Hybrid couplings of small-scale systems to large-scale dynamics

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Hybrid deterministic/stochastic systems

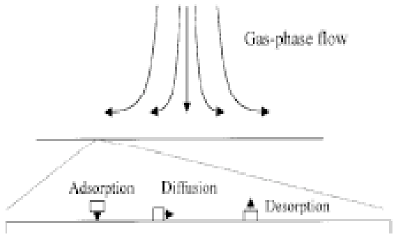
1. Microscopically active interface or boundary layer interacting with an adjacent "bulk" fluid phase.

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

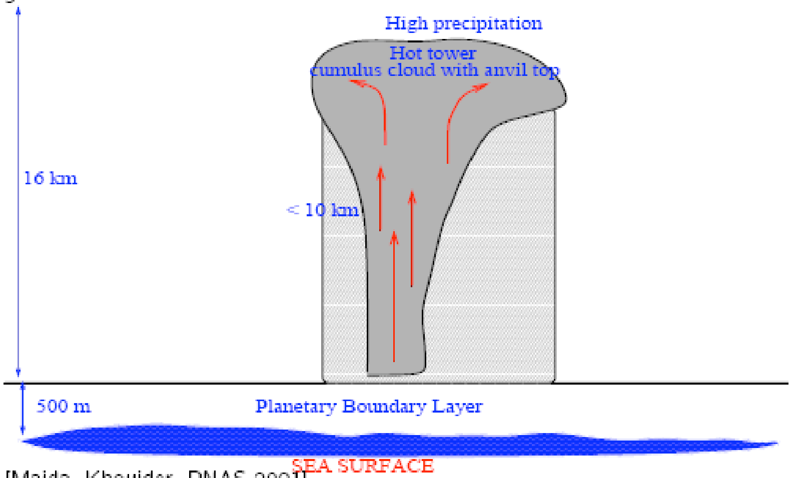
Fluids equations at the macroscopic level coupled with kinetic or stochastic equations ruling the evolution of the fluid microstructure at the meso- or micro- scale, e.g. FENE-type models or coupled Monte Carlo with fluid dynamics.

3. Stochastic Phase-Field models. Solidification, dendritic growth in alloys.

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

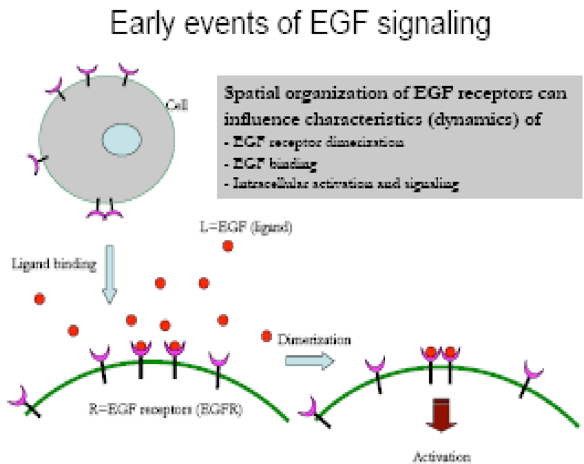


Atmosphere/Ocean applications: Tropical convection; sub-grid scale effects



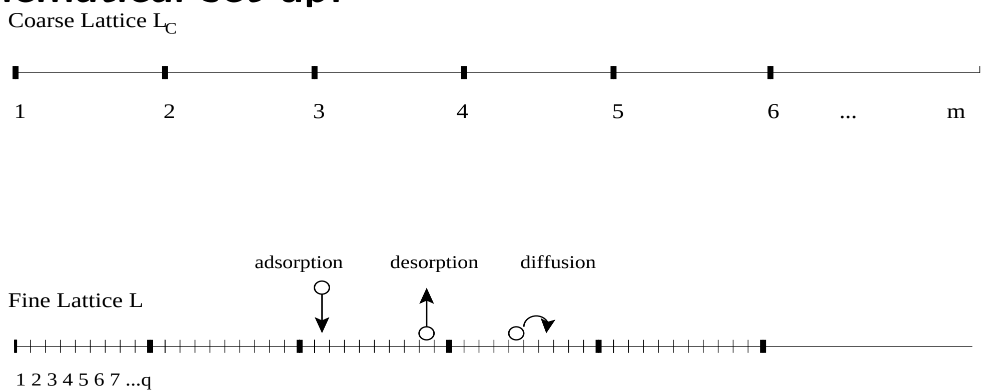
[Majda, Khouider, PNAS 2001],
[Khouider, Majda, Katsoulakis PNAS 2003].

Cell Biology: Epidermal Growth Factor binding/dimerization



"noisy" intercellular communication; synchronization

Mathematical set-up:



$$\begin{aligned} \partial_t X &= F[X,\sigma] \quad \text{(PDE/ODE system)} \\ \partial_t E g(\sigma) &= E L_X g(\sigma) \quad \text{(stochastic model)} \end{aligned}$$

X: Fluid/thermodynamic variables defined on top grid

L_X: generator of the subgrid stochastic process σ defined on the lower grid (subgrid). g: observable, σ: local coverage

Some challenges and questions:

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

- Model reduction: deterministic vs. stochastic closures; when is stochasticity important?

- In general there is no clear scale separation: need hierarchical coarse-graining.

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

- Stochastic boundary conditions

MODEL SYSTEM

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

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

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

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

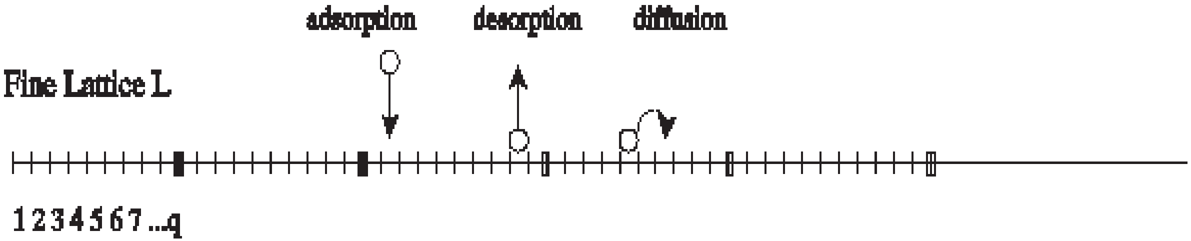
Two-way coupling:

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

Special case: well-mixed, catalytic reactors (CSTR)

M. Katsoulakis (UMass), A. Majda (Courant), A. Sopasakis (UMass) *Nonlinearity* (2006), *Contemp. Math.* (2007), ...

Stochastic lattice model: **Arrhenius** adsorption/desorption dynamics



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

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

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

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

ODE for the large scales:

$$\begin{aligned} \text{CGL:} \quad & f(\vec{X},\sigma) = (a(\bar{\sigma}) + i\omega)\vec{X} - \gamma|\vec{X}|^2\vec{X} + \widehat{\gamma}\vec{X}^* \\ \text{Bistable:} \quad & f(X,\sigma) = a(\bar{\sigma})X + \gamma X^3, \\ \text{Saddle:} \quad & f(X,\sigma) = a(\bar{\sigma}) + \gamma X^2, \\ \text{Linear:} \quad & f(X,\sigma) = a\bar{\sigma} + b - cX \end{aligned}$$

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

Later: Coupling via a stochastic boundary condition: balance of fluxes

I. Deterministic closures of hybrid systems

- Mean field approximations (one-point statistics)
- **Stochastic averaging** (time scale separation)

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

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

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

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

$\mu^x{}_{\text{equil}}$ ivariant (Gibbs) measure $\sim$ stoch. dynamics

Within framework of **Markov processes with two time scales**:

In math, Khasminskii, Kurtz, Papanicolaou,... In EE, Phillips and Kokotovic,... In AOS, Majda, Timofeyev, Vanden-Eijnden,...

Remarks

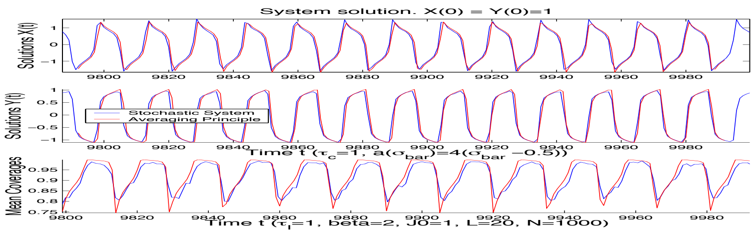
1. Theorem $\rightarrow \epsilon \ll 1$; how big can we take ϵ?

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

   • Analytical calculations for special cases; can also be pre-computed? (not really...)

   • On-the-fly comput.approach: W. E and B. Engquist (HMM); Y. Kevrekidis (Equation Free)

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



However...

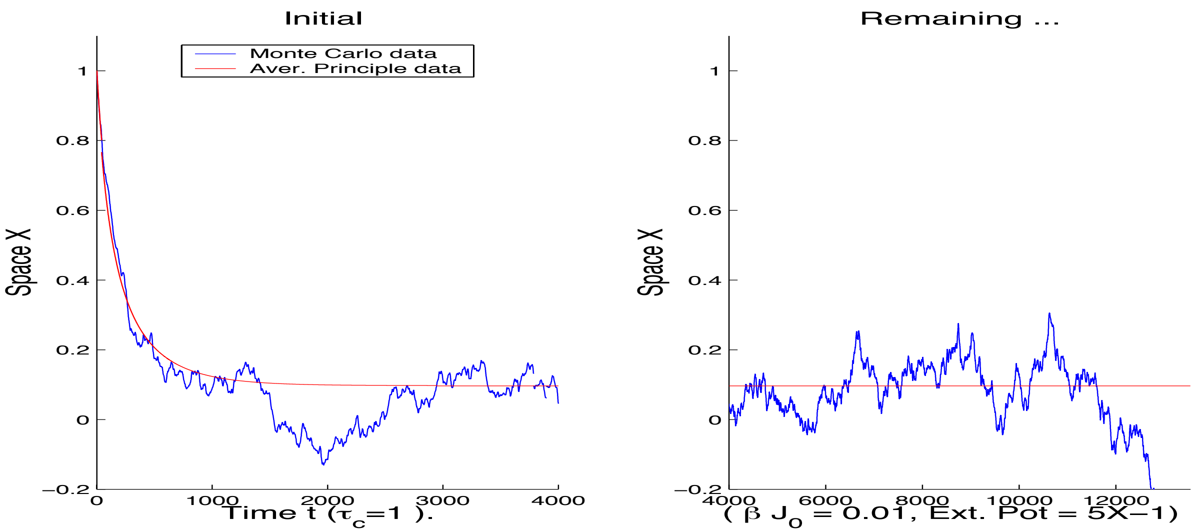
3. Finite time interval derivation [0, T] for averaged equations:

$$\max_{t \in [0,T]} \|X^\epsilon(t) - X_{\mathsf{avg}}(t)\| = C_T o_\epsilon(1)$$

   large deviations from the averaged equation at long-time intervals [Freidlin-Wentzell for SDE].

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

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



Phase transitions in hybrid systems: strong particle/particle interactions

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

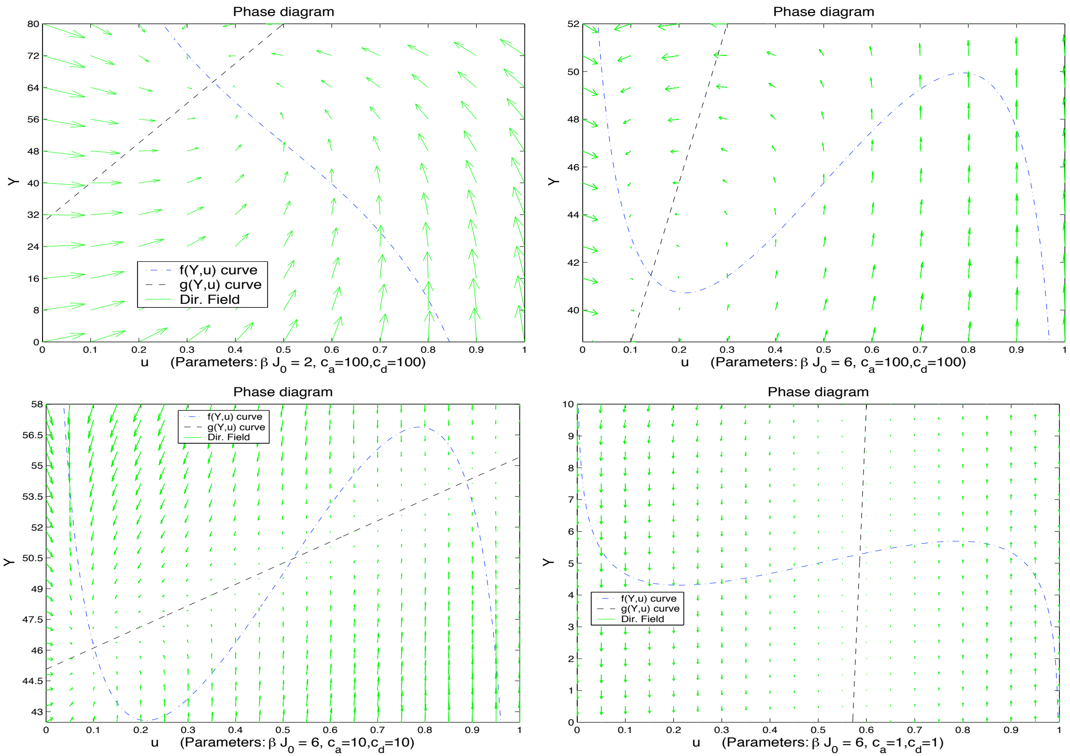
Step 1: mean field approximation (one-point statistics):

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

- one stable state (weak interactions); stochasticity is not important

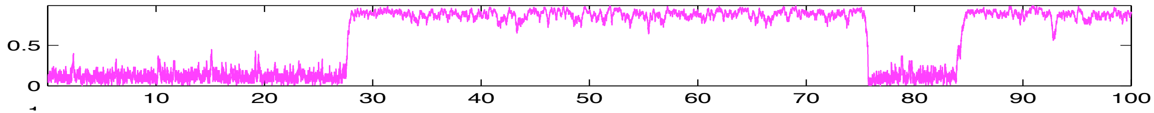
- bistable, excitable, oscillatory regimes (strong interactions)

  Fitzhugh-Nagumo type system

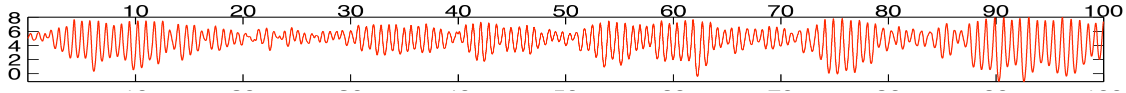


Step 2: Mean field approx. suggests:

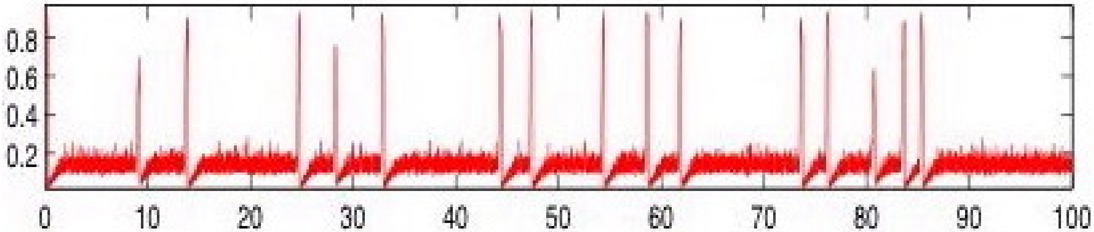
Bistability $\longrightarrow$ random switching.



Oscillatory regime $\longrightarrow$ random oscillations



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

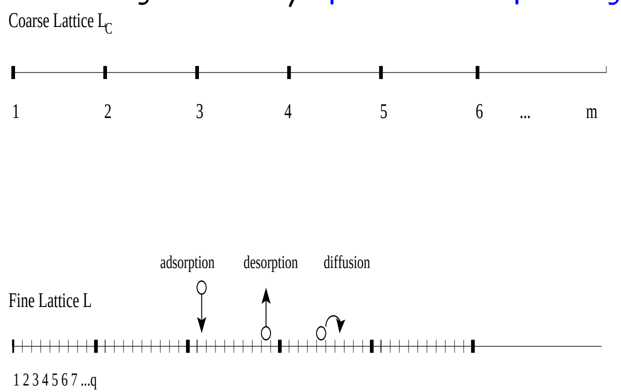


a. Need model reduction through suitable closure.

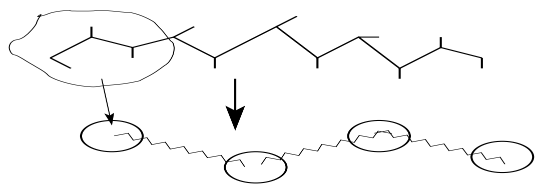
b. Deterministic vs. stochastic closures; stochasticity can be important.

Coarse-Graining (*and reconstruction*) of extended microscopic particle systems

1. Stochastic lattice dynamics/spatial adaptivity in KMC



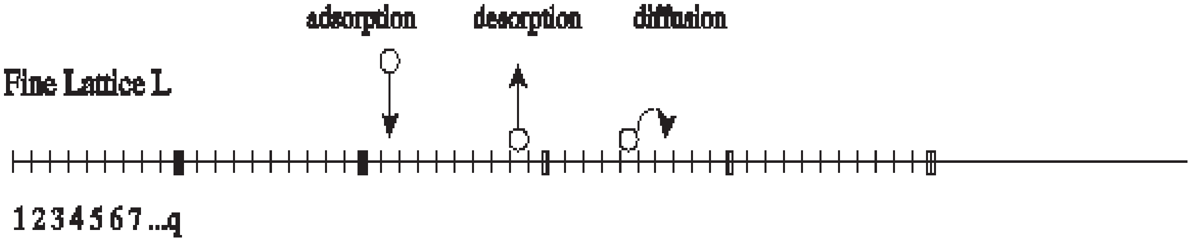
2. Coarse-graining of polymers.



Microscopics $\mapsto$ CG system $\mapsto$ Reconstructed Microscopics

Hierarchical coarse-graining of stochastic processes

Construct a **stochastic process** for a hierarchy of "mesoscopic" length or time scales that includes fluctuations properly.



Coarse observable (why this one?)

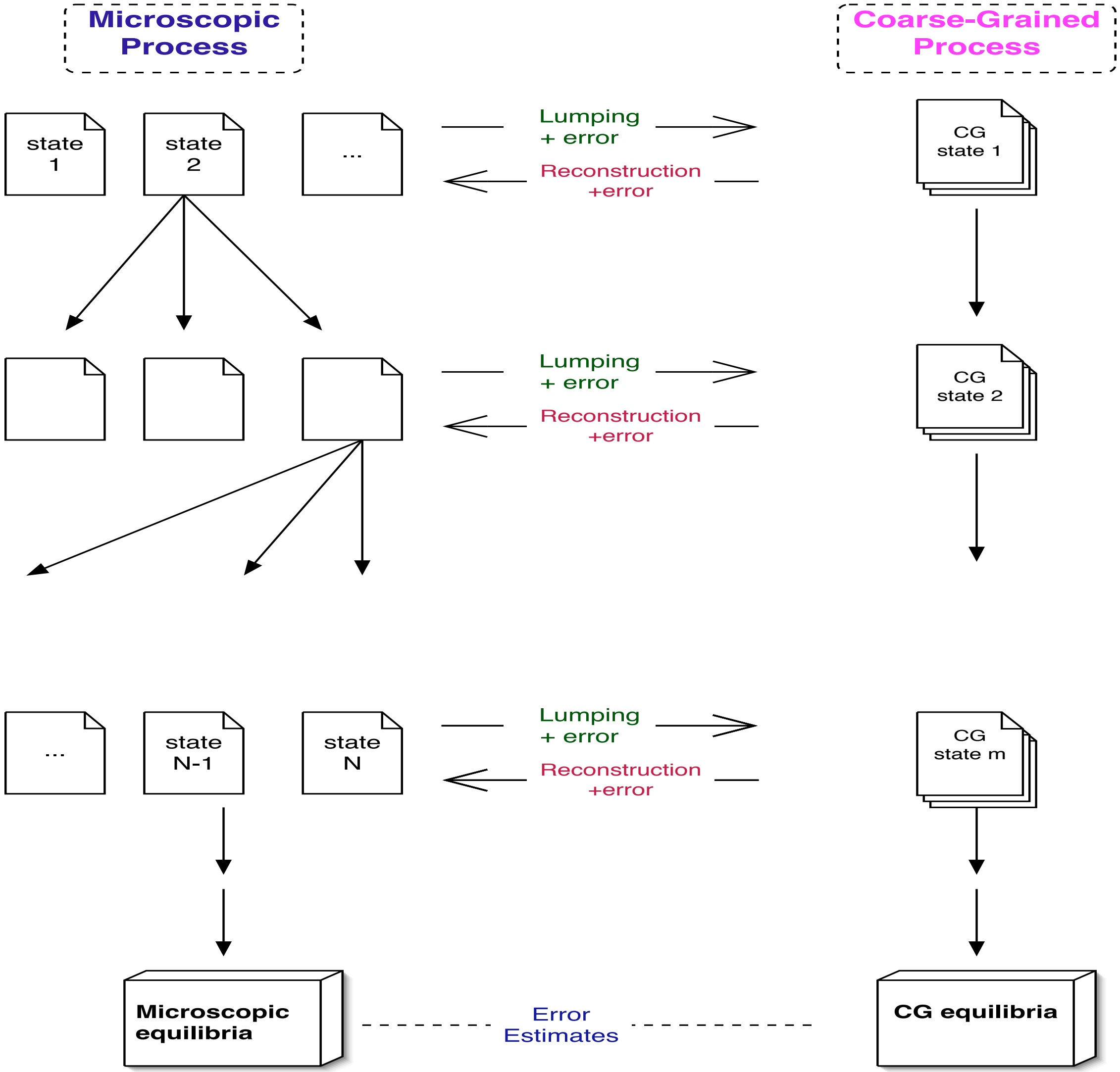
$$\eta_t(k) = \mathbf{T}\sigma_t(k) := \sum_{y \in D_k} \sigma_t(y)$$

In general it is **non-markovian**

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

[K., Majda, Vlachos, PNAS (2003)]

[K., Plechac, Sopasakis, SIAM Num. Analysis (2006)]


Microscopic Process
Coarse-Grained Process
state 1
state 2
...
Lumping + error
Reconstruction +error
CG state 1
Lumping + error
Reconstruction +error
CG state 2
...
state N-1
state N
Lumping + error
Reconstruction +error
CG state m
Microscopic equilibria
Error Estimates
CG equilibria

Error I–Loss of information during coarse-graining

[K., José Trashorras (Paris IX), *J. Stat. Phys.* (2006)]

- $\mu_{m,q,\beta}(t)$: 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,

$$\mathcal{R}\left(\mu_{m,q,\beta}(t) \,|\, \mu_{N,\beta} o F(t)\right) = O_T(\epsilon^2)\,, \quad t \in [0, T]$$

where

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

and the "small" parameter ϵ is

$$\epsilon \equiv C\beta \frac{q}{L} \|V'\|_\infty$$

Information Theory interpretation The relative entropy describes the increase in descriptive complexity of a random variable due to "wrong/incomplete information".

Mathematical Difficulty: $\mathbf{T}\sigma_t(k) = \sum_{y \in D_k} \sigma_t(y)$. is not a Markov process–has "memory"

Elements of the proof:

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

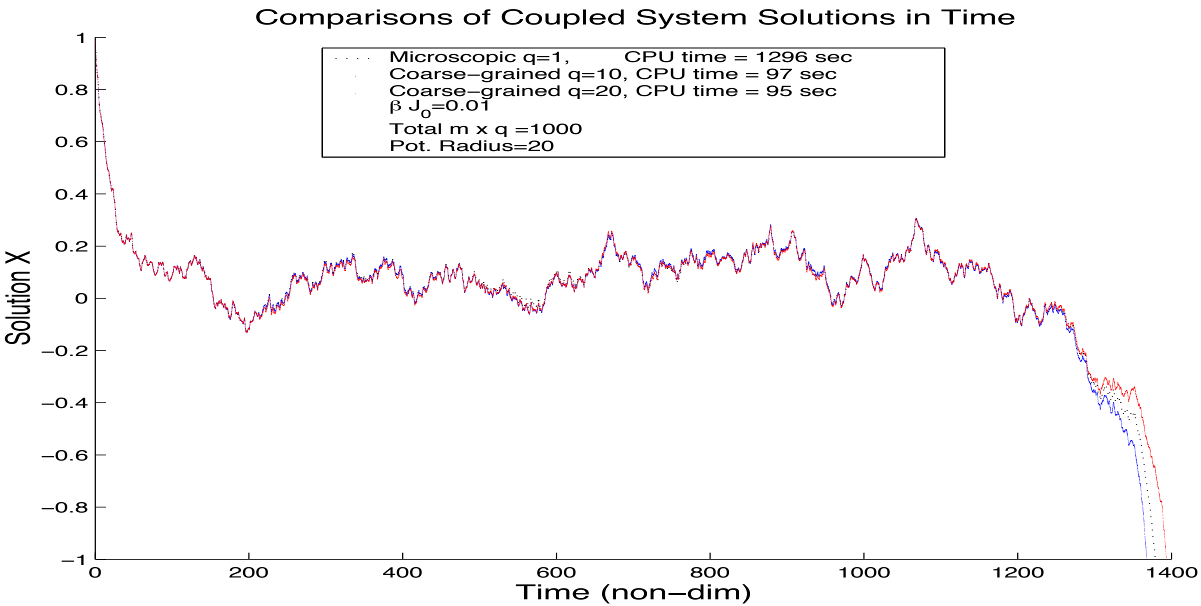
- $\mathbf{T}(\gamma_t)_{t \geq 0}$ and $(\eta_t)_{t \geq 0}$ have the same distribution
- Since σ_t, γ_t are Markov, the Radon-Nikodym derivative of their distributions is:

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

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

Fitzhugh-Nagumo type system; comparison of

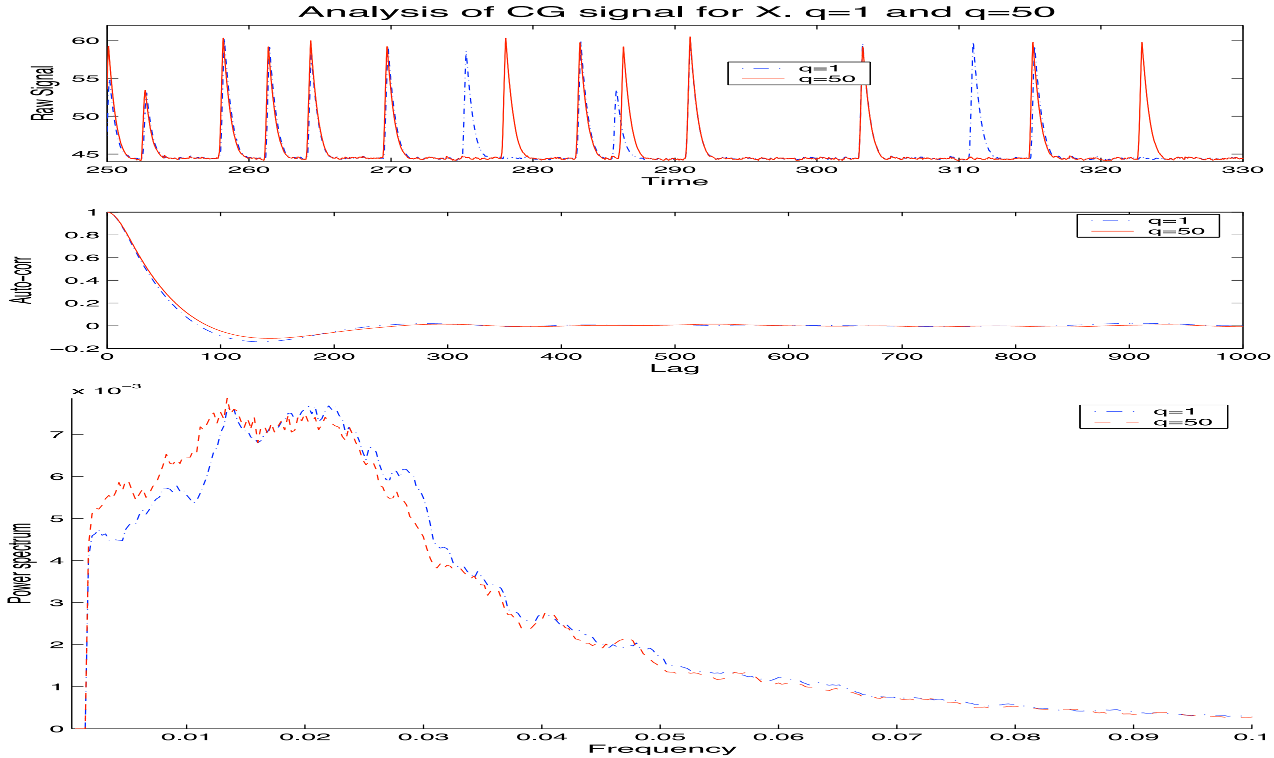
DNS of the hybrid system, $q = 1$

vs.

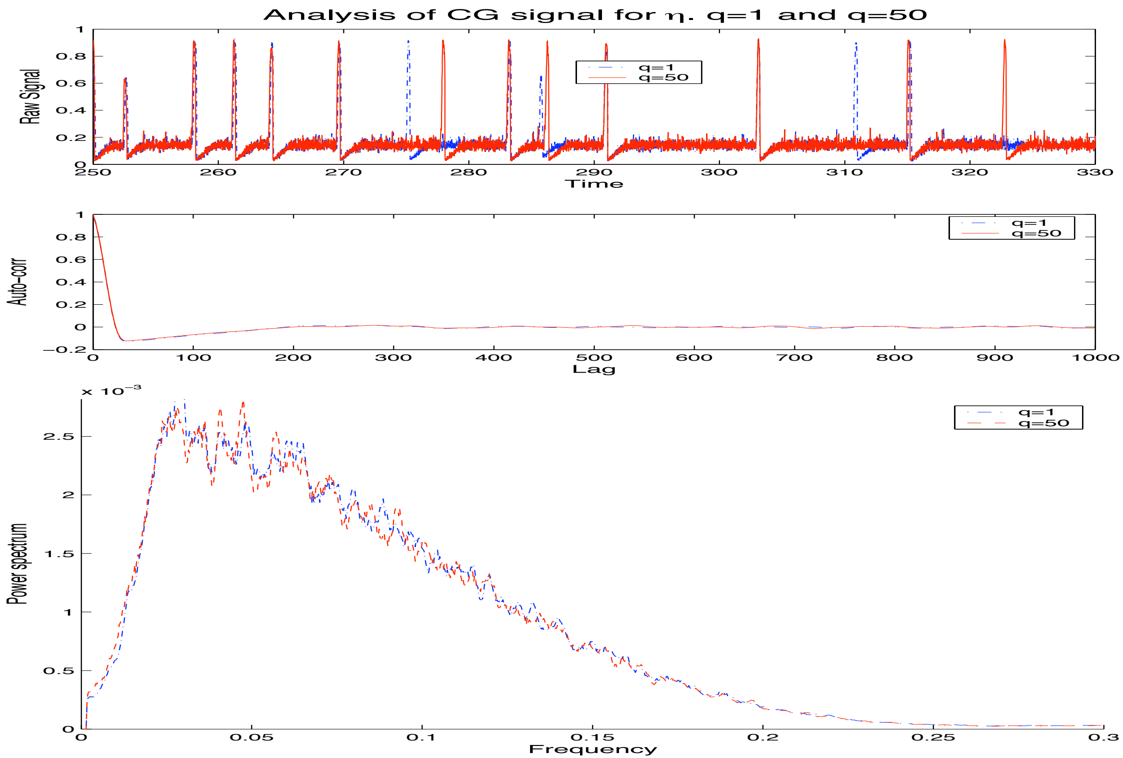
Coarse-Grainings $q = 50$

Space/Time time series analysis:

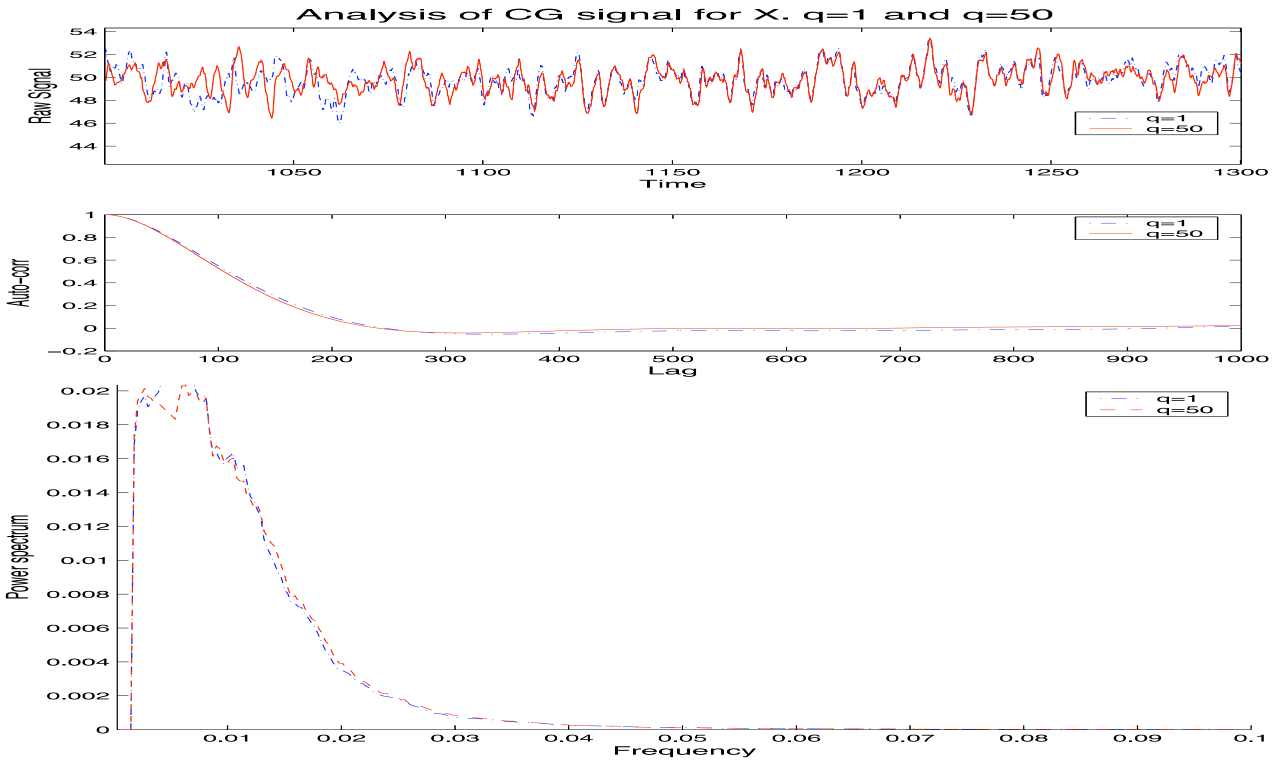
Excitable regime:



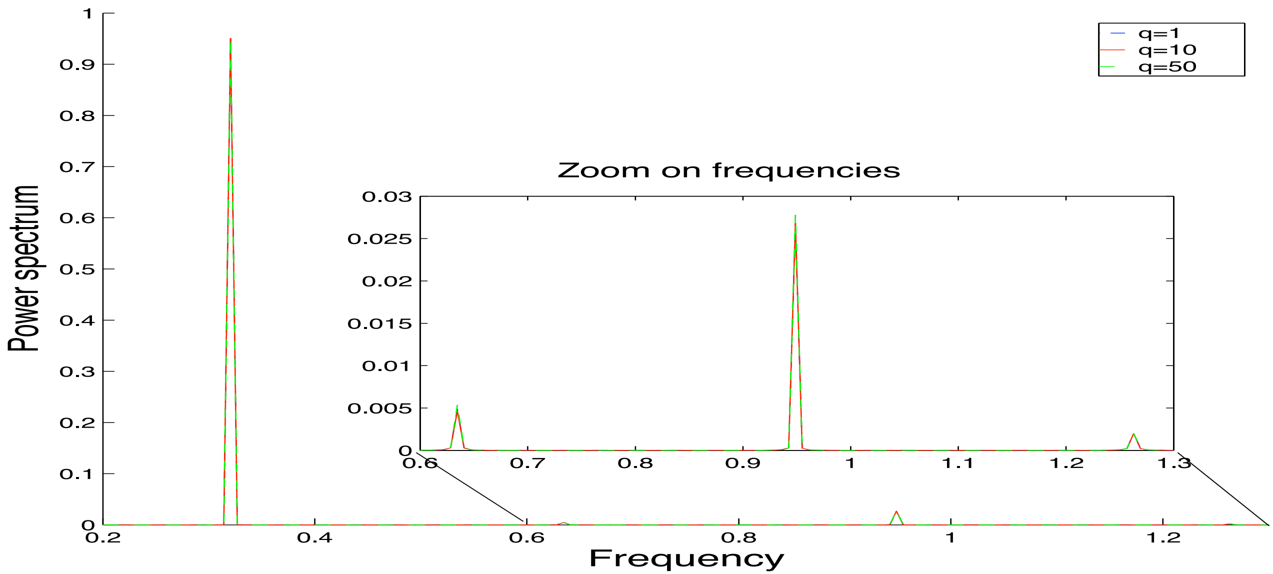
Excitable regime:



Oscillatory regime:

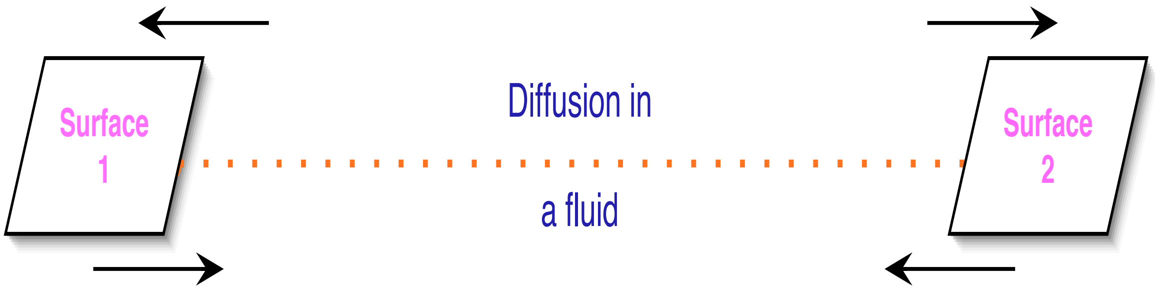


Oscilatory regime-Spatial Power Spectrum:



III. Hybrid couplings through a boundary condition

[K., Sopasakis, Vlachos (Chem Engr., UDel)]

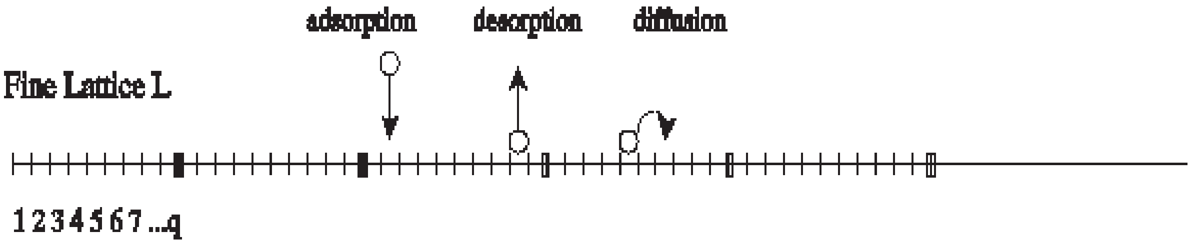


In the interior: Diffusion of microscopic particles in a fluid; no interactions, fickian diffusion.

On each surface: Microscopic stochastic dynamics.

- adsorption to the surface from the fluid
- desorption from the surface to the fluid

Arrhenius adsorption/desorption dynamics



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

Adsorption rate: $c_a(x, \sigma, \rho) = k_a \rho(0, t)(1 - \sigma(x))$

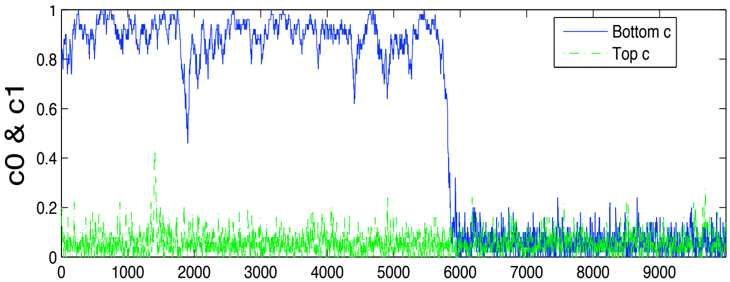
Desorption rate: $c_d(x, \sigma, \rho) = k_d(1 - \rho(0, t))\sigma(x) \exp\left[-\beta U(x)\right]$,

$\rho = \rho(x, t)$ the particle density in the fluid.

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

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

Phase transitions (clustering) and random switching on each surface:



- Microscopic modeling: diffusion $\sim$ random walk of independent particles with exclusion (jump only at empty sites).

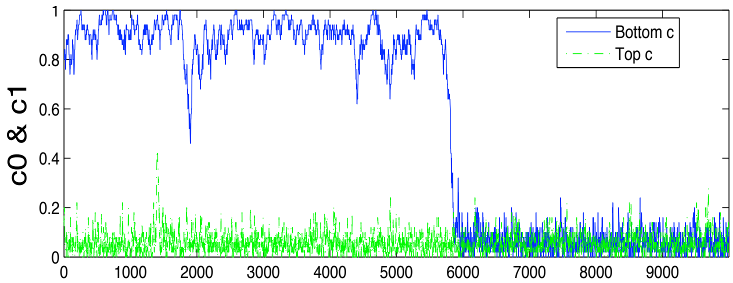
- "Synchronization" of surfaces, depending on their distance or other parameters? Cross-correlations, joint PDFs, etc. Microscopic sims are costly.

- Hybrid vs. microscopic modeling?

Hybrid modeling:

$$\rho_t = D\Delta\rho\,, \qquad \frac{\partial \rho}{\partial x}|_{\text{bdry}} = \text{Adsorption rate} - \text{Desorption rate}\,.$$

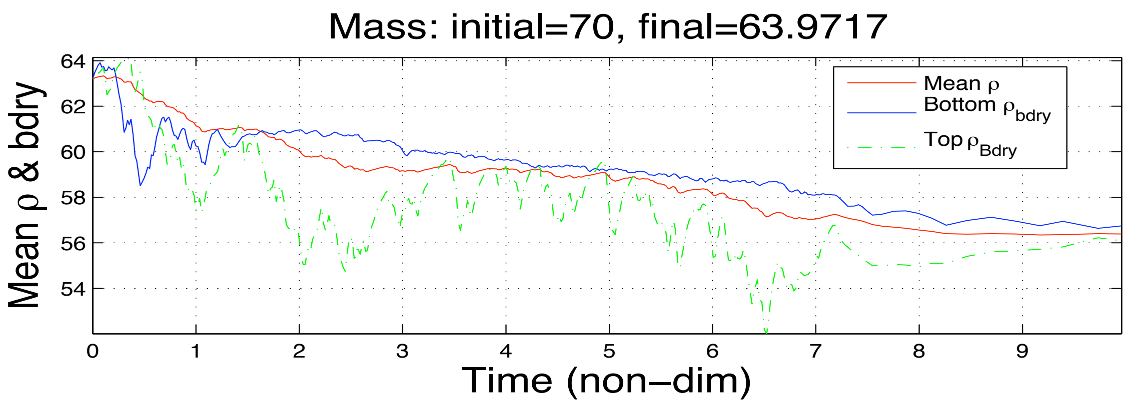
However: density on the surfaces jumps when phase transitions are present:



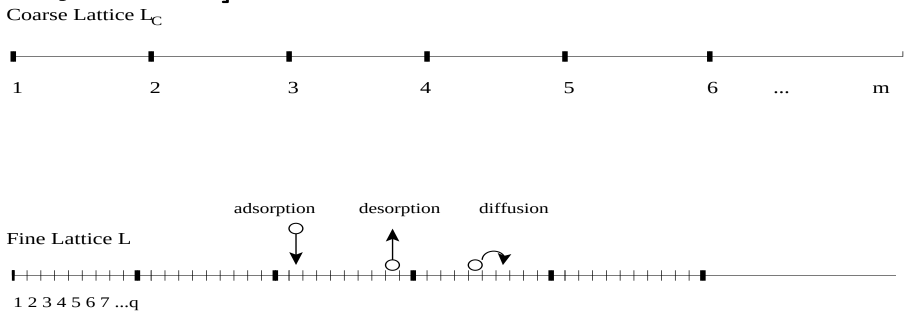
Thus: $\frac{\partial \rho}{\partial x}|_{\text{bdry}} \sim \sum_i \delta(t - t_i)$

- All modes of the solution are excited (at least at the boundaries)

- Numerical hybrid scheme loses mass in time:



1. Coarse-grained simulation of the diffusion: [K., Vlachos, J. Chem. Phys. 2003]



CG is <u>exact</u> in the fickian diffusion case.

2. Hierarchical hybrid simulation: