Mathematical and Computational challenges in Stochastic/Deterministic Hybrid Systems

Markos A. Katsoulakis

University of Massachusetts, Amherst

Joint work with:

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

Related work:

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

A. Szepessy(KTH, Sweden), J.Trashorras(Paris IX),

D. Tsagkarogiannis(UMass $\rightarrow$ MPI-Leipzig), D.G. Vlachos(Chem. Eng. Delaware)

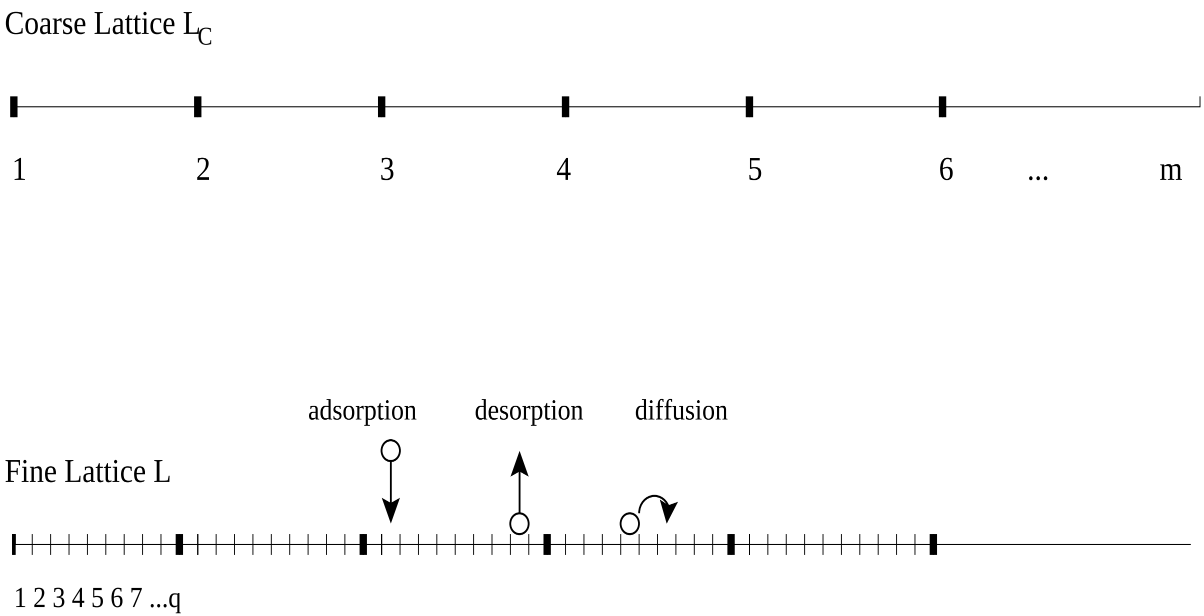
Some hybrid deterministic/stochastic systems

1. Microscopically active interface or boundary layer interacting with an adjacent "bulk" fluid phase.

2. Rheology of polymers: *micro-macro* models.

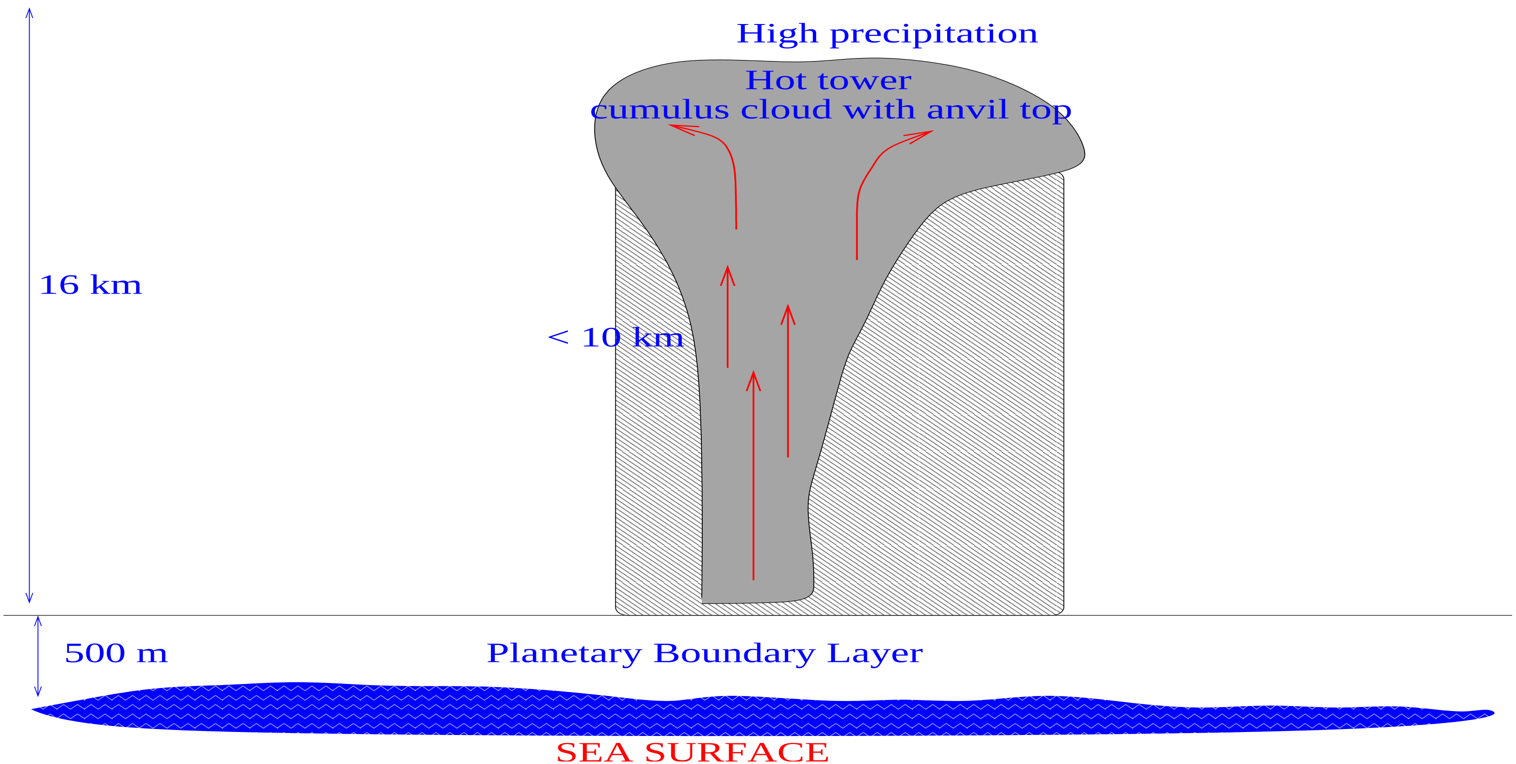
Fluids equations at the macroscopic level coupled with kinetic or stochastic equations ruling the evolution of the fluid microstructure at the meso- or micro- scale, e.g. FENE-type models or coupled Monte Carlo with fluid dynamics.

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



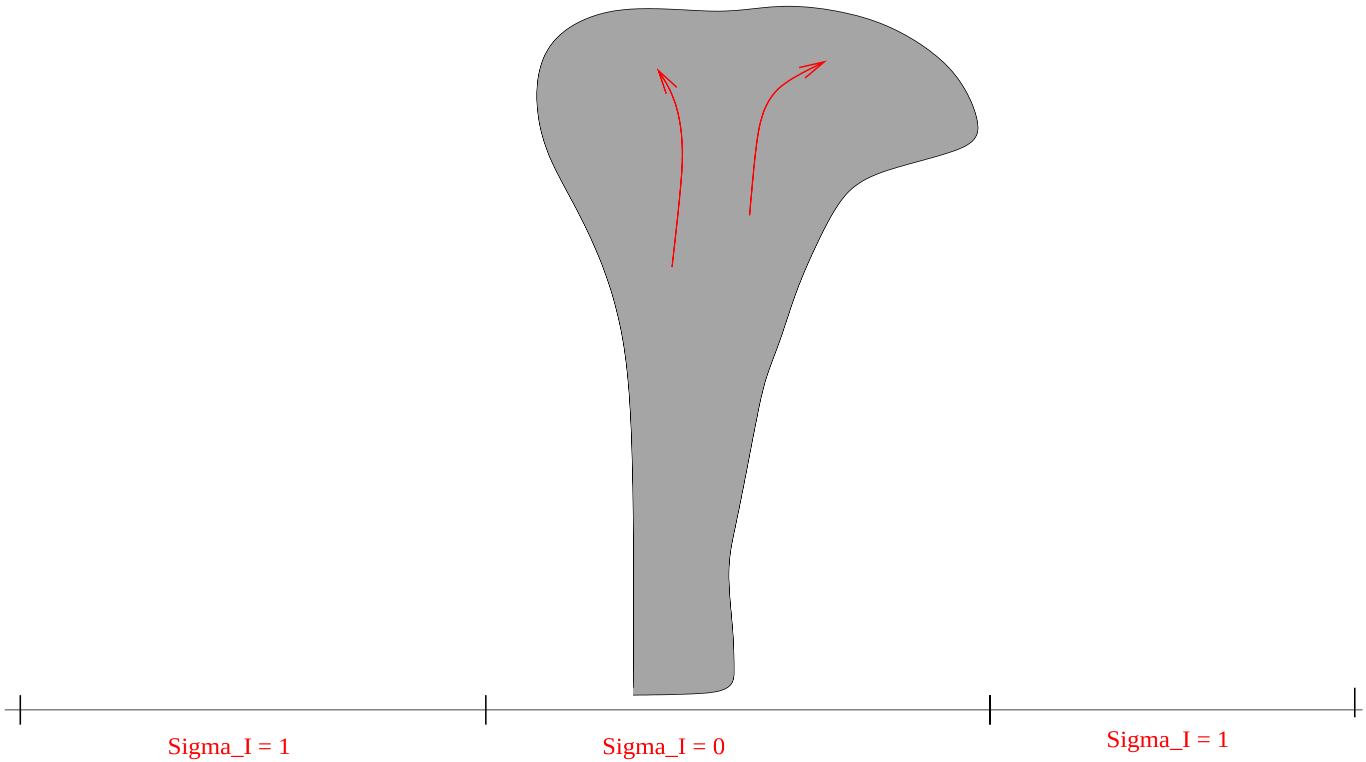
[Vlachos, Schmidt, Aris, J. Chem. Phys 1990]

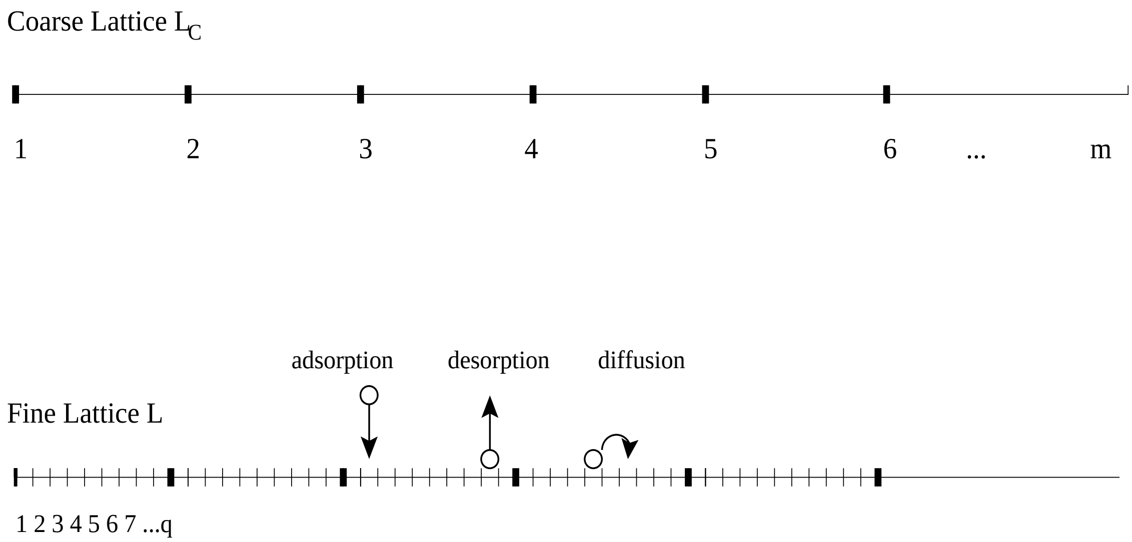
Atmosphere/Ocean applications: Tropical convection.



[Majda, Khouider, PNAS 2001]

“Particles” and sub-grid scale effects:





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

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

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 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

$$\partial_t X = f(X, \bar{\sigma}) \quad \text{(ODE)}$$

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

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

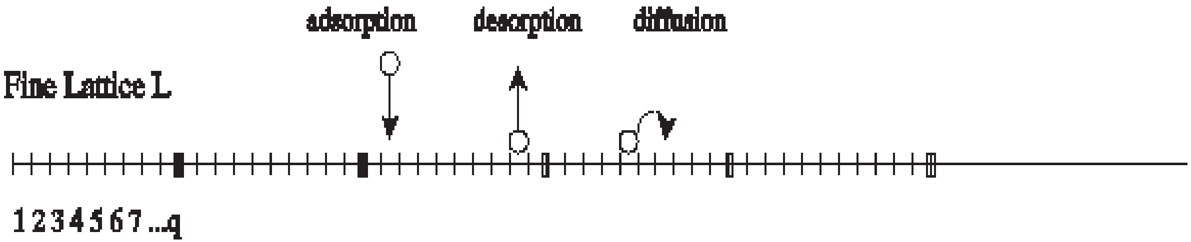
$f(x) = f(x, \bar{\sigma})$: scalar bistable, saddle node, or spatially homogeneous complex Ginzburg-Landau equation (Hopf bifurcations), etc.

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

Special case: well-mixed, CSTR reactors

[Vlachos et al, J. Chem. Phys 1990].

Arrhenius adsoprtion/desorption dynamics:



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

Jump rate: $c(x, \sigma, X) = c_0 \exp\Big[-\beta\Big(U_0 + U(x)\Big)\Big]$

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

$U_0(x) + U(x)$: Energy barrier a particle has to overcome in jumping from a lattice site to the gas phase.

- Interaction energy at x:

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

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

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

I. Deterministic closures

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

$$\partial_t X = f(X, \bar{\sigma}) \quad \text{(ODE)}$$

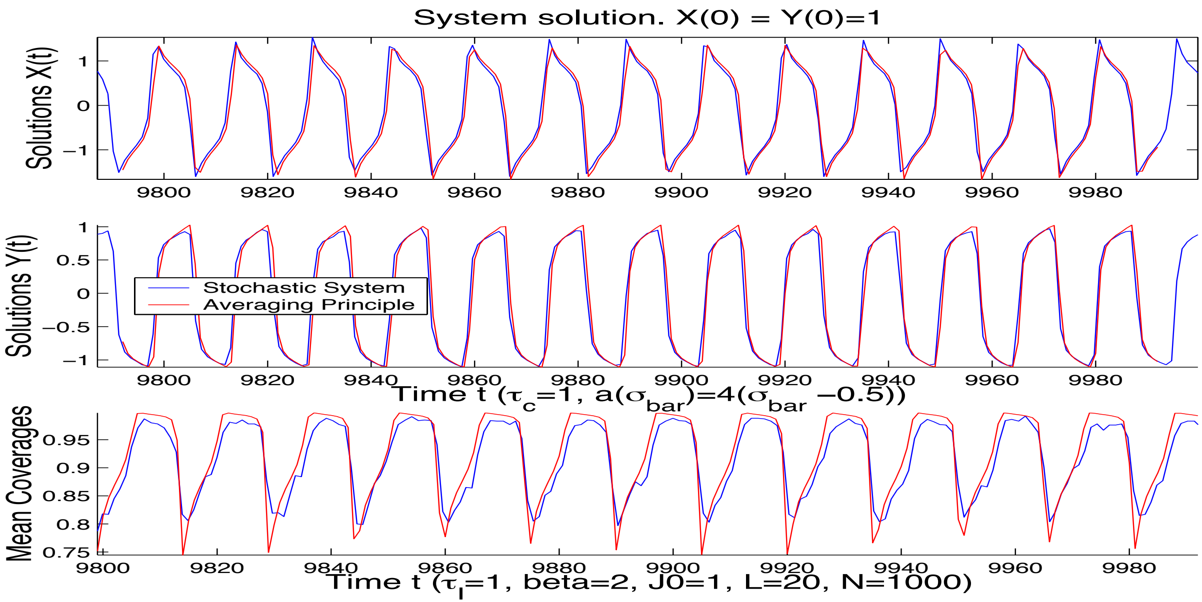
$$\partial_t E f(\sigma) = \frac{1}{\epsilon} E L_X f(\sigma) \quad \text{(stochastic lattice model)}$$

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

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

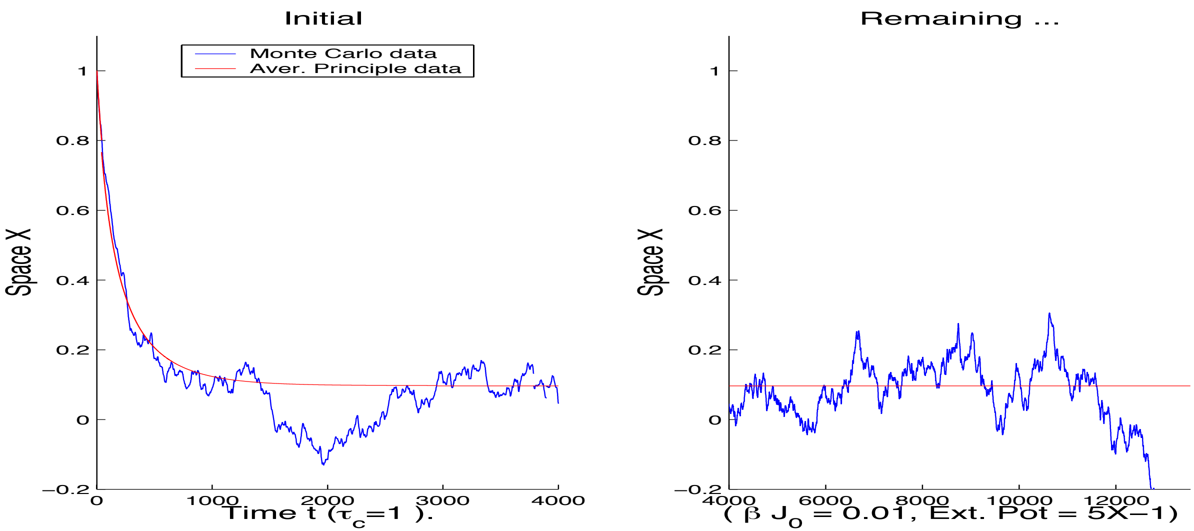
provided:

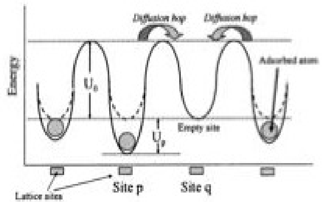
1. $\epsilon \ll 1$
2. No phase transitions in the microscopic model (i.e. weak interactions)
3. Finite time interval derivation.



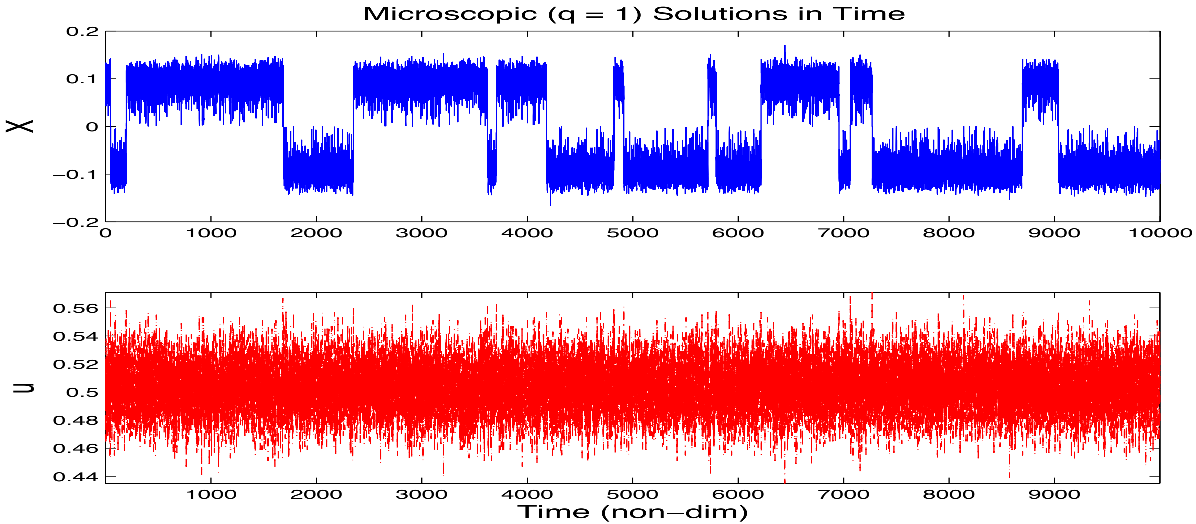
When stochastic fluctuations become important?

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





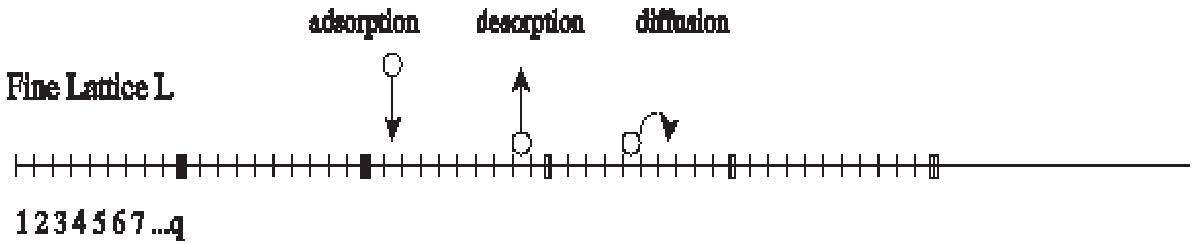
External ODE: $f(X,\sigma) = a(\bar{\sigma})X + \gamma X^3$, (Bistable)



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

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

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



Coarse observable (why this one?)

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

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

Step 1: From the microscopics:

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

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

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

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

• Determine the *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)

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

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

Birth-Death type process, with interactions.

Step 2: Ergodicity at every coarse level q:

Detailed balance for coarse Gibbs states:

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

Coarse-grained Hamiltonian

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

Coarse-grained prior distribution:

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

Error I–Loss of information during coarse-graining

[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,

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

where

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

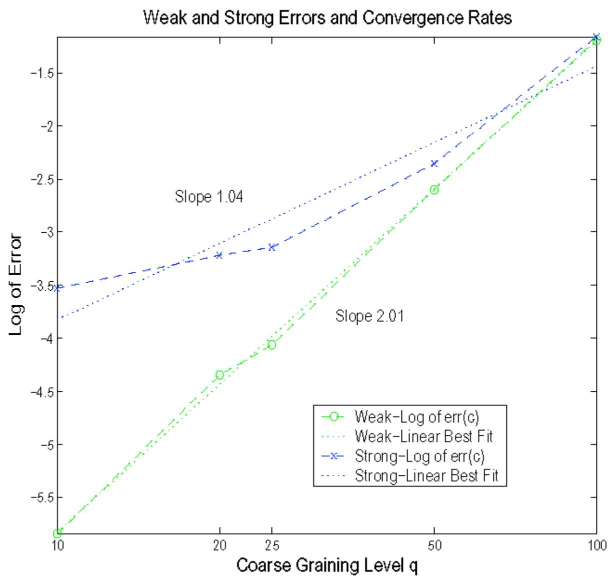
Information Theory interpretation: The relative entropy describes the increase in descriptive (in terms of a D-nary alphabet) complexity of a random variable due to "wrong information".

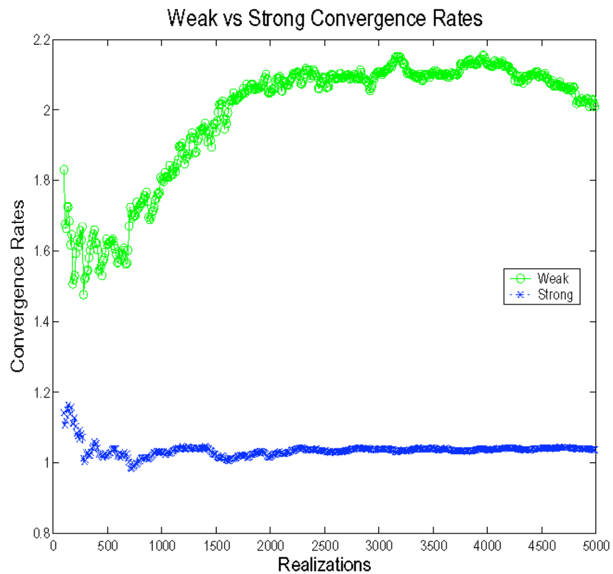
Elements of the proof:

1. Microscopic reconstruction from the coarse process, with controlled error.
2. Error estimation from coarse-graining of interactions & fluctuations.
3. Variational formulation of the relative entropy.

Error Analysis II

1. Improved order of convergence $O(q/L)^2$ using rigorous cluster expansions; **Higher-order corrections:** relation to RG.
2. Weak convergence estimates (easier to verify numerically).





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

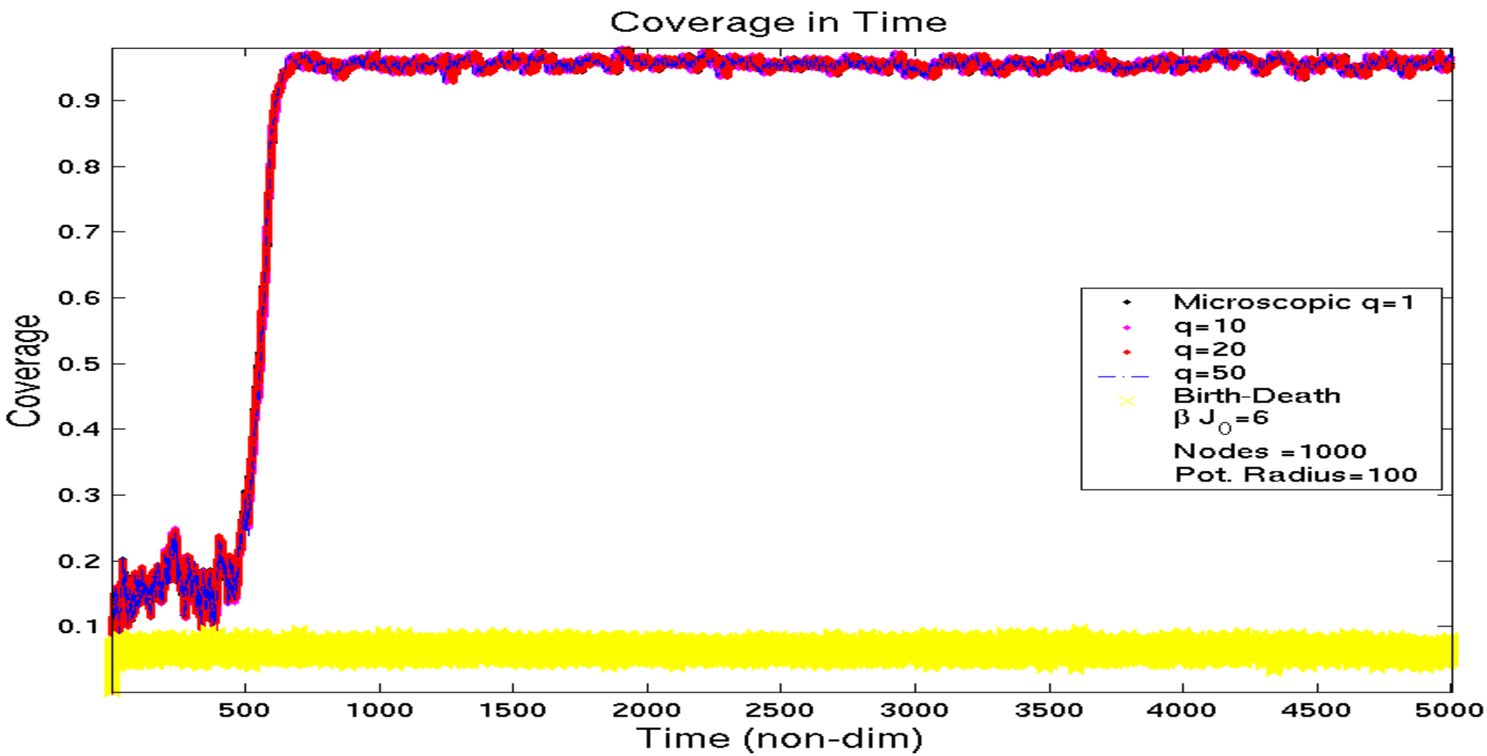
TABLE 7.2
Approximation of $\bar{\tau}_T$, $\mathcal{R}\left(\rho^q_\tau \mid \mathbf{T}_* \rho_\tau\right)$ *and relative error.*

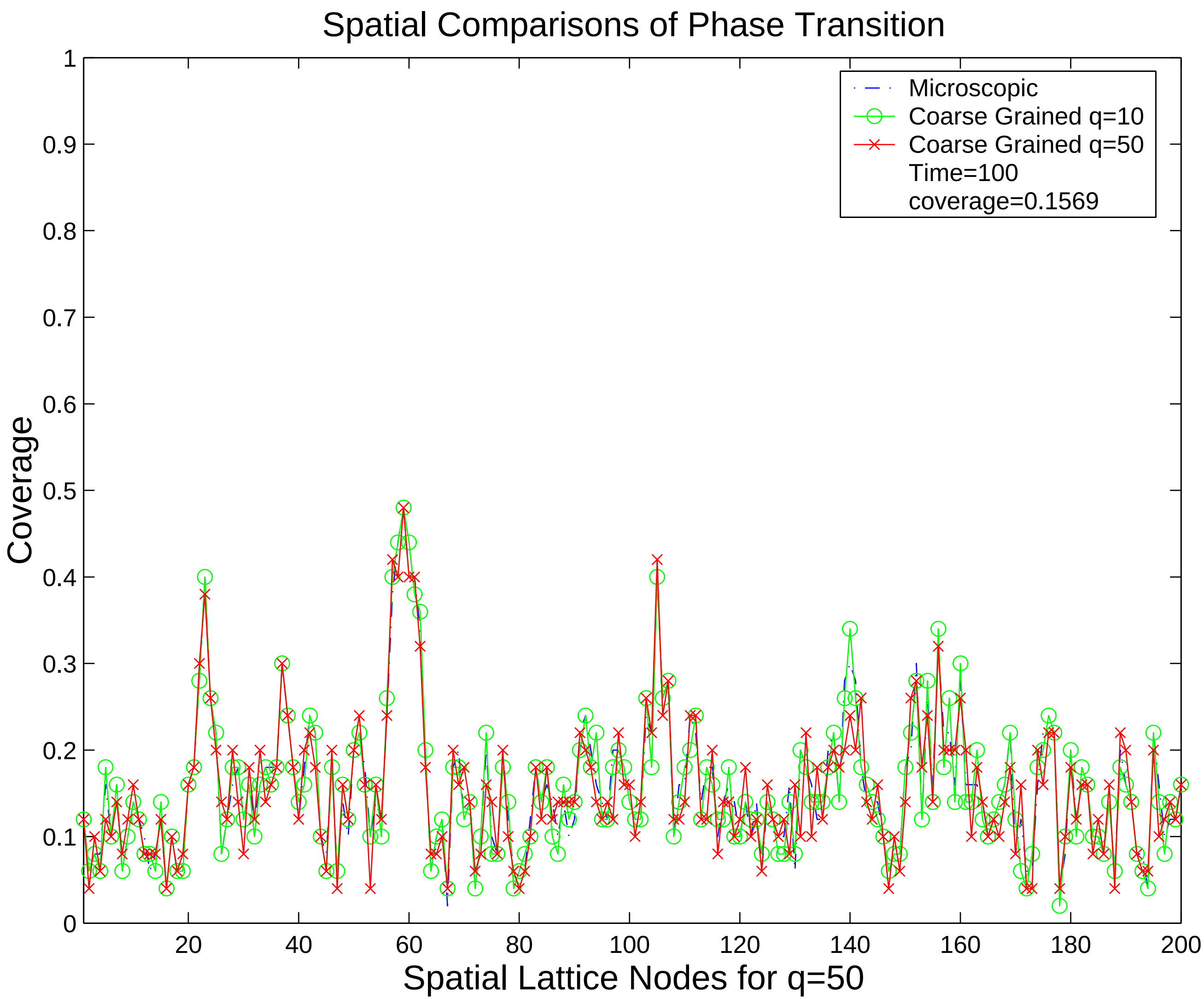
table21

L	q	$\bar{\tau}_T$	$\mathcal{R}\left(\rho^q_\tau \mid \mathbf{T}_* \rho_\tau\right)$	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

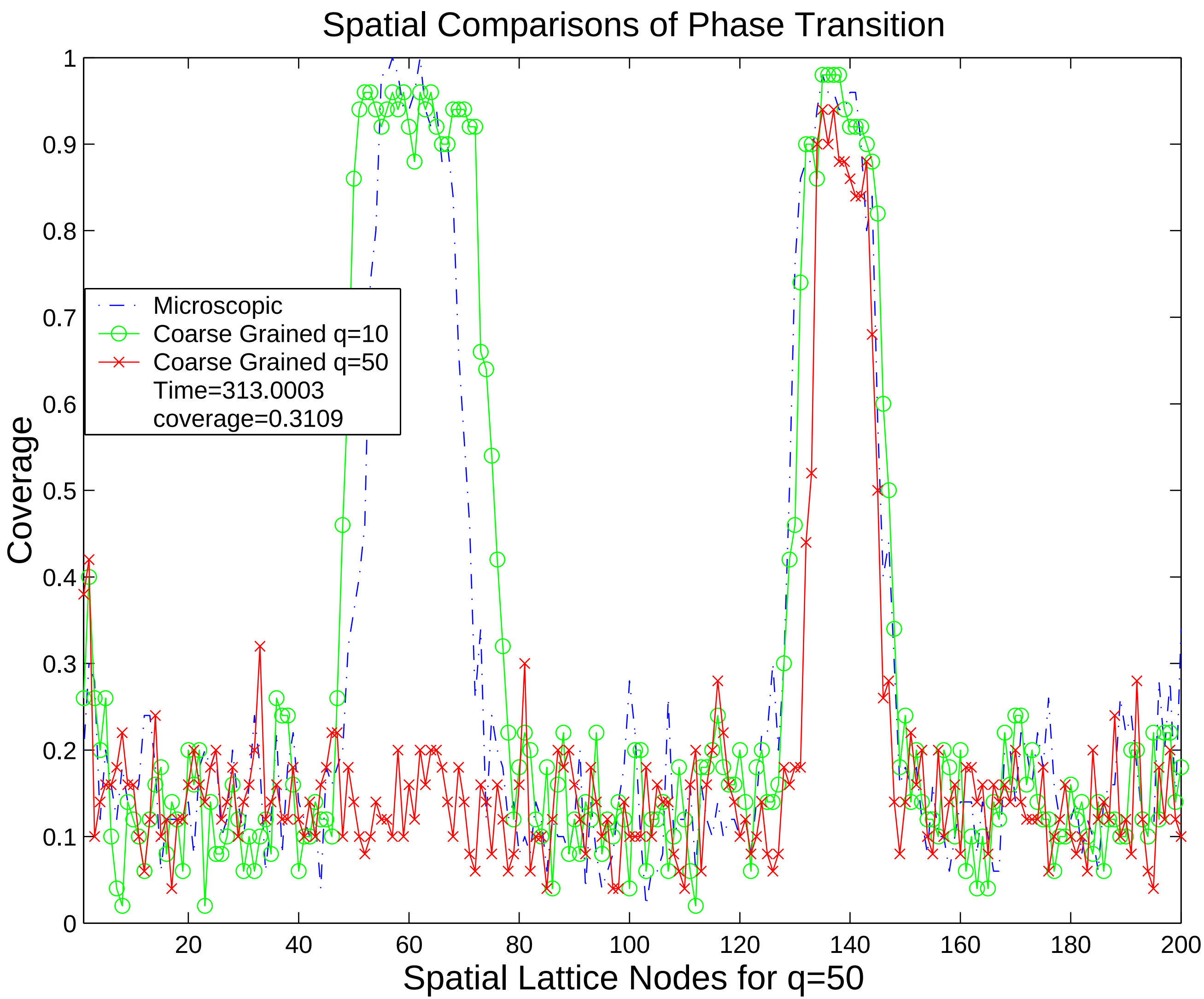
• CPU savings: at least $O(q^2)$ or more.

Demonstration: Rare events and metastability

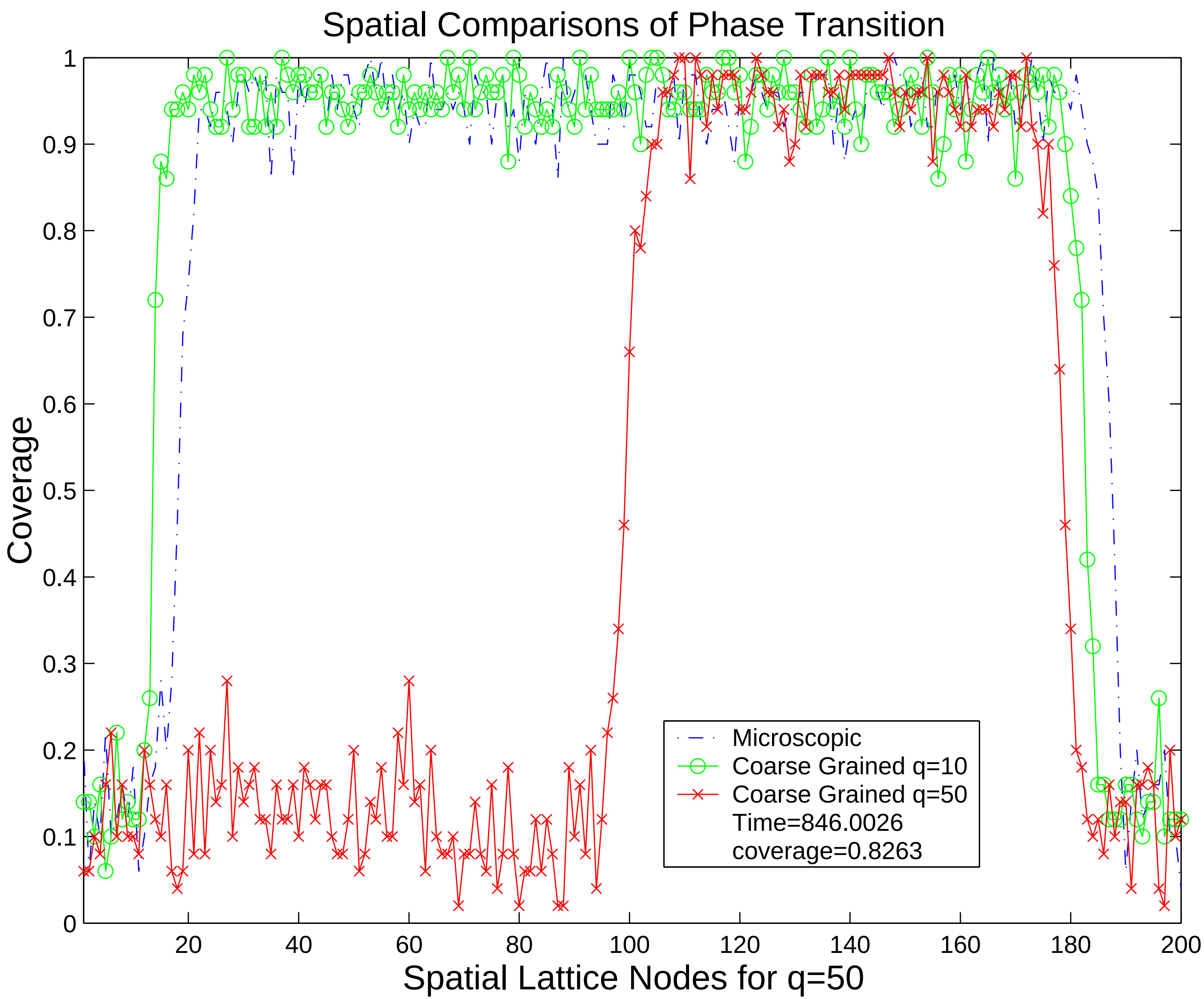




Spatial Comparisons of Phase Transition
Coverage
Spatial Lattice Nodes for q=50
Microscopic
Coarse Grained q=10
Coarse Grained q=50
Time=100
coverage=0.1569
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
20
40
60
80
100
120
140
160
180
200



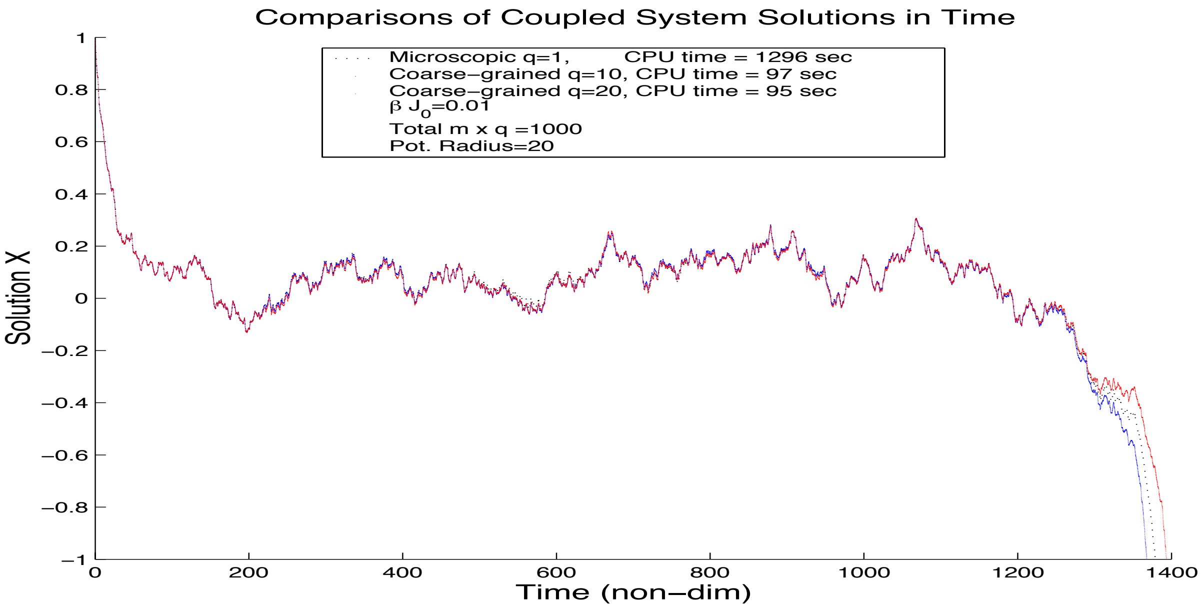
Spatial Comparisons of Phase Transition
Coverage
Spatial Lattice Nodes for q=50
Microscopic
Coarse Grained q=10
Coarse Grained q=50
Time=313.0003
coverage=0.3109
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
20
40
60
80
100
120
140
160
180
200


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

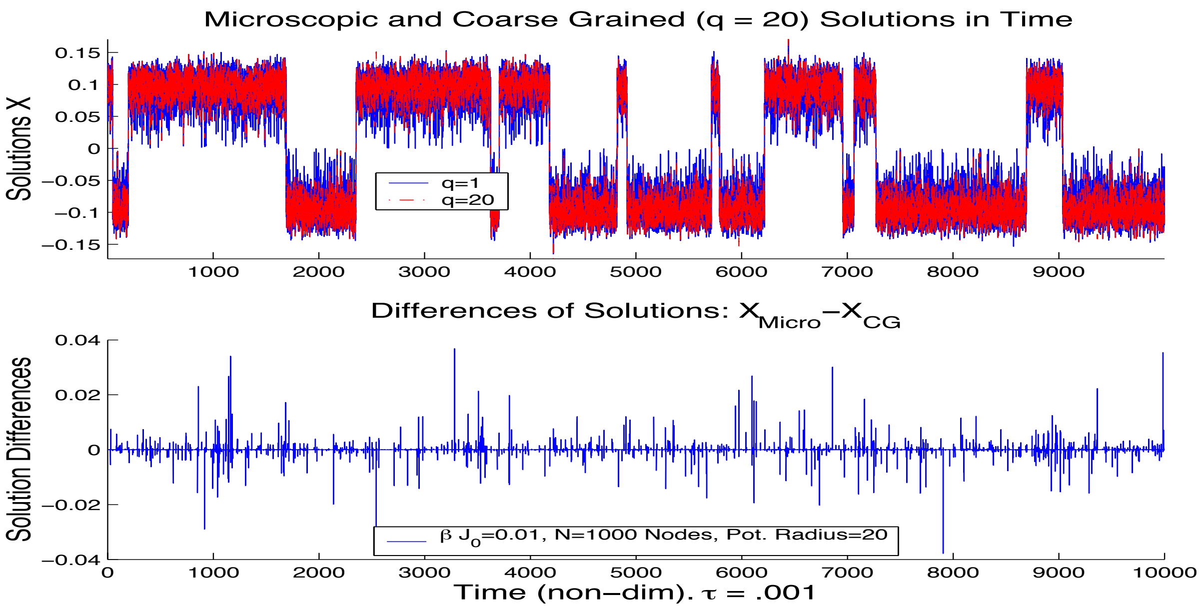
II. Stochastic coarse-graining in hybrid systems

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

1. Blow-up:



2. Externally-driven phase transitions:



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

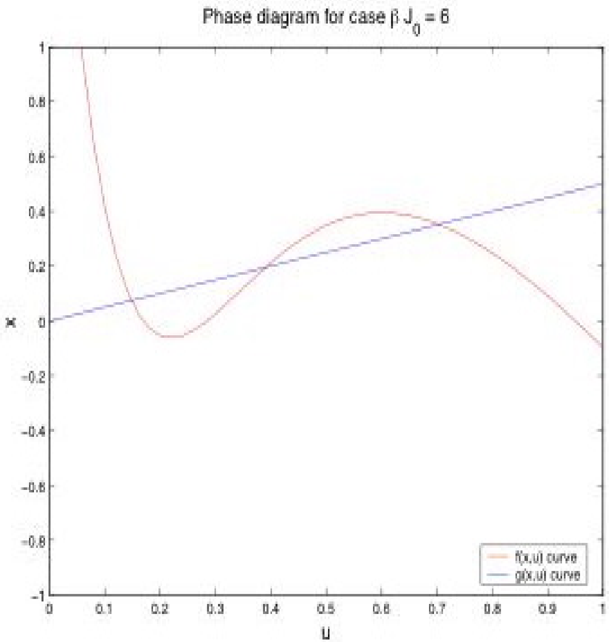
$$\frac{d}{dt}X = f(X, \overline{\sigma}) = a\bar{\sigma} + b - cX$$
$$\frac{d}{dt}Ef(\sigma) = E\mathcal{L}_X f(\sigma)\,, \quad h = h(X)$$

Step 1: mean field approximation (ODEs):

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

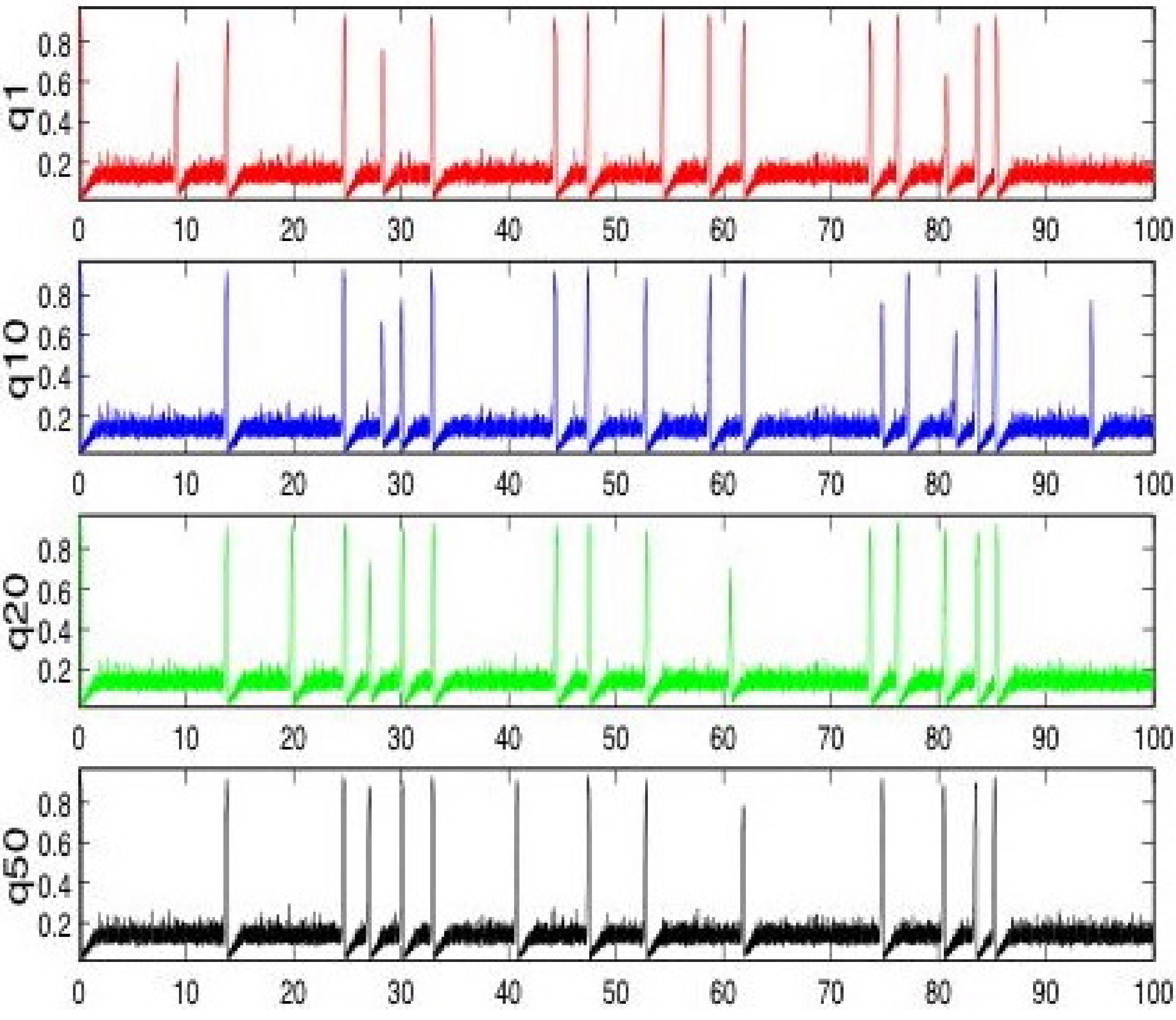
- one stable state (weak interactions J_0); stochasticity is not important
- bistable, excitable, oscillatory regimes (strong interactions)

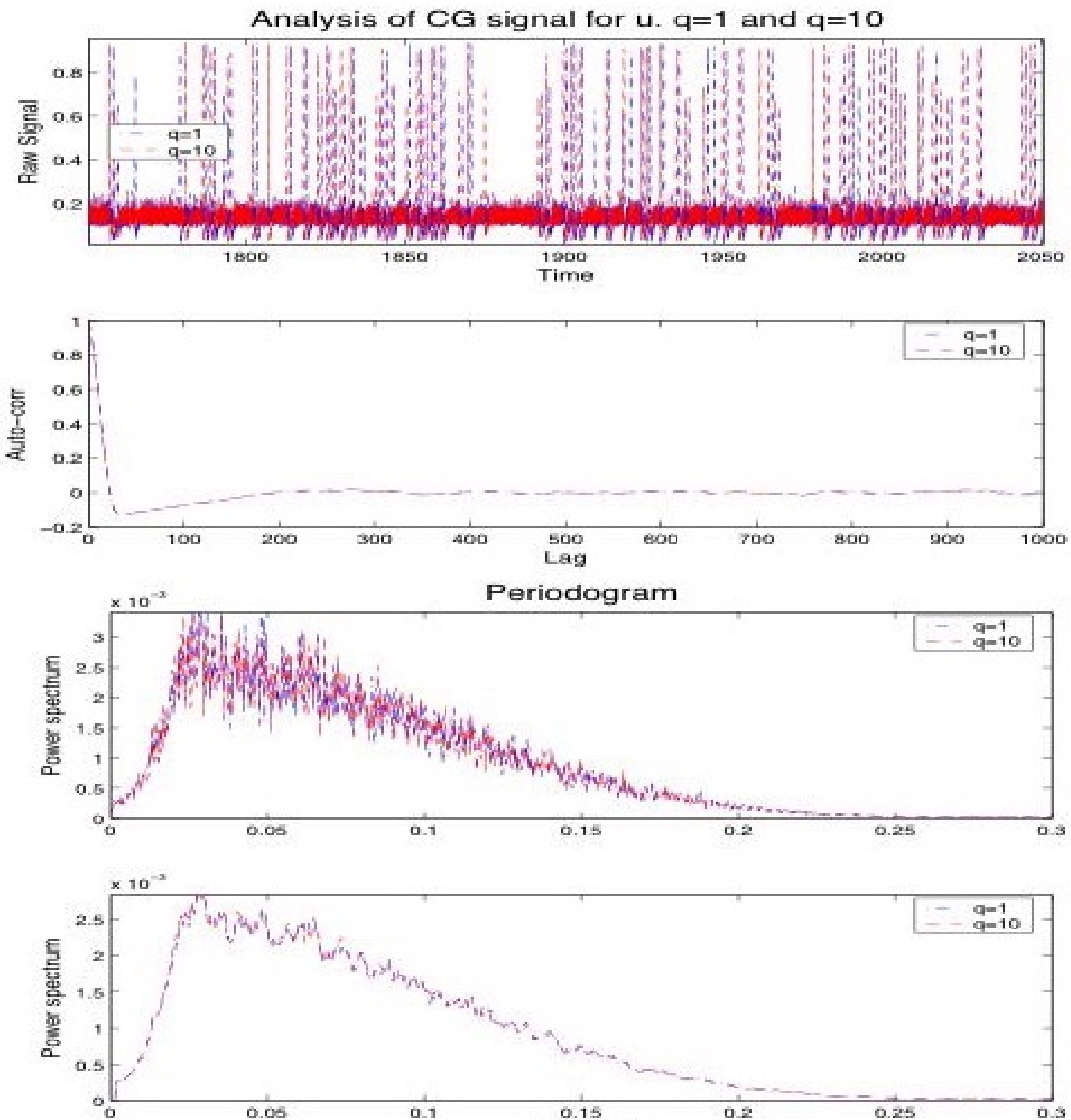
  Fitzhugh-Nagumo type system



Step 2: For the full hybrid system the mean field approx. suggests:

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


q1
q10
q20
q50
0.2
0.4
0.6
0.8
0
10
20
30
40
50
60
70
80
90
100


Analysis of CG signal for u. q=1 and q=10
Raw Signal
Time
q=1
q=10
Auto-corr
Lag
Periodogram
Power spectrum
x 10^-3

An even simpler toy hybrid model:

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

with uniform Curie-Weiss interactions: $J(x-y) = J_0$:

- Intermittency, bistability, (random) oscillations
- Due to the ODE coupling it is more susceptible to noise than the uncoupled spin flip Curie-Weiss.
- Asymptotics (law of large numbers, large deviations, central limit theorm) using the tools of the uncoupled system.

Hybrid Stochastic/Deterministic systems

1. Khouider, Majda, K., PNAS (2003).
2. K., Majda, Sopasakis, Comm. Math. Sci. (2004).

Coarse-grained models

1. K., Majda, Vlachos, J. Comp. Phys. (2003)
2. K., Majda, Vlachos, PNAS (2003).
3. K., Vlachos, J. Chem. Phys. (2003).
4. K., Plecháč, Tsagkarogiannis, J. Stat. Phys., (2005).

Adaptivity within the coarse-grained hierarchy

1. Chaterjee, K., Vlachos, Phys. Rev. E (2005).
2. Chaterjee, Vlachos, K., J. Chem. Phys. (2004).
3. Chaterjee, Vlachos, K., J. Chem. Phys. (2005). (*MC coarse-graining in time, binomial τ-leap*)