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

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Stochastic spatial evolutionary games

Joint work with:

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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 $S = \{1, 2\}$,

<table>
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<tr>
<th>agent $x$</th>
<th>strategy 1</th>
<th>strategy 2</th>
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<tbody>
<tr>
<td>strategy 1</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>strategy 2</td>
<td>0</td>
<td>5</td>
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-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 $\sigma$

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

**Dynamics-strategy revision:** Continuous Time Markov process \( \{\sigma_t\} \):


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

- **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 \( \Sigma = \{1, 2, \ldots, m\} \) with transition rates

\[
Q = \begin{pmatrix} q(x,y) \end{pmatrix}_{x,y \in \Sigma}
\]

Building blocks of the continuous time chain:

- **Residence time** \( \tau_x \): time spent by the process \( X_t \) at \( x \); random waiting time between consecutive jumps.

\[
P(\tau_x > t) = \exp(-\lambda(x)t), \quad \lambda(x) \geq 0
\]

- "Skeleton" Markov Chain

\[
p(x,y) = P(X_{\tau_x} = y \mid X_0 = x), \; y \neq x
\]

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)
Transition Probability $p(x,y)$

No depend. on the Past $1,...,k-1$

Present State $= x$

Possible Future State $= y$

Past States $= x_k$

$k = 1,2,...,k-1$

Residence Time: $\tau_x$

expon. distributed: $\lambda(x)$

Possible Future State $= z$

Possible Future State $= w$

Transition Probability $p(x,y)$

No depend. on the Past $1,...,k-1$
Some typical rates $c(x,\sigma,k)$:

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<th>Innovative</th>
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<td>Imitative</td>
<td>$F(u(x,\sigma,k) - u(x,\sigma,\sigma(x)))$</td>
<td>$F(u(x,\sigma,k))$</td>
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- **Innovative vs Imitative**: Innovative rates can introduce any strategy, even if not currently used in the population, i.e.
  $$c(x,\sigma,k) > 0 \quad \text{for all } x,\sigma,k$$

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

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

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

-Metropolis MCMC algorithm.

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

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

- **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:

\[
w(x, y, \sigma, k) := W(x, y) \delta_{\sigma(y)}(\{k\})
\]

- 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. \( \sigma \):

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

- Asymptotic closure: does

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

  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,

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

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

$$\frac{\partial}{\partial t} f(t, u, i) = \sum_{k \in S} c(u, k, i, f) f(t, u, k) - f(t, u, i) \sum_{k \in S} c(u, i, k, f)$$

$$f(0, u, i) = f_0(u, i)$$

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

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

1. \( c^\gamma(x, \sigma, k) = F(u(x, \sigma, k) - u(x, \sigma, \sigma(x)) \)
   \[
   = F \left( \sum_{x \in \mathbb{T}^{d,\gamma}} \gamma^d \mathcal{J} (\gamma(x - y)) a(k, \sigma(y)) - \sum_{x \in \mathbb{T}^{d,\gamma}} \gamma^d \mathcal{J} (\gamma(x - y)) a(\sigma(x)) \right) \\
   \xrightarrow{\gamma \to 0} F \left( \sum_{l \in S} a(k, l) \mathcal{J} \ast f(u, l) - \sum_{l \in S} a(i, l) \mathcal{J} \ast f(u, l) \right) \\
   = : c(u, i, k, f) \\
   \]

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

\[
\langle \pi^\gamma, g \rangle (\sigma) = \frac{1}{N} \sum_{x \in \Lambda} g(\gamma x, \sigma(x)) : 
\]
\[ L_\gamma \langle \pi^\gamma, g \rangle (\sigma) = \sum_{k \in S} \int_{\Lambda \times S} c(u, i, k, \pi^\gamma(\sigma)) (g(u, k) - g(u, i)) \pi^\gamma(\sigma, dudi) \]

3. Martingale representation theorem:

\[ \langle \pi_t^\gamma, g \rangle = \langle \pi_0^\gamma, g \rangle + \int^t_0 ds \sum_{k \in S} \int_{\Lambda \times S} c(u, i, k, \pi_s^\gamma) (g(u, k) - g(u, i)) \pi_s^\gamma(dudi) + M_{t, \gamma}^g \]

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

\[ \langle f_t, g \rangle = \langle f_0, g \rangle + \int^t_0 ds \sum_{k \in S} \int_{\Lambda \times S} c(u, i, k, f_s) (g(u, k) - g(u, i)) f_s(u, i)dudi \]
Connections to well-mixed systems and Mean Field theories, e.g. [Benaim, Weibull *Econometrica* (2003)]

For uniform interactions between agents, **exact closure for**:

- **Aggregate empirical 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 \(\Lambda\).

- For uniform interactions, \(c^\gamma(x, \sigma, i)\) depends only on \(\eta_i^N\) since,
  \[
  u(x, \sigma, k) := \sum_{y \in \Lambda} W(x, y) a(k, \sigma(y)) = \sum_{i \in S} a(k, i) \eta^N(i)
  \]
  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 $\eta^N_t(i)$ is itself a Markov process
(not always true!)

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

where $\eta^{j,k}$ is a new state induced from $\eta$ 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 $J = 1$, we have

$$\rho(i) := \int f(u, i) du = J \ast f(i)$$

so $c(u, k, i, f)$ is independent of $u$: $c^M(k, i, \rho) := c(u, k, i, f)$
From the IDEs we obtain

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

**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 $a_{12} = a_{21} = 0$,

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

- IDEs:

  Replicator: \[ \frac{\partial p}{\partial t} = (1 - p)J * pF(\beta(J*p - h)) \]
  \[ -p(1 - J * p) F(\beta(h - J * p)) \]

  Logit: \[ \frac{\partial p}{\partial t} = l(\beta(J*p - h)) - p \]

  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

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

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**

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**FIG. 7.** Contour plots containing examples of the morphology obtained for the model (2.9) with $k_r$ nonzero. Both plots are for the same initial data but the right-hand plot is for a later time than the left-hand plot. The right-hand plot demonstrates the tendency of the labyrinths to organize into larger scale structures at later times.

For future work, we will explore similar issues for mesoscopic models with Arrhenius dynamics as well as (2.9).

So far in this section, we have validated our spectral method by making comparisons of our computational results with derived asymptotic results. In all cases, the simulation results were in excellent agreement with the theoretical prediction. Thus, combined with the comparisons made in Section 3 with a finite difference numerical scheme, we see that the spectral method is indeed a very powerful and reliable numerical approach to the solution of mesoscopic models. Finally, we briefly mention some of the results that are obtainable with our spectral scheme in other parameter regimes, such as when the reaction rate $k_r$ is nonzero; in such a case complex patterns tend to develop [20]. A typical example computed in this case can be seen in Fig. 7 where a labyrinthine pattern is observed; the plot on the right is at a later time than the plot on the left. As we typically observe at later times in such simulations, the small structures tend to organize into larger structures and more regular patterns. Further details of such simulations will appear in future publications.

**5. CONCLUSIONS**

In this paper we have developed spectral-based algorithms for mesoscopic equations modeling surface processes and shown their greatly enhanced efficiency as compared to more traditional finite difference schemes. We validated the accuracy of the spectral schemes through comparison with asymptotic scalings and growth laws. We have also reviewed the derivation of mesoscopic models for pattern formation from the underlying microscopic mechanisms and discussed the connections of mesoscopic theories with well known models such as the Cahn–Hilliard equation and its variants.

Mesoscopic theories such as the ones discussed here in the context of surface processes are applicable to numerous areas including polymers, smart materials, biological systems, and complex fluids. We intend to further pursue the development of spectral schemes for such problems in future work.

• Metastability, tunneling and large deviations [Dirr, Manzi, Tsagkarogiannis, 2009]
**PDE approximation:** Spatial rescaling $J_\epsilon(x) = \epsilon^{-d} J(x/\epsilon)$. For small $\epsilon$ and we have

$$J_\epsilon * f \approx f + \frac{\epsilon^2}{2} J_2 \Delta f$$

**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:

\[ \lambda_L(k) = \beta(1-p_0)p_0\tilde{J}(k) - 1 \quad \text{vs.} \quad \lambda_R(k) = \beta(1-p_0)p_0\tilde{J}(k) \]

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

2. Stochastic lattice dynamics/ KMC

**Examples:** Catalysis, epitaxial growth, micromagnetics, etc.

Patterning through self-assembly

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”.

• $\sigma \in S_N = (\Sigma)^\Lambda_N$ – the microscopic configuration space.

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

A. Microscopic equilibrium Gibbs measure

\[ \mu_{N,\beta}(d\sigma) = \frac{1}{Z_{N,\beta}} e^{-\beta H_N(\sigma)} P_N(d\sigma), \]

\[ P_N(d\sigma) = \prod_{x \in \Lambda_N} \rho(d\sigma(x)). \]

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

\[ \mu^c(d\eta) := \mu\{\sigma \in S_N \mid T(\sigma) = \eta\} \]

New CG Hamiltonian:

\[ e^{-\beta H^c(\eta)} = \mathbb{E}[e^{-\beta H_N} \mid \eta] \equiv \int_{S_N} e^{-\beta H_N(\sigma)} P_N(d\sigma \mid Q), \]

Computing \( H^c(\sigma) \) directly \( \implies \) integration on a high-dimensional space.
Solution: Approximate $H^c$ or better $\mu^c$ by a convergent expansion in a small parameter.

\[ \bar{H}_m(\eta) = \bar{H}_m^{(0)}(\eta) - \frac{1}{\beta} \log \mathbb{E}[e^{-\beta(H_N - \bar{H}_m^{(0)})} | \eta] = \bar{H}_m^{(0)}(\eta) + \bar{H}_m^{(1)}(\eta) + NO(\epsilon^3). \]

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

K., Plechac, Rey-Bellet, Tsagkarogiannis, [M$^2$AN, ’07]
Lattice Dynamics:

(a) deposition – spin-flip, strategy update
(b) diffusion + interactions – agent migration

CG Monte Carlo Hierarchy:

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

In general, it is non-markovian.

**Stochastic closures**: when can we write a new approximating Markov process for $\eta_t$:

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

  $$L_c g(\eta) = \sum_{k \in A_c} c_a(k, \eta) \left[ g(\eta + \delta_k) - g(\eta) \right] +$$

  $$c_d(k, \eta) \left[ g(\eta - \delta_k) - g(\eta) \right].$$

- **Coarse-grained** rates and Detailed Balance: $\overline{c_a}^{(\alpha)}$ and $\overline{c_d}^{(\alpha)}$

**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:

\[ \mathcal{R}(\pi_1 | \pi_2) = \int_S \log \frac{d\pi_1}{d\pi_2} \pi_1(d\sigma). \]

II. Observables: Bounds on the weak error:

\[ \mathbb{E}_{T_{X_0}}[f(TX_T)] - \mathbb{E}_{Q_0}[f(Q_T)] \]

Bounds in terms of the “small” parameter

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

B. Microscopic Reconstruction – Reverse CG map

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:

\[ \mathcal{R} (\mu | \nu) := \frac{1}{N} \sum_{\sigma} \log \left\{ \frac{\mu(\sigma)}{\nu(\sigma)} \right\} \mu(\sigma) \]

\[ \mathcal{R} \left( \bar{\mu}_M^{(\alpha)} | \mu_{N,\beta} T^{-1} \right) = O \left( \epsilon^{\alpha+2} \right). \]

- **Tσ = Projection** on coarse variables = \( \sum_{y \in D_k} \sigma(y) \).

III. Traffic flow: Look-ahead dynamics


**Goal:** Explore different traffic scenarios using a flexible compu-
tional 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?

Asymmetric simple exclusion process with Arrhenius look-ahead dynamics

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

Configuration: $\sigma = \{\sigma(x) \mid x \in \Lambda \subset \mathbb{Z}^d\}$, $|\Lambda| = N$: 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 $x + 1$. 

Fig. 1. Simple schematic of the look-ahead rule (for $L = 4$ cells) pertaining to vehicle motion in the lattice for three different traffic examples. The process automatically simulates effects such as braking, acceleration, and simple exclusion rule through the interaction potential $U(x, \sigma)$ (2.2) for the provided range, $L$.

To overcome in changing from one state to another. This energy barrier is found by calculating the potential energy of each vehicle based on (3.1) and performing a move only if that energy is higher than a given threshold. (Note that these dynamics are different from the usual Metropolis dynamics, where a move is encouraged whenever the energy difference between the current position and the new position is high enough.)

During such a spin-exchange between nearest neighbor sites $x$ and $y$ the system will actually allow the order parameter $\sigma(x)$ at location $x$ to exchange value with the one at $y$. This is interpreted as advancing a vehicle from the site at $x$ to the empty site at $y$. Note that based on the construction of our potential $U$ it is not possible to move from an occupied site to another occupied cite; see Figure 1. In general, the rate at which a process will do this for spin-exchange Arrhenius dynamics is

\[
 c(x, y, \sigma(x, y)) =
 \begin{cases}
 c_0 \exp[-U(x, \sigma) - U(y, \sigma(x))] & \text{if } y = x + 1, \\
 0 & \text{otherwise}
 \end{cases}
\]

The parameters comprising the dynamics here are $c_0 = 1/\tau_0$ (2.5) with $\tau_0$ the characteristic or relaxation time for the process and $U(x, \sigma)$ as in (2.2).

Overall given (2.4) and the dynamics just described the probability of spin-exchange between $x$ and $y$ during time $[t, t + \Delta t]$ is

\[
 c(x, y, \sigma(x, y)) \Delta t + O(\Delta t^2).
\]

Clearly for one-lane traffic corresponds to either $x - 1$ or $x + 1$ in (2.4). Note that the exchange, due to the specific construction of the interaction potential $J$ in (2.3), can take effect if and only if the location at $x$ is occupied while the location at $y$ is not. A simple schematic of the lattice and some simple interactions are provided in Figure 1. At the same time, vehicles are restricted (exclusion rule) with performing...
• **Transition rate:** $c(x \rightarrow x + 1, \sigma) = c_0 \exp\left[ -\beta U(x, \sigma) \right]$

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** $L$; $V : \mathbb{R} \rightarrow \mathbb{R}$ has compact support,
  \[ J(x - y) = \frac{1}{L} V\left(\frac{x - y}{L}\right). \]

- **strong interactions** $J \rightarrow$ 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


• Attractive interaction $\rightarrow$ 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

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)

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

\[ c(x, t) \approx \text{local average } V_N(x, t), \quad \text{as } N \to \infty, \]

\[ \partial_t c + c_0 \partial_x \left[ e^{-U} c(1 - c) \right] = 0, \quad \text{where } U(x) = \int_x^1 V(x - y) c(y) \, dy. \]
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,

$$\partial_t c + c_0 \partial_x \left[ c(1 - c) \right] = 0, \text{ for look-ahead pot. } V(x) = 0.$$
3. Comparisons to higher-order dispersive conservation laws:

Include more complexity at the individual level:
-multiple lanes, entrances/exits, different types of vehicles.

![3-lane highway with entrances & exits](image)

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

- 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

References:

*Multi-lane models:* Alperovich, Sopasakis, J. Stat. Phys. ’08,

*Non-oscillatory central schemes for the mesoscopic PDE:* Kurganov, Polizzi, Networks Heter. Med. ’09.
REFERENCES

Reviews


Coarse-grained and Hybrid models


Error analysis and adaptivity

Temporal CG