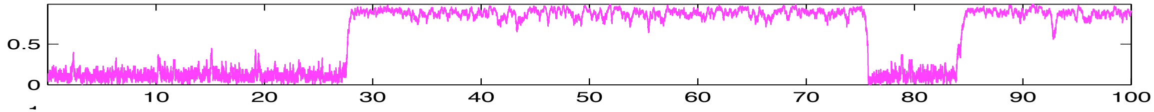
  Fitzhugh-Nagumo type system



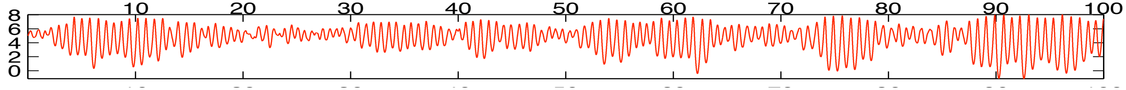
Phase diagram
Y
u (Parameters: β J0 = 2, ca=100,cd=100)
f(Y,u) curve
g(Y,u) curve
Dir. Field
Phase diagram
Y
u (Parameters: β J0 = 6, ca=100,cd=100)
Phase diagram
Y
u (Parameters: β J0 = 6, ca=10,cd=10)
f(Y,u) curve
g(Y,u) curve
Dir. Field
Phase diagram
Y
u (Parameters: β J0 = 6, ca=1,cd=1)
f(Y,u) curve
g(Y,u) curve
Dir. Field

Step 2: Mean field approx. suggests:

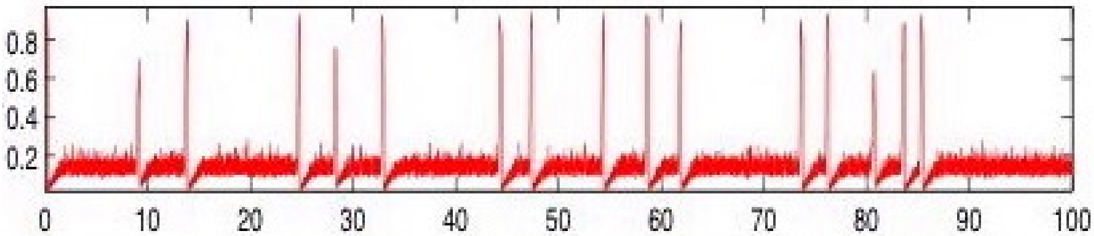
Bistability $\longrightarrow$ random switching.



Oscillatory regime $\longrightarrow$ random oscillations



Excitability $\longrightarrow$ strong **intermittency** regime



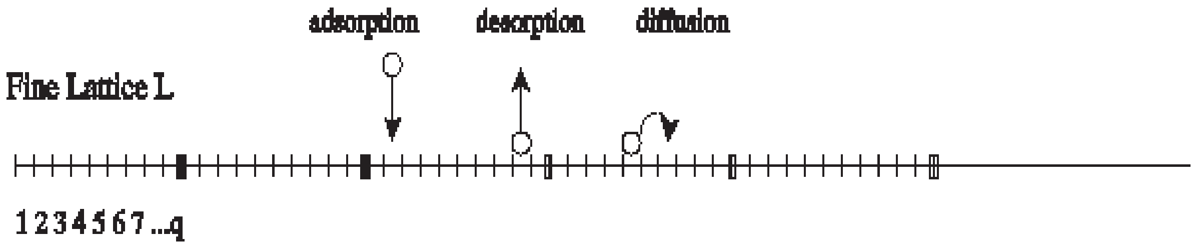
a. Need model reduction through suitable closure.

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

2. Hierarchical coarse-graining of stochastic processes

[Katsoulakis, Majda, Vlachos, PNAS (2003), JCompPhys (2003), JChemPhys(2003)]

Construct a **coarse-grained stochastic process** for a hierarchy of “mesoscopic” length or time scales that retains fluctuations.



Coarse observable (why this one?)

$$\eta_t(k) = \sum_{y \in D_k} \sigma_t(y) \, .$$

In general it is **non-markovian**

Stochastic closures: can we write a new approximating Markov process for η_t?

Examples of continuous coarse-grained models

Deterministic PDE: Ginzburg-Landau models, lattice Boltzmann, etc.

Stochastic PDE: Cahn-Hilliard-Cook, diblock co-polymer models, etc.

Examples of discrete coarse-grained models

CG of macromolecules: model "superatoms" of 10-20 atoms in polymers, proteins etc; fitting of parametrized potentials against DNS for given observables

Renormalization Group Methods

Step 1: From the microscopics:

$$\frac{d}{dt}Eg(\eta) = E\sum_{k\in\Lambda_c}\left\{\sum_{x\in D_k} c(x,\sigma)\big(1-\sigma(x)\big)\right\}\times \Big[g(\eta+\delta_k)-g(\eta)\Big] + E\sum_{k\in\Lambda_c}\left\{\sum_{x\in D_k} c(x,\sigma)\sigma(x)\right\}\times \Big[g(\eta-\delta_k)-g(\eta)\Big]\,.$$

<u>"Closure" argument:</u> Express as a function of the coarse variables the terms

$$\left\{\sum_{x\in D_k} c(x,\sigma)\ldots\right\}$$

- $\sum_{x\in D_k} c(x,\sigma)\big(1-\sigma(x)\big) = \big(q-\eta(k)\big) := c_a(k,\eta)$
- $\sum_{\mathbf{x}\in\mathbf{D_k}} \mathbf{c}(\mathbf{x},\sigma)\sigma(\mathbf{x}) \overset{??}{=} \mathbf{c_d}(\mathbf{k},\eta)$

Note that

$$\sum_{x\in D_k} c(x,\sigma)\sigma(x) = \sum_{x\in D_k}\sigma(x)\,\mathrm{exp}\left[-\beta\Big(U_0+U(x)\Big)\right],$$

where

$$U(x) = \sum_{z\neq x, z\in\Lambda} J(x-z)\sigma(z) - h$$

$$\begin{aligned}
\sum_{z\neq x, z\in\Lambda} J(x-z)\sigma(z) &= \sum_{k\in\Lambda_c}\sum_{z\neq x, z\in D_k} J(x-z)\sigma(z) \\
&= \sum_{z\neq x, z\in D_l} J(x-z)\sigma(z) + \\
&\qquad \sum_{k\neq l, k\in\Lambda_c}\sum_{z\in D_k} J(x-z)\sigma(z) \\
&:= I + II\,.
\end{aligned}$$

Term I: interactions within the cell D_l.

Term II: interactions of $x \in D_l$ with particles in other coarse cells D_k, $k \neq l$.

Coarse-grained potential

$$\bar{J}(k,l) = m^2 \int\int_{D_l \times D_k} J(r-s)drds\,,$$

$|D_l \times D_k| = 1/m^2$.

Includes all contributions of pairwise microscopic interactions between coarse cells and within the same coarse cell.

Wavelet-based coarse graining (with vanishing moments). Advantages: Nonstandard form [Beylkin, Coifman, Rokhlin], accurate quadratures [Beylkin].

Term II $= \sum_{\substack{k\in\Lambda_c \\ k\neq l}} \bar{J}(l,k)\eta(k) + O\left(\frac{q}{L}\right)$

Term I $= \bar{J}(0,0)\Big(\eta(l) - \sigma(x)\Big) + \frac{1}{2L+1} O\left(\frac{q}{L}\right)$

q: level of coarse-graining

L: interaction range

Similar error estimates for singular potentials. Improved estimates using the decay of J.

Desorption rate:

$$c_d(k,\eta) \approx \eta(k) \exp\left[-\beta\Big(U_0 + \bar{U}(k)\Big)\right]$$

where we dropped the term $\mathbf{O}(\frac{\mathbf{q}}{\mathbf{L}})$ in: $U(x) = \bar{U}(l) + O\left(\frac{q}{L}\right)$,

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

- When **L** $>>$ **q** the coarse grained variable η is "approximately" a Markov process.

Expected form of the generator:

Birth-Death type process,

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

- **Coarse-grained** rates:

Adsorption rate of a single particle in the k-coarse cell

$$c_a(k,\eta) = q - \eta(k)$$

Desorption rate (approximate–error estimates)

$$c_d(k,\eta) = \eta(k)\exp\Big[-\beta\Big(U_0 + \bar{U}(k)\Big)\Big]$$

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

Birth-Death type process, with interactions.

Step 2: Ergodicity at every coarse level q:

Detailed balance for coarse Gibbs states:

Gibbs measure: $\mu_{m,q,\beta}(d\eta) = \frac{1}{Z_{m,q,\beta}} \exp(-\beta \bar{H}^{\mathbf{0}}(\eta)) P_{m,q}(d\eta)$

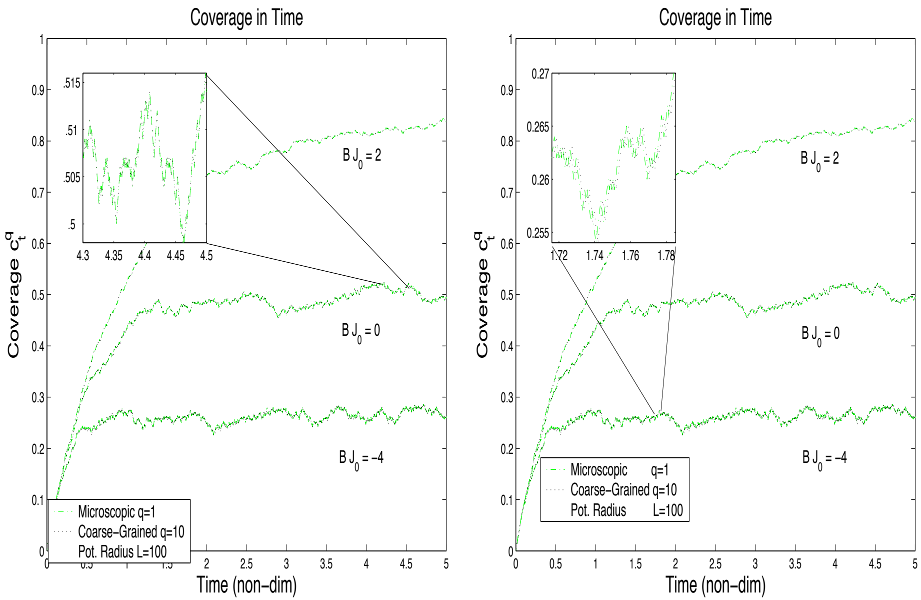
Coarse-grained Hamiltonian

$$\bar{H}^{\mathbf{0}}(\eta) = -\frac{1}{2} \sum_{l} \sum_{k, k \neq l} \bar{J}(k,l)\eta(k)\eta(l) - \frac{\bar{J}(0,0)}{2} \sum_{l} \eta(l)\big(\eta(l)-1\big) + \sum_{l} \bar{h}(l)\eta(l)$$

Coarse-grained prior distribution:

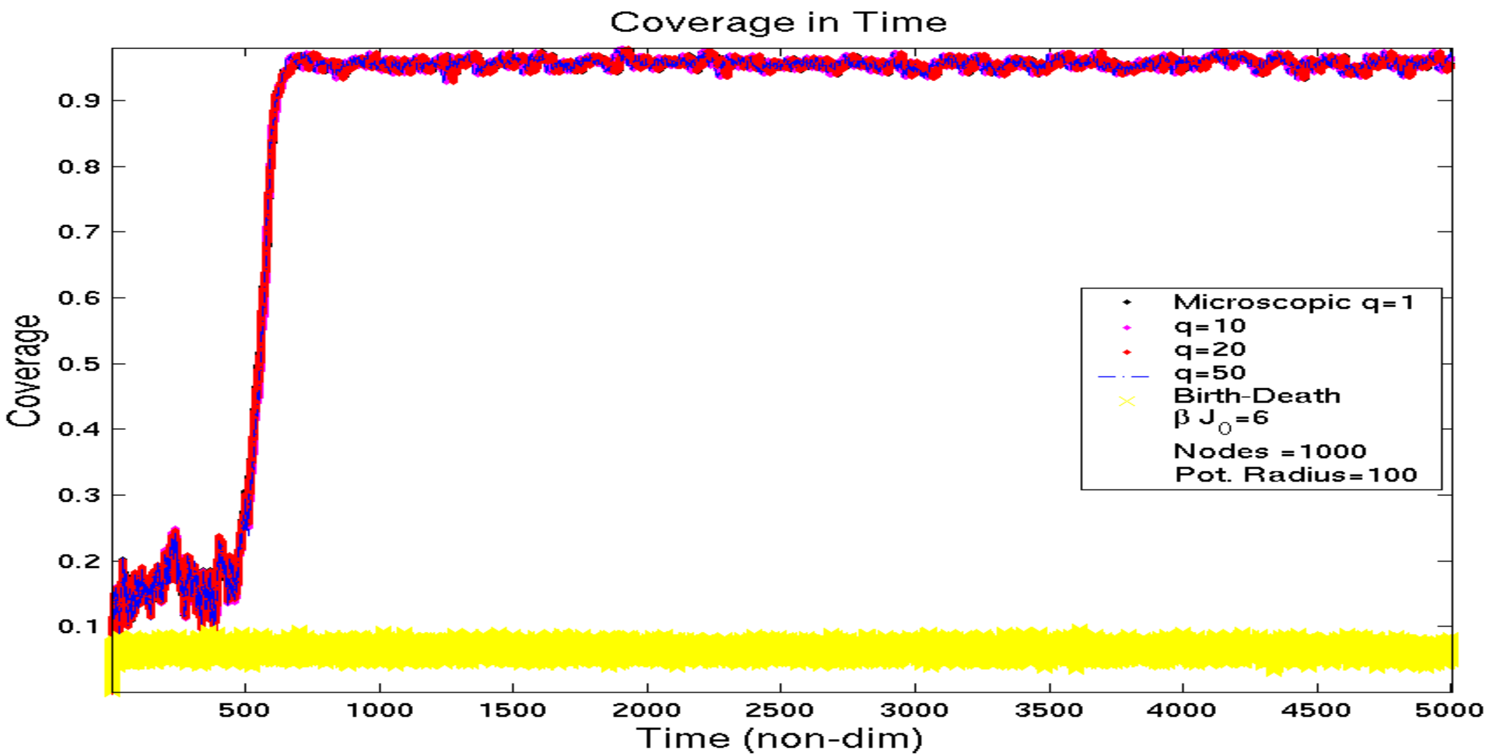
$$P_{m,q}(\eta) = \prod_{k} \rho_q(\eta(k)), \quad \rho_q(\eta(k)=\lambda) = \frac{q!}{\lambda!(q-\lambda)!} \left(\frac{1}{2}\right)^q$$

Higher-order corrections: Relation to RG, cluster expansions.


Coverage in Time
Coverage in Time
Coverage c_t^q
Time (non–dim)
B J0 = 2
B J0 = 0
B J0 = −4
Microscopic q=1
Coarse–Grained q=10
Pot. Radius L=100
Microscopic q=1
Coarse–Grained q=10
Pot. Radius L=100

- CPU savings: at least $O(q^2)$ or more.

Rare events and metastability



Analysis and numerics: Transient and long-time comparisons

Error I–Loss of information during coarse-graining

[with José Trashorras (Paris IX)]

- $\mu_{m,q,\beta}(t)$: Coarse-grained PDF at time t.
- $\mu_{N,\beta}(t)$: Projection of the microscopic PDF at time t on the coarse observables.
- q: level of coarse-graining
- L: # of interacting neighbors

Then,

$$\mathcal{R}\left(\mu_{m,q,\beta}(t)\,|\,\mu_{N,\beta} o F(t)\right) = O_T(\frac{q}{L})\,, \quad t \in [0,T]$$

where

$$\mathcal{R}\,(\mu\,|\,\nu) := \frac{1}{N}\sum_{\sigma} \log\left\{\frac{\mu(\sigma)}{\nu(\sigma)}\right\}\mu(\sigma) \quad .\diamond$$

Information Theory interpretation: The relative entropy describes the increase in descriptive (in terms of a D-nary alphabet) complexity of a random variable due to “wrong information”.

Distance between two probability measures

- Convergence in TV

$$||\pi_1 - \pi_2||_{TV} = \sup_A |\pi_1(A) - \pi_2(A)| = \sup_f \left| \int f(\sigma)\pi_1(d\sigma) - \int f(\sigma)\pi_2(d\sigma) \right|$$

- Relative entropy of $\pi_1(\sigma)$ and $\pi_2(\sigma)$

$$\mathcal{R}\left(\pi_1 \,|\, \pi_2\right) = \sum_{\sigma \in \mathcal{S}} \pi_1(\sigma) \log \frac{\pi_1(\sigma)}{\pi_2(\sigma)} \,.$$

$$\begin{aligned} \mathcal{R}\left(\pi_1 \,|\, \pi_2\right) &\geq 0 \quad \text{and,} \\ \mathcal{R}\left(\pi_1 \,|\, \pi_2\right) &= 0 \quad \text{if and only if } \pi_1(\sigma) = \pi_2(\sigma) \text{ for all } \sigma \in \mathcal{S}. \end{aligned}$$

Bounds:

$$2||\pi_1 - \pi_2||_{TV}^2 \leq \mathcal{R}\left(\pi_1 \,|\, \pi_2\right) \leq ||\pi_1 - \pi_2||_{TV} + \frac{1}{2}||\frac{\pi_1}{\pi_2} - 1||_{\pi_2,2}^2$$

Other lower bounds from variational characterisation:

$$\mathcal{R}\left(\pi_1 \,|\, \pi_2\right) = \sup_{f \in L^\infty(\mathcal{S})} \left\{ \langle \pi_1, f \rangle - \log \langle \pi_2, e^f \rangle \right\}$$

Difficulty: $F(\sigma_t)(k) = \sum_{y \in D_k} \sigma_t(y)$. is not a Markov process.

Elements of the proof:

1. γ_t: Markovian reconstruction of the microscopic process σ_t from the coarse process η_t with controlled error:

- $(F(\gamma_t))_{t\geq 0}$ and $(\eta_t)_{t\geq 0}$ have the same distribution
- Since σ_t, γ_t are Markov, the Radon-Nikodym derivative of their distributions is:

$$\frac{d\mathcal{D}^{\sigma}_{[0,T]}}{d\mathcal{D}^{\gamma}_{[0,T]}}((\rho_t)_{t\in[0,T]}) = \exp\left\{\int_0^T [\lambda_\sigma(\rho_s) - \lambda_\gamma(\rho_s)]ds - \sum_{s\leq T} \log \frac{\lambda_\sigma(\rho_{s-})p_\sigma(\rho_{s-},\rho_s)}{\lambda_\gamma(\rho_{s-})p_\gamma(\rho_{s-},\rho_s)}\right\}$$

2. Variational formulation of the relative entropy and contraction:

$$R\Big(\mu o F \,|\, \nu o F\Big) \leq R\Big(\mu \,|\, \nu\Big)$$

3. Error estimation in the rates from coarse-graining of interactions.

Remark: Reconstruction processes have computational interest, e.g. adaptivity, etc.

Error Control II – Error Estimates for observable

-with: P. Plechac (Warwick), A. Sopasakis; A. Szepessy (KTH).

ϕ: micorscopic observable

ψ: coarse grained observables

such that $\phi(\sigma) := \psi(F(\sigma))$ e.g. $\phi(\sigma) =$ average over lattice

microscopic process: σ,

reconstructed process: γ (still in the microscopic lattice)

coarse-grained process: η

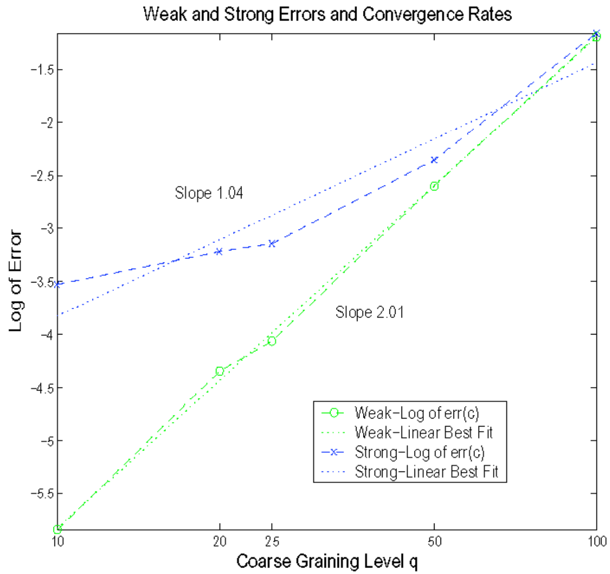
Then for any $0 < T < \infty$

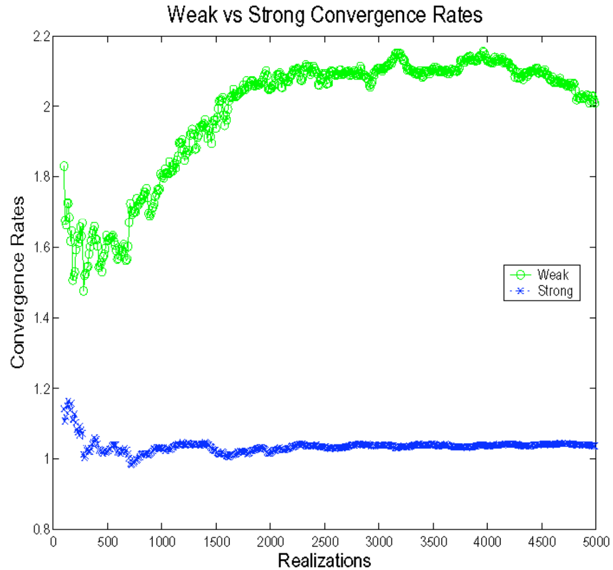
$$|E\phi(\sigma_T) - E\phi(\gamma_T)| \leq C_T(\frac{q}{L})^2\,,$$

and

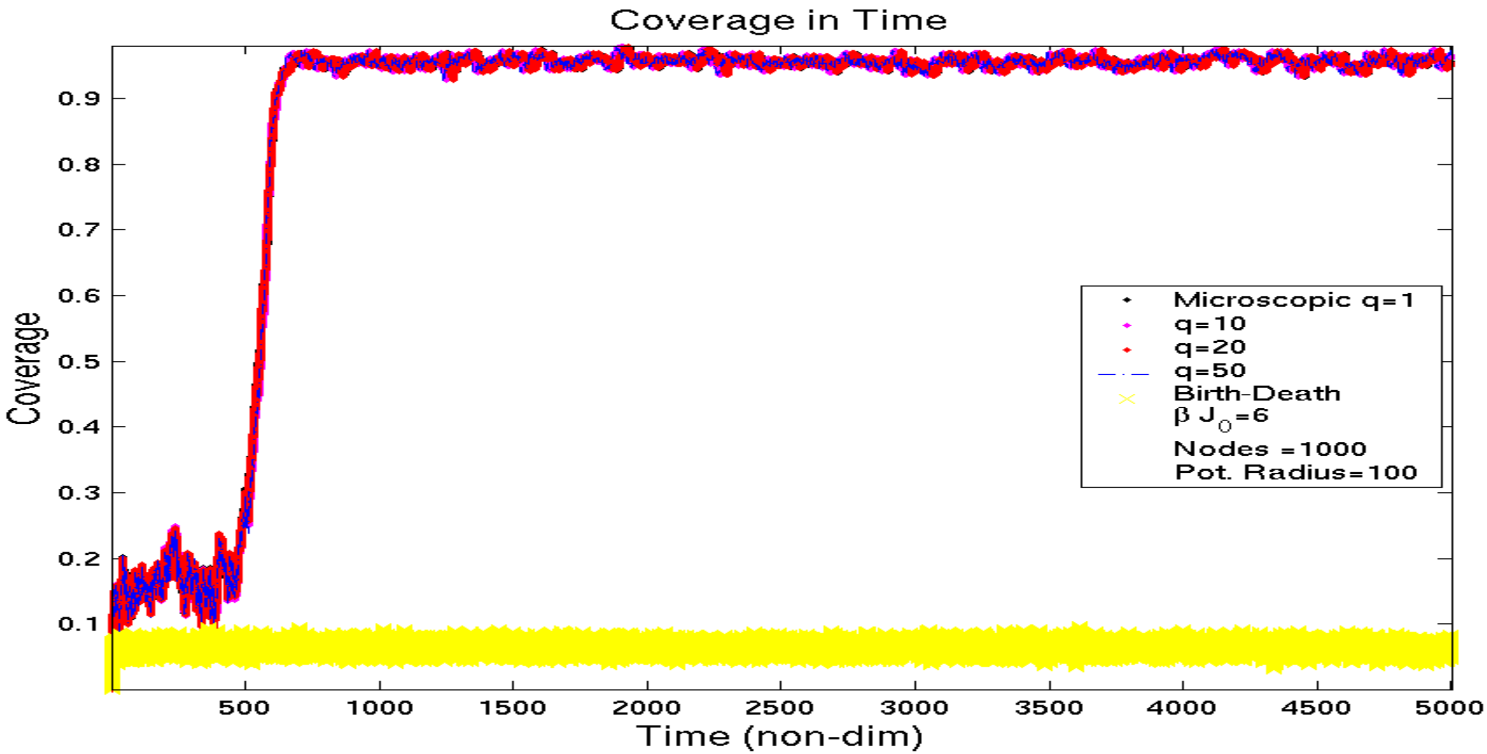
$$|E\psi(F(\sigma_T)) - E\psi(\eta_T)| \leq C_T(\frac{q}{L})^2\,,$$

where the constant C_T is independent of q and L but depends on T.


Weak and Strong Errors and Convergence Rates
Log of Error
Coarse Graining Level q
Slope 1.04
Slope 2.01
Weak−Log of err(c)
Weak−Linear Best Fit
Strong−Log of err(c)
Strong−Linear Best Fit
-1.5
-2
-2.5
-3
-3.5
-4
-4.5
-5
-5.5
10
20
25
50
100


Weak vs Strong Convergence Rates
Convergence Rates
Realizations
Weak
Strong
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000

Demonstration: Rare events and metastability



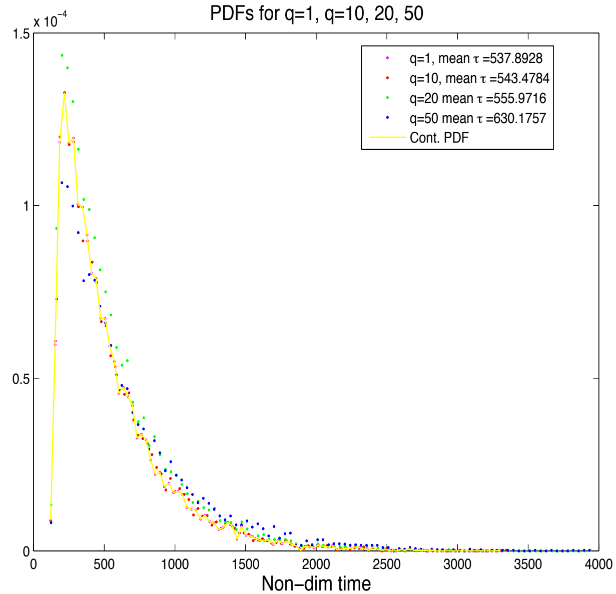
errctable

c_a	L	$q=5$	$q=10$	$q=20$
.07	100	.0591	.0733	.1134
	40	.0820	.0880	.1113
	20	.1508	.2214	.1832
.09	100	.0186	.0563	.0480
	40	.0678	.0749	.1064
	20	.1760	.1767	.1812
1	100	.0010	.0010	.0025
	40	.0036	.0040	.0054
	20	.0016	.0043	.0065

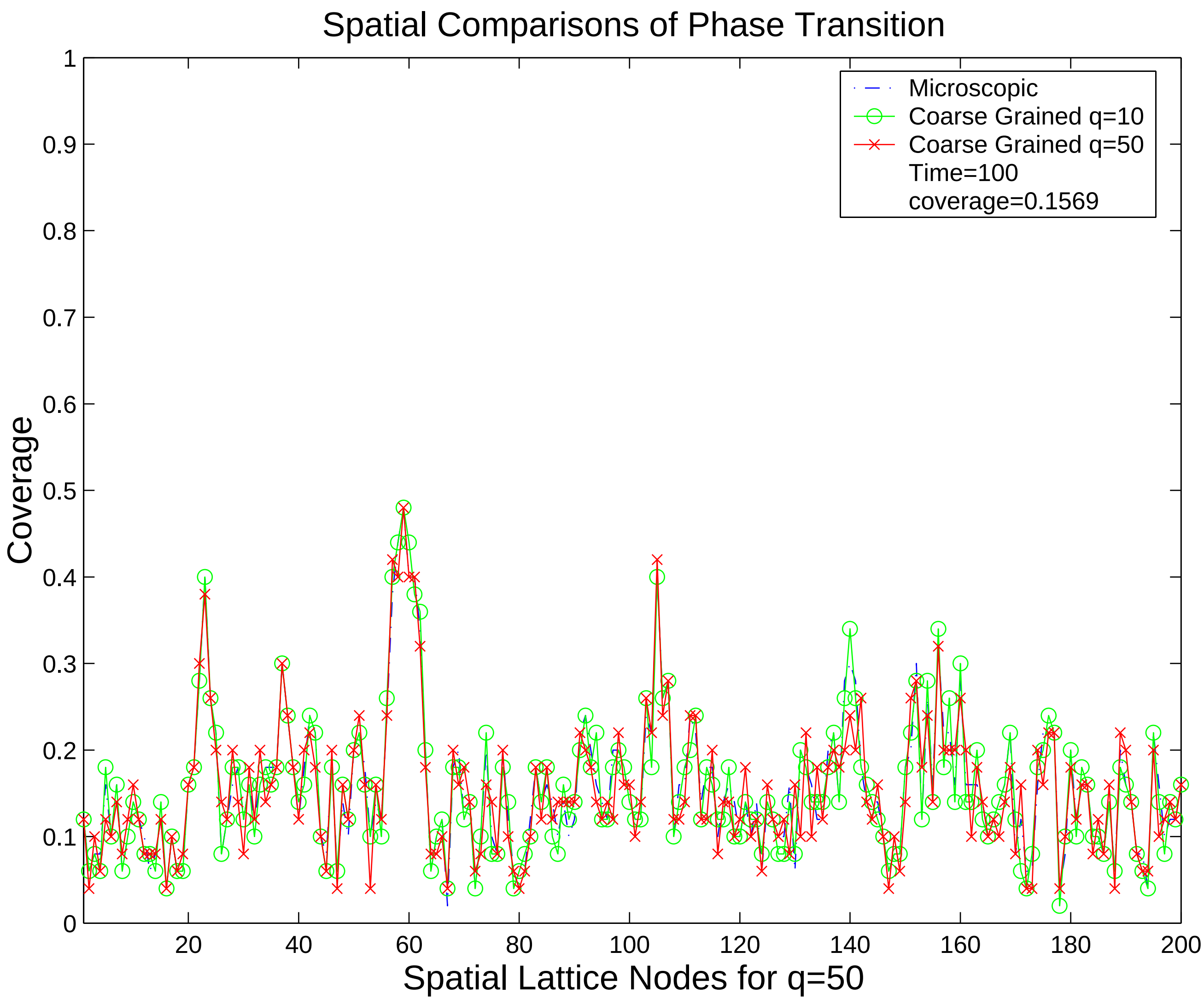
TABLE 7.2
Approximation of $\bar{\tau}_T$, $\mathcal{R}\left(\rho_\tau^q \mid \mathbf{T}_* \rho_\tau\right)$ and relative error.

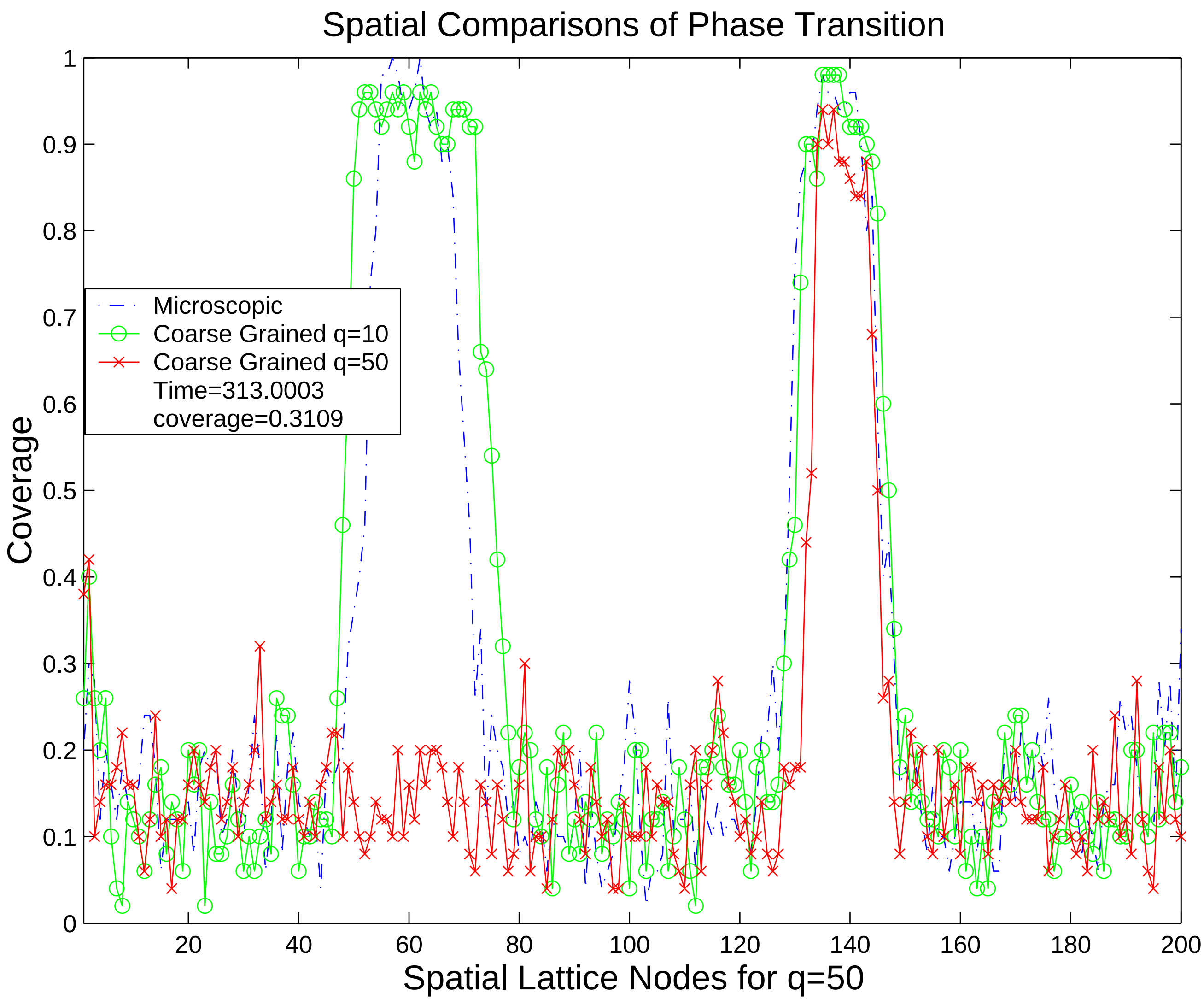
table21

L	q	$\bar{\tau}_T$	$\mathcal{R}\left(\rho_\tau^q \mid \mathbf{T}_*\rho_\tau\right)$	Rel. Err.	CPU [s]
100	1	532	0.0	0	309647
100	2	532	0.003	0.01%	132143
100	4	530	0.001	0.22%	86449
100	5	534	0.003	0.38%	58412
100	10	536	0.004	0.82%	38344
100	20	550	0.007	3.42%	16215
100	25	558	0.010	4.91%	7574
100	50	626	0.009	17.69%	4577
100	100	945	0.087	77.73%	345

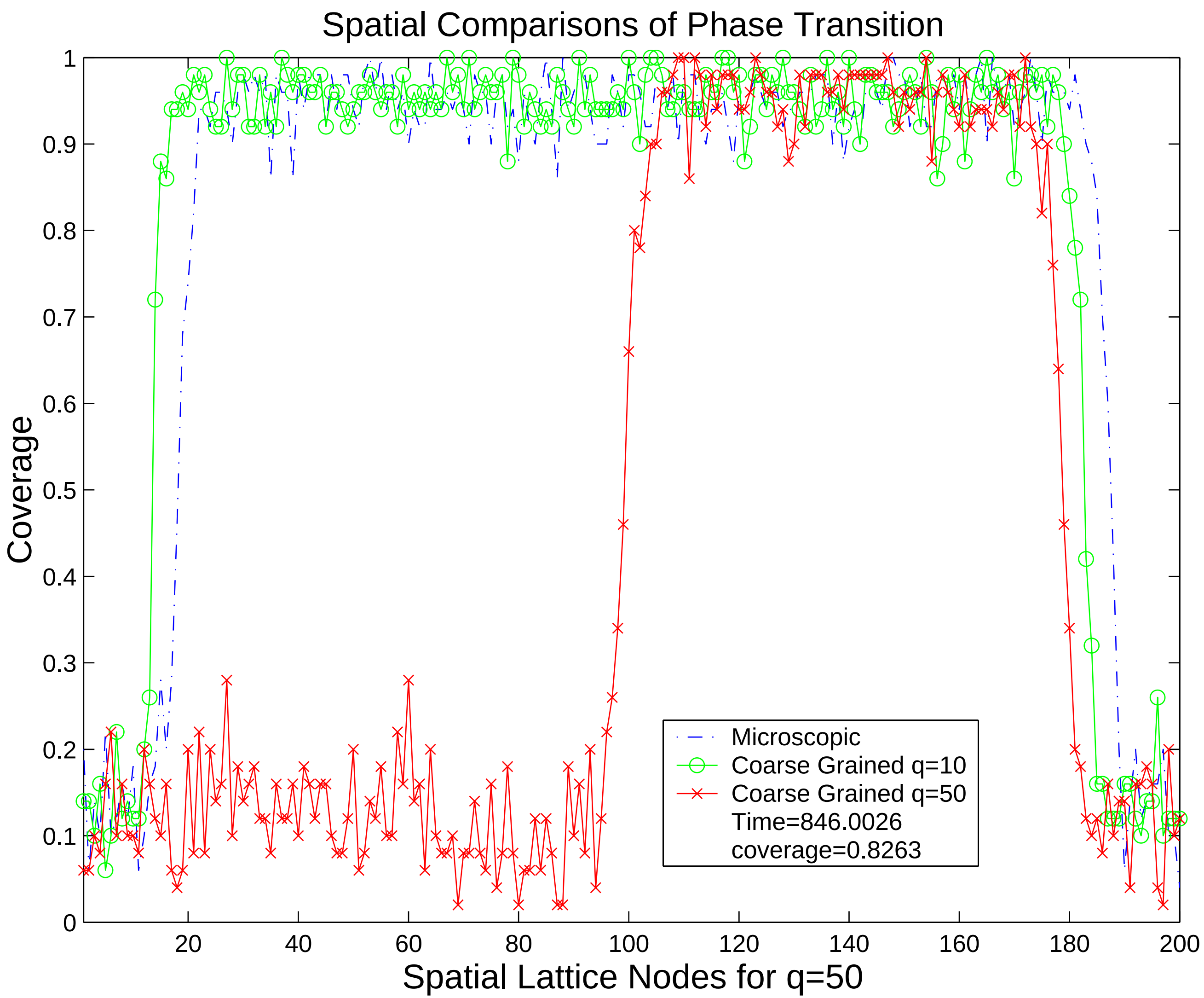


Probability Density Function (PDFs) comparisons between different coarse graining q. The mean times for each PDF are shown in the figures. All PDFs comprised of 10000 samples.


Spatial Comparisons of Phase Transition
Microscopic
Coarse Grained q=10
Coarse Grained q=50
Time=100
coverage=0.1569
Coverage
Spatial Lattice Nodes for q=50
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
20
40
60
80
100
120
140
160
180
200



Spatial Comparisons of Phase Transition
Coverage
Spatial Lattice Nodes for q=50
Microscopic
Coarse Grained q=10
Coarse Grained q=50
Time=313.0003
coverage=0.3109
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
20
40
60
80
100
120
140
160
180
200



Spatial Comparisons of Phase Transition
Coverage
Spatial Lattice Nodes for q=50
Microscopic
Coarse Grained q=10
Coarse Grained q=50
Time=846.0026
coverage=0.8263
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
20
40
60
80
100
120
140
160
180
200

Error Analysis III: beyond the interaction range?

[with Rey-Bellet, Plechac, Tsagkarogiannis]

Cluster expansions around the coarse Hamiltonian $\bar{H} = \bar{H}^0$

Higher-order corrections: multi-body interactions, relation to Renormalization Group calculations.

- explicit expressions for higher order corrections

$$\bar{H}^{(0)}(\eta) + \bar{H}^{(1)}(\eta) \dots \bar{H}^{(\alpha)}(\eta) + \mathrm{O}(\epsilon^{\alpha+1})$$

1. A priori error estimate

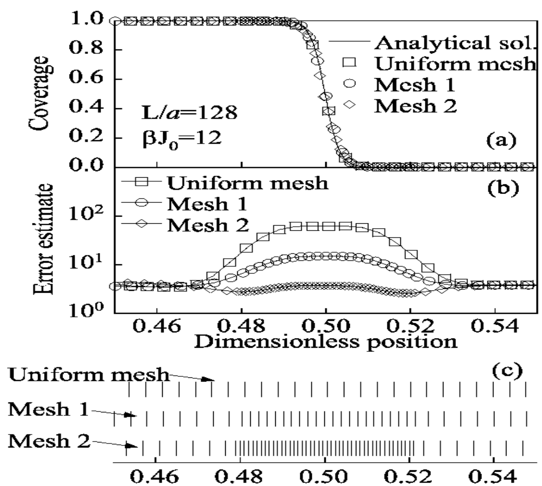
$$\frac{1}{N}\mathcal{R}\left(\bar{\mu}^{(\alpha)}_{M,q,\beta} \,|\, \mu_{N,\beta} o F\right) :=$$

$$\frac{1}{N}\sum_{\eta \in \mathcal{S}^c_{M,q}} \log\left(\frac{\mu^{(\alpha)}_{M,q,\beta}(\eta)}{\mu_{N,\beta}(\{\sigma \,|\, \mathbf{T}\sigma = \eta\})}\right) \mu^{(\alpha)}_{M,q,\beta}(\eta) = \mathrm{O}\left(\epsilon^{\alpha+2}\right) .$$

2. A posteriori error estimate–Adaptivity in CG

Cluster expansions → sharp a posteriori estimates for the relative entropy. The residuum operator $R(.)$ is given by the terms $\bar{H}^{(1)}$ and depends only on the coarse variable η:

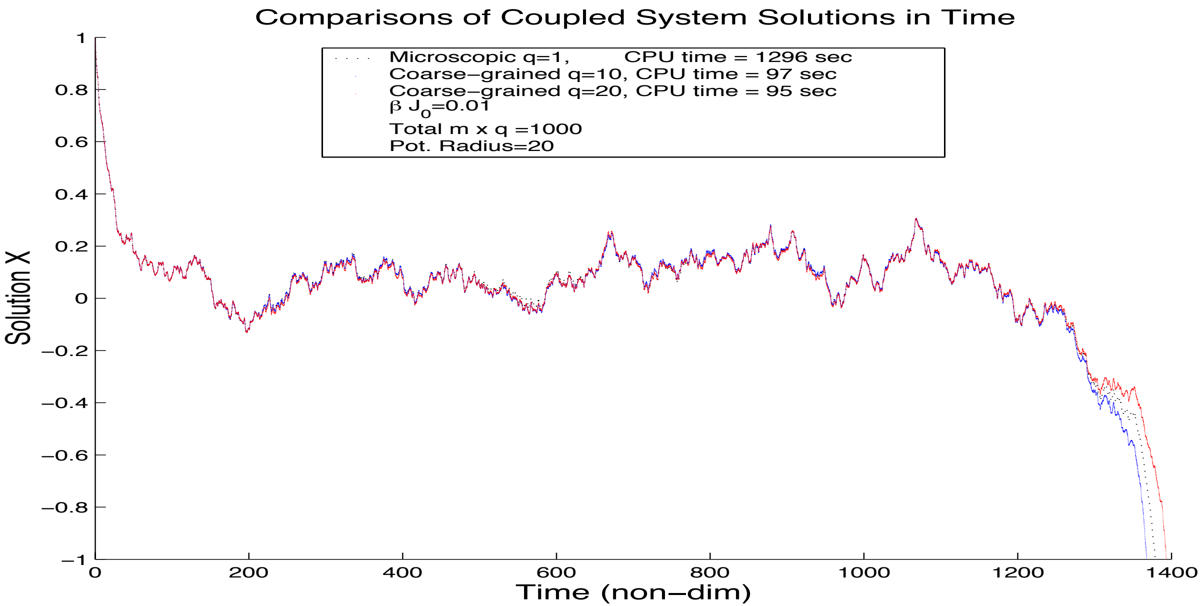
$$\mathcal{R}\left(\mu_{m,q}^{(0)} \,|\, \mu_N o F\right) = E_{\bar{G}^{(0)}}[R(\eta)] + \log\left(E_{\mu_{m,q}^{(0)}}[e^{R(\eta)}]\right) + O\left(\frac{q}{L}\right)^3$$



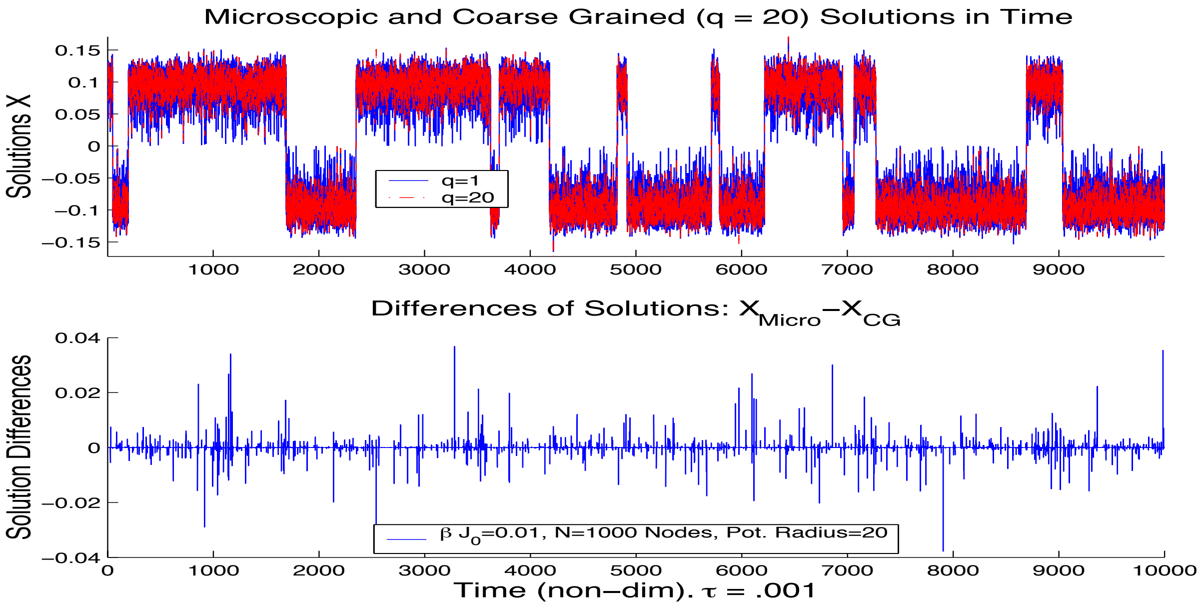
II. Stochastic coarse-graining in hybrid systems

Deterministic closures fail in long time intervals, or when phase transitions are present; revisit the earlier examples:

1. Blow-up:



2. Bistable ODE:



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

Fitzhugh-Nagumo type system; comparison of

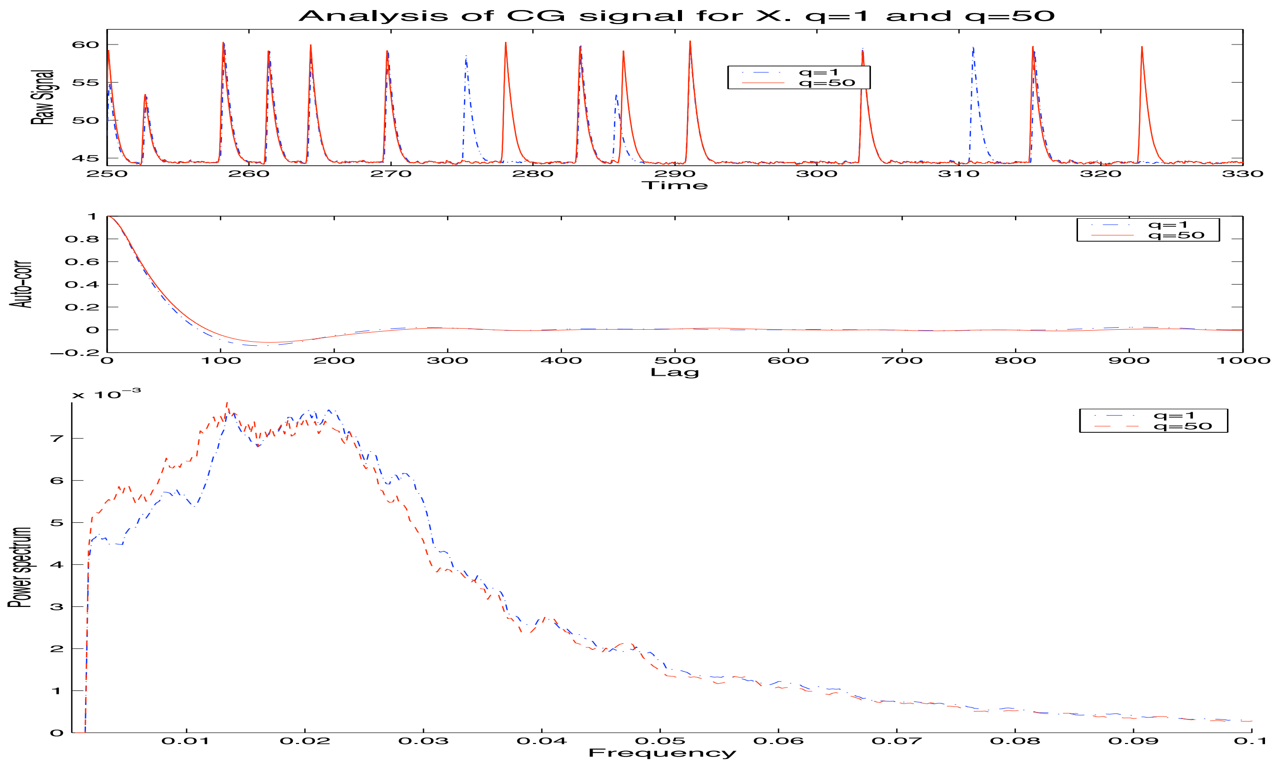
DNS of the hybrid system, $q = 1$

vs.

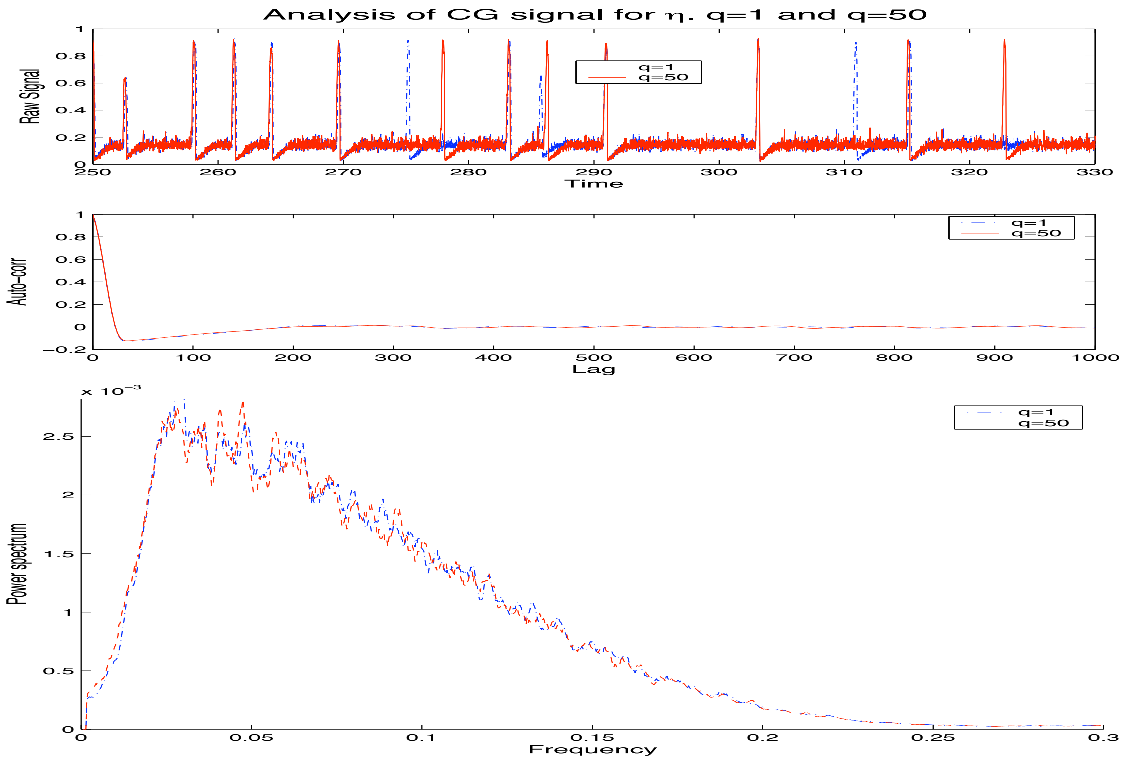
Coarse-Grainings $q = 50$

Space/Time time series analysis:

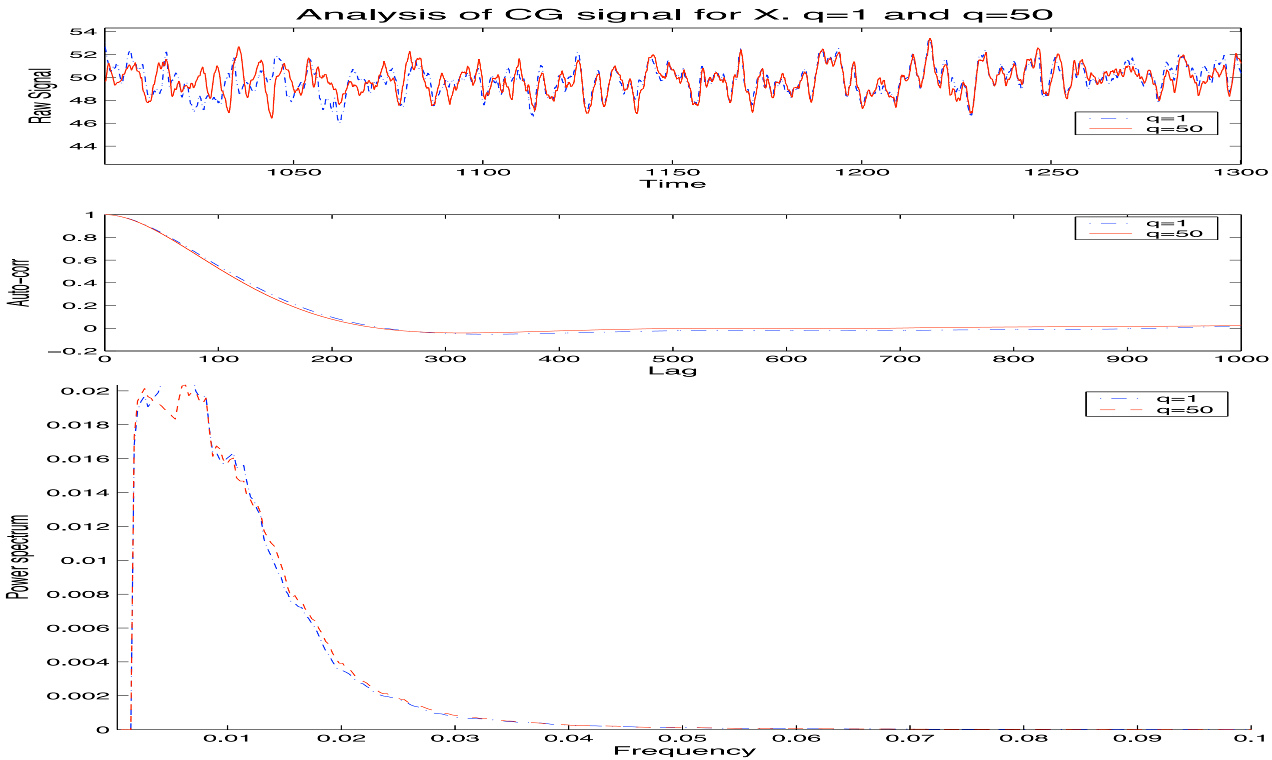
Excitable regime:



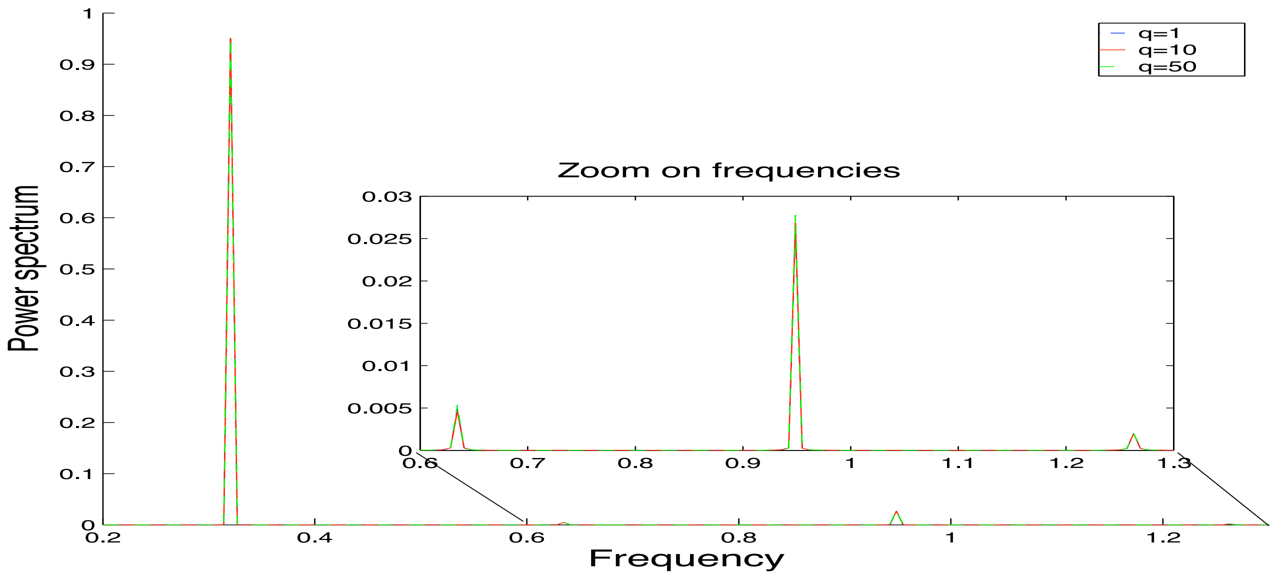
Excitable regime:



Oscillatory regime:



Oscilatory regime-Spatial Power Spectrum:



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