From individual interactions to hierarchical mesoscale models for agent-based, complex dynamics

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Stochastic spatial evolutionary games

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Supported in part by:

-National Science Foundation

Main themes:

- "Microscopic", agent-based models accounting for individual interactions and behaviors; phenomenology.

  - People, groups, organizations

  - Social animals, swarms, cells.

  Role of stochasticity in the micro-scale modeling; spatial evolutionary games, extended systems

  Methods: Stochastic processes, statistical mechanics, Kinetic Monte Carlo

- Mesoscopic models for large, spatially-distributed populations; PDE-limits, "dynamic law of large numbers"

  Methods: Statistical Mechanics + Nonlinear PDE and related numerics.

- Hierarchical mesoscopic models, accounting for:

  - stochasticity at the mesoscale,

  - variable granularity of the mesoscale description.

  Methods: Hierarchical coarse-graining and related numerical methods

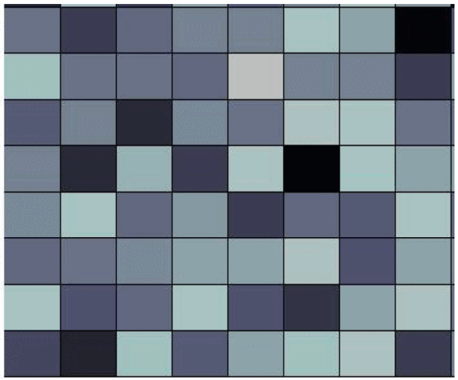
I. Spatial Evolutionary Games: Interactions among individual agents usually involve space, e.g.

- where to live
- from what sellers to buy (proximity?)

Interactions may induce spatial patterns of segregation-much larger than the single agent-scale.

Spatial evolutionary game: Agents with possible strategies, $S = \{1, \cdots, s\}$, on the graph $\Lambda \subset \mathbb{Z}^d$.

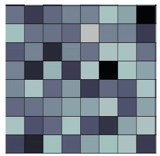
Order parameter: At each site $x \in \Lambda$, an agent uses a strategy denoted by $\sigma_\Lambda(x) \in S$



Payoff function $a(i,j)$: $i-$ vs. $j-$ strategy, $i,j \in S$, e.g. for $S = \{1,2\}$,

		x's neigbhor	
		strategy 1	strategy 2
agent x	strategy 1	3	0
	strategy 2	0	5

-payoff does not depend on whether the players are called player I or player II



Configuration: $\sigma_\Lambda = \{\sigma(x) : x \in \Lambda\}$

High-dimensional state space: $\Xi_\Lambda := S^\Lambda$ (all configurations).

Local interactions: $\mathcal{W}(x,y)$ intensity of the interaction among neighbors:

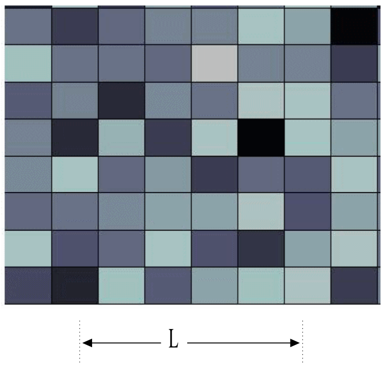
$$\sum_y \mathcal{W}(x-y) \approx 1$$

Examples:

- $\mathcal{W}(x,y) \ = 1/|\Lambda|$ (uniform-mean field)

- "nearest neighbor interaction" : $\mathcal{W}(x,y) = \begin{cases} \frac{1}{2d} & \text{if } \|x-y\| = 1 \\ 0 & \text{otherwise} \end{cases}$

- Kac-type potentials with range $L = \gamma^{-1}$: $\mathcal{W}_\gamma(x,y) = \gamma^d \mathcal{J}(\gamma \|x-y\|)$, e.g. $\mathcal{J}(r) \sim e^{-br^2}$



Total payoff for site x with strategy $\sigma(x) = i$ given the strategy configuration σ

$$u(x, \sigma, i) := \sum_{y \in \Lambda} \mathcal{W}(x, y) a(i, \sigma(y))$$

Framework in [P. Young, *Princeton Univ. Press* (1998)].

Dynamics-strategy revision: Continuous Time Markov process $\{\sigma_t\}$:

[Szabo, Fath, *Phys. Reports* (2007)]

- $c(x, \sigma, k)$ – switching rate of agent x from strategy $\sigma(x)$ to k when the configuration is σ

- Generator: $Lf(\sigma) = \sum_{x \in \Lambda} \sum_{k \in S} c(x, \sigma, k) \left(f(\sigma^{x,k}) - f(\sigma) \right)$

  where

  $\sigma^{x,k}$ new config. $\sim$ agent at x switches from $\sigma(x)$ to k.

Continuous Time Monte Carlo (CTMC)

Construct a continuous-time Markov Chain in configuration space $\Sigma = \{1, 2, ..., m\}$ with transition rates

$$Q = \Big(q(x, y) \Big)_{x,y \in \Sigma}$$

Building blocks of the continuous time chain:

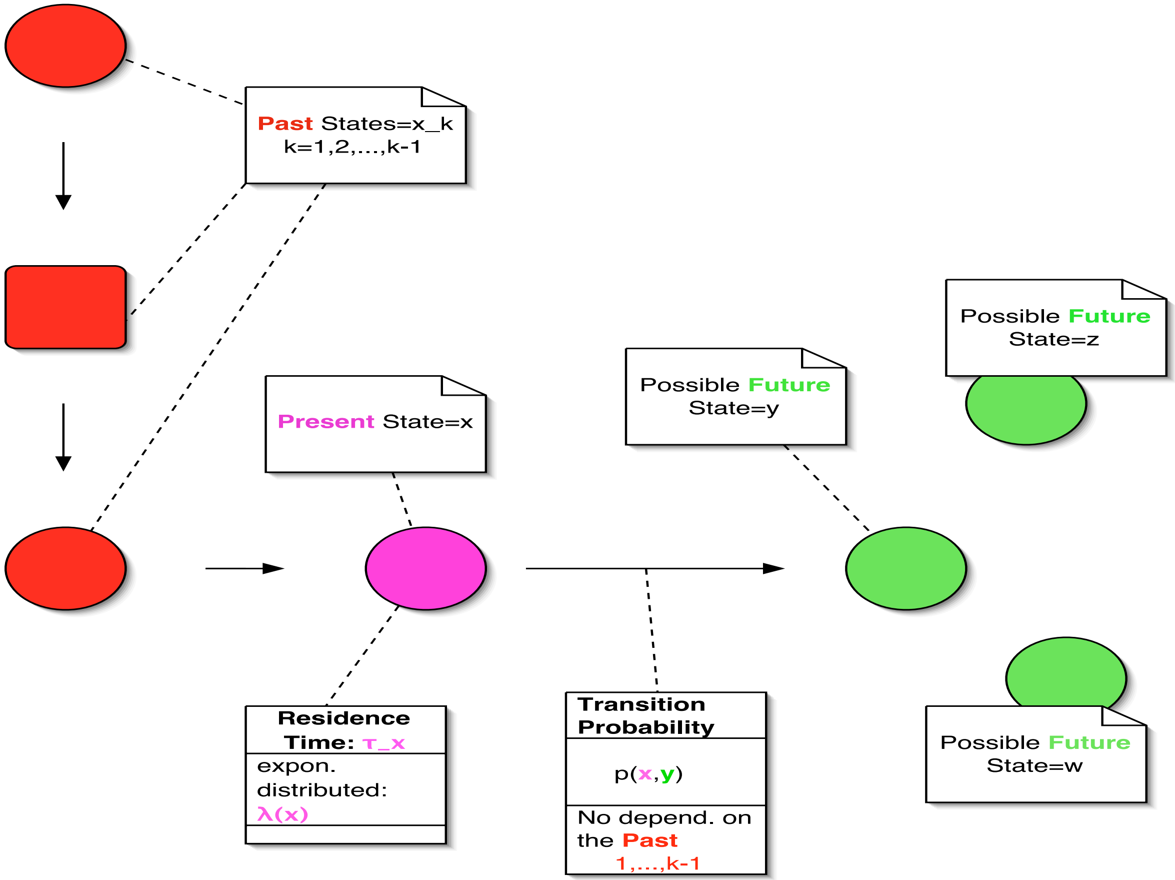
- Residence time τ_x: time spent by the process X_t at x; random waiting time between consecutive jumps.

$$P(\tau_x > t) = \exp\left(-\lambda(x)t\right), \quad \lambda(x) \geq 0$$

- "Skeleton" Markov Chain
$$p(x, y) = P(X_{\tau_x} = y \,|\, X_0 = x)\,, y \neq x$$
we set $p(x, x) = 0$.

Pseudo-algorithm based on exponential clock and "skeleton" Markov chain.

References: Gillespie (chemical reactions); Bortz, Kalos, Lebowitz (Ising-type systems)



Past States=x_k
k=1,2,...,k-1
Present State=x
Possible Future State=y
Possible Future State=z
Possible Future State=w
Residence Time: τ_x
expon. distributed: λ(x)
Transition Probability
p(x,y)
No depend. on the Past 1,...,k-1

Some typical rates $c(x, \sigma, k)$:

	Comparing	Targeting
Innovative	$F(u(x,\sigma,k) - u(x,\sigma,\sigma(x)))$	$F(u(x,\sigma,k))$
Imitative	$\sum_{y\in\Lambda} w(x,y,\sigma,k)F(u(x,\sigma,k) - u(x,\sigma,\sigma(x)))$	$\sum_{y\in\Lambda} w(x,y,\sigma,k)F(u(x,\sigma,k))$

- Innovative vs Imitative: Innovative rates can introduce any strategy, even if not currently used in the population, i.e.

$$c(x, \sigma, k) > 0 \qquad \text{for all} \quad x, \sigma, k$$

- Targeting vs Comparing: Rate depends on the payoff of target strategy, vs. on both the current and target payoffs.

Examples of Rates

- **Comparing** & **Innovative**: $c(\sigma, x, k) = F(u(x, \sigma, k) - u(x, \sigma, \sigma(x)))$

$$c(\sigma, x, k) = \max\left\{1, \exp\left[\left(u(x, \sigma, k) - u(x, \sigma, \sigma(x))\right)\right]\right\} > 0$$

-Metropolis MCMC algorithm.

-detailed balance, Gibbs states for symmetric $a(i, j)$; corresponds to the "Hamiltonian"

$$H(\sigma) = -\frac{1}{2} \sum_{x,y} \mathcal{W}(x, y) a(\sigma(x), \sigma(y))$$

- **Targeting** & **Innovative**: $c(\sigma, x, k) = F(u(x, \sigma, k))$

$$c(\sigma, x, k) = \frac{\exp(u(x, \sigma, k))}{\sum_l \exp(u(x, \sigma, l))} > 0$$

"logit rule" or "Gibbs sampler "or "Glauber "dynamics.

-detailed balance, same Gibbs states as Metropolis.

- **Comparing & Imitative:** (Replicator)

  $c(\sigma, x, k) = w(x, y, \sigma, k)\ F(u(x, \sigma, k) - u(x, \sigma, \sigma(x))$

  – Probability of an individual at site x meeting y among $k-$strategies in his neighborhood:

  $$w(x, y, \sigma, k) := \mathcal{W}(x, y)\delta_{\sigma(y)}(\{k\})$$

  – Probability of imitation $\sim$ payoff increase upon abandoning $\sigma(x)$ and adopting k, e.g.

  $$F(r) = \max\{r, 0\}$$

$$c(\sigma, x, k) = \sum_{y \in \Lambda} w(x, y, \sigma, k) \max\{u(x, \sigma, k) - u(x, \sigma, \sigma(x), 0)\}$$

2. Why mesoscopic PDE approximation: tools to explore the implications of spatial interactions and different agent dynamics in evolutionary games

Discretized density for each strategy:

- Empirical measure for a given config. σ:

$$\pi^\gamma(\sigma; du, di) := \frac{1}{|\Lambda|} \sum_{x \in \Lambda} \delta_{(\gamma x, \sigma(x))}(du di)$$

- Asymptotic closure: does

$$\pi^\gamma(\sigma_t; du, di) \to f(t, u, i) du di \text{ in probability}$$

  and f solves some PDE?

- "dynamic" Law of Large Numbers; suppression of small-scale fluctuations

Theorem 1. *(Long Range Interactions and Periodic BCs)*

If $\mathcal{W}_\gamma(x,y) = \gamma^d \mathcal{J}(\gamma\,\|x-y\|)$

Then,

$$\lim_{\gamma\to 0} \pi_t^\gamma(du,di) = f(t.u,i)\,du di \text{ in probability}$$

uniformly for $t \in [0,T]$ *and* f *solves: for* $u \in \mathbf{T}^d, i \in S$

$$\begin{aligned} \frac{\partial}{\partial t} f(t,u,i) &= \sum_{k\in S} \mathbf{c}(u,k,i,f) f(t,u,k) - f(t,u,i) \sum_{k\in S} \mathbf{c}(u,i,k,f) \\ f(0,u,i) &= f_0(u,i) \end{aligned}$$

For instance, when $c^\gamma(x,\sigma,k) = F\Big(u(x,\sigma,k) - u(x,\sigma,\sigma(x)\Big)$

$$\mathbf{c}(u,i,k,f) := F\left(\sum_{l\in S} a(k,l)\mathcal{J}*f(u,l) - \sum_{l\in S} a(i,l)\mathcal{J}*f(u,l)\right)$$

"Proof":

$$
\begin{aligned}
1.\quad c^{\gamma}(x,\sigma,k) &= F(u(x,\sigma,k) - u(x,\sigma,\sigma(x)) \\
&= F\left(\sum_{x\in\mathbf{T}^{d,\gamma}} \gamma^d \mathcal{J}\ \ (\gamma(x-y))\, a(k,\sigma(y)) - \sum_{x\in\mathbf{T}^{d,\gamma}} \gamma^d \mathcal{J}\ \ (\gamma(x-y))\, a(\sigma(x),\right. \\
&\underset{\gamma\to 0}{\longrightarrow} F\left(\sum_{l\in S} a(k,l)\mathcal{J}*f(u,l) - \sum_{l\in S} a(i,l)\mathcal{J}*f(u,l)\right) \\
&= : \mathbf{c}(u,i,k,f)
\end{aligned}
$$

2. Generator's action on mesoscale observables (e.g. a local average),

$$
\langle \pi^{\gamma}, g\rangle(\sigma) = \frac{1}{N}\sum_{x\in\Lambda} g\Big(\gamma x, \sigma(x)\Big)\ :
$$

$$L_\gamma \langle \pi^\gamma, g \rangle (\sigma) = \sum_{k \in S} \int_{\mathbf{\Lambda} \times S} \mathbf{c}(u,i,k,\pi^\gamma(\sigma)) \left(g(u,k) - g(u,i)\right) \pi^\gamma(\sigma, dudi)$$

3. Martingale representation theorem:

$$\begin{aligned} \langle \pi_t^\gamma, g \rangle &= \left\langle \pi_0^\gamma, g \right\rangle + \int_0^t ds \sum_{k \in S} \int_{\mathbf{\Lambda} \times S} \mathbf{c}(u,i,k,\pi_s^\gamma) \left(g(u,k) - g(u,i)\right) \pi_s^\gamma(dudi) \\ &\quad + M_t^{g,\gamma} \end{aligned}$$

4. As $\gamma \to 0$, $M_t^{g,\gamma} \to 0$, $\pi_t^\gamma(dudi) \to f(t,u,i)dudi$ and

$$\langle f_t, g \rangle = \langle f_0, g \rangle + \int_0^t ds \sum_{k \in S} \int_{\Lambda \times S} \mathbf{c}(u,i,k,f_s) \left(g(u,k) - g(u,i)\right) f_s(u,i) dudi$$

Connections to well-mixed systems and Mean Field theories, e.g. [Benaim, Weibull *Econometrica* (2003)]

For uniform interactions between agents, exact closure for:

- Aggregate emprical measure

$$\eta^\gamma(i) := \frac{1}{|\Lambda|} \sum_{x\in\Lambda} \delta_{\sigma(x)}(\{i\})$$

  which counts the proportion of agents with strategy i in the whole domain Λ.

- For uniform interactions, $c^\gamma(x,\sigma,i)$ depends only on η_i^N since,

$$u(x,\sigma,k) := \sum_{y\in\Lambda} \mathcal{W}(x,y) a(k,\sigma(y)) = \sum_{i\in S} a(k,i)\eta^N(i)$$

  so we can define

$$c(j,k,\eta^N) := c^\gamma(x,\sigma,k)\,, \quad \text{for all} \quad j=\sigma(x)\,.$$

- Therefore the aggregate $\eta_t^N(i)$ is itself a Markov process (not always true!)

$$L^{M,n}g\left(\eta\right) = \sum_{k\in S}\sum_{j\in S} n^d \eta(j)c(j,k,\eta)(g(\eta^{j,k}) - g(\eta))$$

where $\eta^{j,k}$ is a new state induced from η by an agent's switching from j to k.

- Multi-type birth and death process for population dynamics

- At the mesoscopic level, the IDEs reduce to the usual ODE of evolutionary game theory, [Weibull, 1995]. We note that if $\mathcal{J}$ =1, we have

$$\rho(i) := \int f(u,i)du = \mathcal{J} * f(i)$$

so $\mathbf{c}(u,k,i,f)$ is independent of u: $\mathbf{c}^M(k,i,\rho) := \mathbf{c}(u,k,i,f)$

From the IDEs we obtain

$$\frac{d\rho_t(i)}{dt} = \sum_{k\in S} \mathbf{c}^M(k,i,\rho)\rho_t(k) - \rho_t(i)\sum_{k\in S} \mathbf{c}^M(i,k,\rho) := F_i(\rho)$$

Spatial evolutionary games: Reaction-Diffusion systems, [Hofbauer, Sigmund, Bull. AMS (2003)].

$$\frac{\partial f}{\partial t} = F(f) + D\Delta f\,, \quad D > 0\,\text{const.}$$

where $F = (F_i)_{i\in S}$ is given by the mean-field (uniform interactions) case.

- $D > 0 \sim$ random exchange of players/strategies w/o interactions; "fast stirring" vs. slow strategy updates [Durrett, SIAM Rev. (1999)]

- (monotone) travelling waves, spatial morphologies.

Example: **Two-strategy case**, where $a_{12} = a_{21} = 0$,

$$\beta = a_{11} + a_{22}\,, \qquad h = \frac{a_{22}}{a_{11} + a_{22}}$$

- **IDEs**:

$$\text{Replicator: } \frac{\partial p}{\partial t} \quad = \quad (1-p)\mathcal{J} * pF(\beta(\mathcal{J}*p - h)) \\ -p\,(1 - \mathcal{J} * p)\,F\,(\beta\,(h - \mathcal{J} * p))$$

$$\text{Logit : } \frac{\partial p}{\partial t} \quad = \quad l(\beta(\mathcal{J} * p - h)) - p$$

where $F(t) = t^+$ and $l(t) = \frac{1}{1+\exp(-t)}$.

- **Space independent stationary solutions**, p_0 steady states of the ODE.

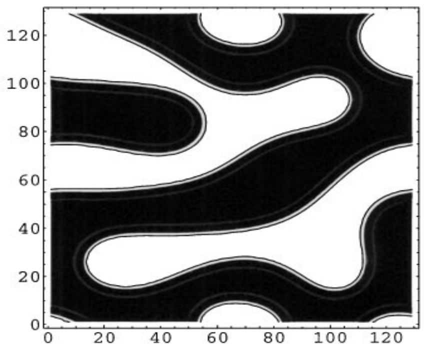
Logit and Statistical Mechanics: $p \mapsto 2p-1 := u$, the logit dynamic yields

$$\frac{\partial u}{\partial t} = -u + \tanh\left(\frac{\beta}{4}(\mathcal{J} * u + (1-2h))\right)$$

which is the Glauber mesoscopic equation:

[DeMasi, Orlandi, Presutti, Triolo, *Nonlinearity* (1994)]

- for $\beta > 0$ high (low temperature): bistability and existence of travelling wave solutions-spatial segregation



- Interface development and curvature dependent evolution [K, Souganidis, *Comm. Math. Phys.*(1995)]; similarities to Allen-Cahn equation.

- Metastability, tunneling and large deviations [Dirr, Manzi, Tsagkarogiannis, 2009]

PDE approximation: Spatial rescaling $\mathcal{J}_\epsilon(x) = \epsilon^{-d}\mathcal{J}(x/\epsilon)$. For small ϵ and we have

$$\mathcal{J}_\epsilon * f \approx f + \frac{\epsilon^2}{2} J_2 \Delta f$$

Replicator:

$$\frac{\partial p}{\partial t} = \beta p(1-p)(p-h) + D(p)\frac{\beta\epsilon^2}{2} J_2 \Delta p$$

where

$$D(p) = [p(1-p) + (1-p)F(p-h) + pF(h-p))]$$

- Bistability (always!), similarity to Allen-Cahn PDE, however...
- Degenerate, nonuniform diffusion: $D(0) = D(1) = 0$.

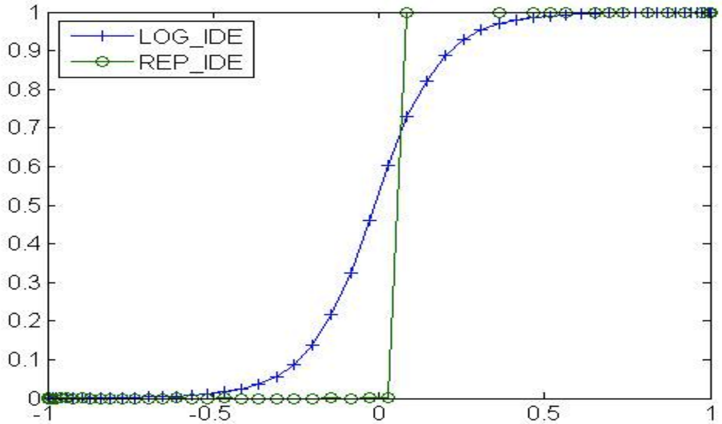
Replicator vs. Logit Dynamics

- Linearized analysis around the unstable equilibrium p_0, **dispersion relations**:

$$\lambda_L(k) = \beta(1-p_0)p_0\hat{\mathcal{J}}(k)-1 \quad \text{vs.} \quad \lambda_R(k) = \beta(1-p_0)p_0\hat{\mathcal{J}}(k)$$

Faster escape from unstable equilibrium for the replicator: sharper interfaces?

- Comparing Standing Waves:

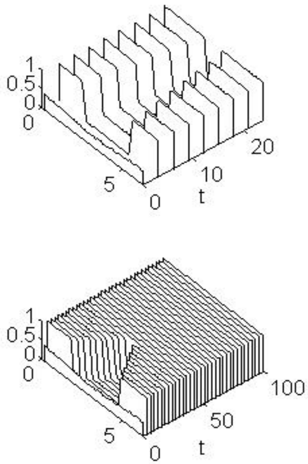


- In logit and other innovative dynamics , there is a nonzero probability to select something not optimal on the "interface". That creates the "mushy" mixed region of a transition.

- In replicator there is a zero probability for actions against the optimal choice. Hence the sharp interface. Similar zero temperature regime in stat. mech.

Constant Diffusion vs. Density Dependent Diffusion

Travelling waves:



Discussion: Hierarchical mesoscopic models

A. Mesoscopic systems as continuous limits

Thermodynamic/Hydrodynamic limits (equilibrium/nonequilibrium)

Coarse quantities: density, average velocity, one-point pdf, etc.

Examples

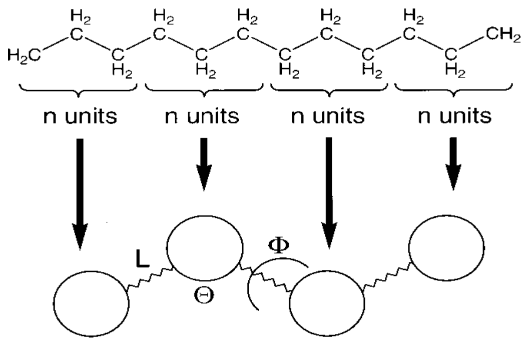
- Deterministic ODE/PDE: Mean-field approximations, Ginzburg-Landau models, kinetic equations, field theories in polymers, etc.

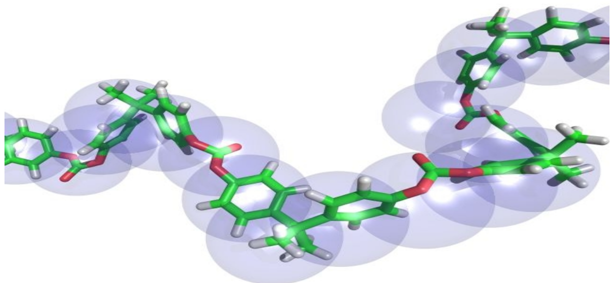
- Stochastic Corrections as SPDEs: Stochastic Allen-Cahn, Cahn-Hilliard-Cook, diblock co-polymer models, etc.

B. Hierarchical Coarse-graining

1. Coarse-graining of polymers; proteins; biomembranes

[Abrams, Kremer *J. Chem. Phys*, (2001)]

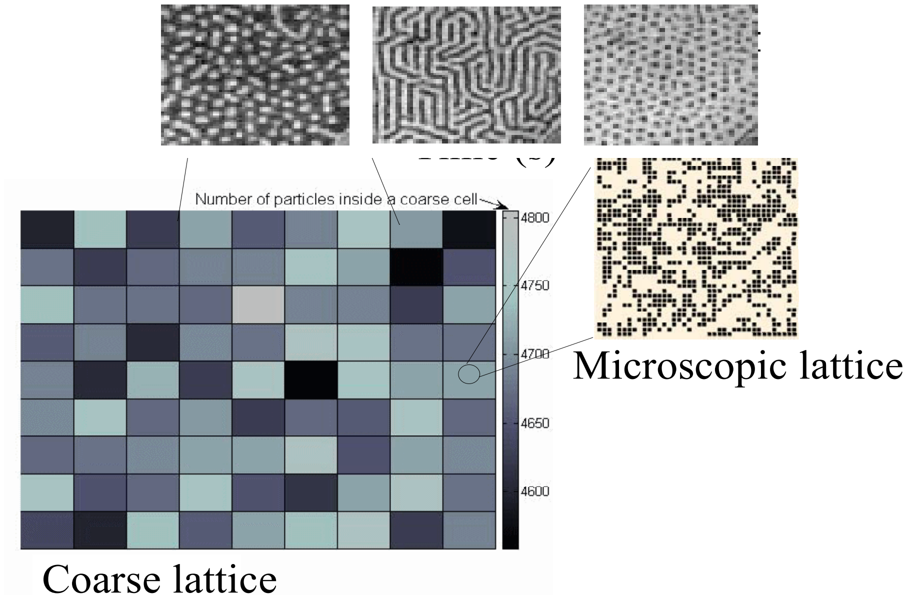




2. Stochastic lattice dynamics/ KMC

Examples: Catalysis, epitaxial growth, micromagnetics, etc.

Patterning through self-assembly



K., Vlachos *J.Chem.Phys.*'03, K., Plechac, Rey-Bellet, *J. Sci. Comp.* '08

Theory and General Mathematical Framework

- N, M – the size of the microscopic and CG systems, respectively.

- q – the parameter that defines the level of coarse-graining, e.g., number of spins in the coarse variable (a block spin) or number of atoms in the "meta-particle".

- $\sigma \in \mathcal{S}_N = (\Sigma)^{\Lambda_N}$ – the microscopic configuration space.

- $\eta = \mathbf{T}\sigma \in \mathcal{S}^c_{M,q}$ – the coarse-graining operator defining configurations on the coarse configuration space.

Basic Steps

A. Microscopic equilibrium Gibbs measure

$$\mu_{N,\beta}(d\sigma) = \frac{1}{Z_{N,\beta}} e^{-\beta H_N(\sigma)} \mathsf{P}_N(d\sigma)\,,$$

$$\mathsf{P}_N(d\sigma) = \prod_{x \in \Lambda_N} \rho(d\sigma(x))\,.$$

B. Coarse-grained measure is given by the projection operator:

$$\mu^c(d\eta) := \mu\{\sigma \in \mathcal{S}_N \,|\, \mathbf{T}(\sigma) = \eta\}$$

New CG Hamiltonian:

$$e^{-\beta H^c(\eta)} = \mathbb{E}[e^{-\beta H_N} \,|\, \eta] \equiv \int_{\mathcal{S}_N} e^{-\beta H_N(\sigma)}\, P_N(d\sigma \,|\, Q)\,,$$

Computing $H^c(\sigma)$ directly $\Longrightarrow$ integration on a high-dimensional space.

Solution: Approximate H^c or better μ^c by a convergent expansion in a small parameter.

$$\bar{H}_m(\eta) = \bar{H}_m^{(0)}(\eta) - \frac{1}{\beta} \log \mathbb{E}[e^{-\beta(H_N - \bar{H}_m^{(0)})} \,|\, \eta] = \bar{H}_m^{(0)}(\eta) + \bar{H}_m^{(1)}(\eta) + N O(\epsilon^3)\,.$$

Cluster expansions developed in statistical physics for controlling measures on high-dimensional spaces.

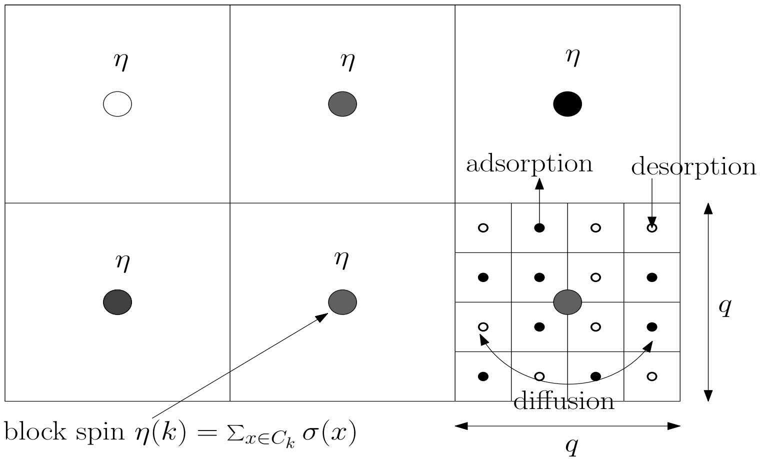
K., Plechac, Rey-Bellet, Tsagkarogiannis, [*M²AN, '07*]

Lattice Dynamics:

(a) deposition – spin-flip, strategy update

(b) diffusion+ interactions – agent migration

CG Monte Carlo Hierarchy:



K., Majda, Vlachos, *Proc. Nat. Acad. Sci.*'03, *JCompPhys*'03;
K., Vlachos *J.Chem.Phys.*'03

Coarse observable at resolution q: $\eta_t(k) = \mathbf{T}\sigma_t(k) := \sum_{y \in D_k} \sigma_t(y)$

In general, it is **non-markovian**.

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

• "Local population" *Birth-Death* type process, with interactions.

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

• **Coarse-grained** rates and Detailed Balance: $\bar{c}_a^{(\alpha)}$ and $\bar{c}_d^{(\alpha)}$

Ergodicity: Are the long-time dynamics reproduced? Rare events?

A. Numerical Analysis of CG

I. Loss of Information: Error control in terms of relative entropy estimates:

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

II. Observables: Bounds on the weak error:

$$\mathbb{E}_{\mathbf{T}X_0}[f(\mathbf{T}X_T)] - \mathbb{E}_{Q_0}[f(Q_T)]$$

Bounds in terms of the "small" parameter

$$\epsilon \,\equiv\, \beta\frac{q}{L}\|\nabla J\|_1$$

B. Microscopic Reconstruction – Reverse CG map

K., Trashorras, JSP '06; K., Plechac, Rey-Bellet, Tsagkarogiannis, [M^{2}AN, '07]; Are, K. Plechac, Rey-Bellet, [SIAM J. Sci. Comp. '08].

Error Quantification in CG Schemes

Theorem: (A priori error analysis)*Loss of information during coarse-graining*

Define the "small" parameter

$$\epsilon \equiv \beta \frac{q}{L} \|\nabla J\|_1$$

- Specific relative entropy:

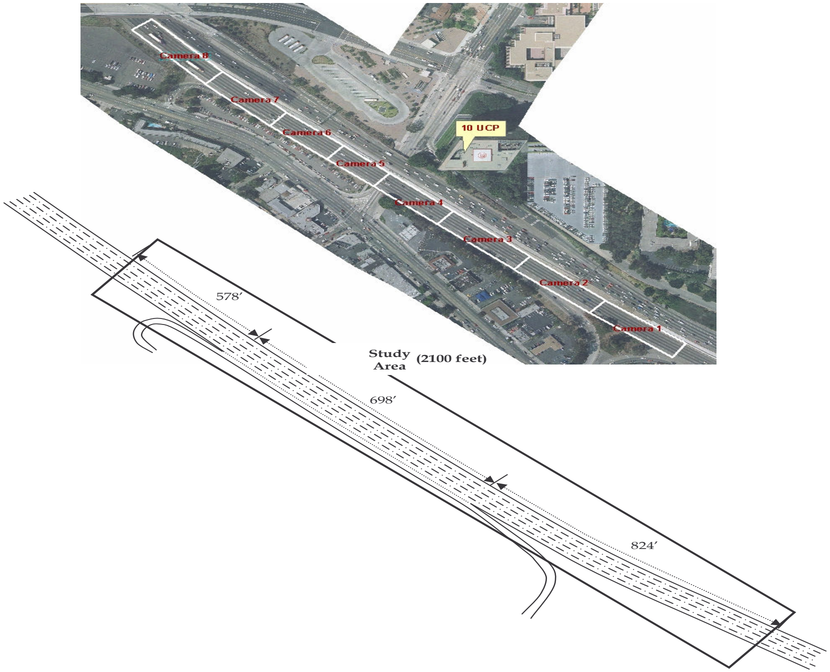
$$\mathcal{R}\left(\mu \,|\, \nu\right) := \frac{1}{N} \sum_{\sigma} \log \left\{ \frac{\mu(\sigma)}{\nu(\sigma)} \right\} \mu(\sigma) \qquad .\diamond$$

$$\mathcal{R}\left(\bar{\mu}^{(\alpha)}_{M,q,\beta} \,|\, \mu_{N,\beta} o \mathbf{T}^{-1}\right) = \mathrm{O}\left(\epsilon^{\boldsymbol{\alpha+2}}\right) .$$

- $\mathrm{T}\sigma =$ **Projection** on coarse variables$= \sum_{y \in D_k} \sigma_(y)$.

K., Trashorras, JSP '06; K., Plechac, Rey-Bellet, Tsagkarogiannis, [M^{2}AN, '07]; Are, K. Plechac, Rey-Bellet, [SIAM J. Sci. Comp. '08].

III. Traffic flow: Look-ahead dynamics



From Federal Highway Administration NGSIM U.S.101 (Hollywood Freeway) Data Analysis report.

Goal: Explore different traffic scenarios using a flexible computational framework, as an additional tool to approaches already in place.

- Individual stochastic dynamics and rules of behavior:

  -interactions with vehicle ahead, speed-up or slow-down

- Include more complexity at the individual level:

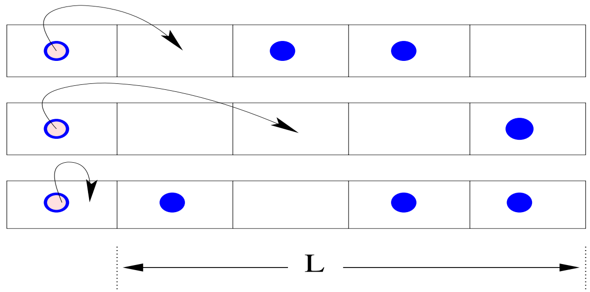
  -multiple lanes, entrances/exits, different types of vehicles.

- Stochasticity: model uncertainty in driver's decisions

- Mesoscale effects, what do we learn from mesoscale modeling?

References: Sopasakis, K., SIAM Appl. Math '06; Alperovich, Sopasakis, J. Stat. Phys. '08, Kurganov, Polizzi, Networks Heter. Med. '09.

Asymmetric simple exclusion process with Arrhenius look-ahead dynamics



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

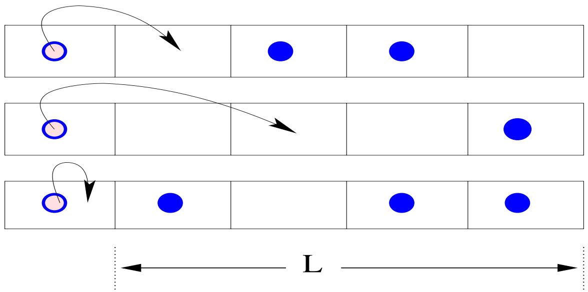
Configuration: $\sigma = \{\sigma(x) \mid x \in \Lambda \subset \mathbf{Z}^d\}$, $|\Lambda| = N$: total number of lattice sites.

Markov Chain modeling with state space

$$\Sigma = \text{set of all configurations } \sigma$$

Dynamics: Sequence of order-parameter exchanges between sites x and $x+1$.

- Transition rate: $c(x \mapsto x+1,\, \sigma) = c_0 \exp\Big[-\beta U(x,\sigma)\Big]$



Arrhenius law: a vehicle's motion is affected by the traffic ahead

- $U(x,\sigma) = \sum_{z \neq x} J(x-z)\sigma(z) - h(x)$.
- J: potential with look-ahead range L; $V : \mathbb{R} \to \mathbb{R}$ has compact support,

$$J(x-y) = \frac{1}{L} V\Big(\frac{x-y}{L}\Big)\,.$$

- strong interactions $J \to$ clustering due to slow-down
- Calibration in 1-d: $c_0 \sim$ max. speed in empty highway, $J \sim$ driver reaction to bumper-to-bumper traffic ahead.

References: Arrhenius diffusion laws in stat. mechanics/chemical engineering

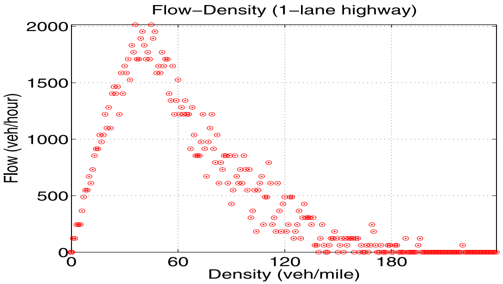
-Arrhenius Energy Barriers is KMC: Kang, Weinberg, J. Chem. Phys. '88, Chem. Rev. '95.

-Mesoscale models: Katsoulakis, Vlachos, Phys.Rev.Lett. '00, J. Chem. Phys. '03.

- Attractive interaction $\mapsto$ backward diffusion, clustering.

- A simplified version is the Cahn-Hilliard equation but w/o mobility depending on the energy barrier, and detailed interactions.

Some numerical experiments: Phase diagram for the complex system



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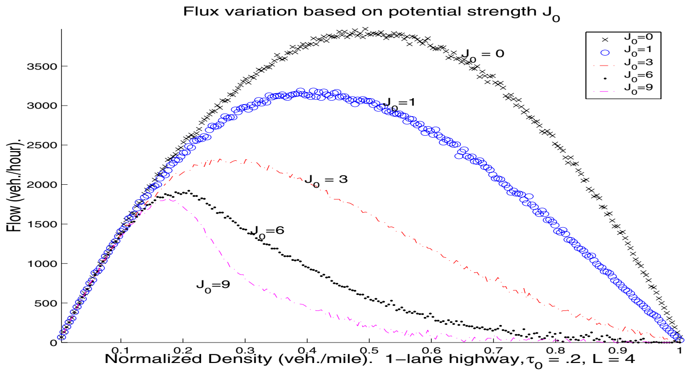


The non-convex form of these figures agrees with observations at higher densities in [Hall, F.L.: Traffic Flow Theory, US Federal Highway Administration, Washington (1996)]

Q: can we get any insights on this behavior?

Mesoscopics: Average behavior and deterministic closures

Consider the local coverage

$$v_N(x,t) = \frac{1}{|B_x|} \sum_{y \in B_x} \sigma_t(y)$$

For Kač potentials (local mean-field limits)

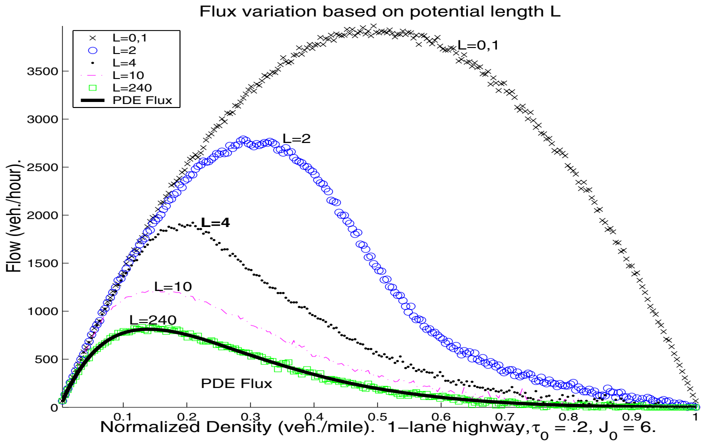
$$J^\gamma(x-y) = \gamma^d V(\gamma(x-y))\,, \qquad \gamma^{-1}: \quad \text{interaction range}$$

$c(x,t) \quad \approx \quad$ local average $\quad v_N(x,t)\,, \quad$ as $\quad N \to \infty\,,$

$$\partial_t c + c_o \partial_x \left[e^{-U} c(1-c) \right] = 0\,, \text{ where } U(x) = \int_x^1 V(x-y) c(y)\, dy\,.$$

The role of mesoscopics:

1. Approximate phase diagram for the complex system; "control" parameters of the problem:



2. Comparison of the agent-based model to earlier PDE-based models: $J = 0$ Lighthill-Whitham model,

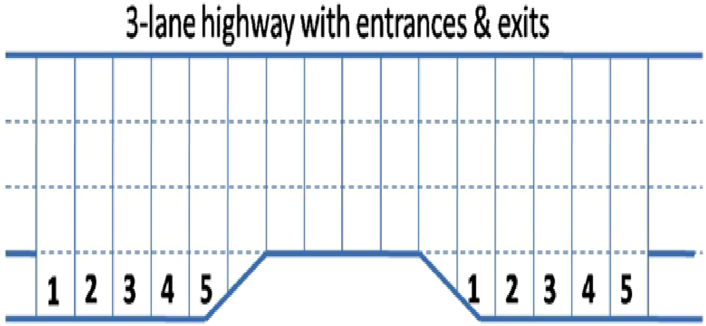
$$\partial_t c + c_o \partial_x \Big[c(1-c) \Big] = 0\,, \text{ for look-ahead pot. } V(x) = 0\,.$$

3. Comparisons to higher-order dispersive conservation laws:

[T. Nagatani, The physics of traffic jams, Rep. Prog. Phys., '02].

Include more complexity at the individual level:

-multiple lanes, entrances/exits, different types of vehicles.



- Transition rate: $c(x \mapsto x+1,\, \sigma) = c_0 \exp\Big[-\beta U(x,\sigma)\Big]$

- anisotropic potential accounts for passing/look-ahead

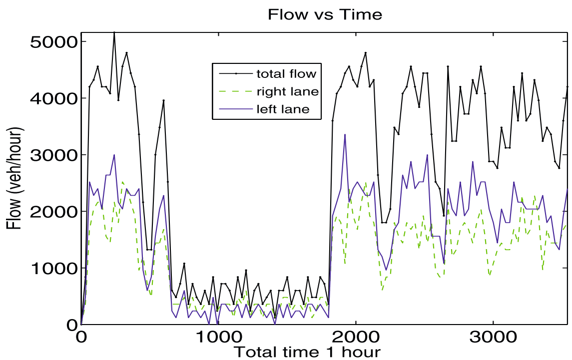
$$U(x,y,\sigma) = U_{la}(x,\sigma) + U_p(x,y,\sigma) + h(x,y,t)$$

$h = h(x,t)$: "external field" in stat. mech. e.g. traffic light, accident, etc.

- Stochasticity: models uncertainty in driver's decisions

- Micro-to-meso-scale phenomena:

  -effect of microscopics (e.g. a virtual accident) on the mesoscopics: initiation of stop-and-go waves



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