Efficient Analysis of Population Protocols and Chemical Reaction Networks

Doctoral Defense

Martin Helfrich

December 5, 2023

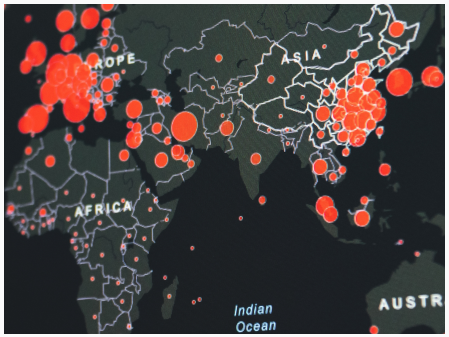
Introduction: Motivation

Introduction: Models

"Population protocols and chemical reaction networks are formal models in which many simple entities interact resulting in a hard to analyse system."

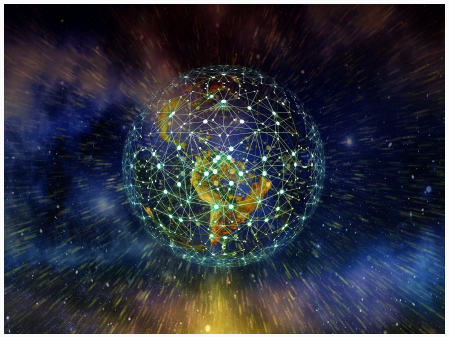
Introduction: Use Cases

Epidemiology

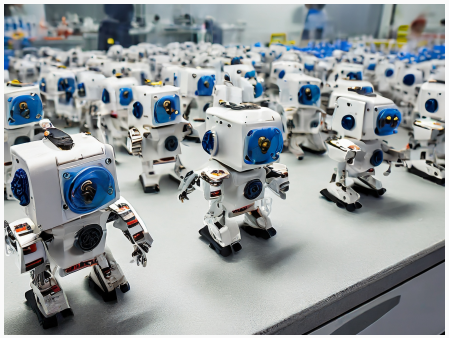


Sensor Networks

Social Networks



PP
CRN



Robot Swarms

Self-Organizing Systems

Drug Discovery

Introduction: Thesis Overview

Goal of Thesis:

Enable efficient (or "practical") analysis of these models via:

1. Theoretical results
2. New efficient analysis methods
3. Easily accessible tools

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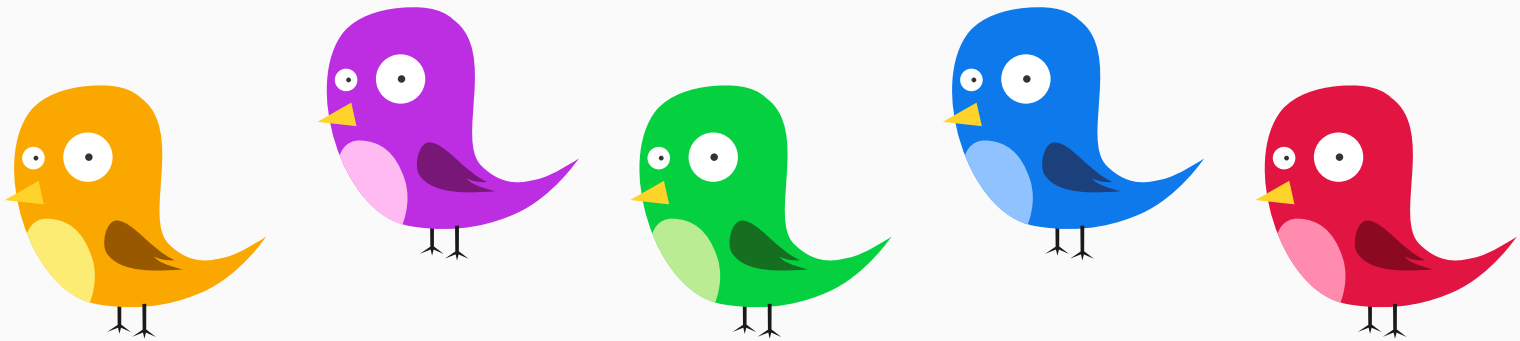
Results of Thesis:

- **Efficient verification of population protocols**
  $\rightarrow$ in this talk: focus on tool Peregrine
- **Synthesis of efficient population protocols**
  $\rightarrow$ not in this talk
- **Efficient transient analysis of chemical reaction networks**
  $\rightarrow$ in this talk: focus on segmental simulation idea

Population Protocols

Population Protocols: Intro

(birds by Michael Blondin)



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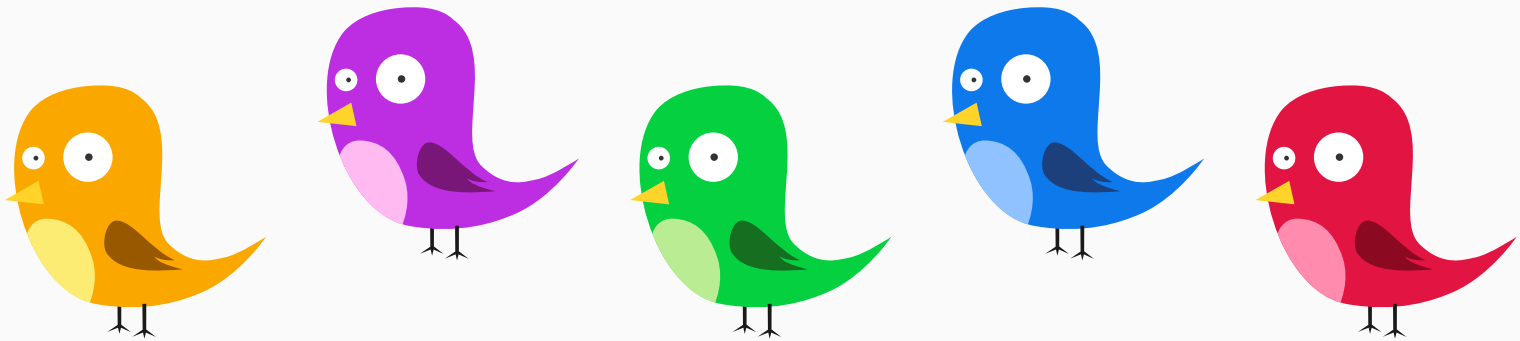

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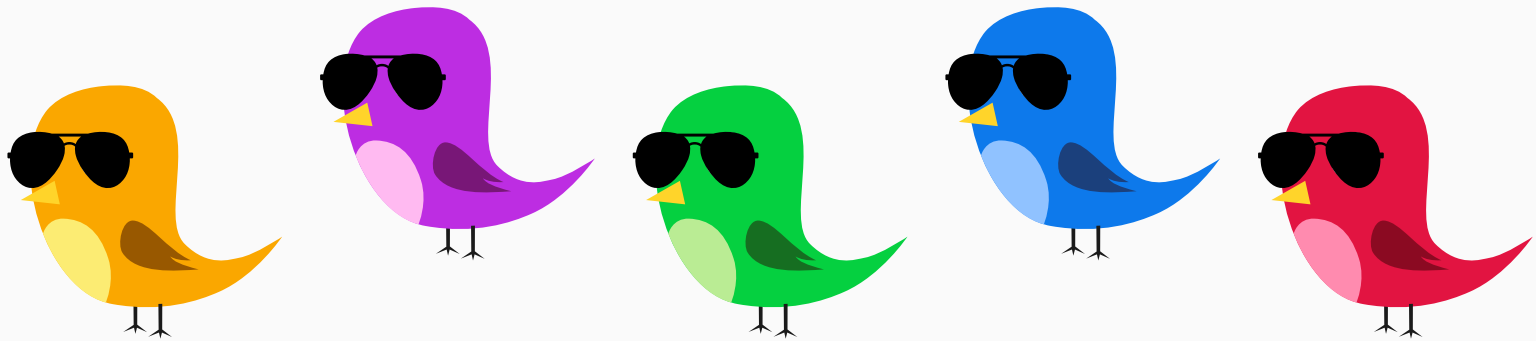

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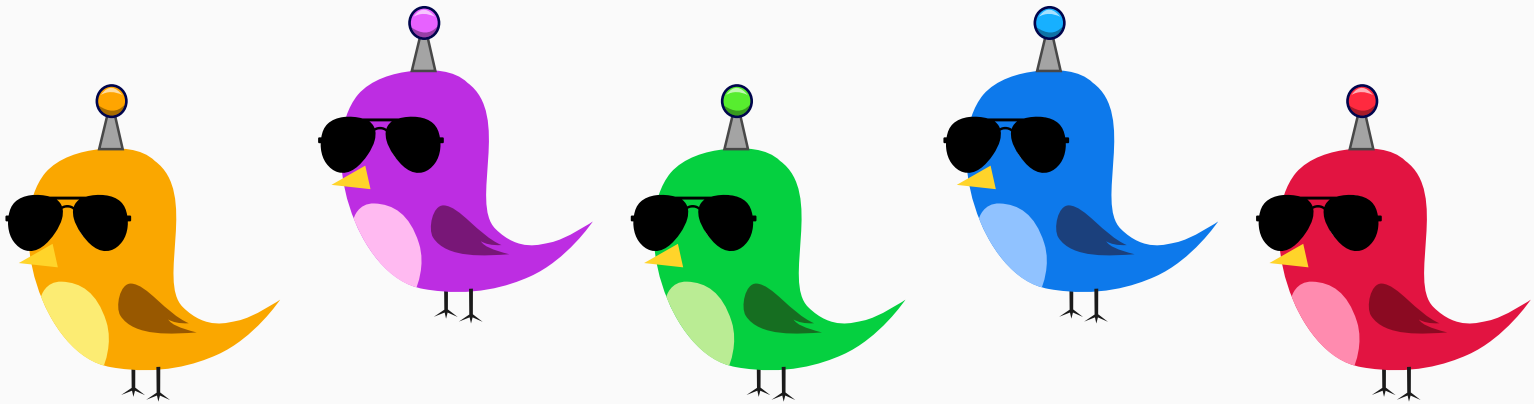

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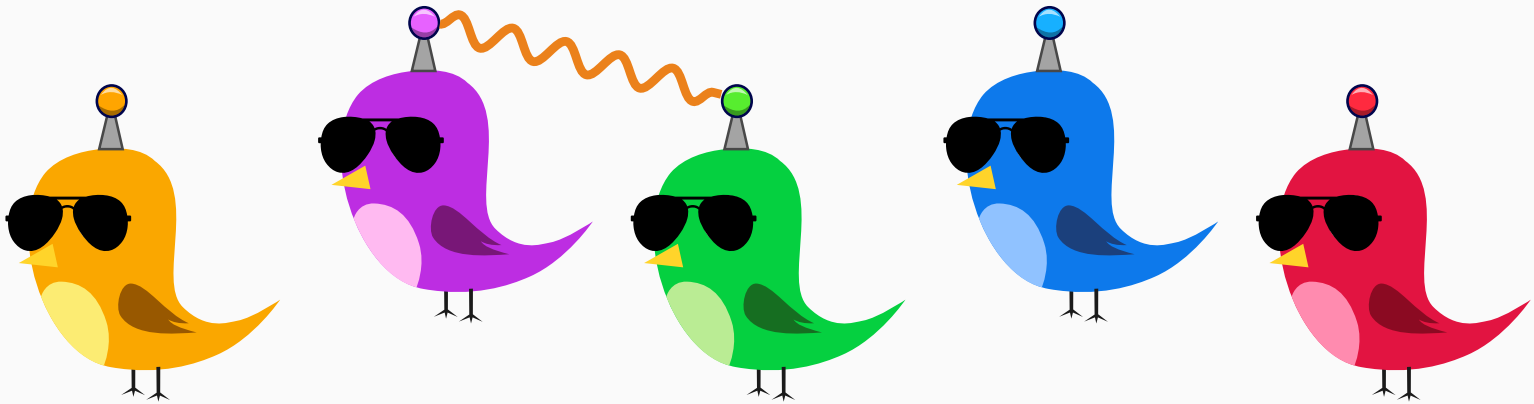

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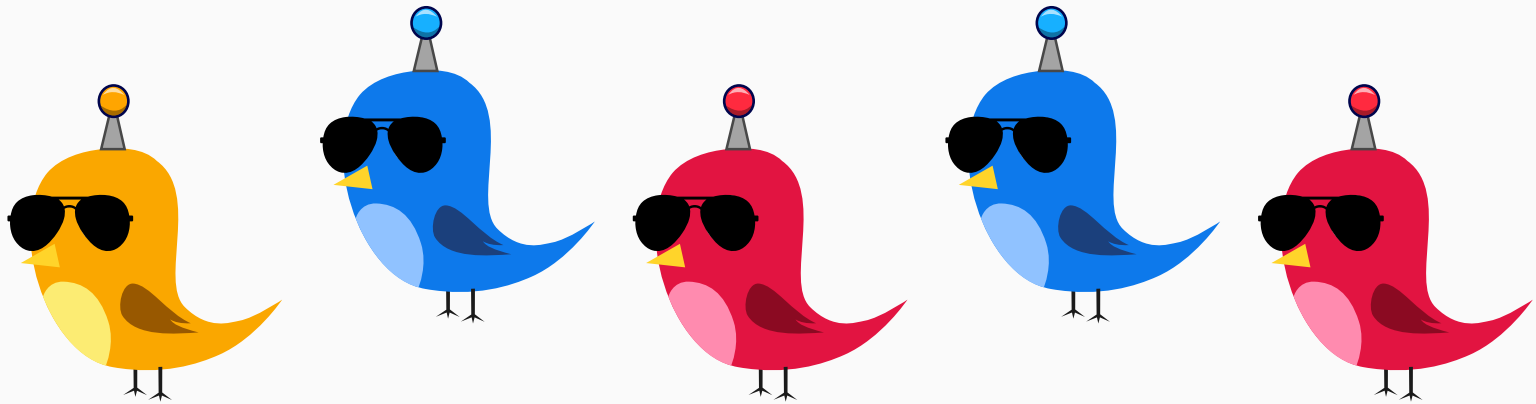

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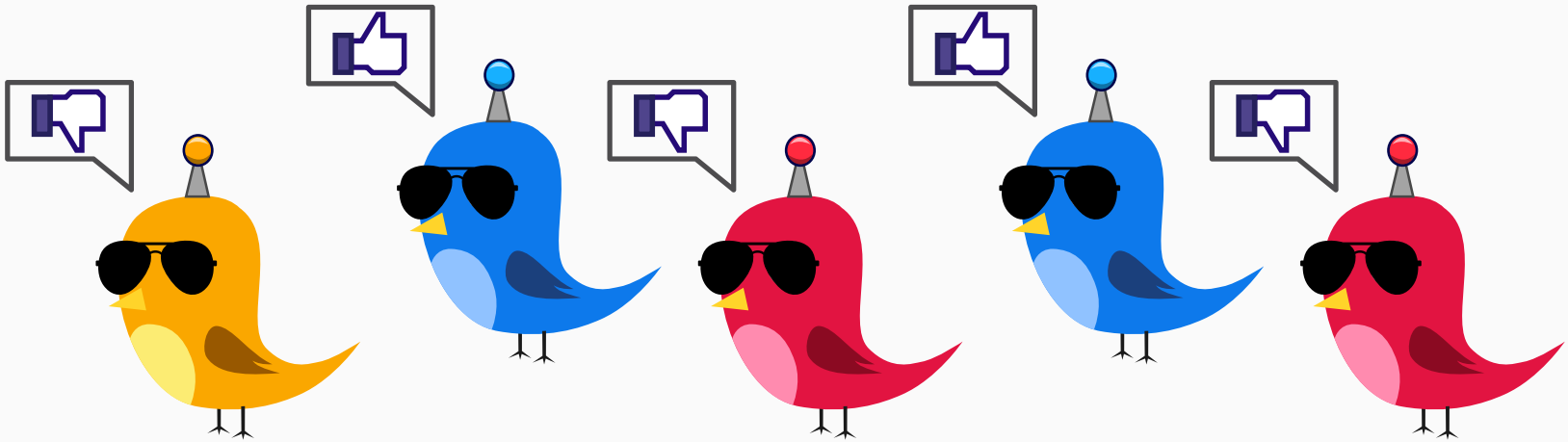

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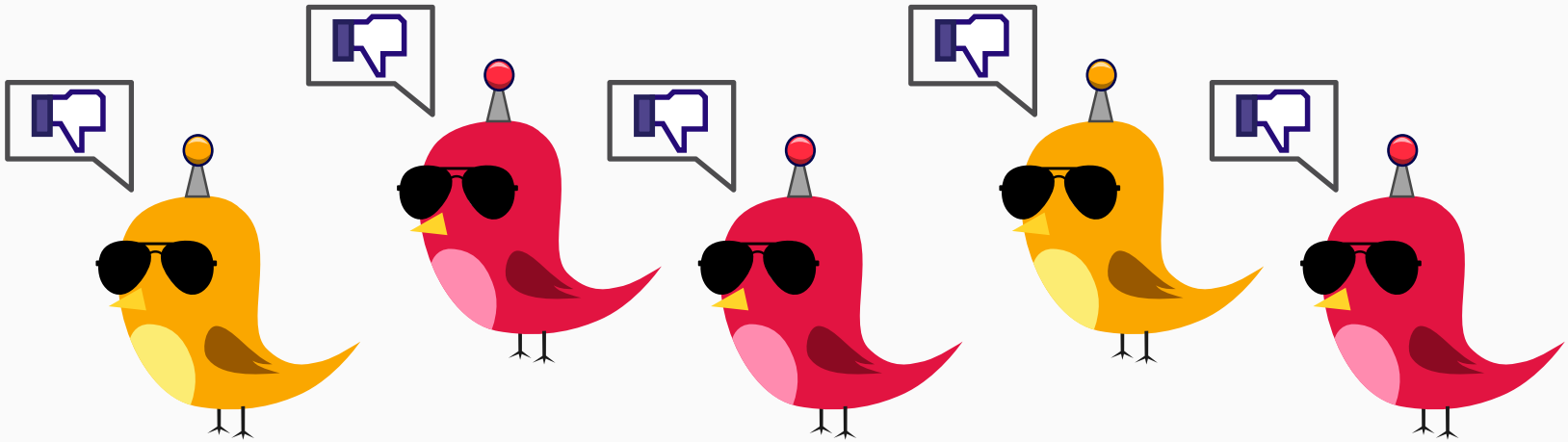

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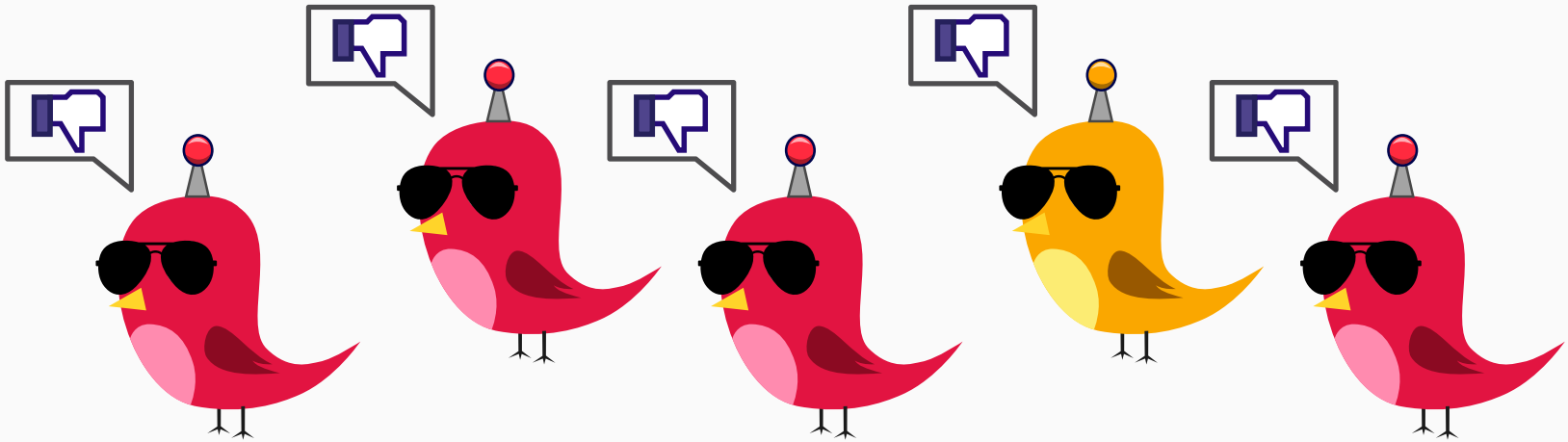

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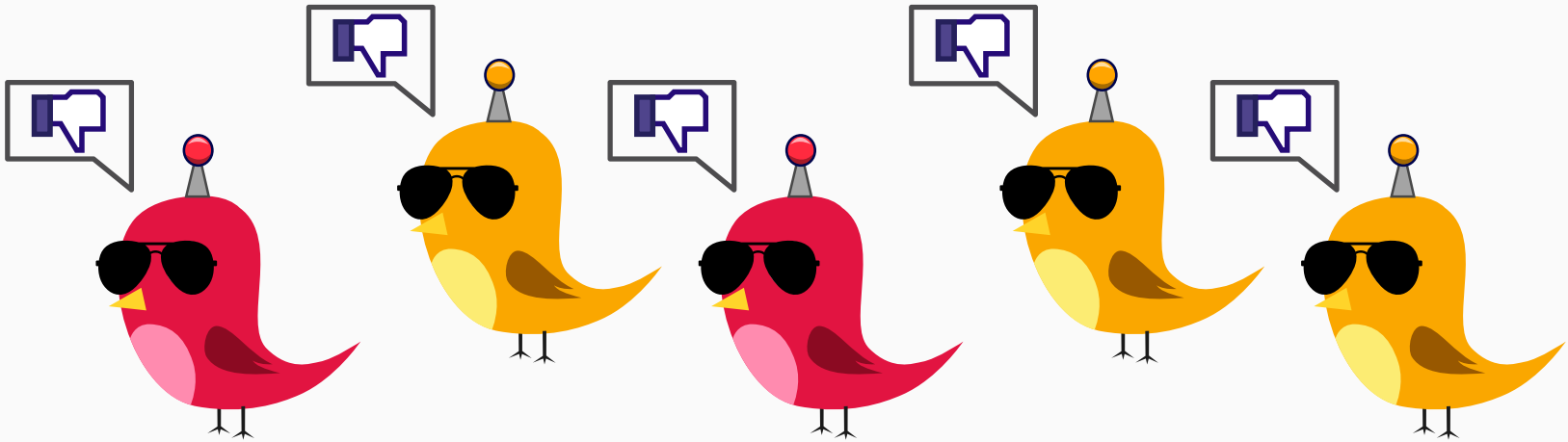

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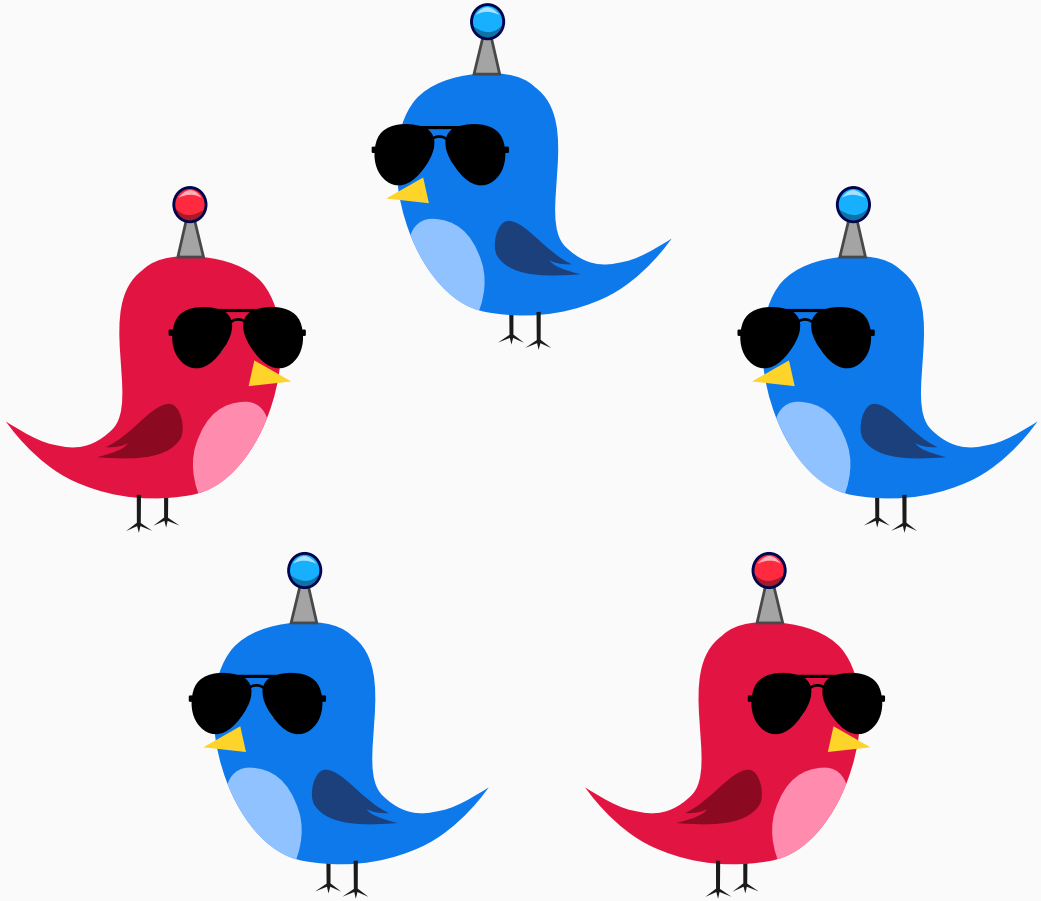

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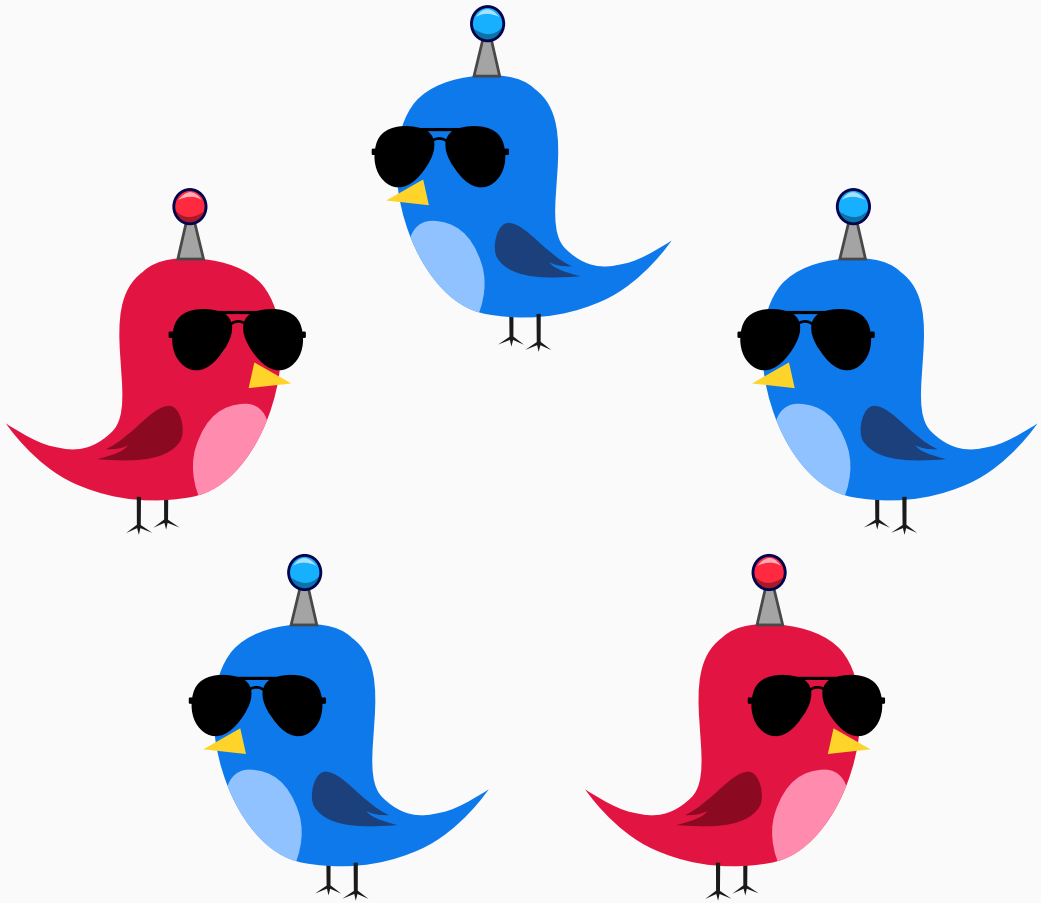

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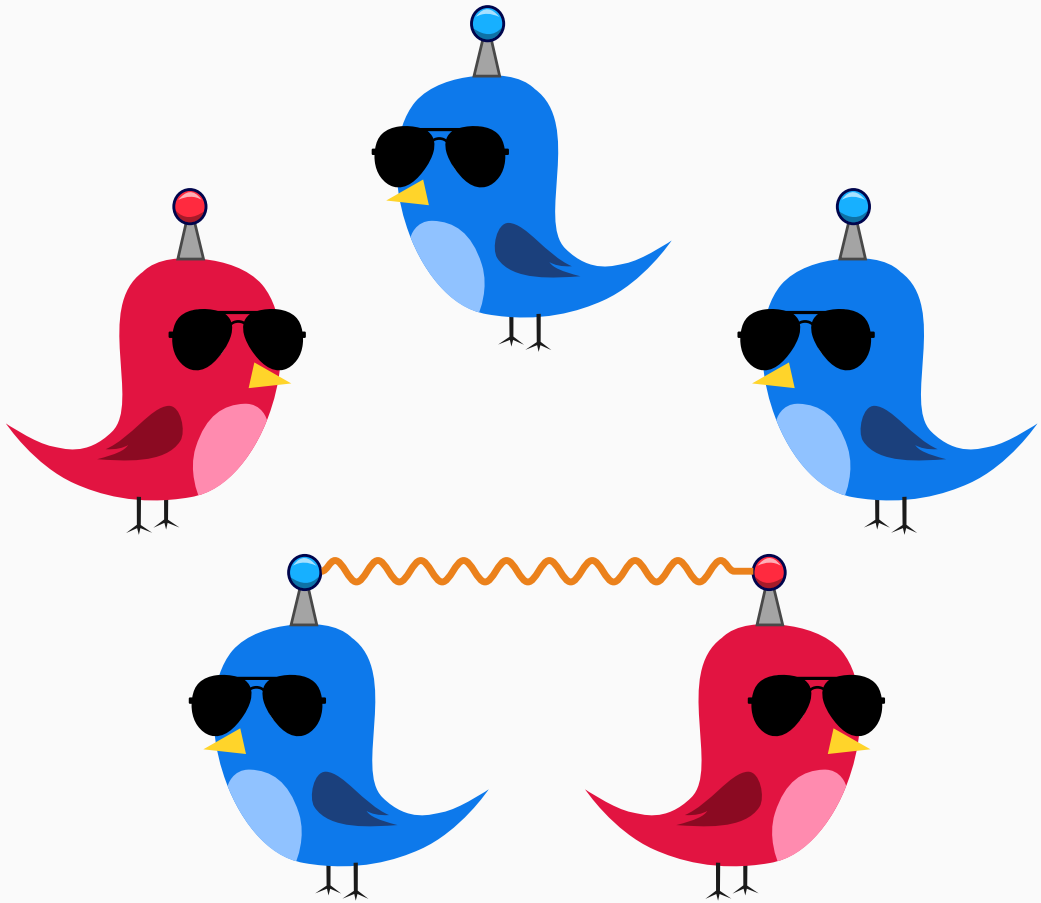

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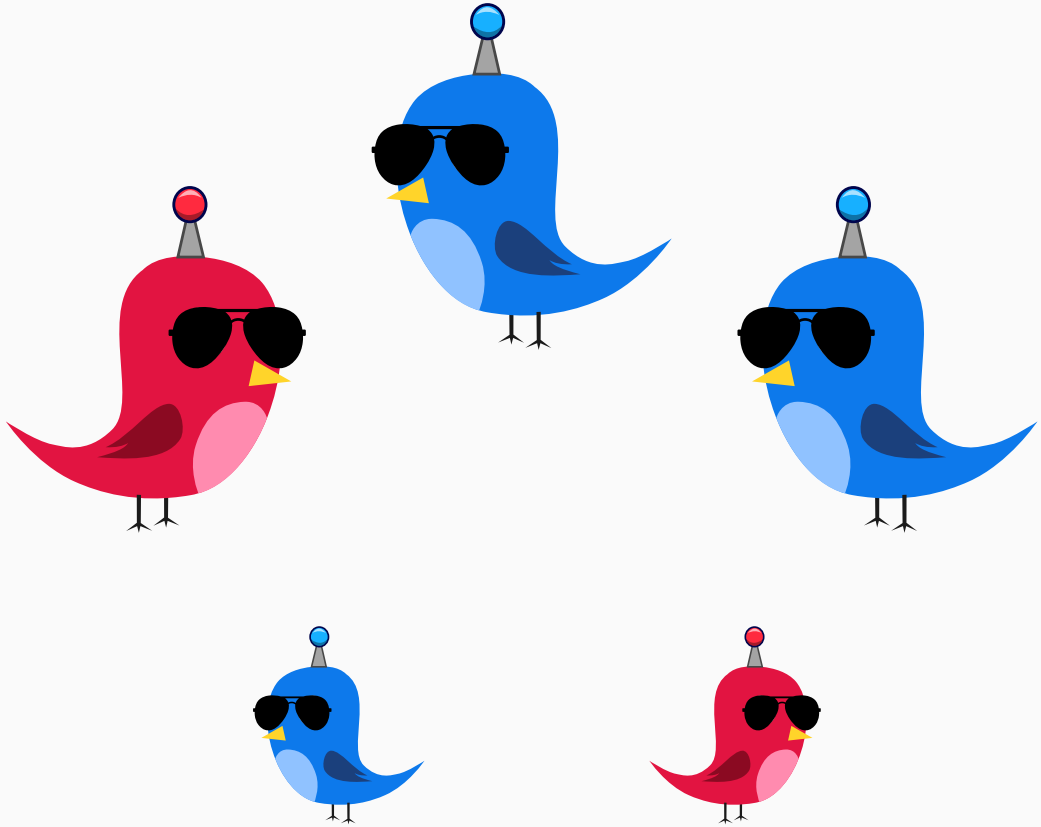

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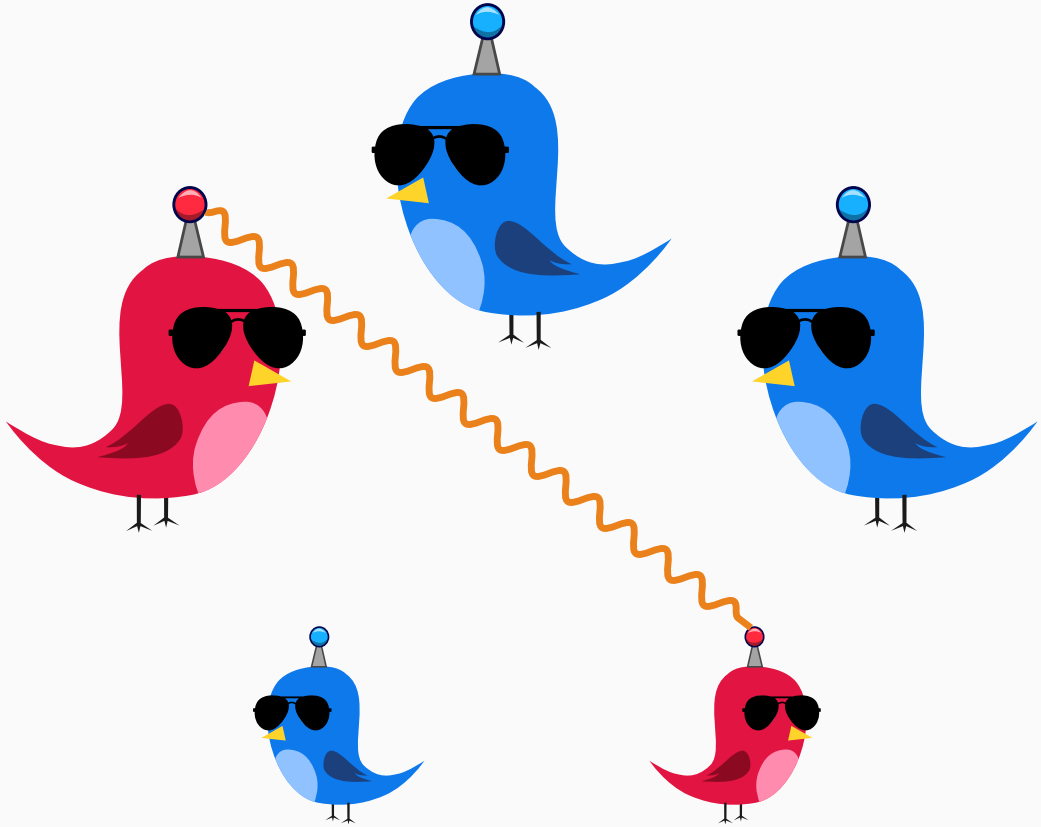

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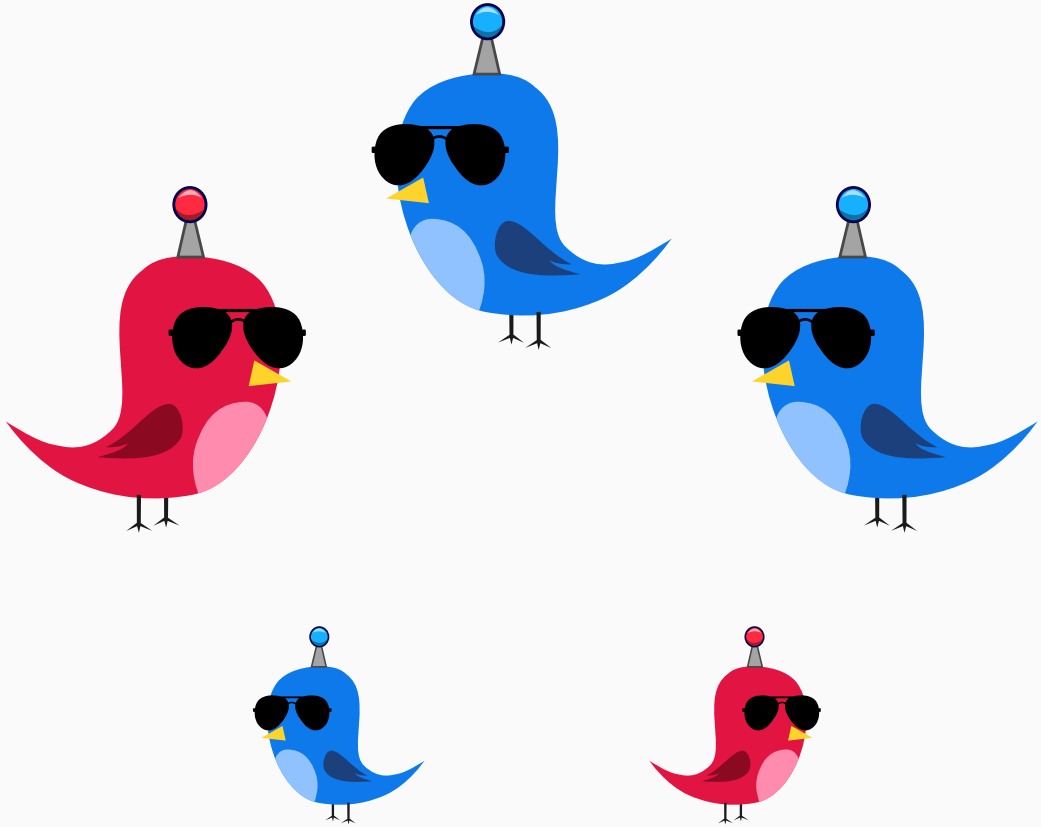

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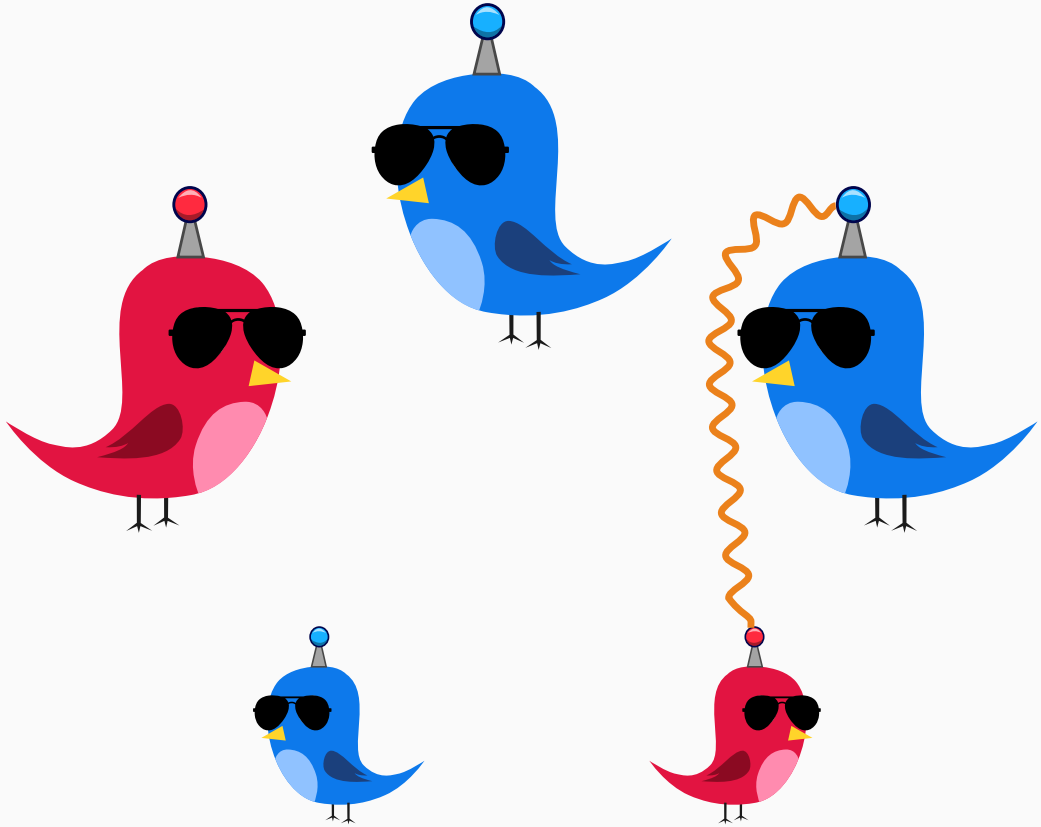

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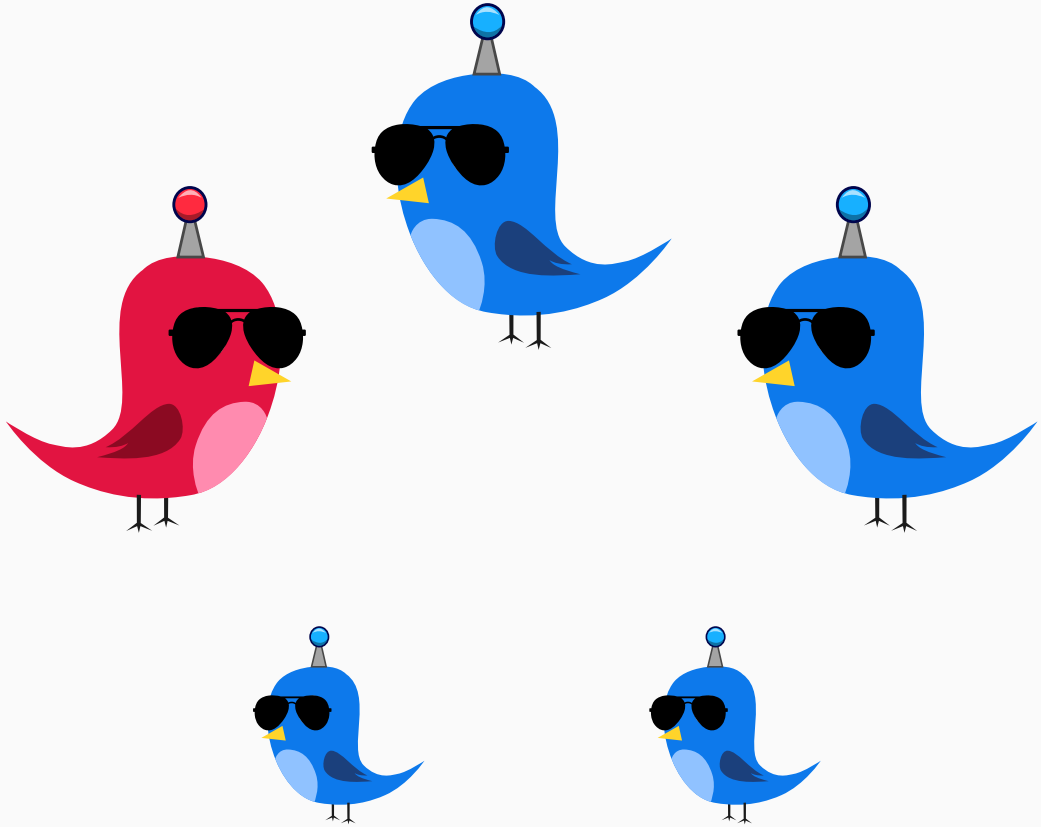

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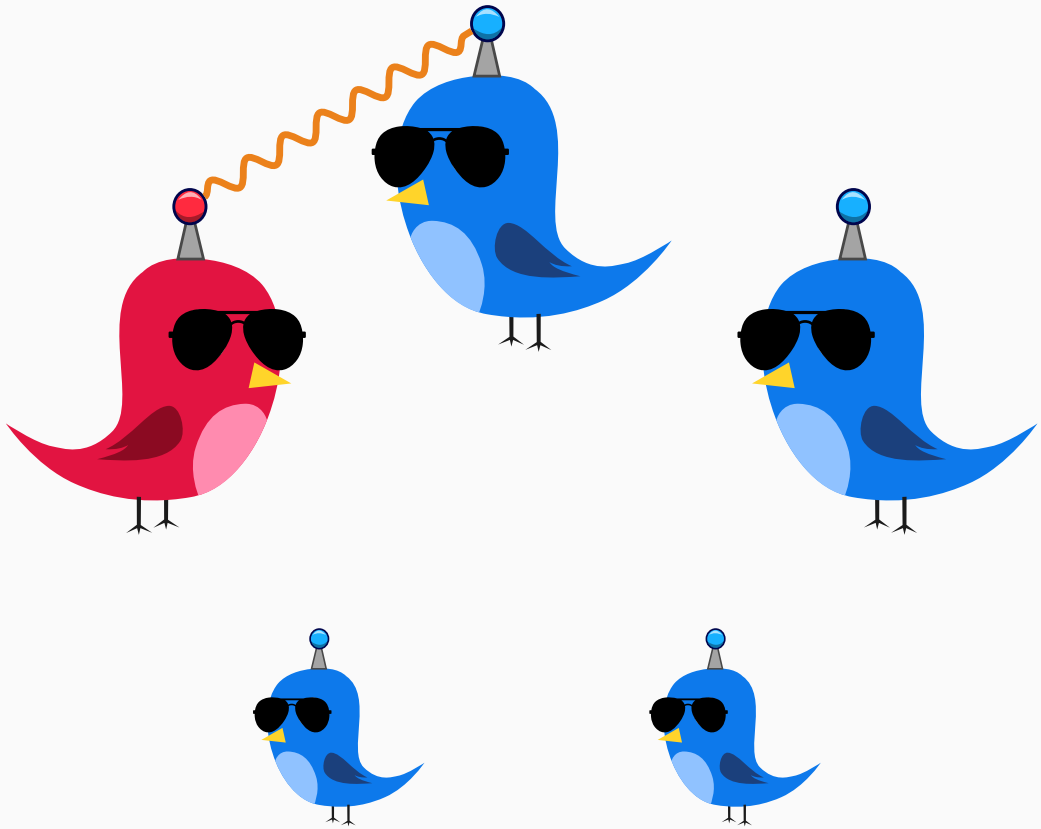

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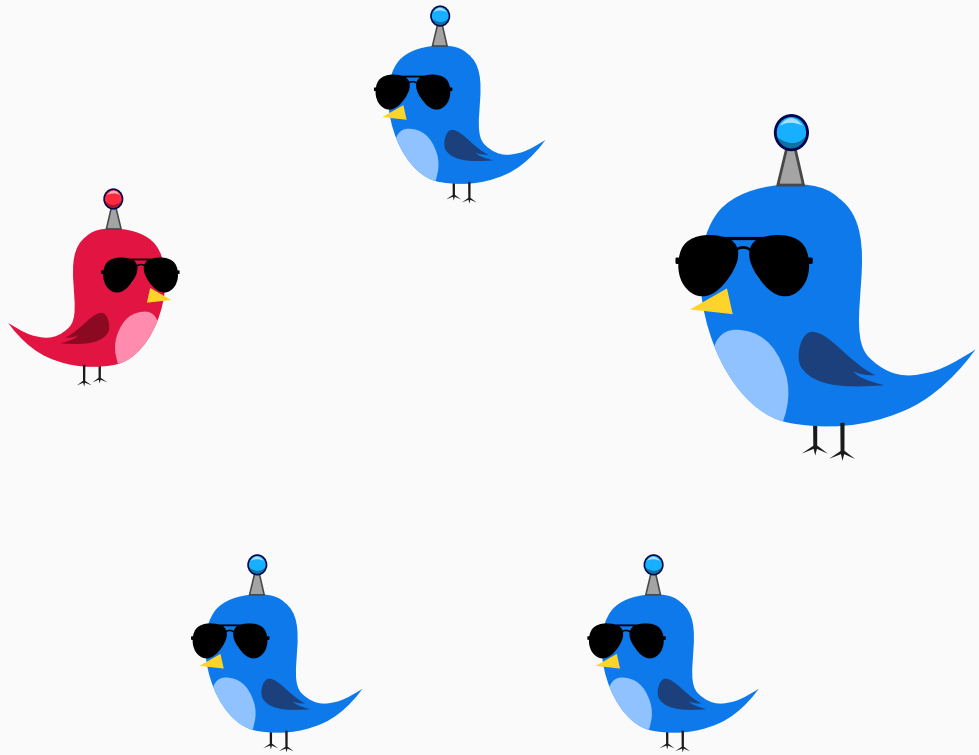

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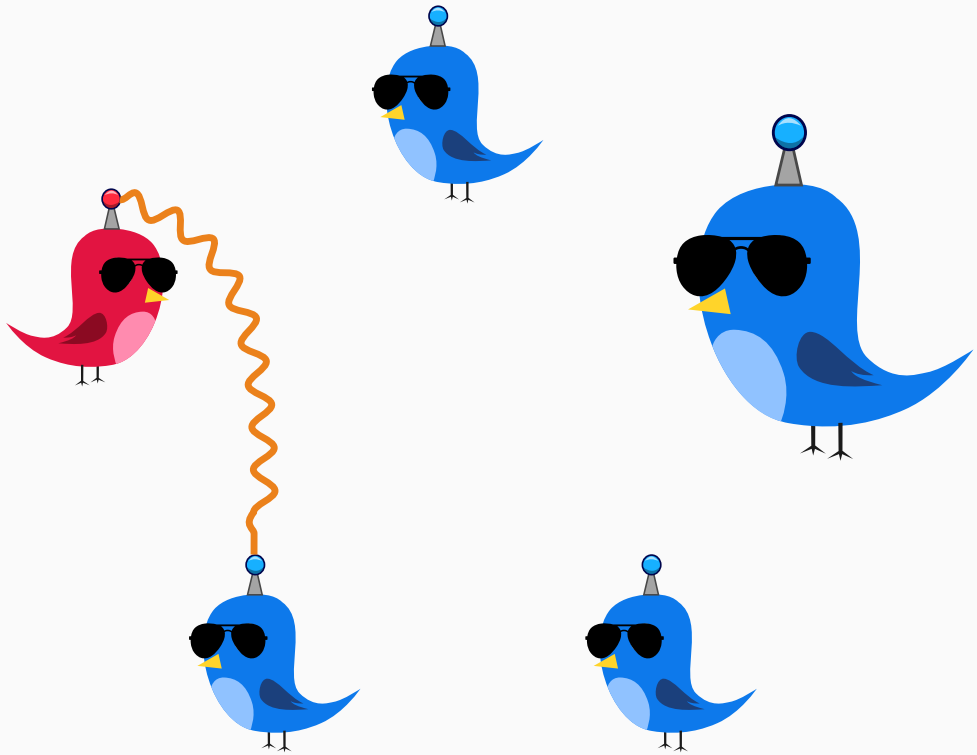

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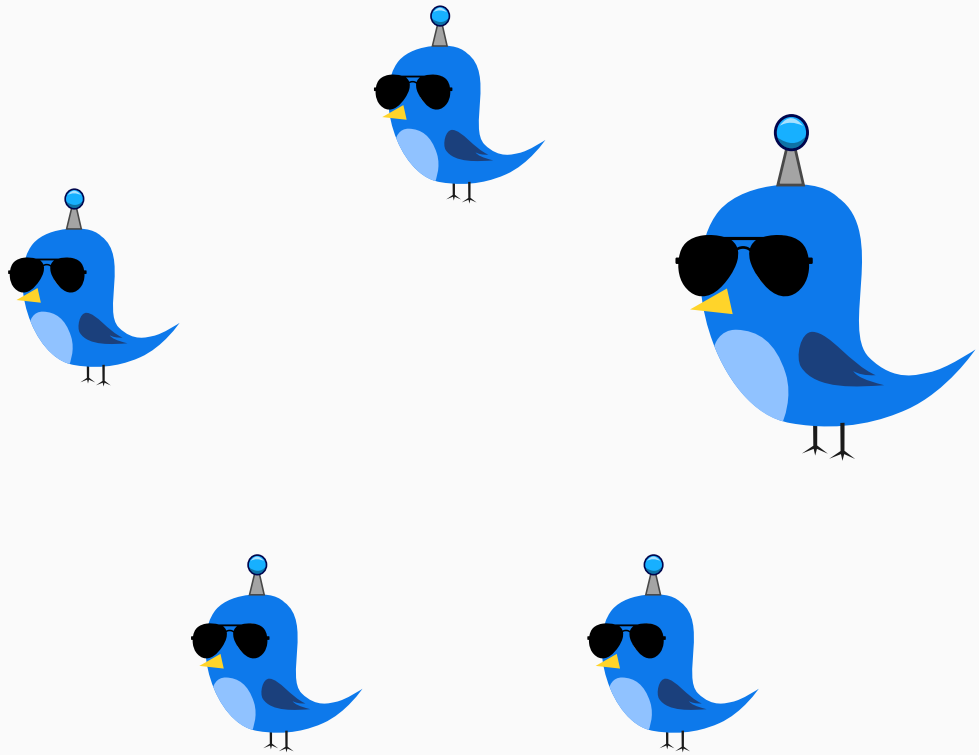

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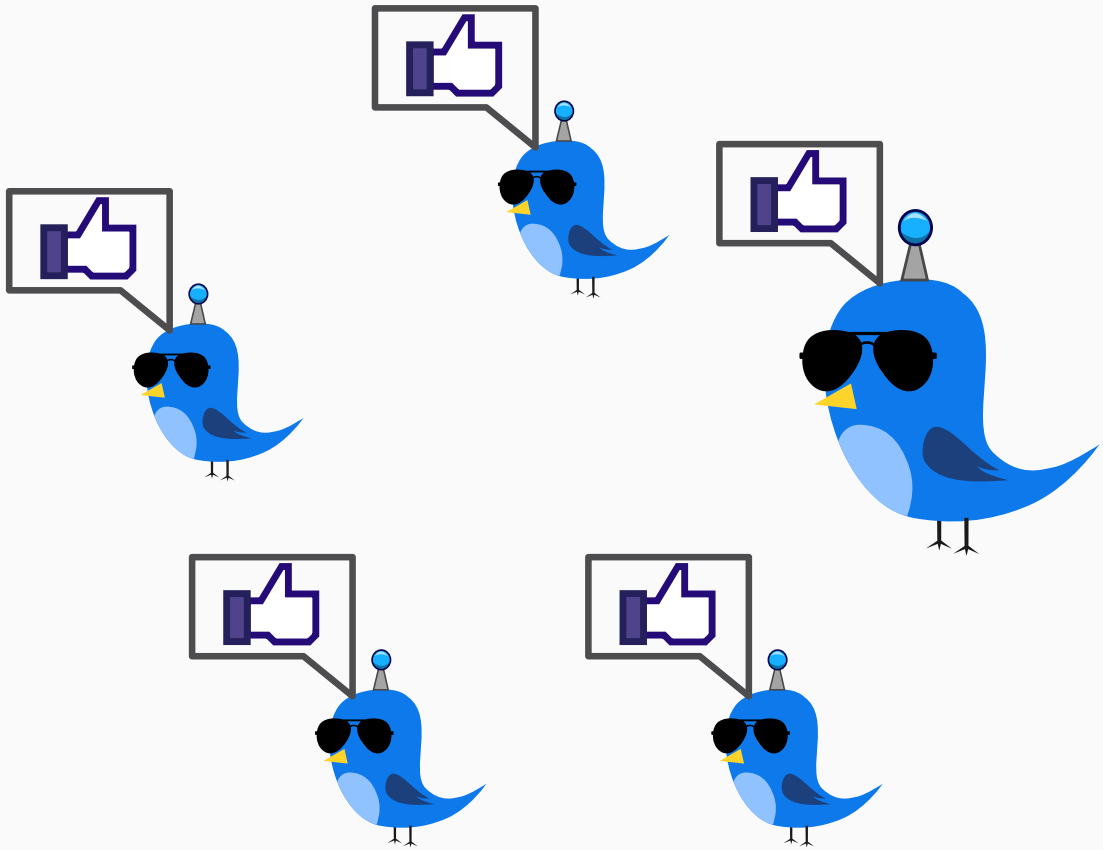

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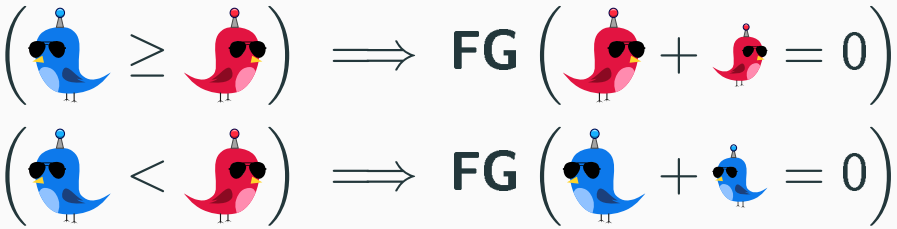
Correctness properties:

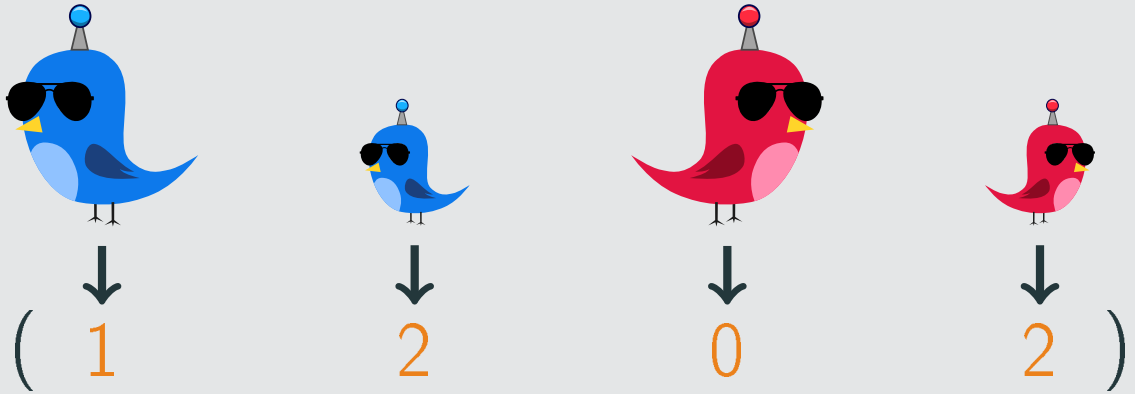


"Birds converge to color of majority."

Population Protocols: Verification Idea

Definition: Configuration

A vector describing the number of agents per state:



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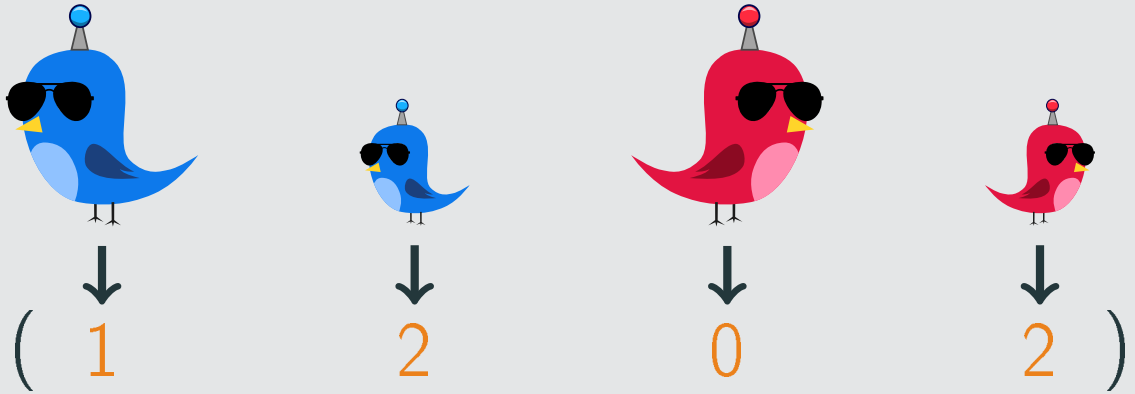

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Correctness proofs are typically structured in stages that trap the system in progressively more constrained subsets of configurations.

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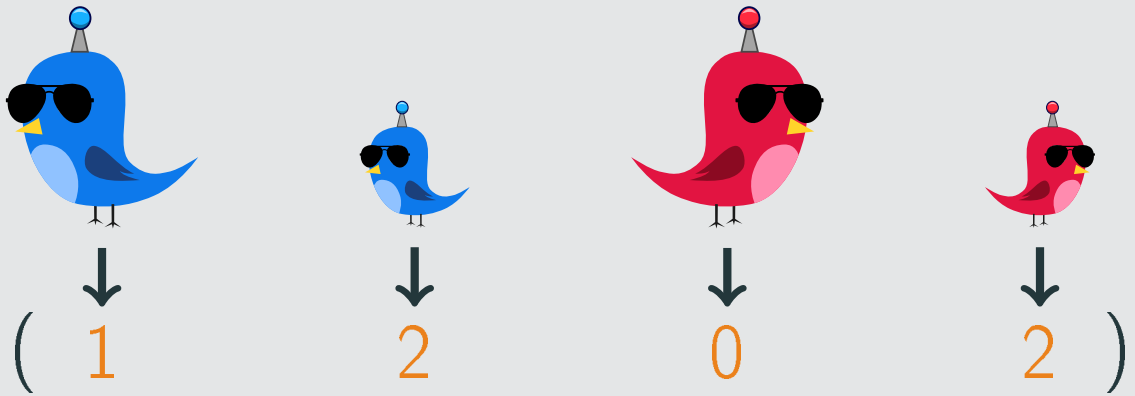

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→ **Idea:** Formalize structure as stage graph!

Population Protocols: Stage Graphs

Definition: Stage Graph

A stage graph for $\varphi_{\text{pre}} \Rightarrow FG\varphi_{\text{post}}$ is a finite DAG satisfying:

1. Each node is an inductive set of configurations, called stage.

"It is impossible to leave stages."

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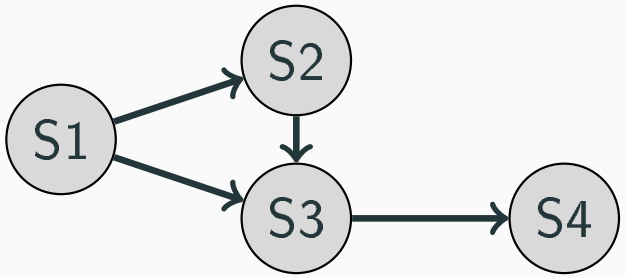

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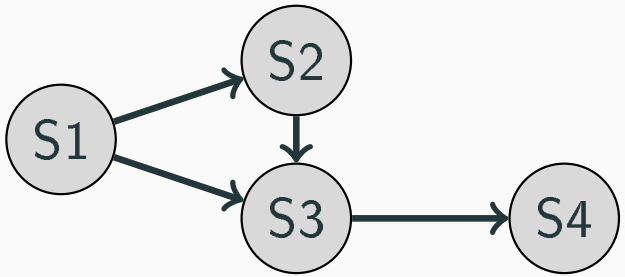

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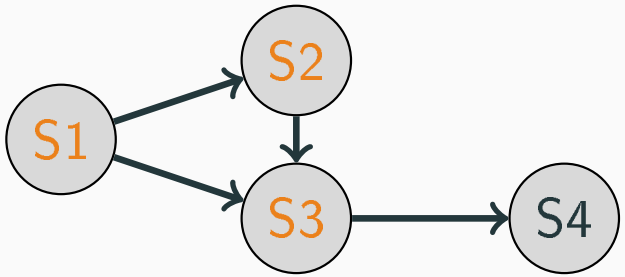

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4. In stages without successors, all configurations satisfy φ_{post}.

   "Finally, the postcondition holds forever."

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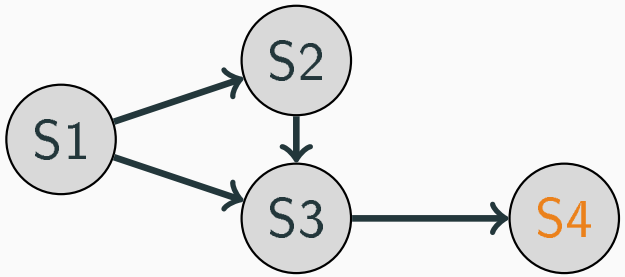

Population Protocols: Results

Theory

A population protocol is correct if and only if there is a stage graph proving it.

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Def: Presburger Stage Graph

A stage graph that is described using only Presburger formulas.

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→ Decidable **but** stage graphs can be huge!

Practice

- Most systems have small stage graphs
- Most systems make progress by "killing" transitions

→ Use heuristics to efficiently construct Presburger stage graphs

Population Protocols: Utility of Stage Graphs

Stage graphs:

- Can be efficiently constructed for most protocols
- Certify liveness properties
- Are independently checkable
- Explain how the protocol works
- Give speed guarantees
- Help to find counter examples

Chemical Reaction Networks

Chemical Reaction Networks

Example: Viral Infection

Species:	$\mathrm{RNA}, \mathrm{DNA}, \mathrm{V}, \mathrm{P}$	
Initial state:	$(1 \times \mathrm{RNA})$	
End time:	200s	
Reactions:	$\mathrm{DNA} + \mathrm{P} \xrightarrow{0.00001} \mathrm{V}$ $\mathrm{RNA} \xrightarrow{1000} \mathrm{RNA} + \mathrm{P}$ $\mathrm{DNA} \xrightarrow{0.025} \mathrm{DNA} + \mathrm{RNA}$ $\mathrm{RNA} \xrightarrow{1} \mathrm{DNA} + \mathrm{RNA}$	$\mathrm{RNA} \xrightarrow{0.25} \emptyset$ $\mathrm{P} \xrightarrow{2} \emptyset$

Chemical Reaction Networks

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- Continuous time (,i.e., behaves like CTMC not DTMC)
- Focus on modeling systems (instead of designing them)

CRN: Transient Analysis

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- Hard because of complex dynamics, state-space explosion, stochasticity, stiffness, multimodality, ...
- Two approaches:
  - Direct (numerical)
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This work

- Goal: Efficiently compute many simulations
- Idea: Use memoization!

CRN: Simulation

Gillespie's stochastic simulation algorithm (SSA) [9]

- Sample one reaction at a time

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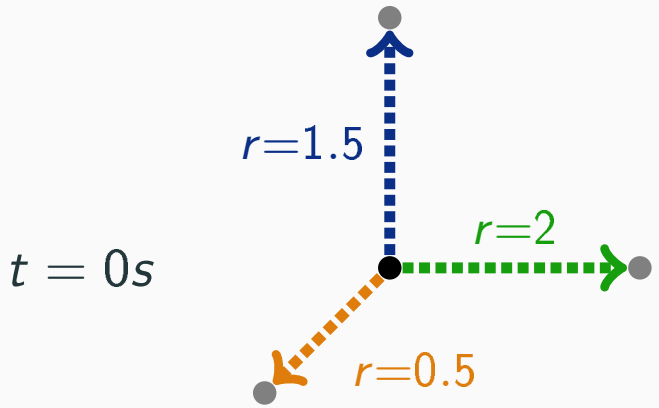
$t = 0s$ $\quad$ $\bullet$ s_{init}

Start in initial state.

CRN: Simulation

Gillespie's stochastic simulation algorithm (SSA) [9]

- Sample one reaction at a time

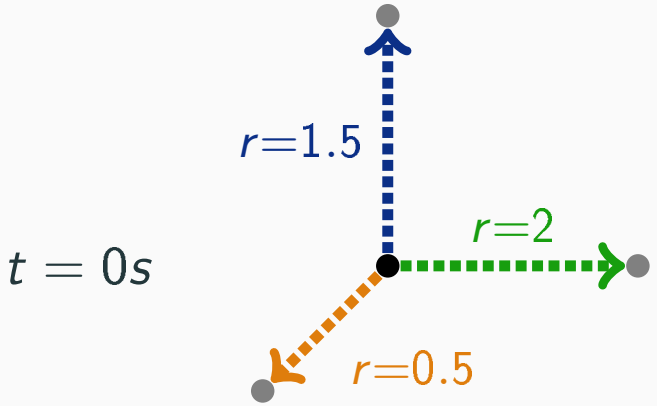


Compute rate of all reactions.

CRN: Simulation

Gillespie's stochastic simulation algorithm (SSA) [9]

- Sample one reaction at a time



Time until the next reaction: $\Delta t \sim EXP(0.5{+}2{+}1.5)$

Probability of reactions: $\frac{0.5}{4}, \frac{2}{4}, \frac{1.5}{4}$

CRN: Simulation

Gillespie's stochastic simulation algorithm (SSA) [9]

- Sample one reaction at a time

$t = 0.18s$

Apply change to both time and state, then repeat.

CRN: Simulation

Gillespie's stochastic simulation algorithm (SSA) [9]

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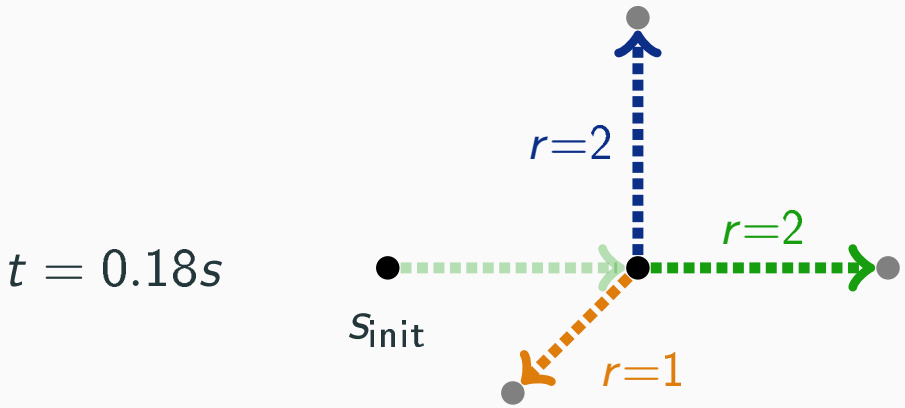

Time until the next reaction: $\Delta t \sim EXP(1{+}2{+}2)$

Probability of reactions: $\frac{1}{5}, \frac{2}{5}, \frac{2}{5}$

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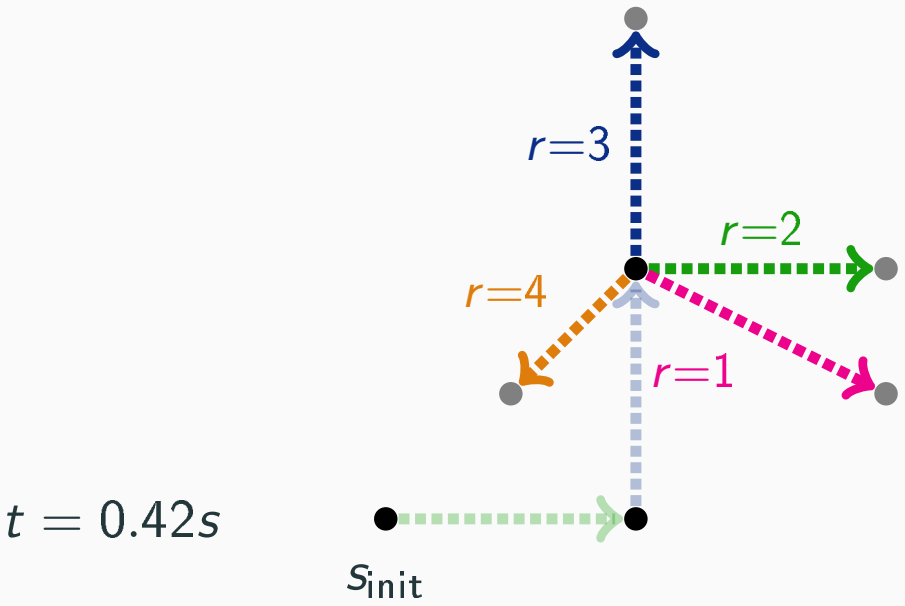
Gillespie's stochastic simulation algorithm (SSA) [9]

- Sample one reaction at a time



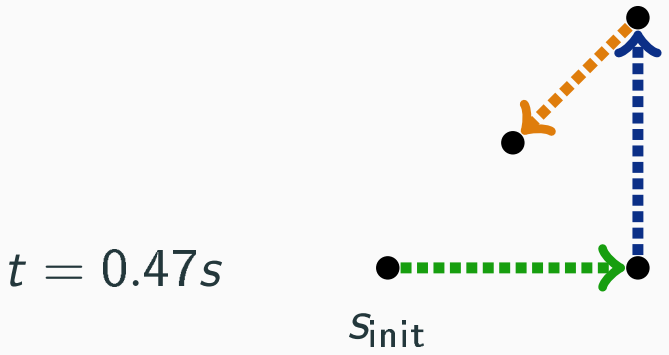
Time until the next reaction: $\Delta t \sim EXP(4+2+3+1)$

Probability of reactions: $\frac{4}{10}, \frac{2}{10}, \frac{3}{10}, \frac{1}{10}$

CRN: Simulation

Gillespie's stochastic simulation algorithm (SSA) [9]

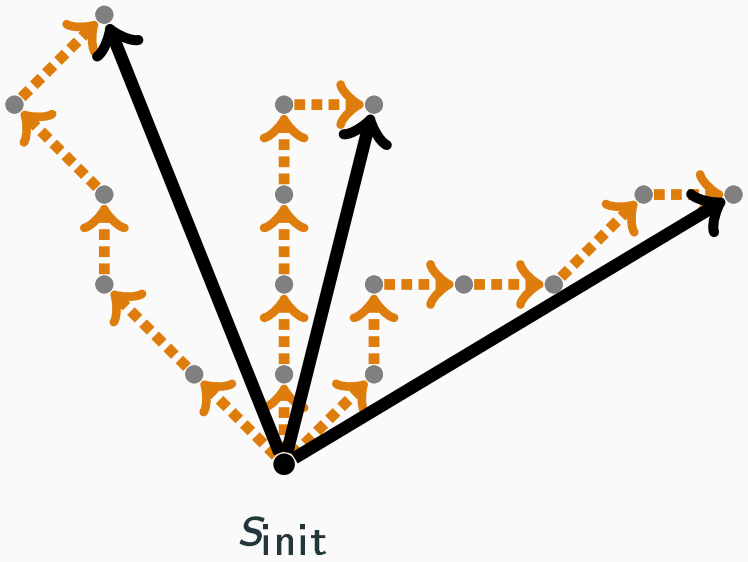
- Sample one reaction at a time
- May take a long time



CRN: Segmental Simulation

Precompute k short trajectories (called segments) for each state.

$\rightarrow$ Simulate by sampling segments instead of single reactions.



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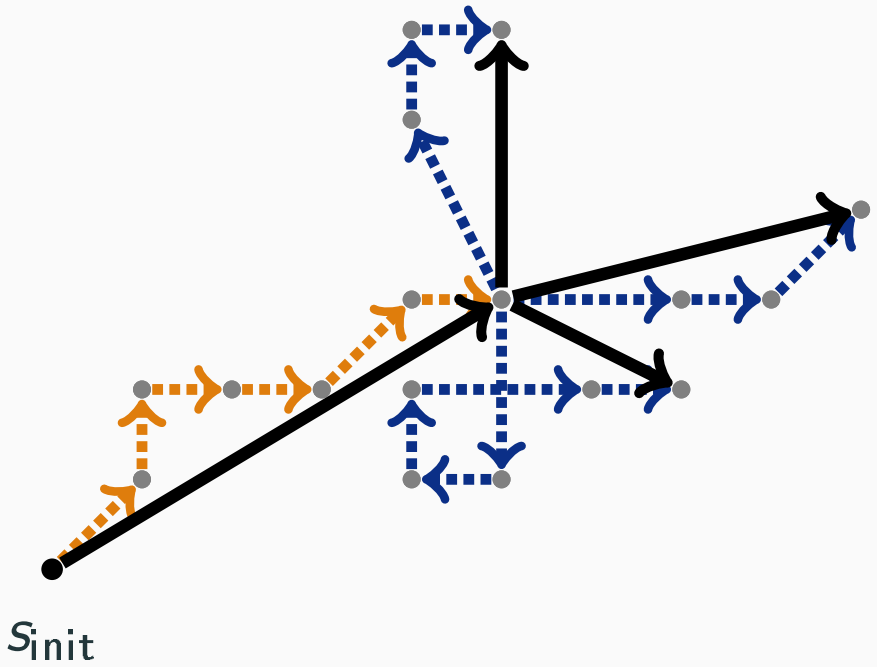

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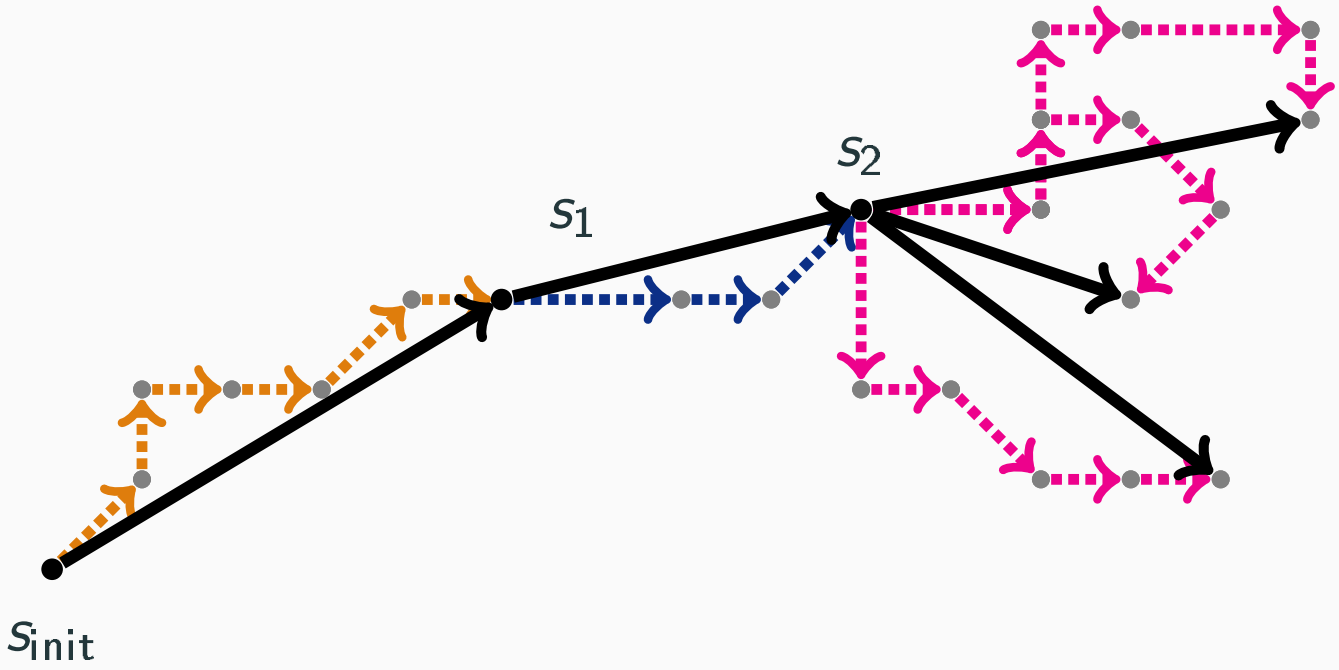

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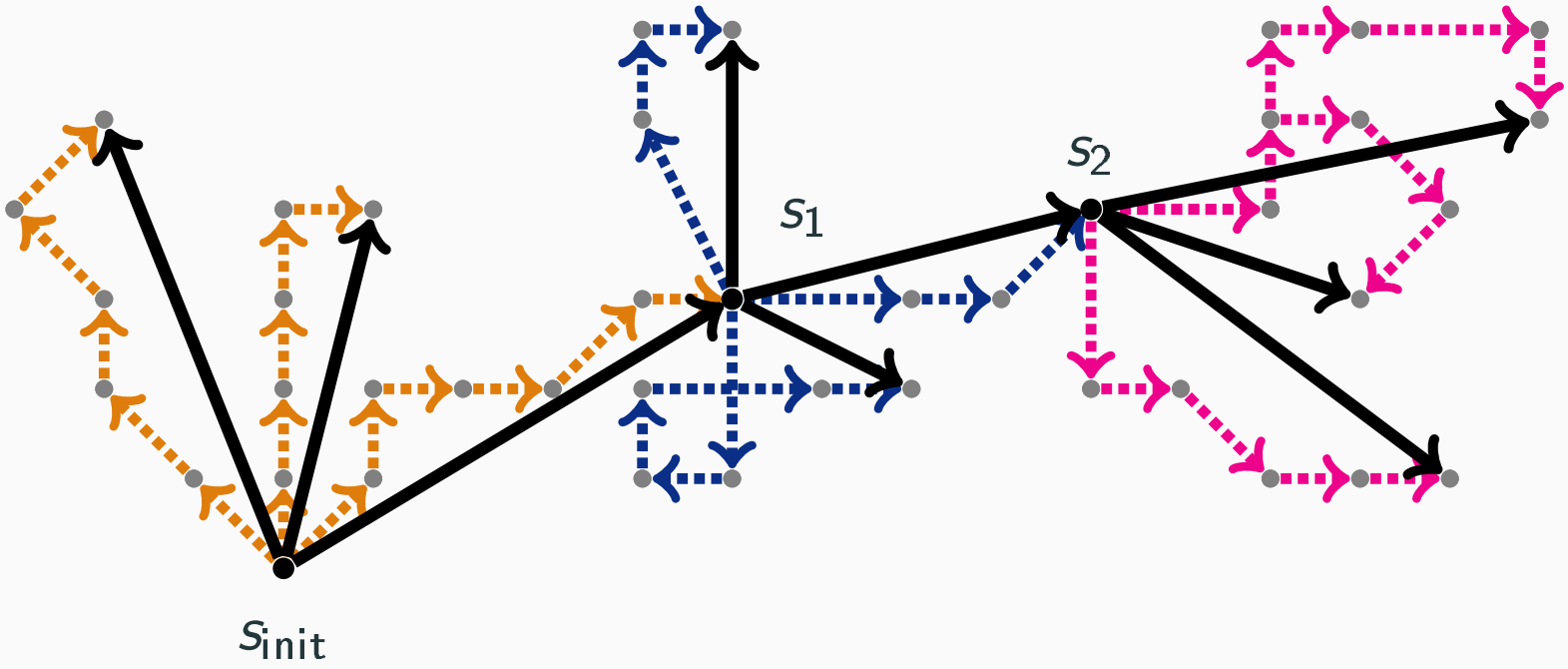

- much faster!

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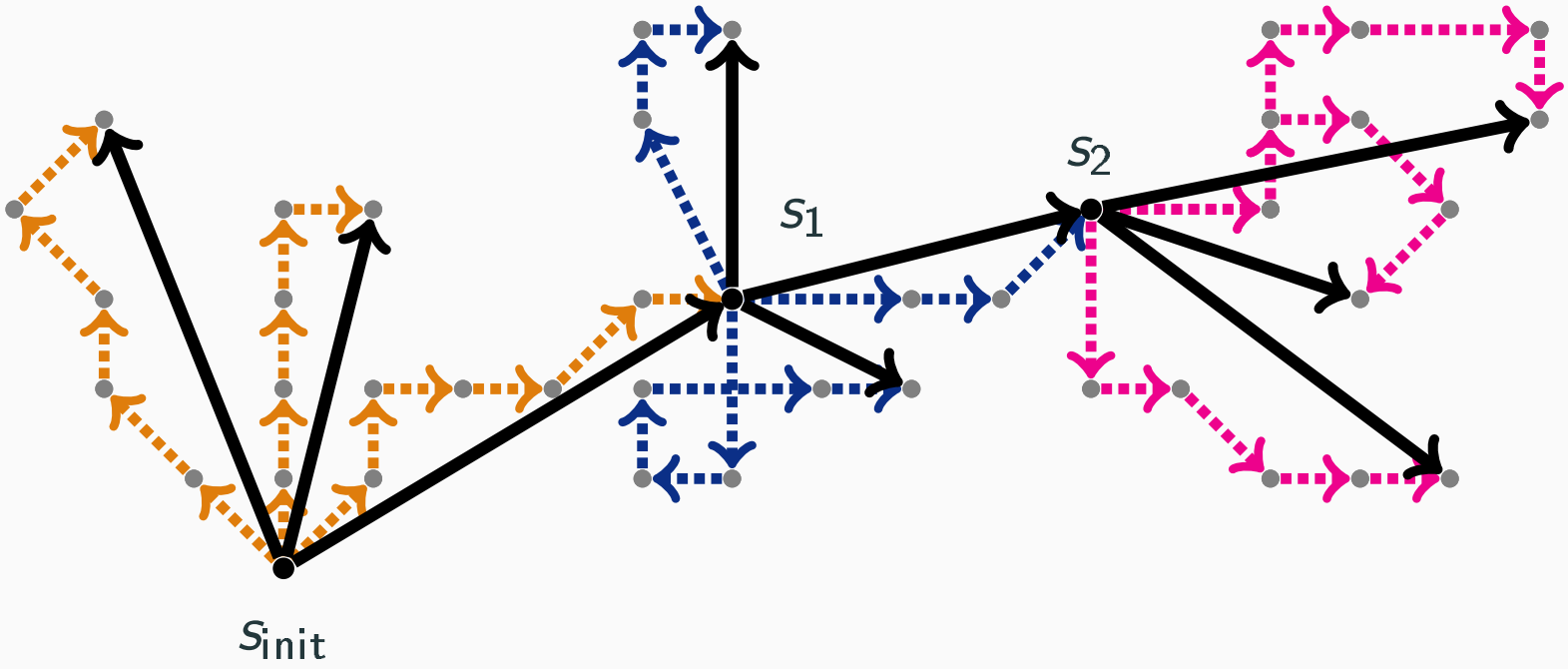

- much faster!
- Problem: many states $\rightarrow$ too inefficient

CRN: Abstraction-Based Segmental Simulation

- Idea: Do not treat every state separately!

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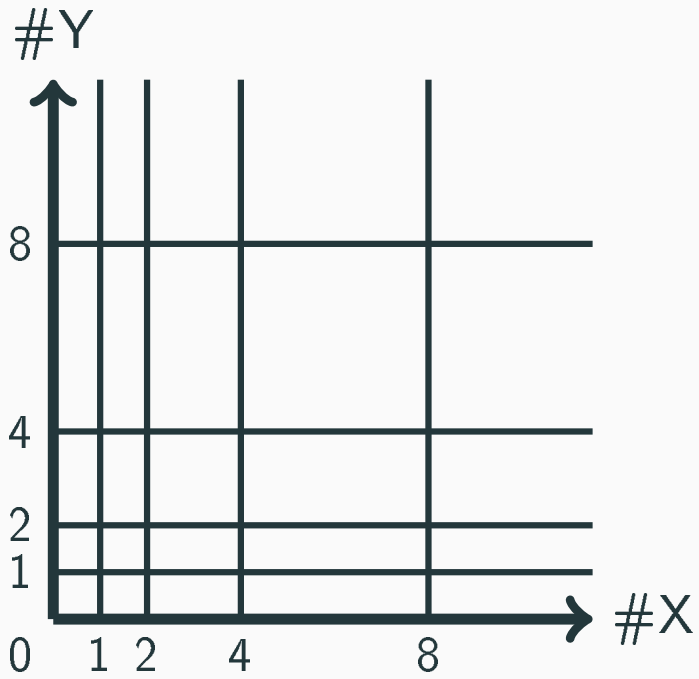
- Population-level abstraction: split state-space into regions (called abstract states)



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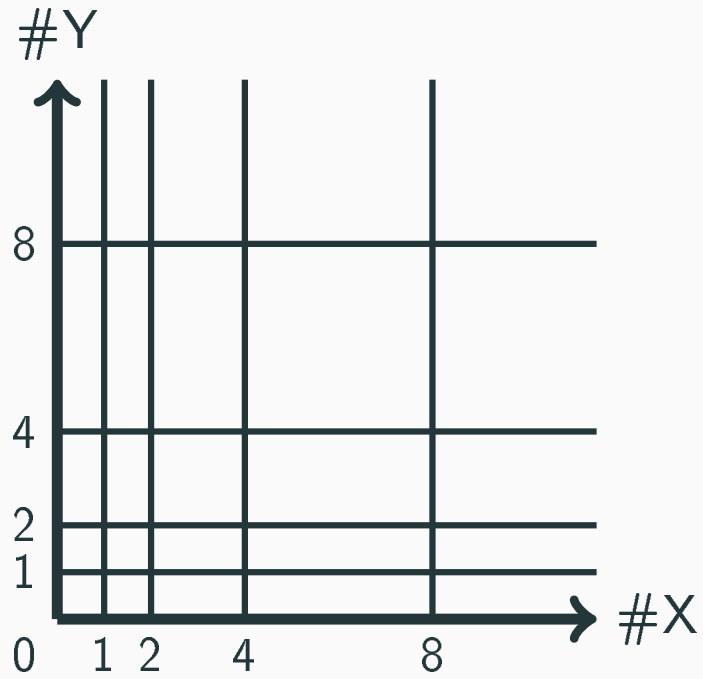

- Choose representative for each abstract state (usually center)

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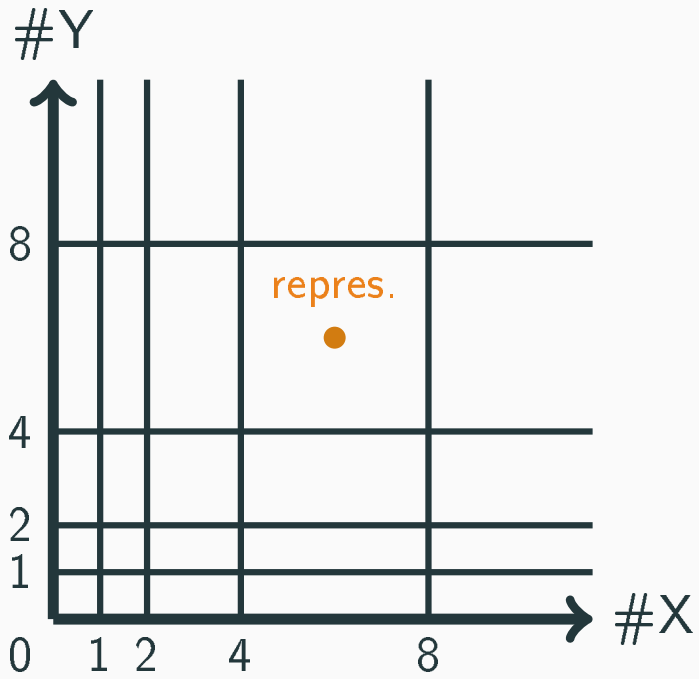

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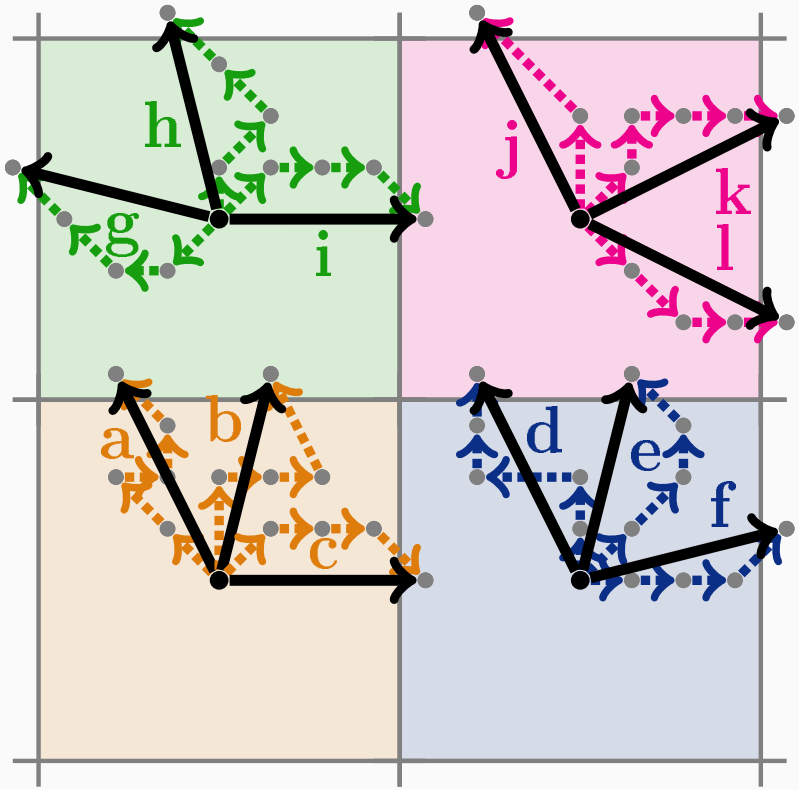

Segments end when they leave the abstract state.

→ Intuition: "*significant change*"

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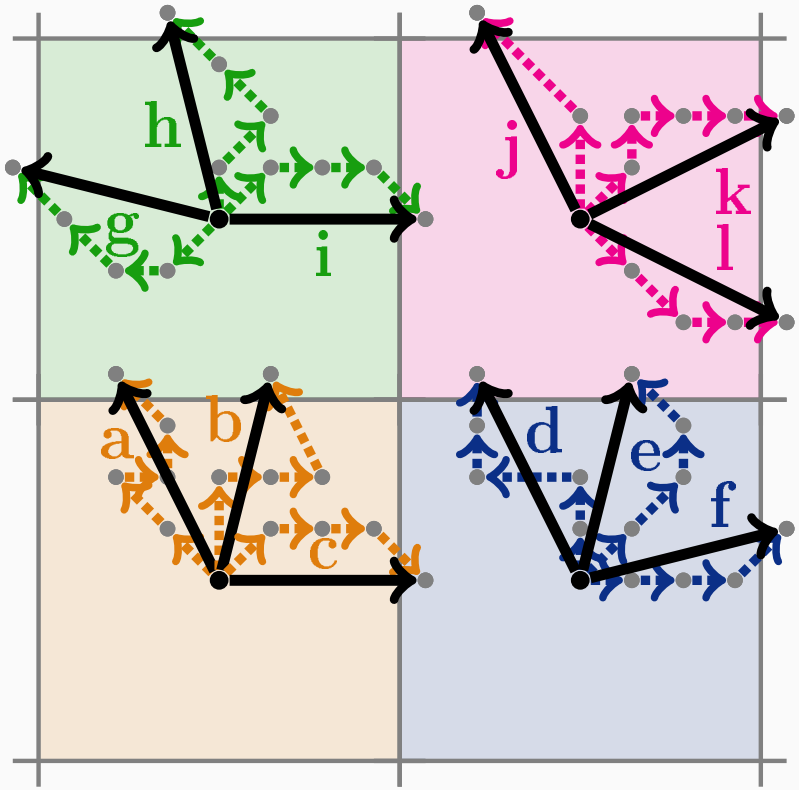
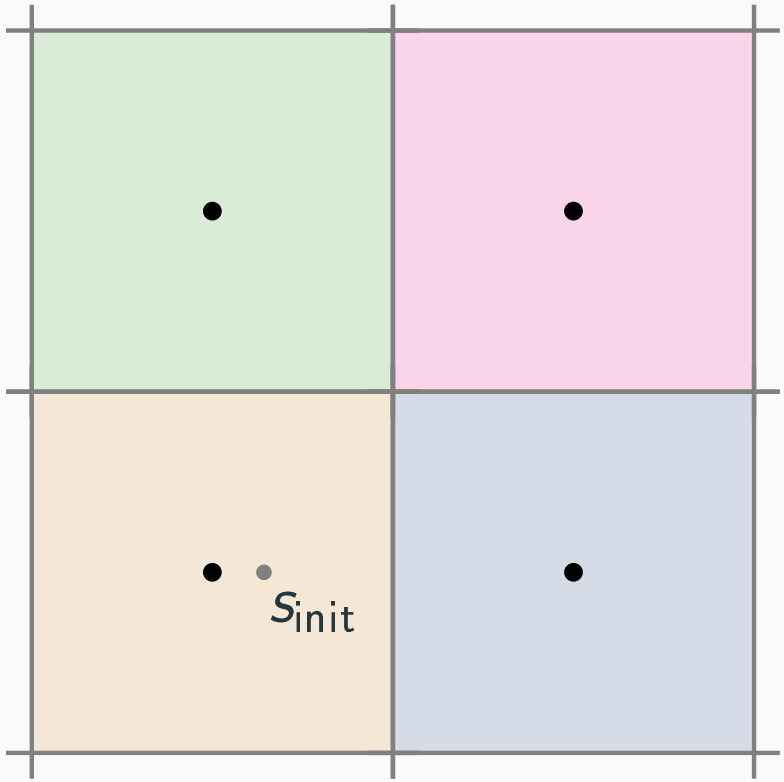


MEMORY
$(k = 3)$



SIMULATION

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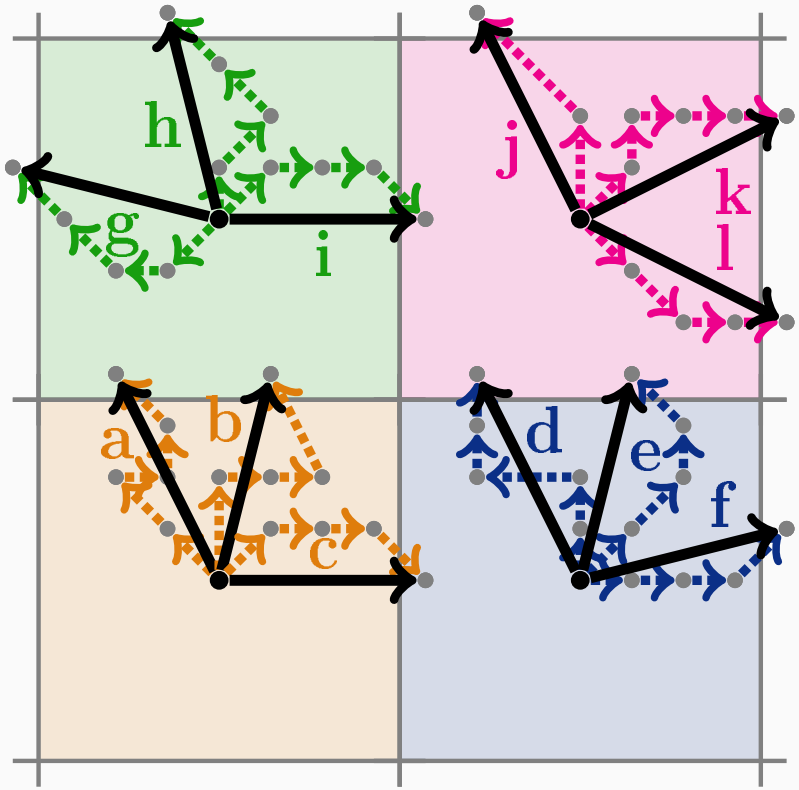

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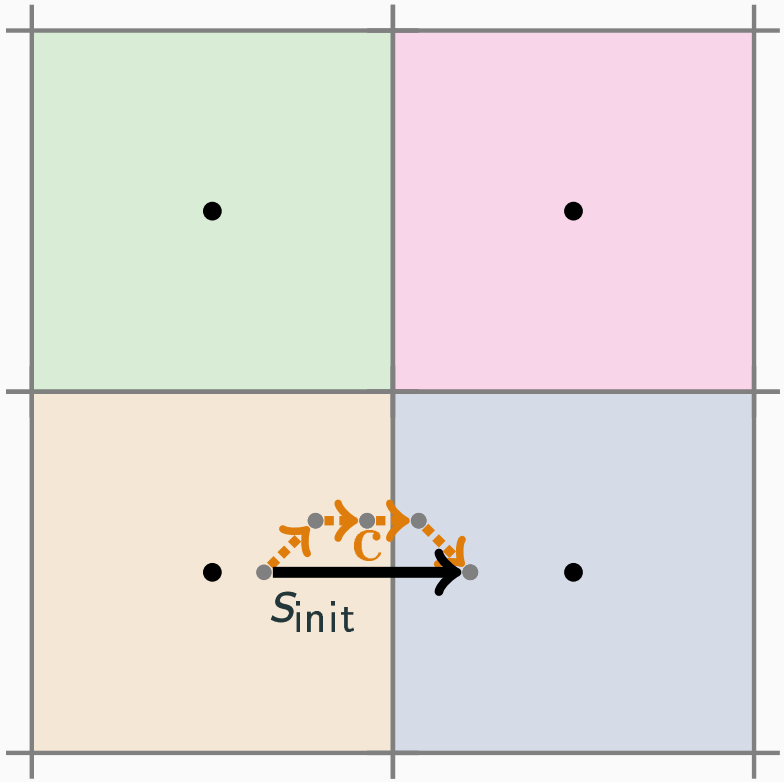

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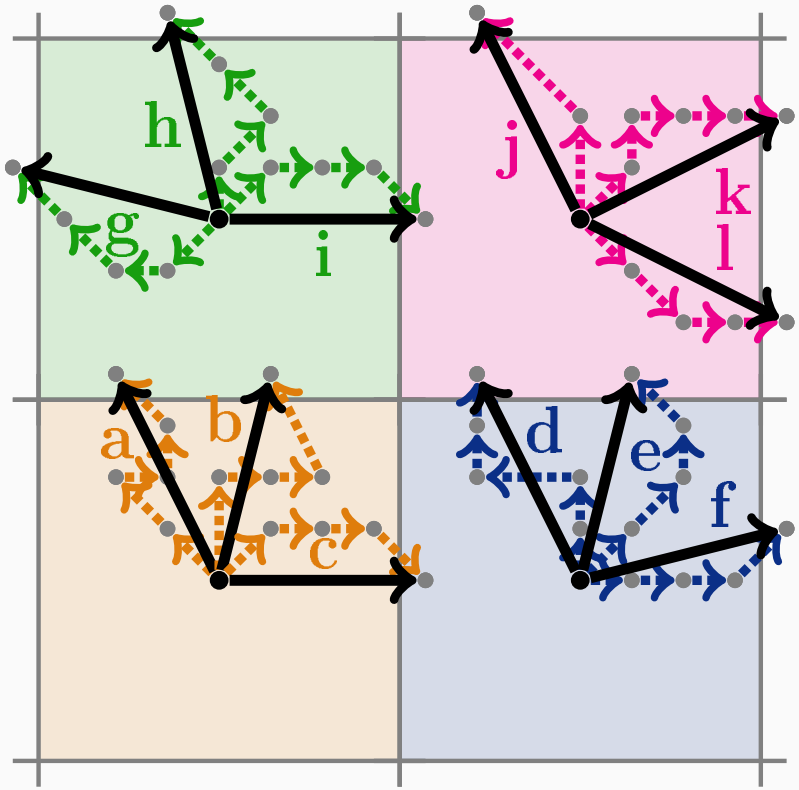

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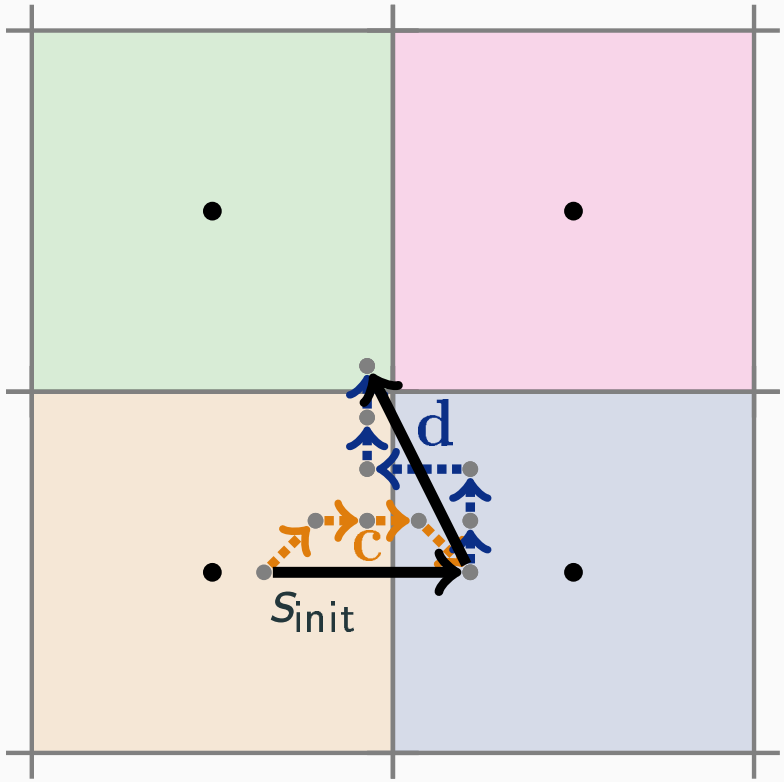

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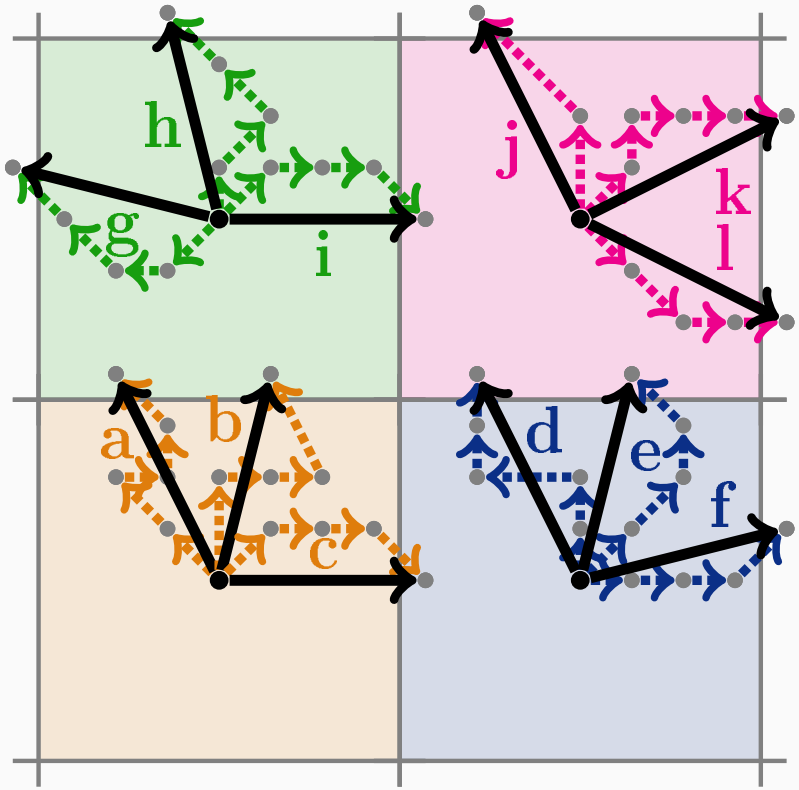

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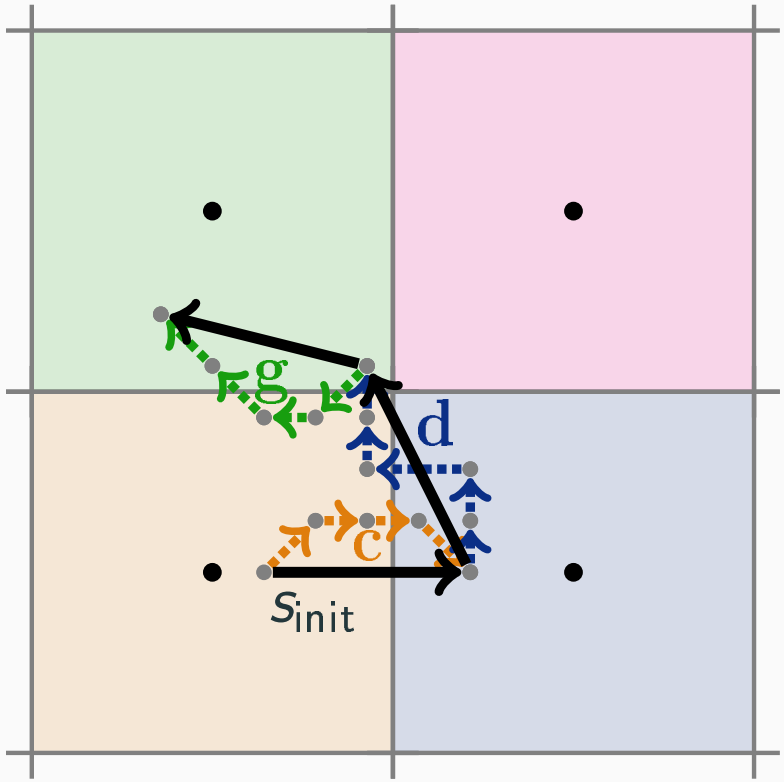

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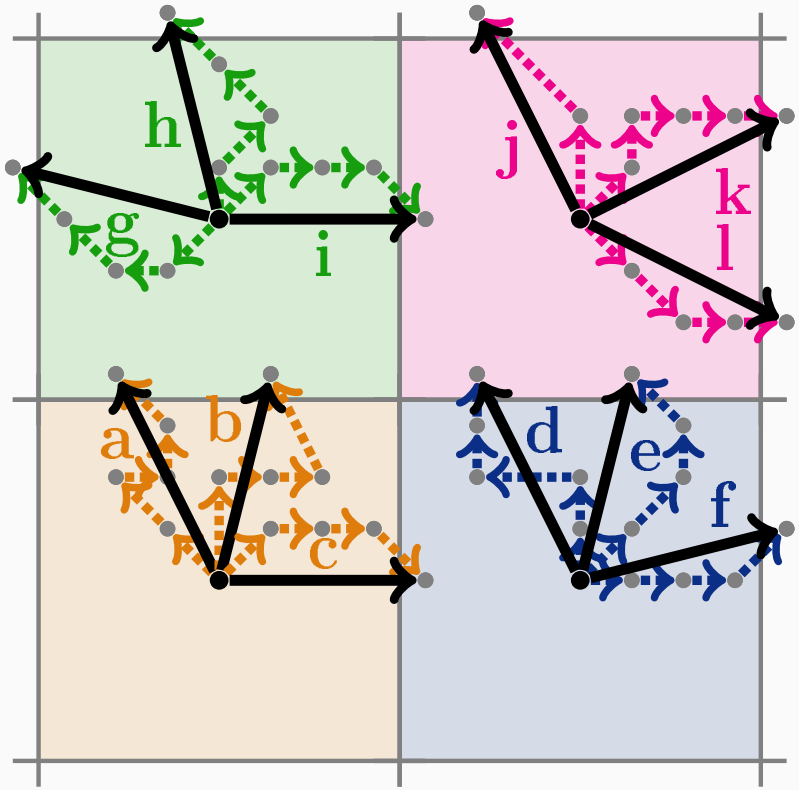

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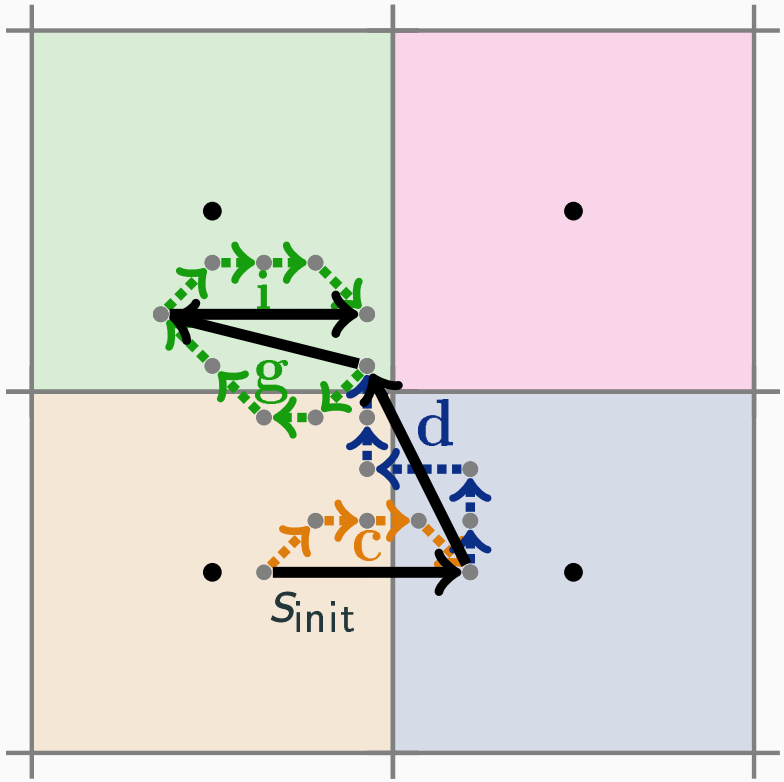

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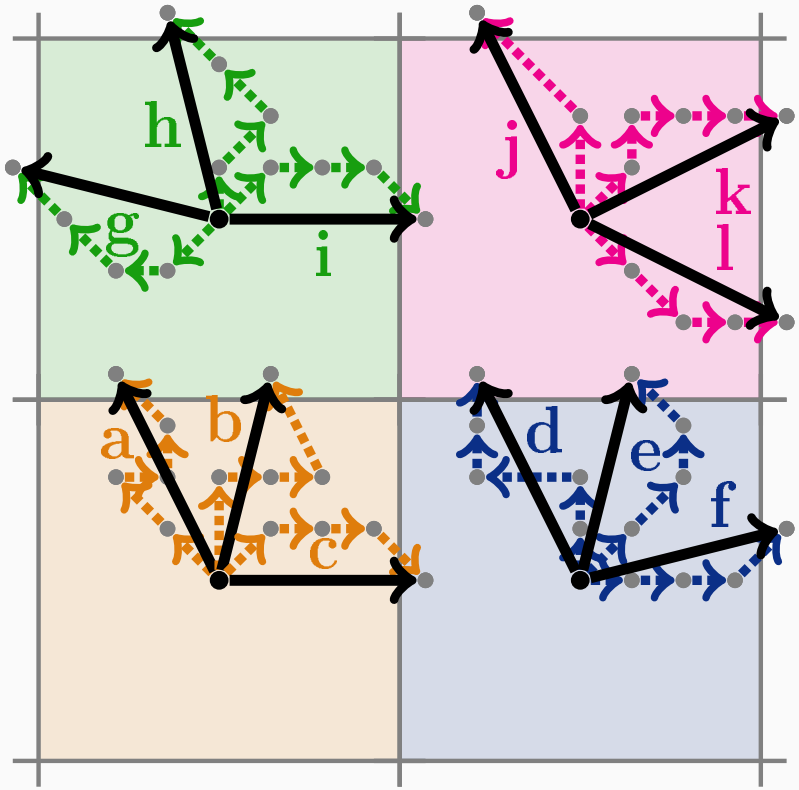

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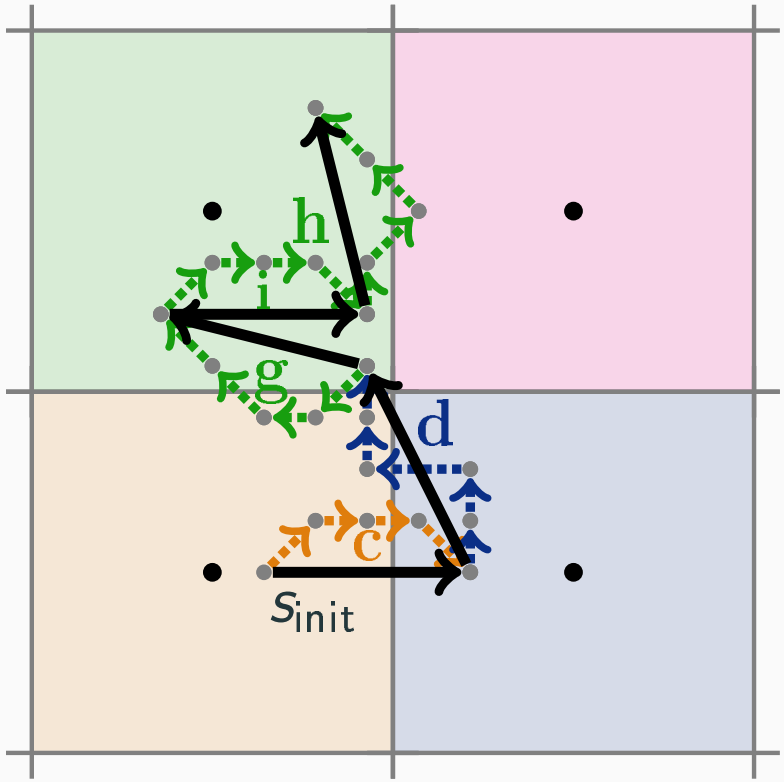

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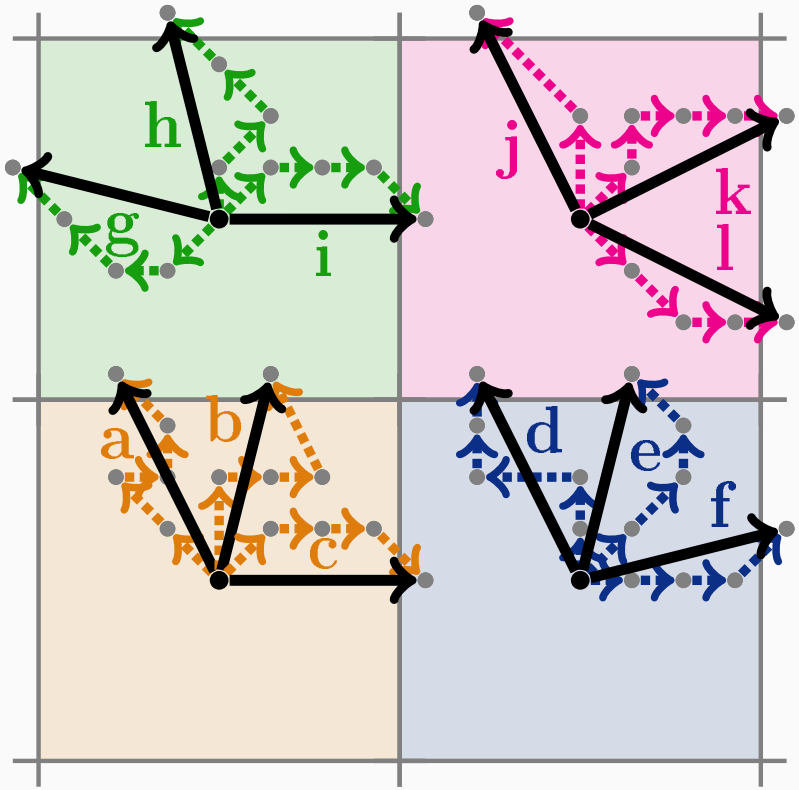

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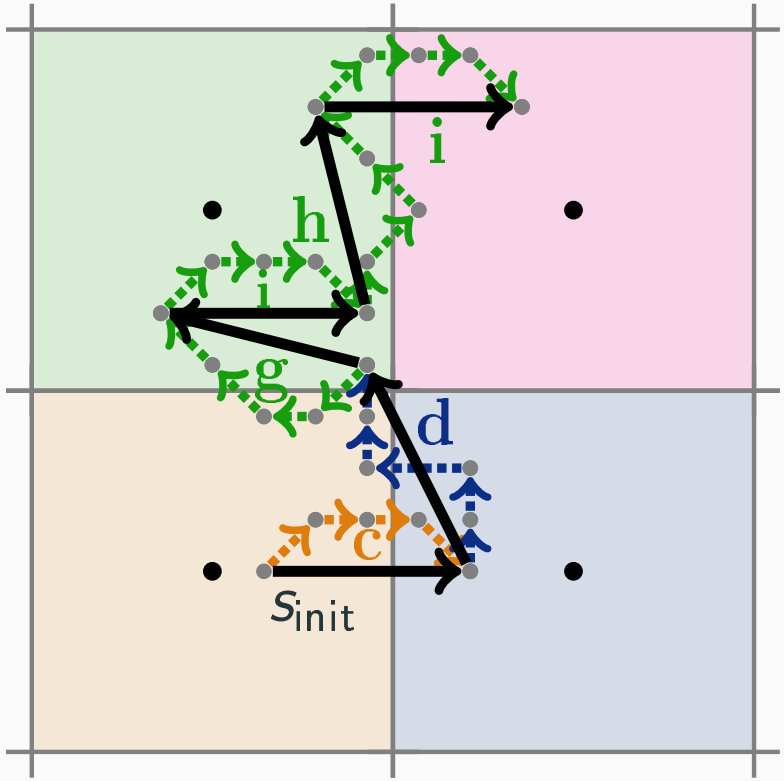

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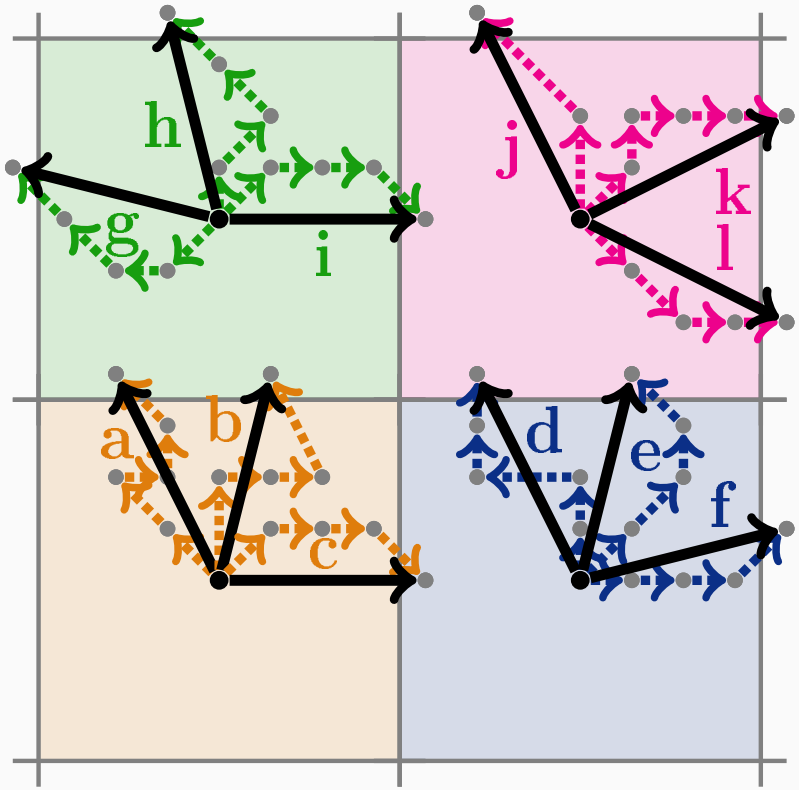

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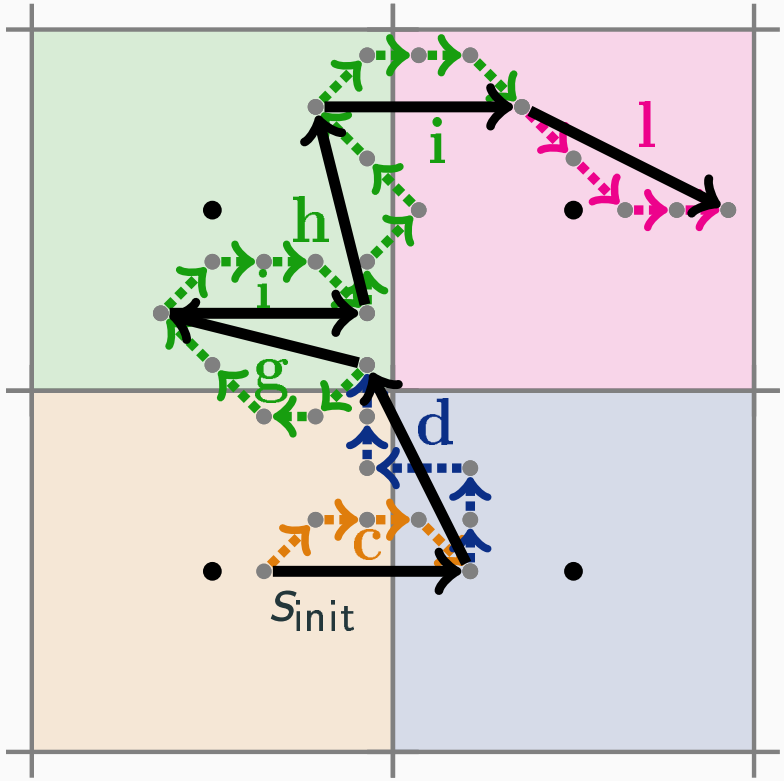

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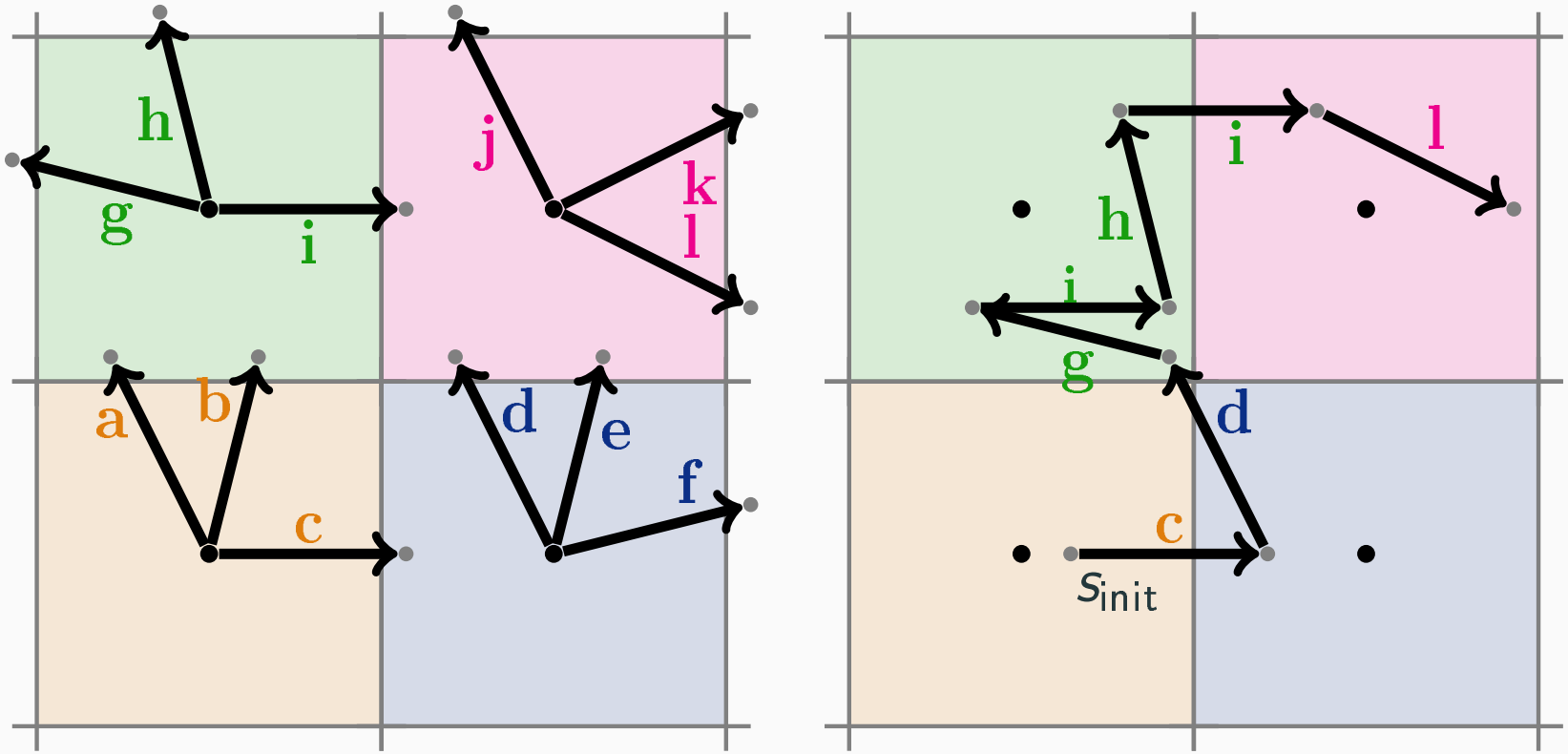

To save memory: Work with summaries instead of segments.

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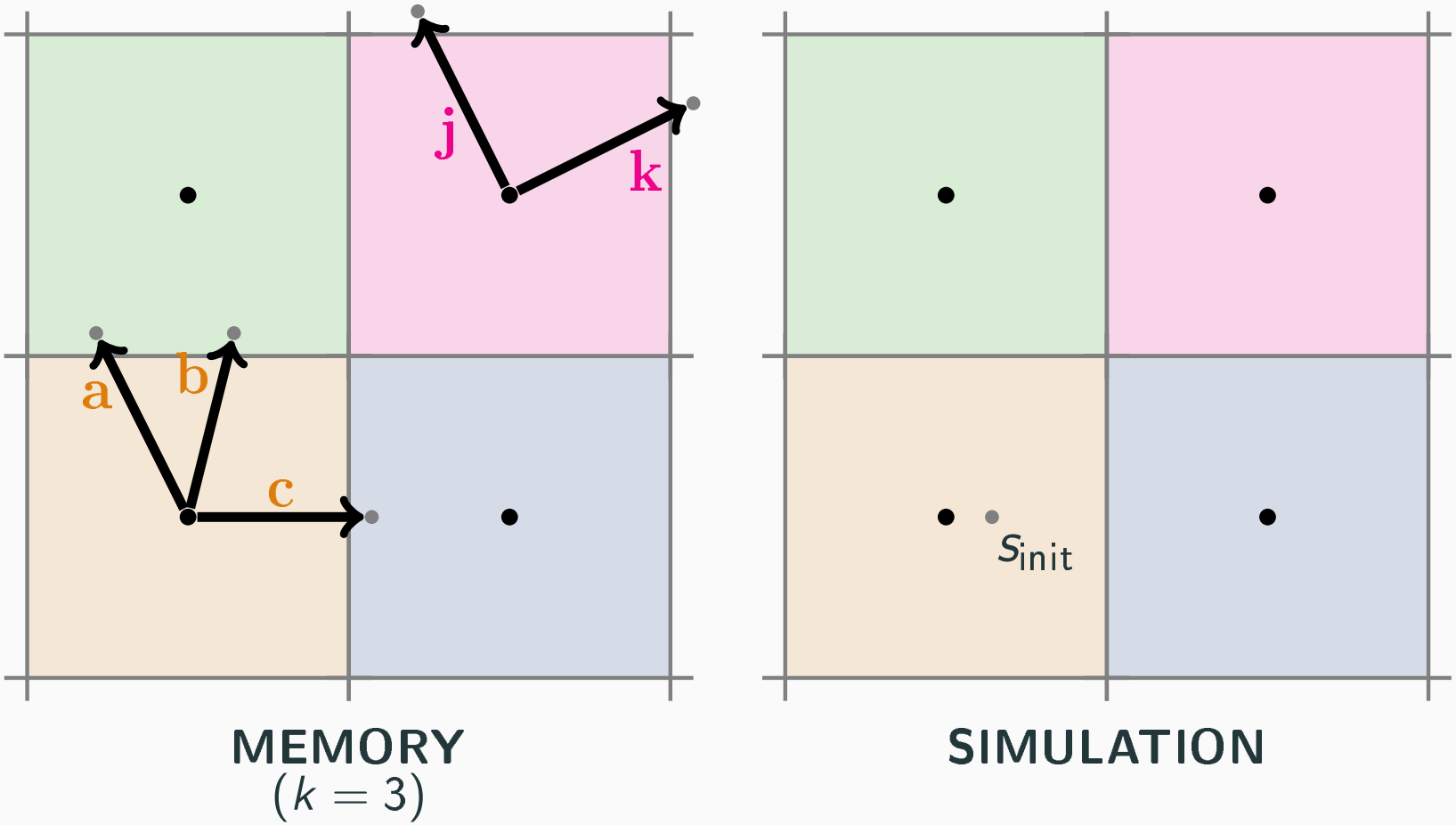

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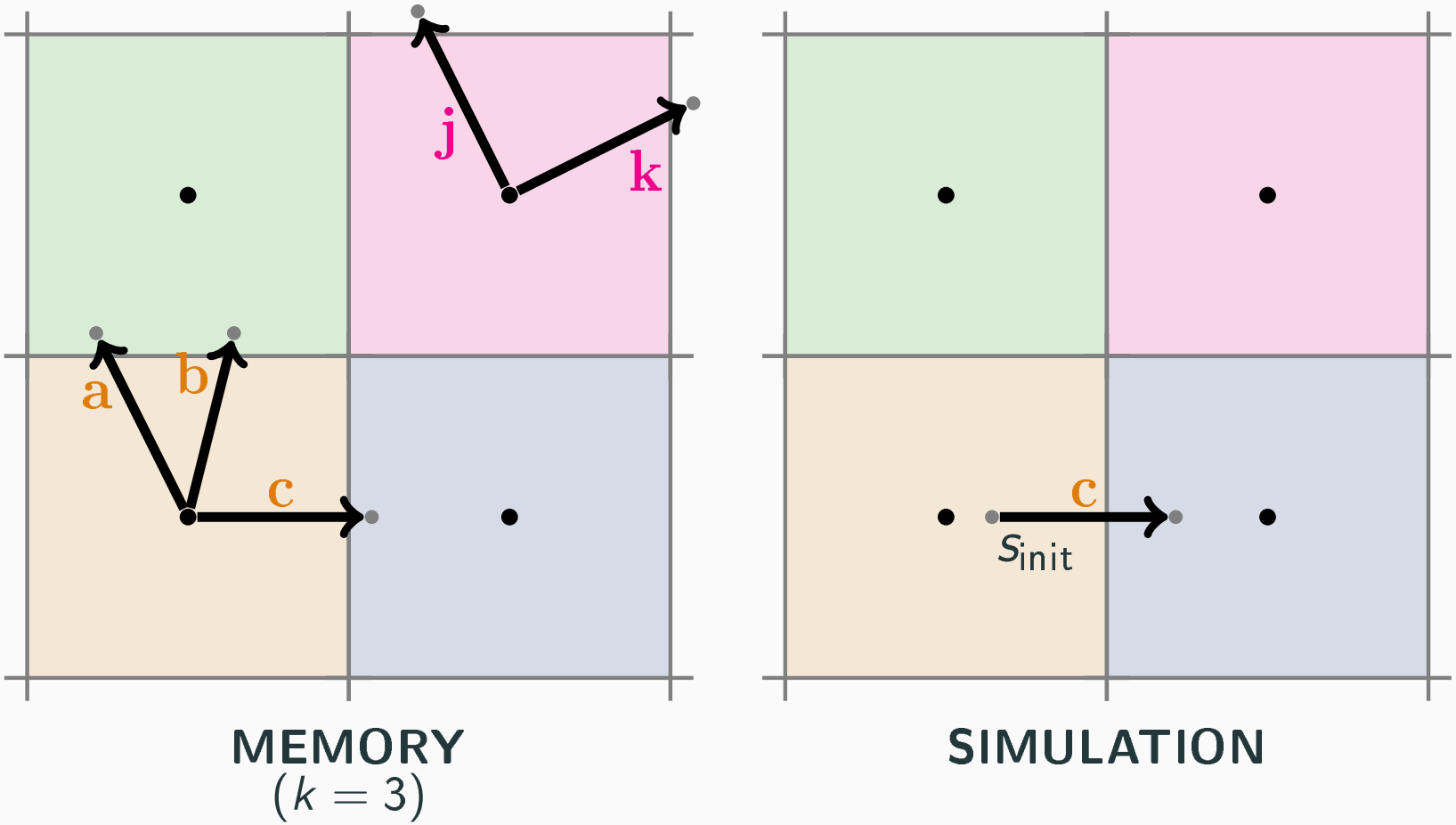

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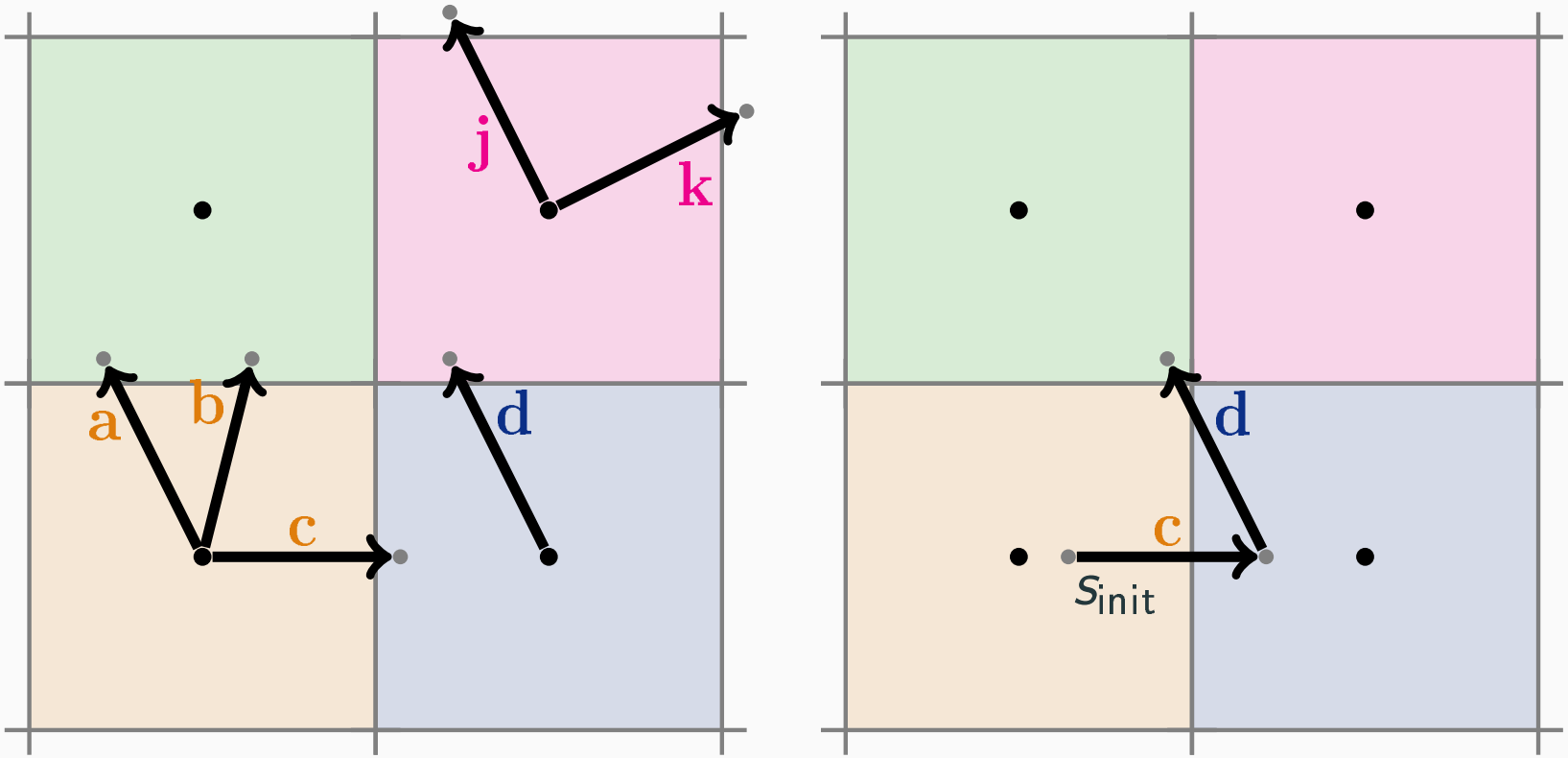

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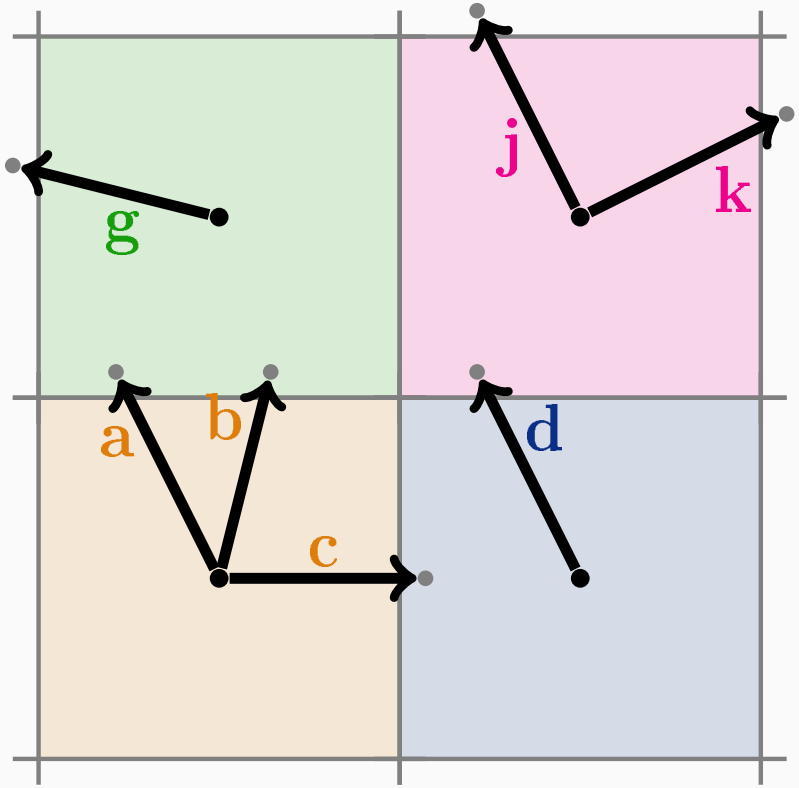

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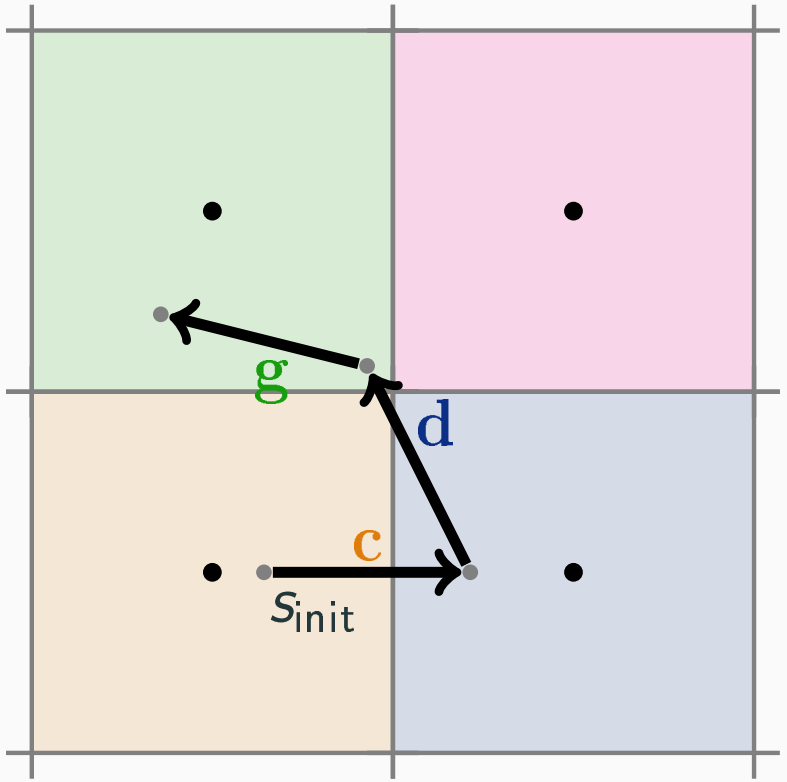

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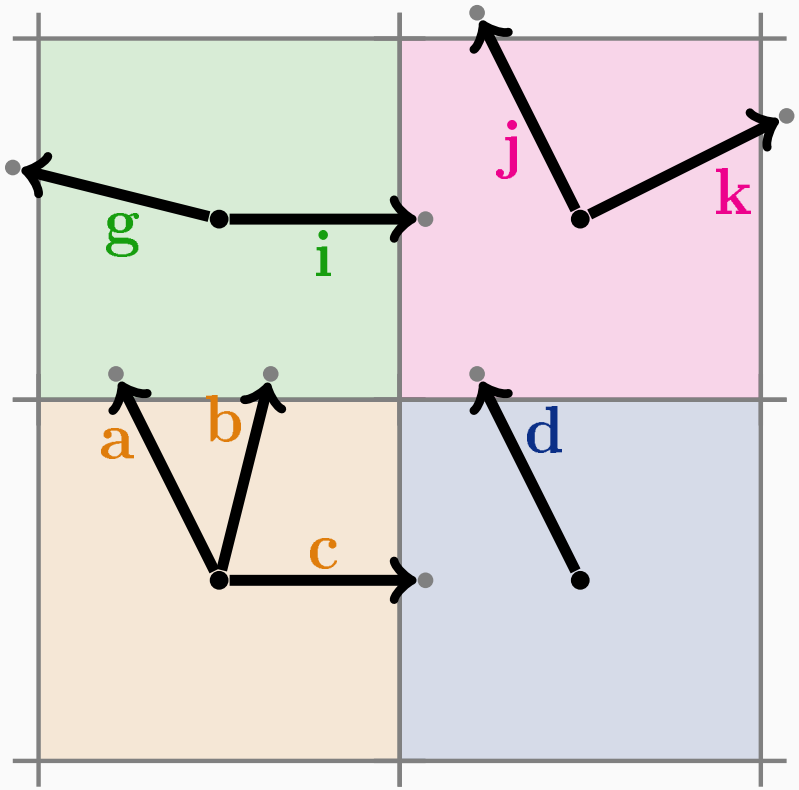

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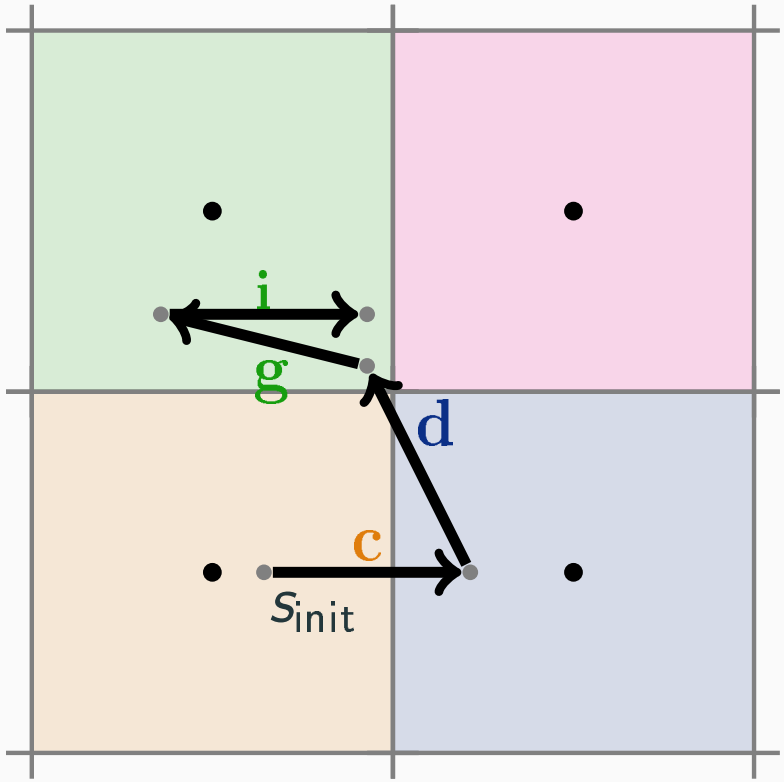

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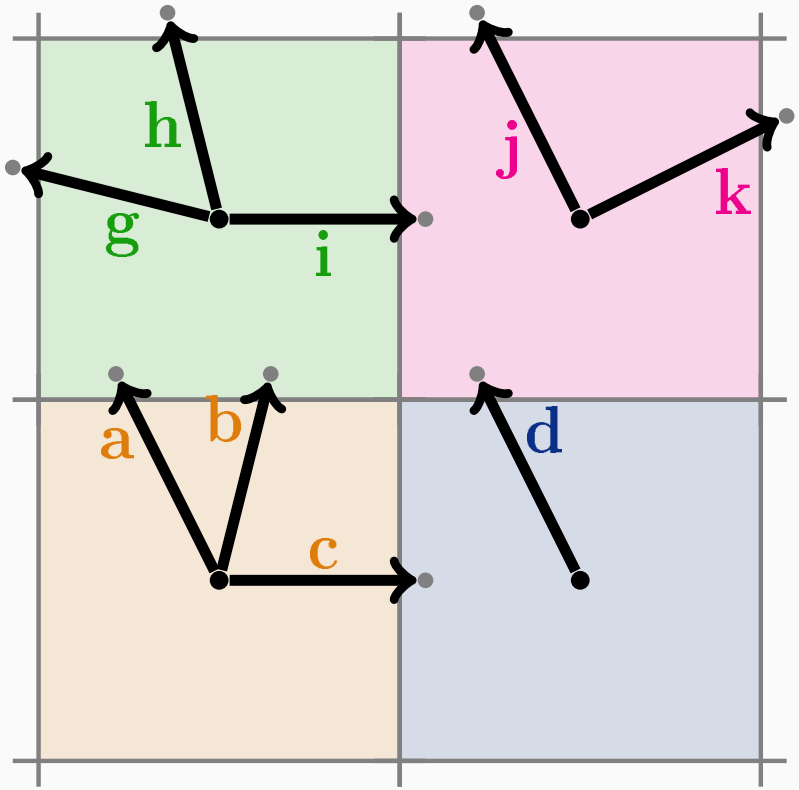

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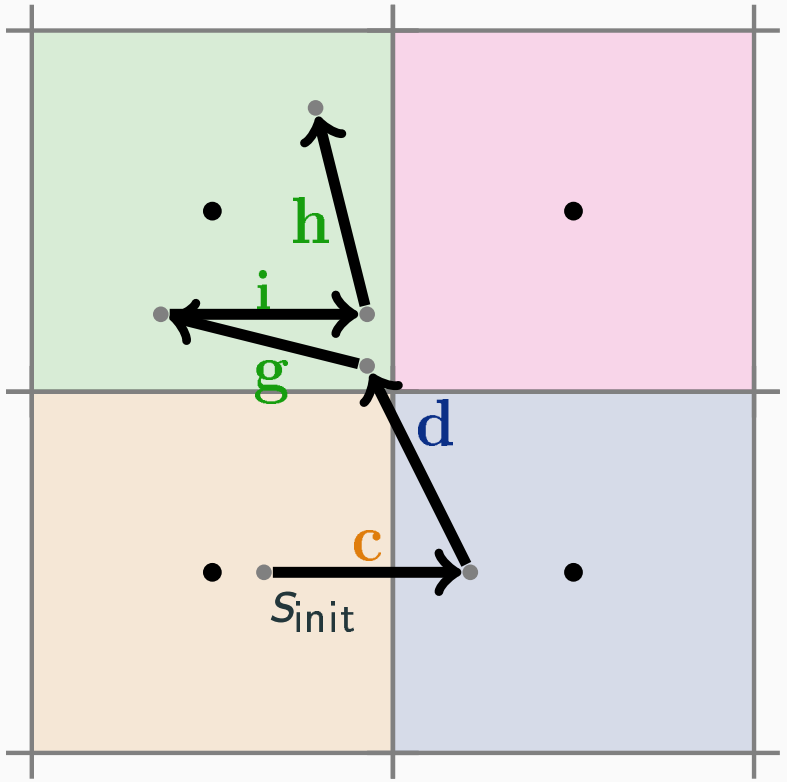

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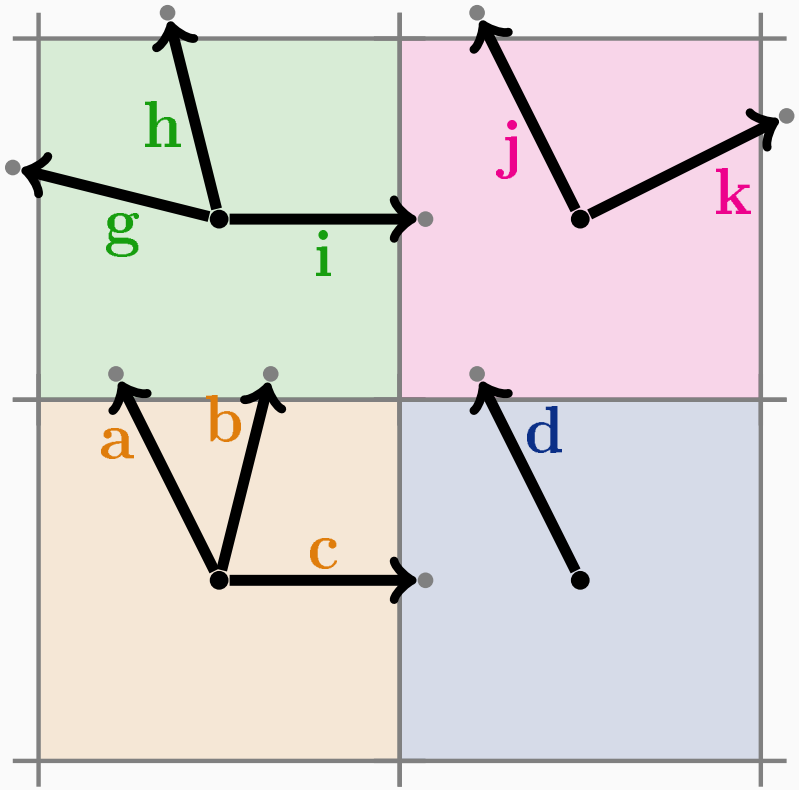

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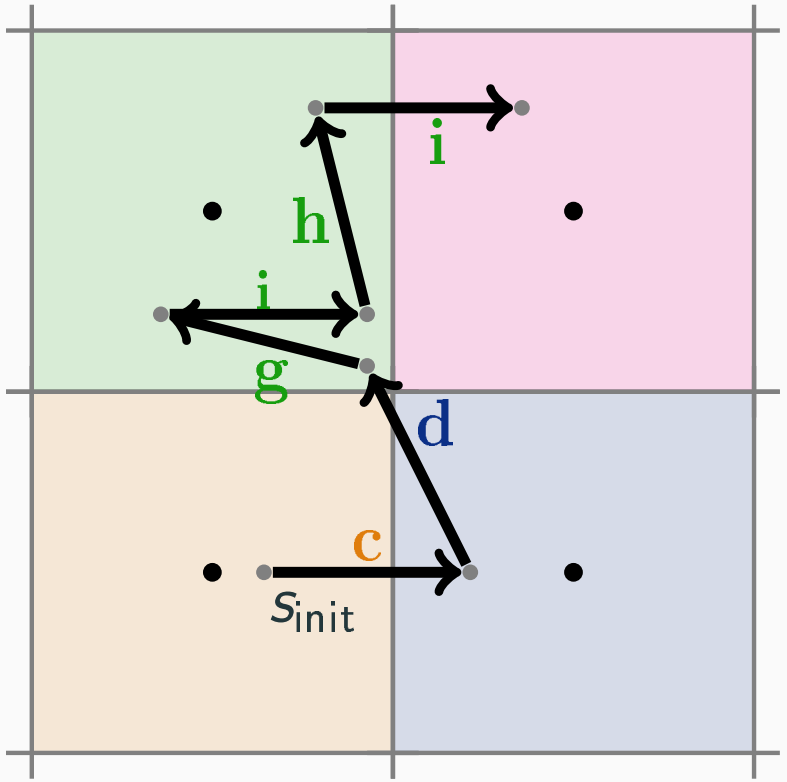

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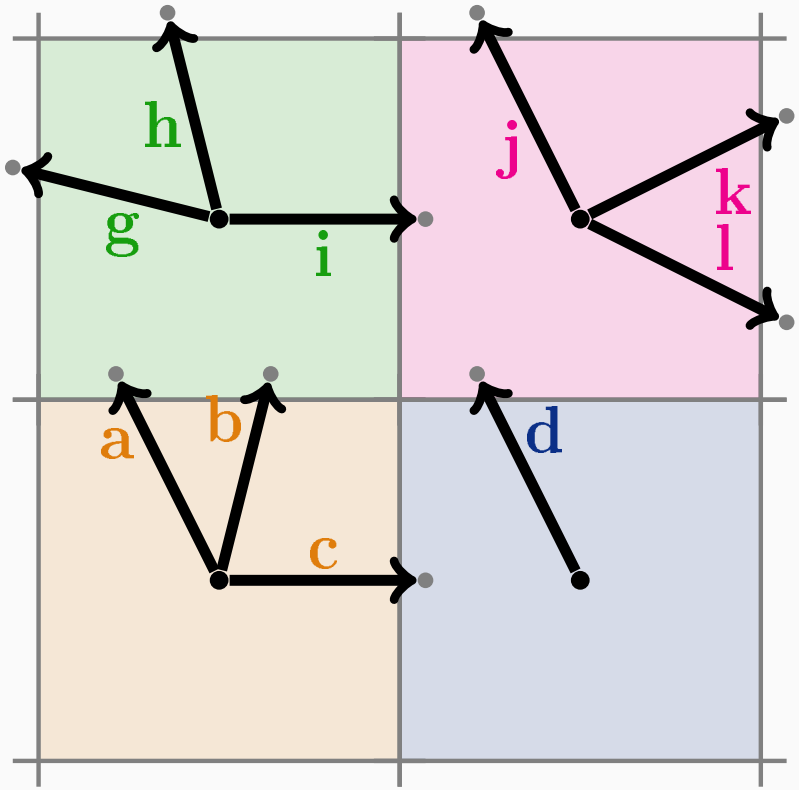

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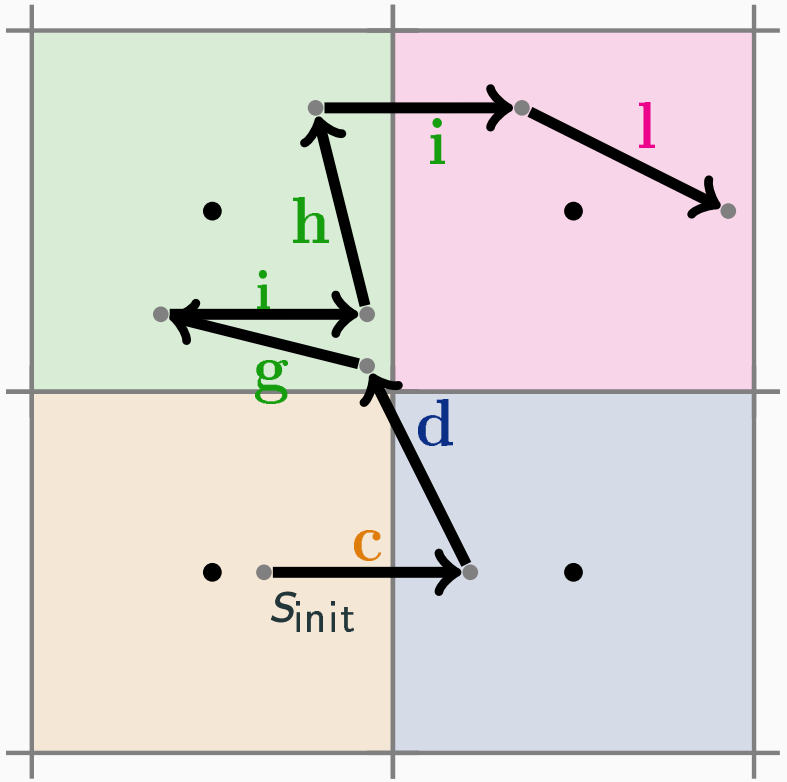

SIMULATION

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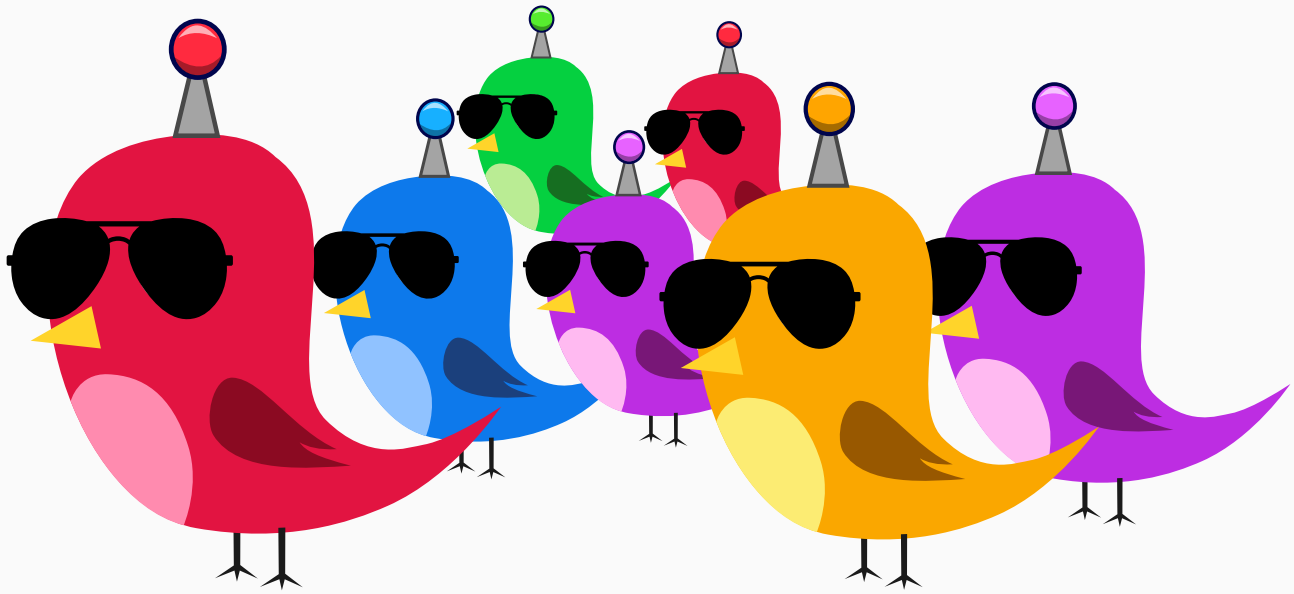
CRN: Conclusion

Segmental simulation:

- Reuses previous simulations to generate new ones
- Is an approximate simulation technique
- Accurately captures dynamics of most systems
- Speeds up transient analysis (up to 4000x faster)
- Efficiently predict the behavior of CRNs

Try it in SAQuaiA!

Thank you



THANK YOU!

My Publications i

First Author:

- Checking Qualitative Liveness Properties of Replicated Systems with Stochastic Scheduling (CAV'20) [3]
- Peregrine 2.0: Explaining Correctness of Population Protocols Through Stage Graphs (ATVA'20) [8]
- Abstraction-Based Segmental Simulation of Chemical Reaction Networks (CMSB'22) [10]

Non-first Author:

- Succinct Population Protocols for Presburger Arithmetic (STACS'20) [2]
- Fast and Succinct Population Protocols for Presburger Arithmetic (SAND'22) [5]

My Publications ii

Others (not part of thesis):

- Automata Tutor v3 (CAV20) [7]
- Decision Power of Weak Asynchronous Models of Distributed Computing (PODC'21) [4]
- Fast and succinct population protocols for Presburger arithmetic (Journal of Comp. and Sys. Sciences 2023) [6]

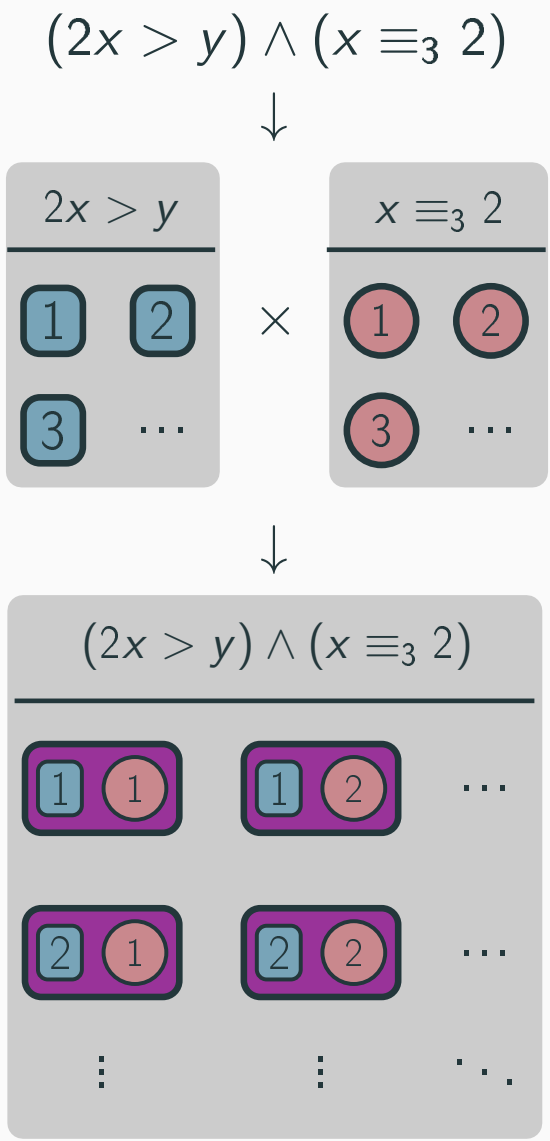
Population Protocol: Synthesis

Our result

For every quantifier-free Presburger formula φ there is an population protocol which

- has $\mathcal{O}(\mathrm{POLY}(|\varphi|))$ states,
  $\rightarrow$ succinct
- for n agents stabilizes in $\mathcal{O}(n^2 \log n)$ expected interactions, and
  $\rightarrow$ fast
- can be constructed efficiently.

Population Protocol: Synthesis (Fast) (by Angluin *et al.* [1])



Population Protocol: Synthesis Idea

Idea:

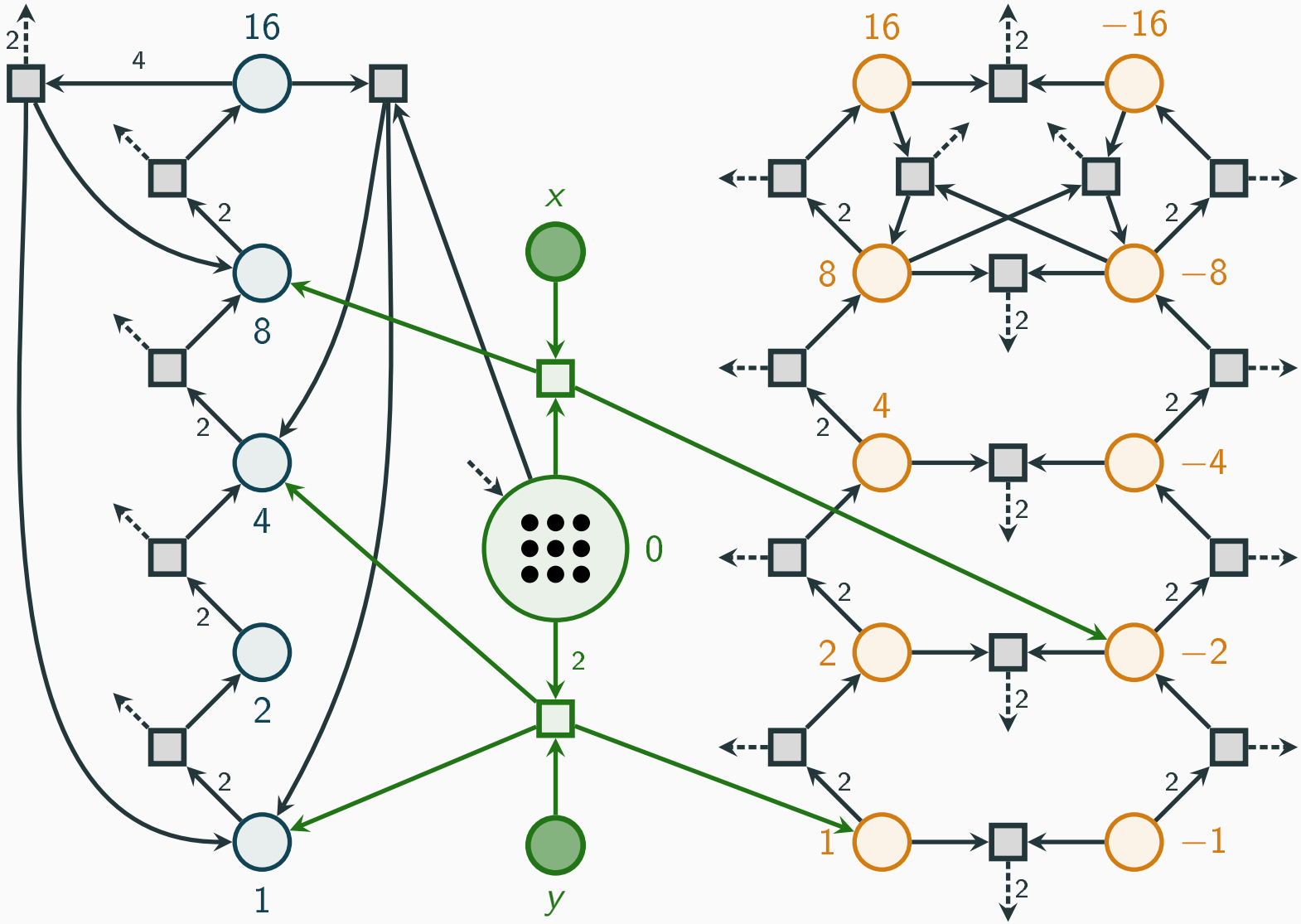
- Binary value representation
  (instead of unary)
- Agents participate in computation of only one atomic formula
  (instead of in all)

Population Computer

Like population protocol but easier to design because:

- k-way transitions
- Helper agents
- More flexible output definition

Population Protocol: Synthesis (Fast and Succinct)



$$8x + 5y \equiv_{11} 4 \quad \vee \quad y - 2x \geq 5$$

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