TOPICS

1. Interacting particle systems;main paradigm: microscopic modelling of surface processes.

2. Derivation of mesoscopic PDE from microscopic dynamics.

3. Rigorous construction of stochastic mesoscopic models: random fluctuations inherited from the microscopics.

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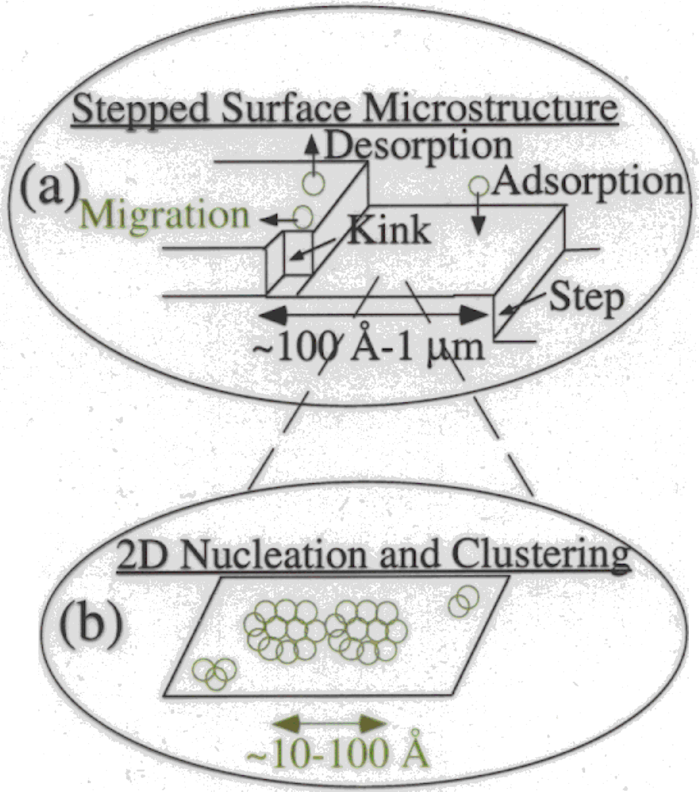
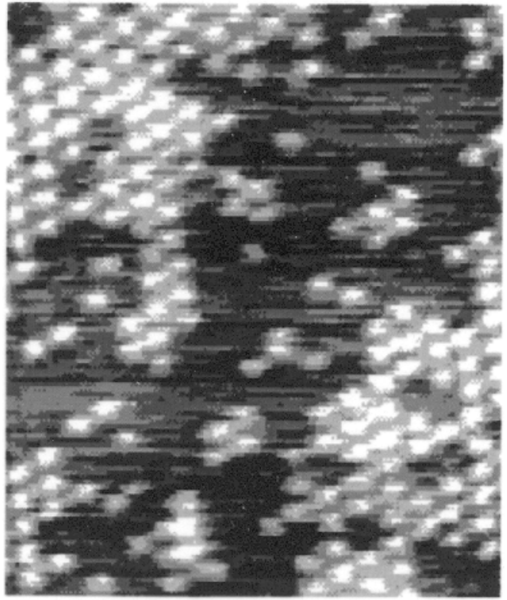
Preprints: www.umass.edu/ markos/home.html

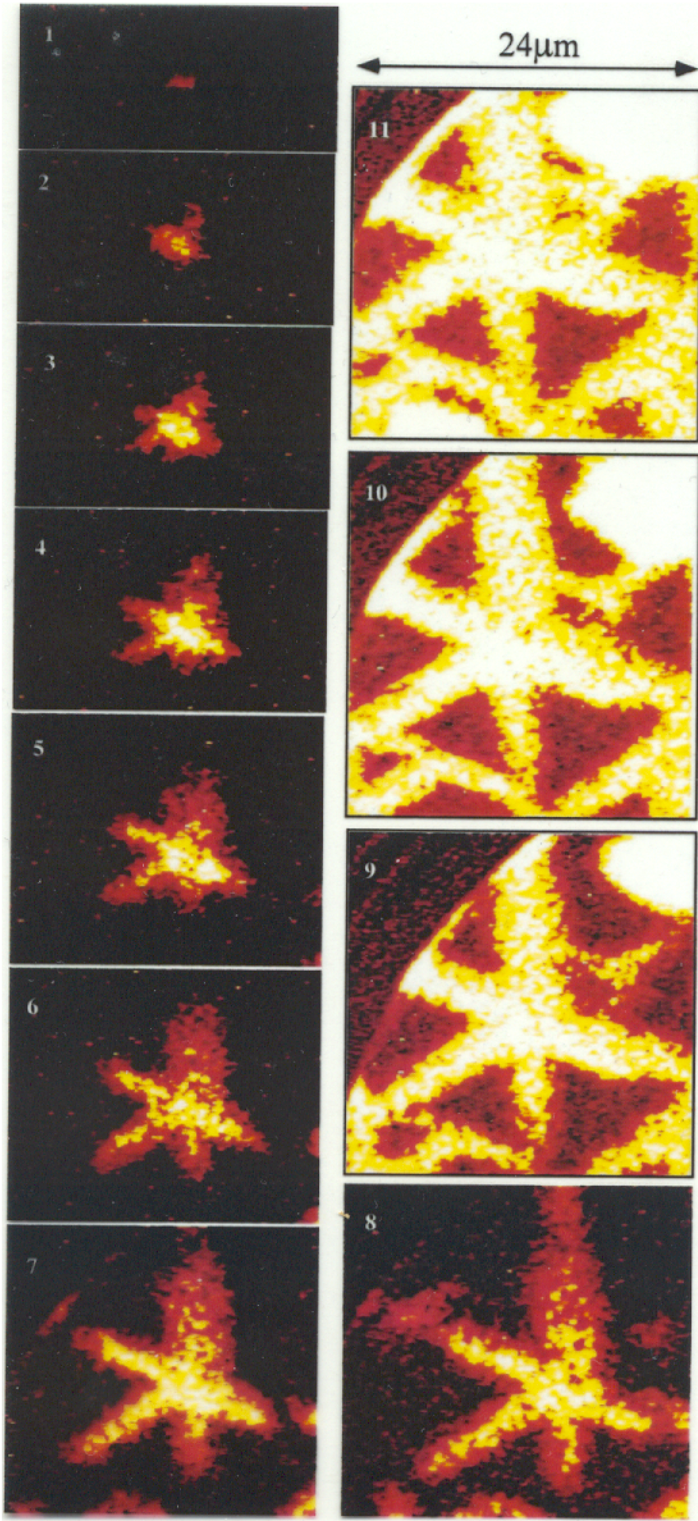

Stepped Surface Microstructure
(a)
Desorption
Adsorption
Migration
Kink
Step
~100 Å-1 μm
2D Nucleation and Clustering
(b)
~10-100 Å

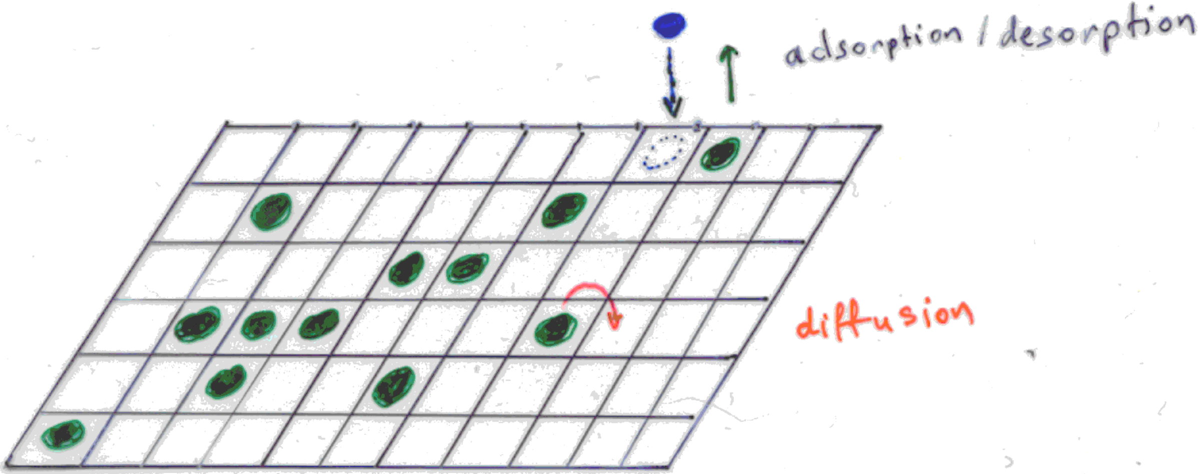
80 Å



Oxygen atoms on Ruthenium (0001)

[J. Wintterlin et. al. Surf. Science 1997]


24μm
1
2
3
4
5
6
7
8
9
10
11



- Single species models (Ising models)
- Multiple species models (Potts models)

MICROSCOPIC MODELS

A. Molecular dynamics, brownian particles.

B. Lattice models, Ising-type systems.

Ising Systems

- *Spin:* $\sigma(x) \in \{0, 1\}$ at the lattice site $x \in \mathbf{Z}^d$ (vacant vs. occupied sites).
- Potts, Heisenberg models: $\sigma(x) \in \{0, 1, ..., q\}$, or $\sigma(x) \in \mathbf{S}^2$.
- *Spin configuration:* $\sigma = \{\sigma(x) \mid x \in \Lambda \subset \mathbf{Z}^d\}$.

- **Hamiltonian:**

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

- h: external field
- J: potential; attractive interactions: $J \geq 0$.

Canonical Gibbs measure:

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

$$P^a_{\beta,\Lambda}(\sigma = \sigma_0) = \frac{1}{Z_{\beta,\Lambda}} \exp\{-\beta H(\sigma_0)\} P^a_\Lambda(\sigma = \sigma_0)$$

Prior distribution (no interactions!):

$$P^a_\Lambda(\sigma = \sigma_0) = \Pi_{x \in \Lambda} P^a(\sigma(x) = \sigma_0(x))$$

where

$$P^a(\sigma(x) = 1) = a \quad \text{and} \quad P^a(\sigma(x) = 0) = 1 - a\,.$$

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

A. Spin Flip Dynamics–Adsorption/Desorption

Spin flips occur at each lattice site x in $[t, t+\Delta t]$ with probability

$$c(x,\sigma)\Delta t$$

- Spin flip rate (Metropolis-type dynamics):

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

  σ^x: configuration after a spin flip at x.
- $\Delta_x H(\sigma) = H(\sigma^x) - H(\sigma)$.
- $\Psi \geq 0$ satisfies the **detailed balance law***:

$$\Psi(r) = \Psi(-r)e^{-r}$$

- Typical choices of Ψ's are:

  $\Psi(r) = (1+e^r)^{-1}$ (Glauber dynamics).
  $\Psi(r) = e^{-r^+}$ (Metropolis dynamics).

Note*: Dynamics obeying detailed balance leave the Gibbs measures invariant.

Arrhenius dynamics:

$$c(x,\sigma) = \begin{cases} c_0 \exp[-\beta(U_0 + U(x))], & \sigma(x) = 1 \\ c_0, & \sigma(x) = 0 \end{cases}$$

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

- Surface binding energy at x: U_0.
- Interaction energy at x:

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

B. Spin Exchange Dynamics–Surface diffusion.

- **Dynamics:** Sequence of spin exchanges with nearest neighbors.

- Spin exchange rate (Metropolis-type dyn.):

$$c(x, y, \sigma) = \Psi(-\beta \Delta_{x,y} H(\sigma)),$$

- $\Delta_{x,y} H(\sigma) = H(\sigma^{(x,y)}) - H(\sigma)$.

  $\sigma^{(x,y)}$:config. after a spin exch. between x, y.

- Detailed balance.

- Typical choices of Ψ's are:

  $\Psi(r) = 2(1 + e^r)^{-1}$ (Kawasaki dynamics).

  $\Psi(r) = e^{-r^+}$ (Metropolis dynamics).

<u>**Arrhenius**</u> dynamics:

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

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

No interactions (J=0, U=0): symmetric or asymmetric <u>random walk</u> for each particle+<u>exclusion rule</u>.

1. MESOSCOPIC THEORIES

Coarse-grainings of the microscopic models at various levels:

a. suppresion of small scale fluctuations (Law of Large Numbers),
b. fluctuations of the coarse-grained quantities (Central Limit Theorem).

Key condition: Long range interaction potential on $\mathbf{Z}^d$, with interaction range $\gamma^{-1} >> 1$:

$$J_\gamma(x-y) = \gamma^d J(\gamma(x-y)) \,.$$

Coarse-graining I : $$v_\gamma(x,t) = \frac{1}{|B_x|} \sum_{y \in B_x} \sigma_t(y)$$

B_x: ball with radius **R** centered at $x \in \mathbf{Z}^d$,

latt. size $= 1 <<$ **R** $<< \gamma^{-1} =$ inter. range.

Asymptotic limit of $v_\gamma(x,t)$ as $\gamma \to 0$;

Local Mean Field Limit. [Lebowitz-Penrose]

Coarse-graining II:

Empirical measure: Defined for each configuration σ:

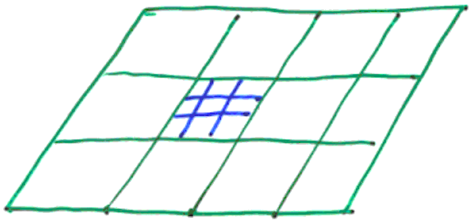
$$\mu_\Lambda(dy, dv, t) = \frac{1}{|\Lambda|} \sum_{x \in \Lambda} \delta_x(dy) \delta_{\sigma_t(x)}(dv) \,.$$

Coarse-grained *random* variable counting the number of spins v contained in a region A. In the $|\Lambda| \to \infty$ limit it will give rise to the (one-point) probability distribution of spins in A:

$$\mu_\Lambda(dy, dv, t) \approx f(x, v, t) dy\, dv \,.$$

Mesoscopic ("kinetic") equation derived from spin flip models of micromagnetics.

Coarse-graining III: [Majda, Vlachos, K.]



M : # of coarse cells
q # of microscopic cells in each coarse cell

Define

$$\eta_t(k) = \sum_{x \in B_k} \sigma_t(x), \quad k \in \{1, \dots, M\}$$

B_k ← coarse cell

$\eta_t(k) \in \{0, 1, \dots, q\}$: # particles per coarse cell

New Markov process — "coarse-grained" process

- Invariant measures, detailed balance
- Correct asymptotics as $M, q \to \infty$ (CGI)
- Incorporation of noise

A. Spin flip dynamics [De Masi, Orlandi, Presutti and Triolo (Glauber dyn.)], [Souganidis, K.]

$[h = 0,\ c(x,\sigma) = \Psi(-\beta\Delta_x H(\sigma))]$

$v_\gamma(x,t) \approx u(\gamma x,t)$ as $\gamma \to 0,\ x \in \mathbf{Z}^N$:

$$u_t = \Psi(-\beta J * u)[1 - u - u \exp(-\beta J * u)]$$

<u>*Arrhenius dynamics*</u>

$$u_t = [1 - u - u \exp(-\beta J * u - \beta h)]$$

Propagation of chaos: For $x \neq y$ and $\gamma \to 0$,

$$E_{\mu_0}\sigma_t(x)\sigma_t(y) \approx E_{\mu_0}\sigma_t(x)E_{\mu_0}\sigma_t(y)$$

[Majda, Khouider]: Mesoscopic models for tropical convection.

B. Spin exchange dynamics

Metropolis-type dynamics [Giacomin, Lebowitz]

$v_\gamma(x, \gamma^{-2}t) \approx u(\gamma x, t)$, $D = \Psi(0)$:

$$u_t - D\nabla \cdot [\nabla u - \beta u(1-u)\nabla J * u] = 0$$

Arrhenius diffusion dynamics

$$u_t - \nabla \cdot \{D \exp(-\beta J * u)[\nabla u - \beta u(1-u)\nabla J * u]\} = 0$$

$$D = \exp(-\beta U_0)\,.$$

Parabolic Arrhenius dynamics [Chen, Vlachos, K.]

Multi-species diffusion models [Chen, Vlachos, K.]

- **Variational formulation**

$$u_t - \nabla \cdot \{\mu[u]\nabla(\frac{\delta E[u]}{\delta u} + h)\} = 0$$

Free energy :

$$E[u] = -\frac{1}{2}\int\int J(r-r')u(r)u(r')drdr' + \int \frac{1}{\beta}H(u)dr$$

Relative Entropy (w.r.to Bernoulli measure):

$$H(u) = u \ln u + (1 - u)\ln(1 - u)$$

Mobility :

$$\mu[u] = \begin{cases} D\beta u(1-u) & \text{Metropolis} \\ D\beta u(1-u)e^{-\beta J*u} & \text{Arrhenius} \\ D\beta u(1-u)e^{-\beta|\nabla J*u|^2/k} & \text{Parab. Arr.} \end{cases}$$

Free energy dissipation :

$$\partial_t E[u] = -\int \mu[u]\left|\nabla\frac{\delta E[u]}{\delta u}\right|^2 dx$$

- $E\,\sigma_t(x) \approx v_\gamma(x,t)$

- $$\frac{d}{dt} E\,\sigma_t(x) = \sum_{y \in N(x)} E\left(\sigma_t(y) - \sigma_t(x)\right) c(x,y,\sigma) \qquad (*)$$

NOT closed!

1. Weak, long range interactions: $J(x-y) = \gamma^d J(\gamma(x-y))$

2. Interaction energy at x:

$$\boxed{U(x) :=} \sum_y J(x-y)\,\sigma_t(y) = \gamma^d \sum_y J(\gamma(x-y))\,\sigma_t(y) \approx$$

("Law of Large #") $$\approx \gamma^d \sum_y J(\gamma(x-y))\,E\,\sigma_t(y) + O(\gamma^{d/2})$$

("Central Limit Thm" correction)

$$\approx \gamma^d \sum_y J(\gamma(x-y))\,v_\gamma(y,t) + O(\gamma^{d/2})$$

$$\approx \int J(x-y)\,u(y,t)\,dy = \boxed{J * u + O(\gamma^{d/2})}$$

random fluctuations

3. All rates depend on $U(x)$, $U(x)-U(y)$, etc...

4. Approximate independence at different lattice sites?

$\Downarrow$

Equation $(*)$ closes...

Relative Entropy Method [Yau ~1991]

A. Local equilibria:

$$\mu^{a}_{\beta,\Lambda}(d\sigma) = \frac{1}{Z_{\beta,\Lambda}} \exp[-\beta H(\sigma)]\, P^{a}_{\Lambda}(d\sigma)$$

$a = u(\gamma x, t)$, u solves the mesosc equation

- "Slowly-varying" parameter a.
- Relative entropy, $R(\mu|\nu) = \int \log\left(\frac{d\mu}{d\nu}\right) d\mu$

B. Show: $R(\mu^{\gamma}_{t} \,|\, \mu^{u(\cdot,t)}_{\beta,\Lambda}) \longrightarrow 0$ as $\gamma \downarrow 0$

Long range interactions $\Rightarrow$ $\mu^{u(\cdot,t)}_{\beta,\Lambda}$ product measure

$\Downarrow$

independence, propagation of chaos, etc...

2. Stochastic Mesoscopic Models and Large Deviations.

The convergence theorems described earlier imply, as $\gamma^{-1} \to \infty$:

$P(v_\gamma$ is close to $u) \to 1$, $\quad u$ solves mesosc. PDE

v_γ: average occupation; γ^{-1}: interaction range.

1. Many physical systems have large but finite # of interacting neighbors.

   What is the above rate of convergence?

2. Can we include random fluctuations from the underresolved scales in the mesoscopic models? Nucleation and metastability.

A. Large Deviation Principle: Singular perturbations of dynamical systems [Friedlin-Wentzell].

Formal asymptotics :

$$P(v^\gamma \text{ is close to } u) \approx \exp\{-\gamma^{-d}(I[u] - \inf_v I[v])\},$$

- γ^{-d}: # of interacting neighbors in $d-$dim.
- $I[u]$: **Action functional**, $I[u] \geq 0$, with "=" iff u is a solution to the mesoscopic surface diffusion equation.

$$I[u] = \int_0^T \int \mu[u]|\nabla H|^2 dxdt\,,$$

where H:

$$u_t - \nabla \cdot \{\mu[u]\nabla(\frac{\delta E[u]}{\delta u})\} = \nabla \cdot \{\mu[u]\nabla H\}\,.$$

[Asselah, Giacomin] (Kawasaki dynamics).

B. Stochastic mesoscopic PDE:

$$u_t - \nabla \cdot \{\mu[u]\nabla(\frac{\delta E[u]}{\delta u})\} + \gamma^{d/2} N_t = 0$$

$$N_t = \nabla \cdot \{\sqrt{2\mu[u]}\dot{W}\}.$$

$\dot{W} = (\dot{W}_1(x,t), ..., \dot{W}_d(x,t))$ is a d-dim. space/time white noise.

- Formal derivation from the microscopics: ∞-dim. Fokker-Planck equation for v^γ. Rigorous derivation?
- The SPDE satisfies a *fluctuation-dissipation* relation, i.e. it is reversible with respect to the (formal) underlying Gibbs measure:

$$\mu_G(du) = Z^{-1} \exp(-\beta\gamma^{-d} E[u]) du$$

- The SPDE and the IPS share the same $I[u]$.
- WKB expansion ([Fleming, James 1992] for SDE):

$$P(\mu^\gamma \approx u) = (1 + \sum_i \gamma^{di}\Phi_i[u]) \exp\{-\gamma^{-d} I[u]\}.$$

[Feng, K.] ∞-dim. Hamilton-Jacobi equation approach.