Computational Physics (P452) Presentation

# Markovian Agent Based Monte Carlo Simulations

## for reaction-diffusion models, population dynamics, and epidemic spreading

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1 Introduction

Theory of Stochastic reactions

2 Applications

3 Conclusion

# Why perform Monte-Carlo Simulations

- They are important in capturing unexpected macroscopic features which may include competing dynamical states with more ease than solving traditional differential equations.
- They can address features driven purely by random noise. Critical microscopic fluctuations can induce strong macroscopic features that cannot be described by deterministic rate equations.
- It allows us to study *structure formation*, as we can visualise spontaneous formation of spatially inhomogeneous structures.
- For complicated systems described by higher order differential equations, Monte-Carlo methods can capture the gross system behaviour with relatively less computational costs.

# Master equation

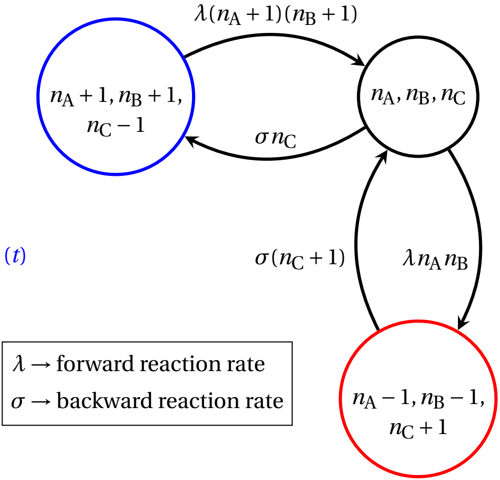
- The transition rates for a Markovian process is,

$$\frac{\partial P_n(t)}{\partial t} = \sum_{m \neq n} \left[ P_m(t)\, w_{m\to n} - P_n(t)\, w_{n \to m} \right]$$

- Consider a reversible reaction: $A + B \underset{\sigma}{\overset{\lambda}{\rightleftharpoons}} C$
- We can construct the master equation as,

$$\begin{aligned} \frac{\partial P_{n_A,n_B,n_C}(t)}{\partial t} &= \lambda\,(n_A+1)\,(n_B+1)\,P_{n_A+1,n_B+1,n_C-1}(t) \\ &\quad + \sigma\,(n_C+1)\,P_{n_A-1,n_B-1,n_C+1}(t) \\ &\quad - (\lambda\, n_A n_B + \sigma\, n_C)\,P_{n_A,n_B,n_C}(t) \\ &= \sum_m L_{mn} P_m(t) \end{aligned}$$

where $L_{nm} = \delta_{nm} \sum_{m' \neq n} w_{n \to m'} - w_{m \to n \neq m} \longrightarrow$ Reduces it to a linear algebra problem in infinitely many dimensions.



$\lambda \rightarrow$ forward reaction rate

$\sigma \rightarrow$ backward reaction rate

# Observables & Ensemble Averages

- Consider an arbitrary obervable quantity $f(n,t)$. Then its time evolution will be given by the following. If $f(n,t) = n_{\mathrm{A}}(t)$, mean particle number of species A, it will evolve as,

$$\frac{\partial\langle f(n,t)\rangle}{\partial t} = \sum_{n} f(n)\,\frac{\partial P_n(t)}{\partial t} \implies \boxed{\frac{\partial\langle n_{\mathrm{A}}(t)\rangle}{\partial t} = \sum_{n_{\mathrm{A}},n_{\mathrm{B}},n_{\mathrm{C}}=0}^{\infty} n_{\mathrm{A}}\,\frac{\partial P_{n_{\mathrm{A}},n_{\mathrm{B}},n_{\mathrm{C}}}(t)}{\partial t}}$$

- Simplifying, we get the Rate equation,

$$\begin{aligned}\frac{\partial\langle n_{\mathrm{A}}(t)\rangle}{\partial t} &= \sum_{n_{\mathrm{A}},n_{\mathrm{B}},n_{\mathrm{C}}=0}^{\infty} n_{\mathrm{A}}\left[\lambda\left(n_{\mathrm{A}}+1\right)\left(n_{\mathrm{B}}+1\right)P_{n_{\mathrm{A}}+1,n_{\mathrm{B}}+1,n_{\mathrm{C}}-1}(t) + \sigma\left(n_{\mathrm{C}}+1\right)P_{n_{\mathrm{A}}-1,n_{\mathrm{B}}-1,n_{\mathrm{C}}+1}(t)\right] \\ &\quad - \sum_{n_{\mathrm{A}},n_{\mathrm{B}},n_{\mathrm{C}}=0}^{\infty} n_{\mathrm{A}}\left[\left(\lambda\, n_{\mathrm{A}} n_{\mathrm{B}} + \sigma\, n_{\mathrm{C}}\right)\right]P_{n_{\mathrm{A}},n_{\mathrm{B}},n_{\mathrm{C}}}(t)\end{aligned}$$

In the first term, we can convert $n_{\mathrm{A}} \to n_{\mathrm{A}}-1, n_{\mathrm{B}} \to n_{\mathrm{B}}-1, n_{\mathrm{C}} \to n_{\mathrm{C}}+1$ and in the second term, $n_{\mathrm{A}} \to n_{\mathrm{A}}+1, n_{\mathrm{B}} \to n_{\mathrm{B}}+1, n_{\mathrm{C}} \to n_{\mathrm{C}}-1$

$$\frac{\partial\langle n_{\mathrm{A}}(t)\rangle}{\partial t} = \sum_{n_{\mathrm{A}},n_{\mathrm{B}},n_{\mathrm{C}}=0}^{\infty}\left[\lambda\left(n_{\mathrm{A}}-1\right)n_{\mathrm{A}} n_{\mathrm{B}} + \sigma\left(n_{\mathrm{A}}+1\right)n_{\mathrm{C}} - \left(\lambda\, n_{\mathrm{A}}^2 n_{\mathrm{B}} + \sigma\, n_{\mathrm{A}} n_{\mathrm{C}}\right)\right]P_{n_{\mathrm{A}},n_{\mathrm{B}},n_{\mathrm{C}}}(t)$$

# Observables & Ensemble Averages

- Opening up the brackets and cancelling terms,

$$\begin{aligned}\frac{\partial\langle n_{\mathrm{A}}(t)\rangle}{\partial t} &= \sum_{n_{\mathrm{A}},n_{\mathrm{B}},n_{\mathrm{C}}=0}^{\infty}\left[\cancel{\lambda n_{\mathrm{A}}^{2} n_{\mathrm{B}}} - \lambda n_{\mathrm{A}} n_{\mathrm{B}} + \cancel{\sigma n_{\mathrm{A}} n_{\mathrm{C}}} + \sigma n_{\mathrm{C}} - \cancel{\lambda n_{\mathrm{A}}^{2} n_{\mathrm{B}}} - \cancel{\sigma n_{\mathrm{A}} n_{\mathrm{C}}}\right] P_{n_{\mathrm{A}},n_{\mathrm{B}},n_{\mathrm{C}}}(t) \\ &= \sum_{n_{\mathrm{A}},n_{\mathrm{B}},n_{\mathrm{C}}}\left[-\lambda n_{\mathrm{A}} n_{\mathrm{B}} + \sigma n_{\mathrm{C}}\right] P_{n_{\mathrm{A}},n_{\mathrm{B}},n_{\mathrm{C}}}(t) = \boxed{-\lambda\langle n_{\mathrm{A}} n_{\mathrm{B}}\rangle + \sigma\langle n_{\mathrm{C}}\rangle = R(t)}\end{aligned}$$

- Here, the time-derivative of the second moment term introduces higher-order correlations. Thus, we are still stuck with an infinite set of linear coupled DEs for moments/correlations.
- Mean Field Approximation: Neglect all two-point/higher correlations, which means

$$\langle n_{\mathrm{A}} n_{\mathrm{B}}(t)\rangle \approx \langle n_{\mathrm{A}}(t)\rangle\langle n_{\mathrm{B}}(t)\rangle$$

  which is reasonable for spatially well-mixed systems or for reactions with abundant reactants where all spatial and time correlations are small relative to the mean densities.

# Markovian Agent Based Monte-Carlo Simulations

- In agent-based Monte Carlo simulations, we implement the microscopic stochastic reaction processes as a Markov chain – the updated configurations depend only on the immediately past states, and transitions between them are governed by predefiined probabilities.
- The underlying conceptual framework consists of stochastic master equations, – directly determining quantities such as particle numbers, their Fourier transforms, correlation functions etc.
- The goal is not to fully reflect a natural system's behavior on all scales, but to properly capture its *emergent qualitative features at sufficiently long times and distances*, including temporal oscillations or spatial structures.

# Simulation Setup

We first need to establish the rules of the world.

- Agents: Indistinguishable passive (or active) particles belonging to a species that are subject to certain reactive processes.
- Simulation space: Particles are allowed to move or hop between sites on a lattice – lattice sites may be constrained by a finite carrying capacity.
- Reactive process: Particles may interact with themselves or with other particles of their own species or another species.

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Now, once the initial setup is completed, we run the simulation.

- At each step, one particle is randomly selected from the space and subjected to reactive processes based on predefined probabilities.
- Time evolution: A Monte Carlo step (MCS) is complete when each particle that was present at the start of the step was selected once on average.
- Observables: We use Master equations to track observables as the simulation evolves.

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    - Diffusion-limited Annihilation Reactions
    - Prey-Predator Models
    - Epidemic Spreading
3. Conclusion

# Diffusion-limited Annihilation reactions

- These are the simplest forms of reaction-diffusion models
- For example, consider single-species coagulation reaction: $2\mathrm{A} \xrightarrow{\lambda} \mathrm{A}$
- Solving for the number density, $n_A$,

$$\frac{\partial\langle n_\mathrm{A}(t)\rangle}{\partial t} = -\lambda\,\langle[n_\mathrm{A}(n_\mathrm{A}-1)](t)\rangle \approx -\lambda\left\langle n_\mathrm{A}^2(t)\right\rangle$$

$$\langle n_\mathrm{A}(t)\rangle = A\,t^{-\alpha} + \epsilon(t) \implies \boxed{\log\langle n_\mathrm{A}(t)\rangle \propto -\log t}$$

# Diffusion-limited Annihilation reactions

**Algorithm 1** Monte-Carlo algorithm for single species annihilation in 1D.

```
Input: Initialize WORLD[$0 : N-1$] = $(1, \dots, 1)$
Output: WORLD
DIFFUSION = 0.25
for $j = 1$ to $N$ do
    $j$ = RANDOMINT($0, N-1$) s.t. WORLD[$j$] == 1    // pick a random non-empty location
    if rand() < DIFFUSION then
        if rand() < 0.5 then
            WORLD[$j-1$], WORLD[$j$] = 1, 0    // go left
        else
            $j = -1$ if $j == N-1$ else $j$
            WORLD[$j+1$], WORLD[$j$] = 1, 0    // go right
        end if
    end if
end for
return WORLD
```

# Single Species Annihilation in 1D

Monte-Carlo simulation of the one-dimensional binary-annihilation reaction with periodic boundary conditions. Hopping probability 25% in either direction. Every site in the inital lattice is occupied by a particle. Note that the theoretical $\langle n \rangle$ value goes to 0 here while the simulation does not, due to the formation of isolated islands where the particles can remain stable for a long time – more likely to happen in a realistic scenario.

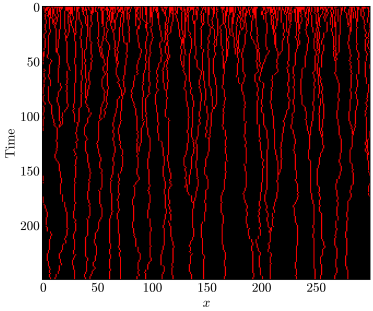

Figure 1: Snapshot of a single simulation run

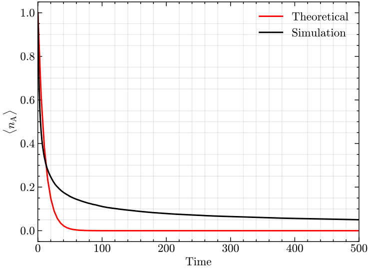

Figure 2: Plot of number density vs. time, averaged over 100 runs. Monte-Carlo error is $\sim 10^{-3}$ is too small to be shown in the plot.

# Two-species Annihilation

- Consider $\mathrm{A} + \mathrm{B} \to \emptyset$
- We need two particles of distinct species to meet for annihilation.
- This leads to slower density decay than the single species model.
- At large time steps, we are left with islands of each species where no reactions occur and all possible interactions are confined to the empty space between them.
- In differential equation form,

$$\frac{\partial \langle n_{\mathrm{B}}(t) \rangle}{\partial t} = \frac{\partial \langle n_{\mathrm{A}}(t) \rangle}{\partial t} = -\lambda \langle [n_{\mathrm{A}} n_{\mathrm{B}}](t) \rangle$$

$$\text{if } \langle n_{\mathrm{A}}(0) \rangle = \langle n_{\mathrm{B}}(0) \rangle \implies \langle n_{\mathrm{A}}(t) \rangle, \langle n_{\mathrm{B}}(t) \rangle \sim t^{-d/2}$$

$$\text{if } \langle n_{\mathrm{A}}(0) \rangle > \langle n_{\mathrm{B}}(0) \rangle \implies \langle n_{\mathrm{B}}(t) \rangle \sim e^{-t}$$

- However, at higher dimensions, mean-field equations cannot correctly capture kinetics in inhomogenous systems. To fix this, we can reverse-engineer the rate equation from the known time-dependence of $\langle n \rangle$, obtaining an effective rate equation

$$\frac{d \langle n_{\mathrm{A}}(t) \rangle}{dt} = -\langle \lambda(t) \rangle \langle n_{\mathrm{A}}(t) \rangle \,.$$

# Two-species Annihilation

**Algorithm 2** Monte-Carlo algorithm for two-species annihilation in 1D.

```
Input: WORLD[$0 : N-1$] = (a, b, a, b, ...)        // Initialise the world with species a & b randomly.
Output: WORLD
DIFFUSION $= 0.25$
for $j = 1$ to $N$ do
    $j =$ RANDOMINT($0, N-1$) s.t. WORLD[$j$] $\neq 0$        // pick a random non-empty location
    if rand() < DIFFUSION then
        if rand() $< 0.5$ then
            If the element on the left ($j-1$) is of the opposite flavour, move and annihilate, else do nothing.
        else
            If the element on the right ($j+1$) is of the opposite flavour, move and annihilate, else do nothing.
        end if
    end if
end for
return WORLD
```

# Two-species Annihilation

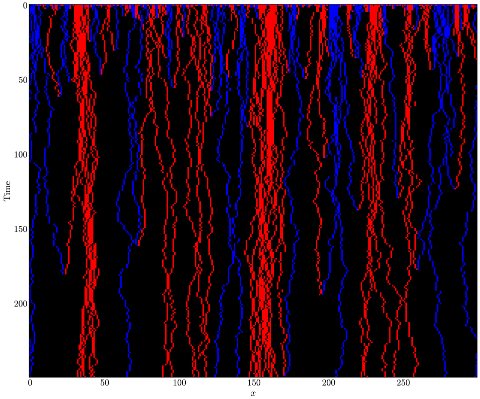

Figure 3: Snapshot of the time evolution of a single simulation in one dimension.

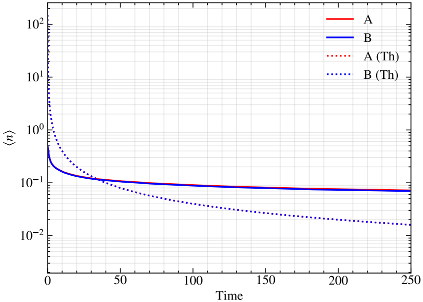

Figure 4: Evolution of mean number density averaged over 1000 runs. The simulation values, like in the last case does not go to zero due to the formation of islands. Monte-Carlo error $\sim 10^{-3}$.

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# Lotka-Volterra Model

- We look at the dynamics of a predator and a prey species interacting on a two-dimensional lattice.
- We setup the world with two species, predators and prey.
- A predator can predate upon the prey and/or die. The prey can only reproduce.

$$A + B \xrightarrow{r_{\text{predation}}} 2A$$

$$\text{For death and birth, } A \xrightarrow{d_{\text{predator}}} \emptyset \text{ and, } B \xrightarrow{b_{\text{prey}}} 2B$$

- In differential equation form,

$$\frac{d(n_{\text{prey}})}{dt} = an_{\text{prey}} - bn_{\text{prey}}n_{\text{predator}}$$
$$\frac{d(n_{\text{predator}})}{dt} = cn_{\text{prey}}n_{\text{predator}} - dn_{\text{predator}}$$

# Lotka-Volterra Simulation

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**Algorithm 3** Pseudocode for the Monte-Carlo algorithm for 2D Lotka-Volterra Simulation, representing one MCS.

---

```
Input: Let WORLD be a 2D array randomly populated with species A (predator) and B (prey) s.t. there are $N$ total particles in the lattice.
Output: WORLD
1. Select a particle $P$ at random. $P$ will be of species $S_P$.
2. Let $E_P$ be the lattice site of $P$.
3. if rand() $< r_{\text{hopping}_S} \rightarrow$ Randomly hop onto one of the neighbouring sites.
4. if $S_P =$ B
    1. if rand() $< b_{\text{prey}} \rightarrow$ generate a new particle of species B .
5. if $S_P =$ A
    1. Remove each particle of species B at $E_P$, $b_i$ and generate a new particle of species A at $E_P$ with probability $r_{\text{predation}}$ each.
    2. if rand() $< d_{\text{prey}} \rightarrow$ remove particle P from $E_P$.
```

# Lotka-Volterra Simulation

- When a few predator particles enter an area abundant with prey, a spreading activity front appears. Here, the predator particles can reproduce rapidly, inducing local population expansion.
- Prey are consumed during this process, leaving a depletion region of low abundance in which predators cannot survive for long.
- Hence, the bulk of surviving predators move toward areas of high prey abundance, leaving behind empty spaces in the lattice where over time species can replenish, thus enabling another activity front to pass through.
- We see a glimpse of this oscillatory structure formation behaviour in the snapshot – patches of blue are invaded by red and pink represents lattice sites containing members of both species.

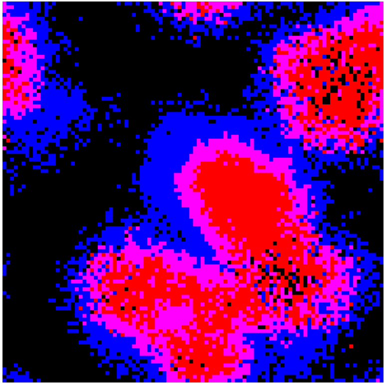

Figure 5: A snapshot of the simulation.

# Lotka-Volterra Simulation

Other than spontaneous structure formation, Lotka-Volterra Simulations can also be used to study other evolutionary ecological dynamics of prey-predator systems.

- We can periodically vary external resources can be used to study the co-evolution of the prey-predator systems.
- At an extinction critical points, the detailed balance conditions are typically violated, and such systems can display an non-equilibrium phase transitions.
- One can track survival traits by assigning numerical trait values to each particle (active agents). By allowing individual particles to pass on their traits to their offsprings, one can observe the effects of **Darwinian adaptation**.
- Hierarchical prey-predator interactions (e.g. a **food chain**), are described by the *May-Leonard Models*, which can be simulated by extending the existing setup.

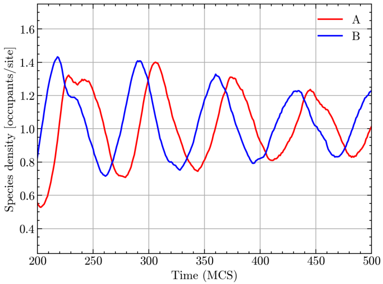

Figure 6: Oscillatory $\langle n_{\text{predator/prey}} \rangle$ obtained for a single Monte-Carlo run – only showing the steady state after 200 MCS. Since this is one Monte-Carlo run, we cannot calculate statistically the error.

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# SIR Modelling

- The susceptible-infectious-recovered (SIR) model is a simplified model for epidemic spreading with recovery/death.
- The population is divided into – infected, susceptible and recovered species, who are immune to re-infection. The dynamics of the world is represented by,

$$\mathrm{I} + \mathrm{S} \xrightarrow{r} \mathrm{I} + \mathrm{I}$$

$$\mathrm{I} \xrightarrow{\gamma} \mathrm{R}$$

- The differential rate equations for the three species will be,

$$\frac{d\langle n_{\mathrm{S}}(t)\rangle}{dt} = -r\langle n_{\mathrm{I}}(t)\rangle\langle n_{\mathrm{S}}(t)\rangle ,$$
$$\frac{d\langle n_{\mathrm{I}}(t)\rangle}{dt} = r\langle n_{\mathrm{I}}(t)\rangle\langle n_{\mathrm{S}}(t)\rangle - \gamma\langle n_{\mathrm{I}}(t)\rangle ,$$
$$\frac{d\langle n_{\mathrm{R}}(t)\rangle}{dt} = \gamma\langle n_{\mathrm{I}}(t)\rangle ,$$

- Detailed numerical analysis will be provided in the report.

# SIR Modelling

- Although the SIR rate equations can accurately capture the course of an epidemic near its peak and for large and well-connected populations, they cannot properly account for two-point (or higher) correlations or spatio-temporal fluctuations.
- These fluctuations stem from environmental variability and the intrinsic stochasticity of the reaction processes, and become important quantitatively at the outset and at the late stage of the epidemic.
- Stochastic fluctuations may drive the system into the absorbing epidemic extinction state during the early stages of the infection outbreak and crucially affect the scaling properties at the epidemic threshold.

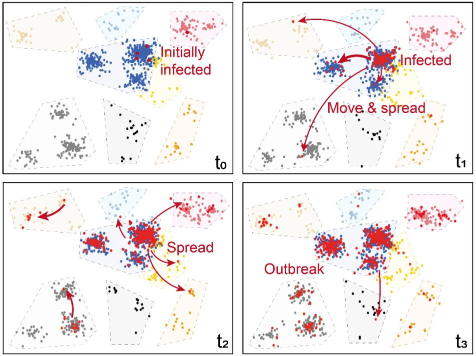

Figure 7: Modelled population mobility and the spread of the disease at four increasing time steps. Source: Chen *et. al.*, 2023.

# SIR Modelling

Here, the dotted lines show the solutions to the coupled differential eqs. Notice how $\langle n_S \rangle$ does not fully go to zero for the simulation with 100 runs – due to islands of susceptible people being formed who do not get exposed to infected people.

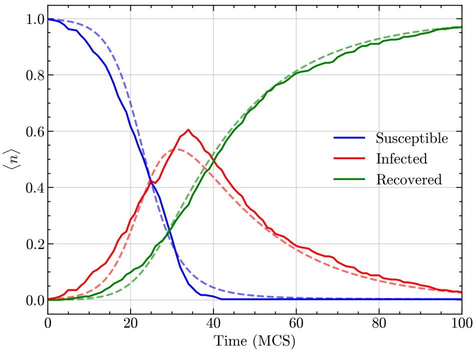

Figure 8: Time evolution of $\langle n \rangle$ for all three species over one Monte-Carlo run ($r = 0.075, \gamma = 0.05$).

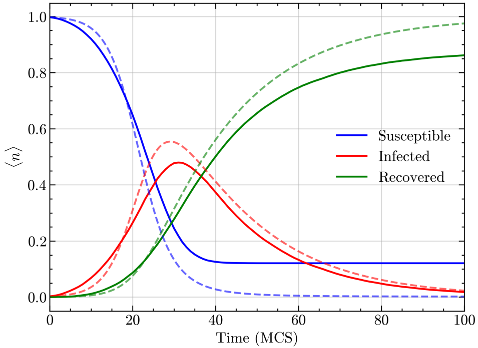

Figure 9: Time evolution of $\langle n \rangle$ for all three species over 100 Monte-Carlo runs ($r = 0.075, \gamma = 0.05$). The error bar is of the order $\sim 10^{-2}$.

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# Caveats of Agent-based Monte Carlo Modelling

- Any quantity of interest should be computed for sufficiently many individual trajectories to ensure that the results are statistically significant and reach the desired accuracy.
- For correlation functions, we can utilise the spatial and temporal symmetries of the system to obtain local correlations by averaging over sufficiently disjoint regions.
- For systems where the lattice size is crucial (eg. ecological or biological systems), one has to trade computational time for more accurate potrayal of the problem in question.
- The models are also heavily dependent on the choice of implementation of the Monte-Carlo algorithm. (eg. multiple site occupancies for annihilation reactions can lead to exponential decay instead of coagulation as expected – as each particle always has another reactant available which removes the binary reaction condition that two particles need to meet).

However it is to note that **sometimes results obtained from Monte-Carlo methods do not always constitute unwanted artefacts, but instead may genuinely reflect model properties which can only be derived stochastically**.

# Summary

- We introduced the Master equation as the underlying framework for Markovian process driven Monte-Carlo Simulations and agent-based simulations of stochastic models that describe bio-chemical reactions, population dynamics, and epidemic spreading.
- The underlying assumption is that much of a complex system's features are irrelevant in capturing the essence of its gross dynamical properties. If necessary, additional complications can be reintroduced at the expense of increased computational costs.
- Monte-Carlo methods are usefull in **visualising the dynamics of simulations** (eg: as we saw in the Lotka-Volterra snapshots) as well as tracking populations sizes whereas differential equations only tell us about the evolution of quantities like population sizes – which is just a numerical value.
- Because of this, features like **structure formation**, which (we have seen in both Lotka-Volterra and reaction-diffusion here) can only be studied using Monte-Carlo simulations.
- Although it is conceptually easy to add more variables and additional dynamical features to a model system, it becomes quickly impractical to properly run parameter sweeps to adequately assess their characteristic regimes. This ultimately constrains the applicability of stochastic simulation models.

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*Thank You*

# Appendix: Stationarity

- In the stationary regime, the configurational probabilities become time-independent, which implies that the net global probability current across all connected configurations, vanishes.
- This detailed-balance condition relates the stationary configurational probabilities with the forward and backward transition rates.
- As $t \to \infty$, let's say we achieve stationarity. This means that

  $$\frac{\partial P_n(\infty)}{\partial t} = \sum_{m \neq n} \left[P_m(\infty)\, w_{m\to n} - P_n(t)\, w_{n\to m}\right] = 0 \implies P_m(\infty)\, w_{m\to n} - P_n(\infty)\, w_{n\to m} = 0$$

  $$\frac{P_n(\infty)}{P_m(\infty)} = \frac{w_{m\to n}}{w_{n\to m}}$$

  This way, we can prove detailed balance.
- For an arbitrary configuration cycle $n_1 \to n_2 \to \dots n_N = n_1$ of length $N-1$ and its reverse $n_N = n_1 \to n_{N-1} \to \dots n_1$, the product of stationary probabilities on the left-hand side cancels, and we obtain the equivalent Kolmogorov criterion, which states that detailed balance holds if and only if

  $$w_{n_1\to n_2}\, w_{n_2\to n_3} \dots w_{n_{N-1}\to n_1} = w_{n_1\to n_{N-1}}\, w_{n_{N-1}\to n_{N-2}} \dots w_{n_2\to n_1}$$