



# High-Performance and Scalable Agent-Based Simulation With BioDynaMo

*Lukas Breitwieser, Ahmad Hesam, Fons Rademakers,  
Juan Gómez Luna, and Onur Mutlu*

<https://arxiv.org/abs/2301.06984>, <https://doi.org/10.1145/3572848.3577480>

ACM SIGPLAN Annual Symposium on Principles and Practice of Parallel Programming  
27 February 2023, Montreal Canada



**ETH** zürich

**SAFARI**

**TU**Delft

# Key problem



Most existing agent-based simulation platforms exhibit **low performance**

# Impact of low performance

# Impact of low performance



Limits the model size and complexity

# Impact of low performance



Limits the model size and complexity



Increases the development time

# Impact of low performance



Limits the model size and complexity



Increases the development time



Limits the capability to optimize parameters  
→ might lead to less optimal solution

# Impact of low performance



Limits the model size and complexity



Increases the development time



Limits the capability to optimize parameters  
→ might lead to less optimal solution



Increases costs

# Our solution: BioDynaMo



BioDynaMo is a **modular and high-performance** agent-based simulation platform written in C++.

<https://biodynamo.org>

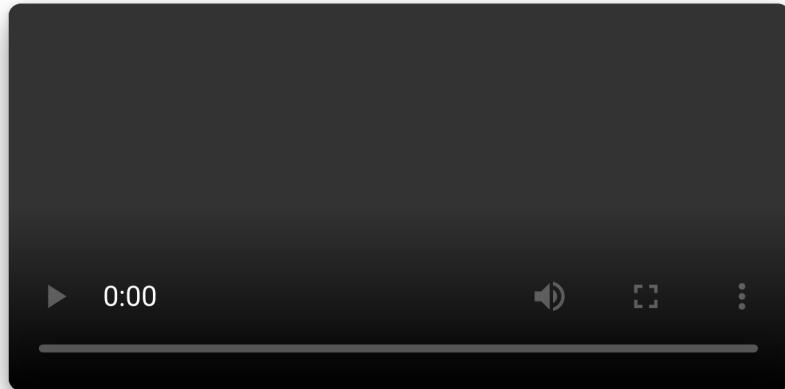


---

# Background

# Example agent-based model

Modeling a swarm of birds

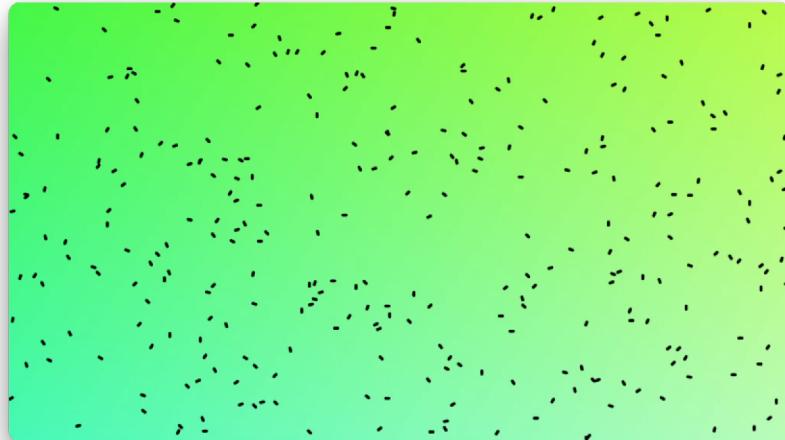


# Example agent-based model

Modeling a swarm of birds

Agent is a bird with the following attributes:

- position
- velocity



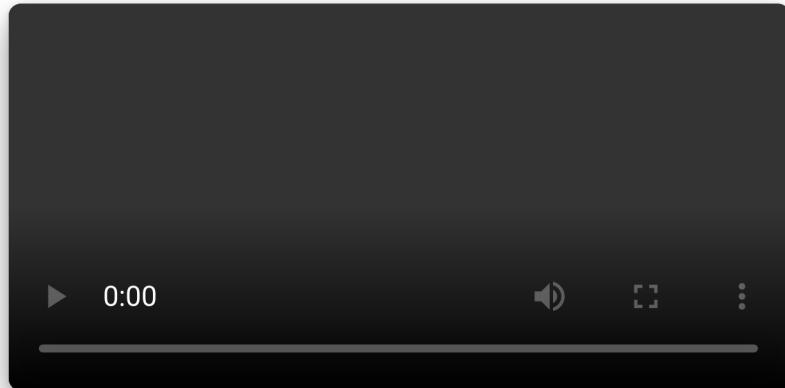
# Example agent-based model

Modeling a swarm of birds

Agent is a bird with the following attributes:

- position
- velocity

and three behaviors



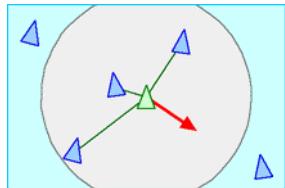
# Example agent-based model

Modeling a swarm of birds

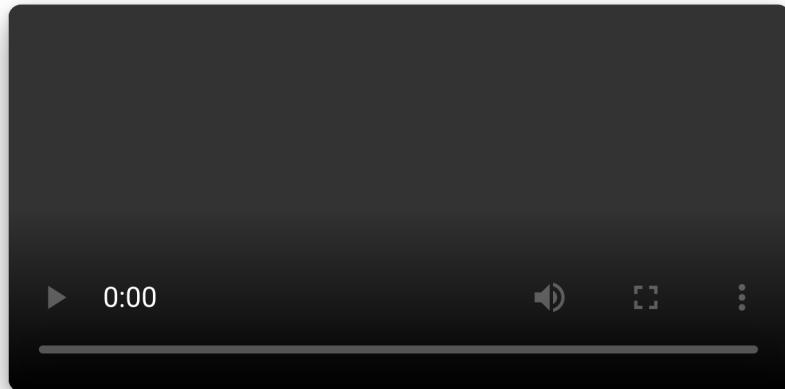
Agent is a bird with the following attributes:

- position
- velocity

and three behaviors



Separation



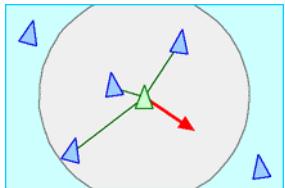
# Example agent-based model

Modeling a swarm of birds

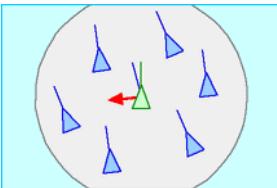
Agent is a bird with the following attributes:

- position
- velocity

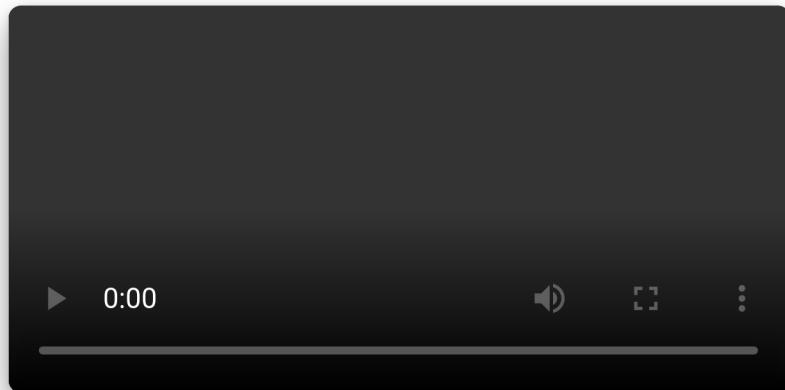
and three behaviors



Separation



Alignment



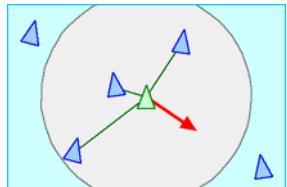
# Example agent-based model

Modeling a swarm of birds

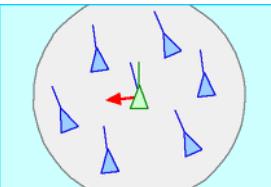
Agent is a bird with the following attributes:

- position
- velocity

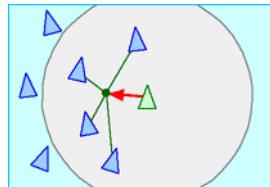
and three behaviors



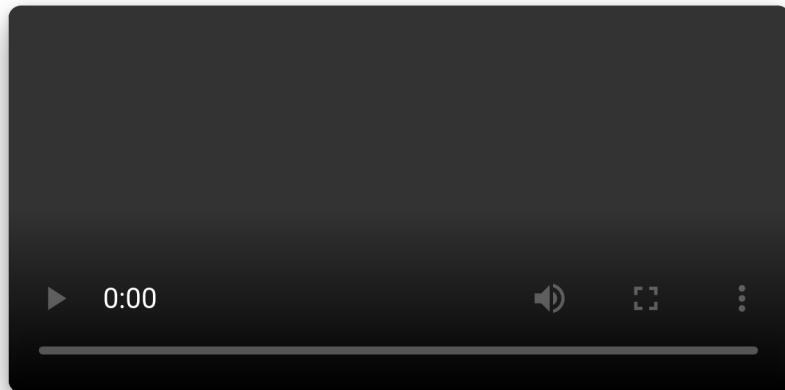
Separation



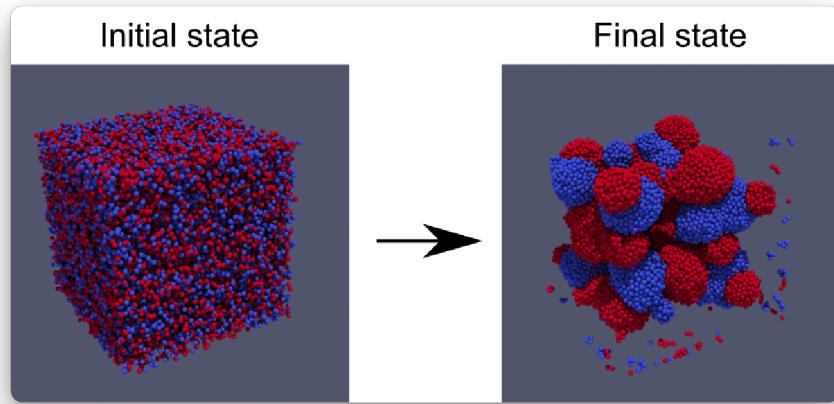
Alignment



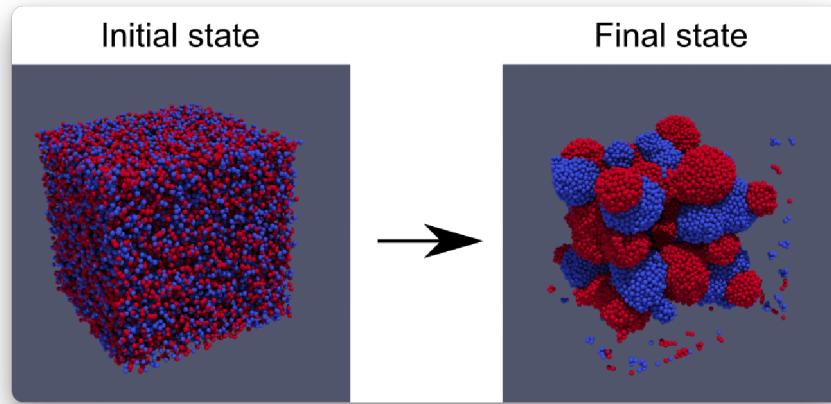
Cohesion



# Cell sorting in BioDynaMo



# Cell sorting in BioDynaMo

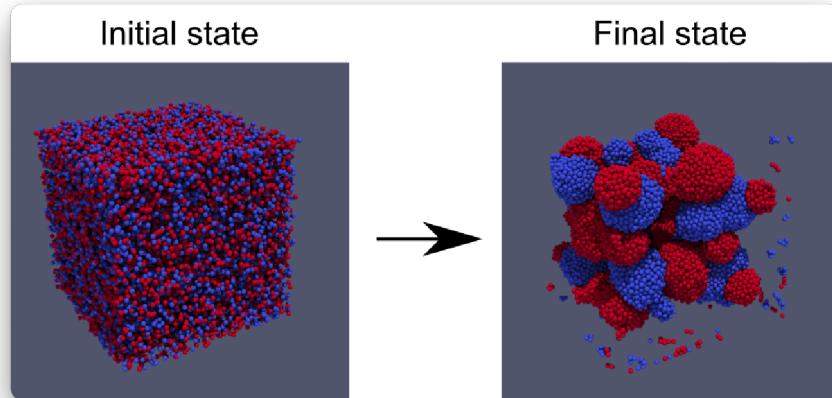


## Agent

Spherical cell with type attribute (red and blue)

## Behaviors

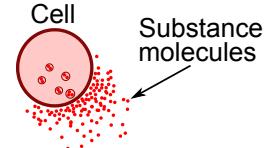
# Cell sorting in BioDynaMo



## Agent

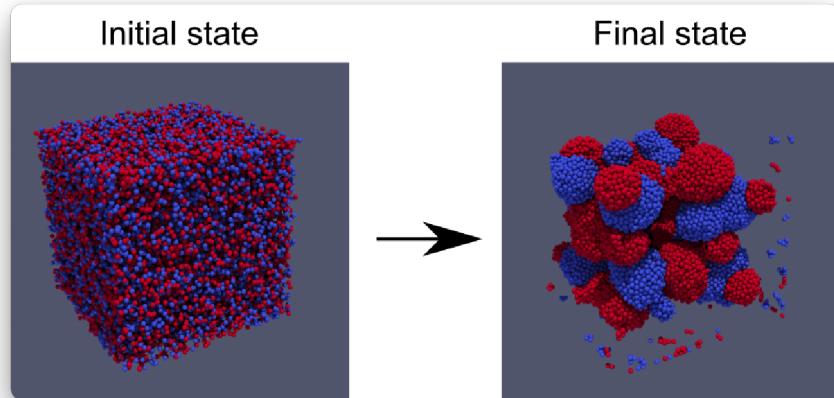
Spherical cell with type attribute (red and blue)

## Behaviors



Substance  
secretion

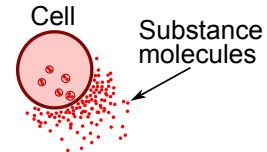
# Cell sorting in BioDynaMo



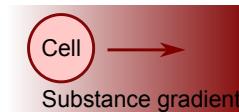
## Agent

Spherical cell with type attribute (red and blue)

## Behaviors

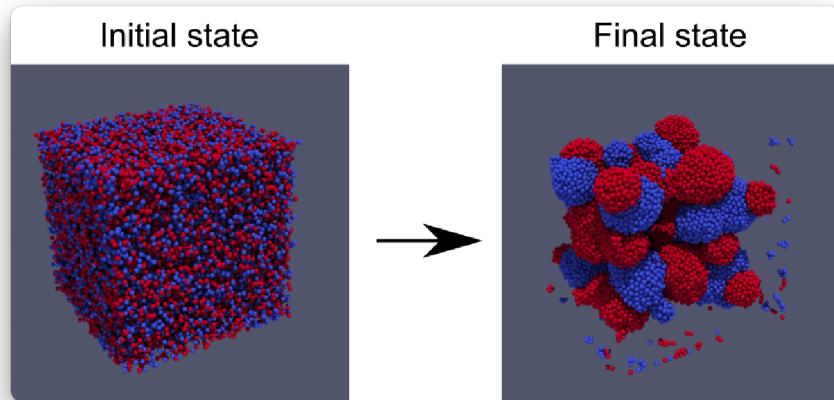


Substance  
secretion



Chemotaxis

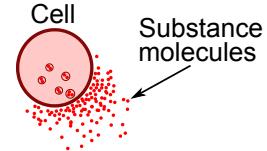
# Cell sorting in BioDynaMo



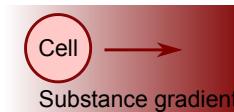
## Agent

Spherical cell with type attribute (red and blue)

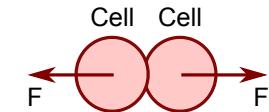
## Behaviors



Substance secretion



Chemotaxis



Mechanical forces

# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11     for each agent {
12         SecreteSubstance(agent);
13         FollowSubstanceGradient(agent);
14         CalculateForces(agent);
15     }
16
17     DiffuseSubstance('purple');
18     DiffuseSubstance('light-blue');
19
20     Visualize();
21 }
```

# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11     for each agent {
12         SecreteSubstance(agent);
13         FollowSubstanceGradient(agent);
14         CalculateForces(agent);
15     }
16
17     DiffuseSubstance('purple');
18     DiffuseSubstance('light-blue');
19
20     Visualize();
21 }
```

# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11    for each agent {
12        SecreteSubstance(agent);
13        FollowSubstanceGradient(agent);
14        CalculateForces(agent);
15    }
16
17    DiffuseSubstance('purple');
18    DiffuseSubstance('light-blue');
19
20    Visualize();
21 }
```

# Cell sorting implementation

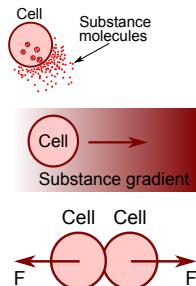
```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11     for each agent {
12         SecreteSubstance(agent);
13         FollowSubstanceGradient(agent);
14         CalculateForces(agent);
15     }
16
17     DiffuseSubstance('purple');
18     DiffuseSubstance('light-blue');
19
20     Visualize();
21 }
```

# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11     for each agent {
12         SecreteSubstance(agent);
13         FollowSubstanceGradient(agent);
14         CalculateForces(agent);
15     }
16
17     DiffuseSubstance('purple');
18     DiffuseSubstance('light-blue');
19
20     Visualize();
21 }
```

# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11     for each agent {
12         SecreteSubstance(agent);
13         FollowSubstanceGradient(agent);
14         CalculateForces(agent);
15     }
16
17     DiffuseSubstance('purple');
18     DiffuseSubstance('light-blue');
19
20     Visualize();
21 }
```



# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11     for each agent {
12         SecreteSubstance(agent);
13         FollowSubstanceGradient(agent);
14         CalculateForces(agent);
15     }
16
17     DiffuseSubstance('purple');
18     DiffuseSubstance('light-blue');
19
20     Visualize();
21 }
```

# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11     for each agent {
12         SecreteSubstance(agent);
13         FollowSubstanceGradient(agent);
14         CalculateForces(agent);
15     }
16
17     DiffuseSubstance('purple');
18     DiffuseSubstance('light-blue');
19
20     Visualize();
21 }
```

# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11     for each agent {
12         SecreteSubstance(agent);
13         FollowSubstanceGradient(agent);
14         CalculateForces(agent);
15     }
16
17     DiffuseSubstance('purple');
18     DiffuseSubstance('light-blue');
19
20     Visualize();
21 }
```

## Fundamental operations

# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11     for each agent {
12         SecreteSubstance(agent);
13         FollowSubstanceGradient(agent);
14         CalculateForces(agent);
15     }
16
17     DiffuseSubstance('purple');
18     DiffuseSubstance('light-blue');
19
20     Visualize();
21 }
```

## Fundamental operations

- Iterate over agents and execute a function

# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11    for each agent {
12        SecreteSubstance(agent);
13        FollowSubstanceGradient(agent);
14        CalculateForces(agent);
15    }
16
17    DiffuseSubstance('purple');
18    DiffuseSubstance('light-blue');
19
20    Visualize();
21 }
```

## Fundamental operations

- Iterate over agents and execute a function
- Determine neighbors

# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');
6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();
10
11    for each agent {
12        SecreteSubstance(agent);
13        FollowSubstanceGradient(agent);
14        CalculateForces(agent);
15    }
16
17    DiffuseSubstance('purple');
18    DiffuseSubstance('light-blue');
19
20    Visualize();
21 }
```

## Fundamental operations

- Iterate over agents and execute a function
- Determine neighbors
- **Iterate over neighbors and execute a function**

# Cell sorting implementation

```
1 // Model initialization
2 AddSubstance('purple');
3 AddSubstance('light-blue');
4 CreateAgentsRandom(number, 'red');
5 CreateAgentsRandom(number, 'blue');

6
7 // Simulation
8 for each iteration {
9     UpdateNeighborSearchIndex();

10    for each agent {
11        SecreteSubstance(agent);
12        FollowSubstanceGradient(agent);
13        CalculateForces(agent);
14    }

15    DiffuseSubstance('purple');
16    DiffuseSubstance('light-blue');

17    Visualize();
18 }
```

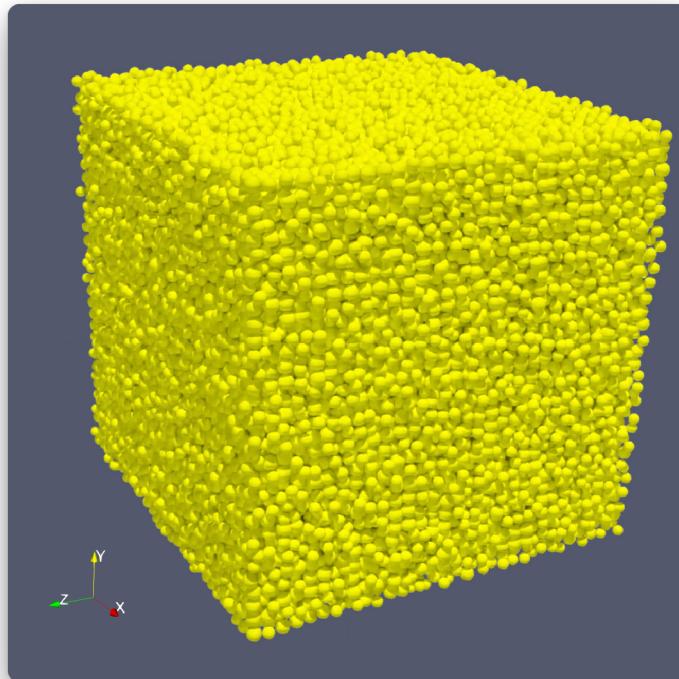
## Fundamental operations

- Iterate over agents and execute a function
- Determine neighbors
- Iterate over neighbors and execute a function
- **Add and remove agents**

# Benchmark simulations

The selected simulations cover a broad spectrum of performance related simulation characteristics

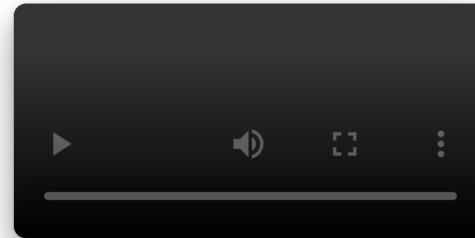
Characteristic	Cell proliferation	Cell clustering	Epidemiology	Neuroscience	Oncology
Create new agents during simulation	x			x	x
Delete agents during simulation					x
Agents modify neighbors				x	
Load imbalance			x	x	
Agents move randomly			x		x
Simulation uses diffusion	x			x	
Simulation has static regions				x	
Number of iterations	500	1000	1000	500	288
Number of agents (in millions)	12.6	2	10	9	10
Number of diffusion volumes	0	54m	0	65k	0



# Benchmark simulations

The selected simulations cover a broad spectrum of performance related simulation characteristics

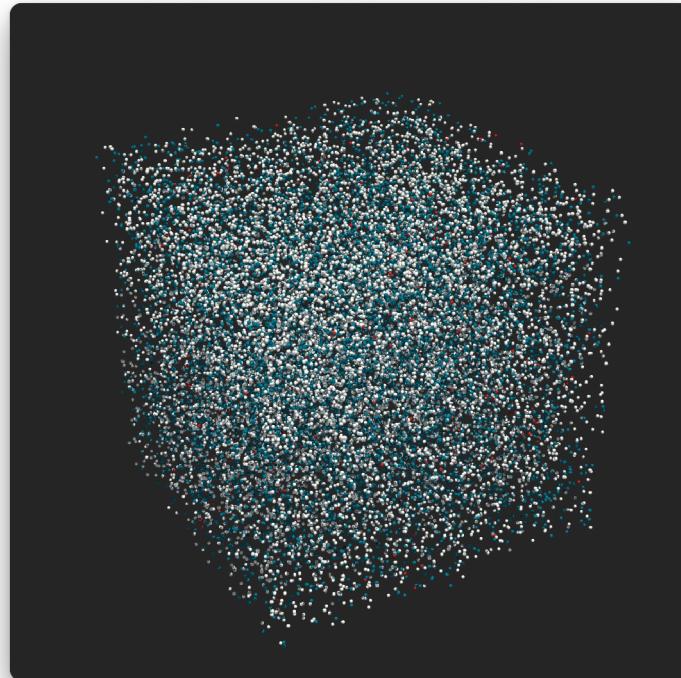
Characteristic	Cell proliferation	Cell clustering	Epidemiology	Neuroscience	Oncology
Create new agents during simulation	x			x	x
Delete agents during simulation				x	
Agents modify neighbors				x	
Load imbalance			x	x	
Agents move randomly		x			x
Simulation uses diffusion		x		x	
Simulation has static regions				x	
Number of iterations	500	1000	1000	500	288
Number of agents (in millions)	12.6	2	10	9	10
Number of diffusion volumes	0	54m	0	65k	0



# Benchmark simulations

The selected simulations cover a broad spectrum of performance related simulation characteristics

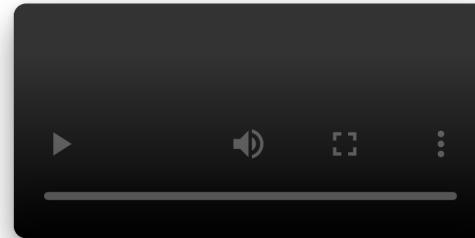
Characteristic	Cell proliferation	Cell clustering	Epidemiology	Neuroscience	Oncology
Create new agents during simulation	x			x	x
Delete agents during simulation					x
Agents modify neighbors			x	x	
Load imbalance		x	x		
Agents move randomly		x			x
Simulation uses diffusion	x			x	
Simulation has static regions				x	
Number of iterations	500	1000	1000	500	288
Number of agents (in millions)	12.6	2	10	9	10
Number of diffusion volumes	0	54m	0	65k	0



# Benchmark simulations

The selected simulations cover a broad spectrum of performance related simulation characteristics

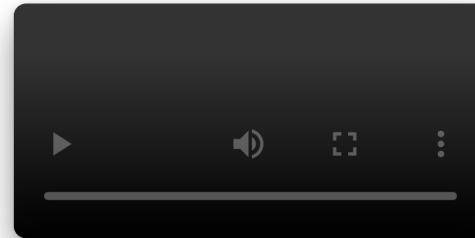
Characteristic	Cell proliferation	Cell clustering	Epidemiology	Neuroscience	Oncology
Create new agents during simulation	x		x	x	x
Delete agents during simulation				x	x
Agents modify neighbors			x	x	
Load imbalance		x	x	x	
Agents move randomly		x	x		x
Simulation uses diffusion	x		x	x	
Simulation has static regions			x	x	
Number of iterations	500	1000	1000	500	288
Number of agents (in millions)	12.6	2	10	9	10
Number of diffusion volumes	0	54m	0	65k	0



# Benchmark simulations

The selected simulations cover a broad spectrum of performance related simulation characteristics

Characteristic	Cell proliferation	Cell clustering	Epidemiology	Neuroscience	Oncology
Create new agents during simulation	x			x	x
Delete agents during simulation				x	x
Agents modify neighbors			x	x	
Load imbalance		x	x		
Agents move randomly		x	x		x
Simulation uses diffusion	x		x		
Simulation has static regions			x		
Number of iterations	500	1000	1000	500	288
Number of agents (in millions)	12.6	2	10	9	10
Number of diffusion volumes	0	54m	0	65k	0



# More details about the simulations and BioDynaMo's modeling features

<https://doi.org/10.1093/bioinformatics/btab649>

*Bioinformatics*, 38(2), 2022, 453–460  
doi: 10.1093/bioinformatics/btab649  
Advance Access Publication Date: 16 September 2021  
Original Paper

OXFORD

---

Systems biology  
**BioDynaMo: a modular platform for high-performance agent-based simulation**

Lukas Breitwieser  <sup>1,2,\*</sup>, Ahmad Hesam <sup>1,3,\*</sup>, Jean de Montigny <sup>1</sup>,  
Vasileios Vavourakis <sup>4,5</sup>, Alexandros Iosif <sup>4</sup>, Jack Jennings <sup>6</sup>, Marcus Kaiser <sup>6,7,8</sup>,  
Marco Manca  <sup>9</sup>, Alberto Di Meglio <sup>1</sup>, Zaid Al-Ars <sup>3</sup>, Fons Rademakers <sup>1</sup>,  
Onur Mutlu <sup>2,10,\*</sup> and Roman Bauer <sup>11,\*</sup>

<sup>1</sup>CERN openlab, IT Department, CERN, Geneva 1211, Switzerland, <sup>2</sup>Department of Computer Science, ETH Zurich, Zurich 8092, Switzerland, <sup>3</sup>Department of Quantum & Computer Engineering, Delft University of Technology, Delft 2628CD, The Netherlands, <sup>4</sup>Department of Mechanical & Manufacturing Engineering, University of Cyprus, Nicosia 2109, Cyprus, <sup>5</sup>Department of Medical Physics & Biomedical Engineering, University College London, London WC1E 6BT, UK, <sup>6</sup>School of Computing, Newcastle University, Newcastle upon Tyne NE4 5TG, UK, <sup>7</sup>Department of Functional Neurosurgery, Ruijin Hospital, Shanghai Jiao Tong University School of Medicine, Shanghai 200025, China, <sup>8</sup>Precision Imaging Beacon, School of Medicine, University of Nottingham, Nottingham NG7 2UH, UK, <sup>9</sup>SCImPulse Foundation, Geleen 6162 BC, The Netherlands, <sup>10</sup>Department of Information Technology and Electrical Engineering, ETH Zurich, Zurich 8092, Switzerland and <sup>11</sup>Department of Computer Science, University of Surrey, Guildford GU2 7XH, UK

\*To whom correspondence should be addressed.  
Associate Editor: Jonathan Wren

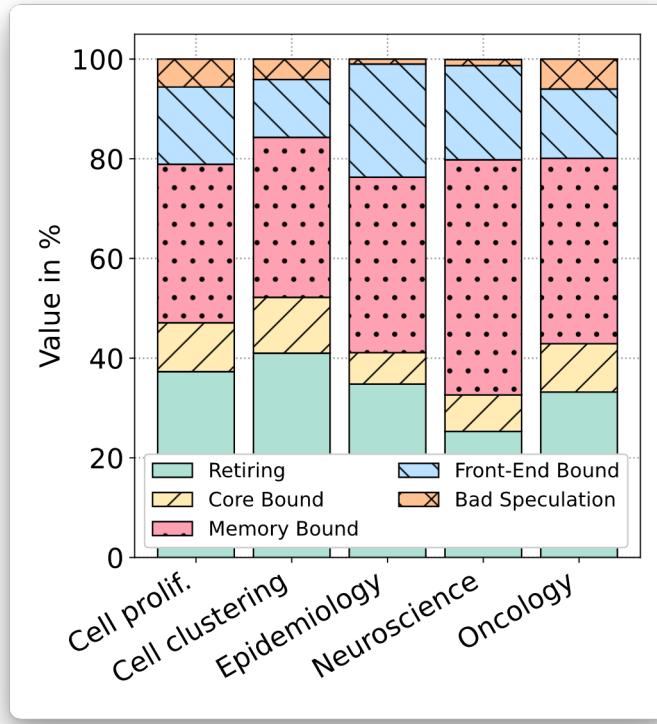
Received on February 4, 2021; revised on September 2, 2021; editorial decision on September 3, 2021; accepted on September 13, 2021

---

# Optimizations

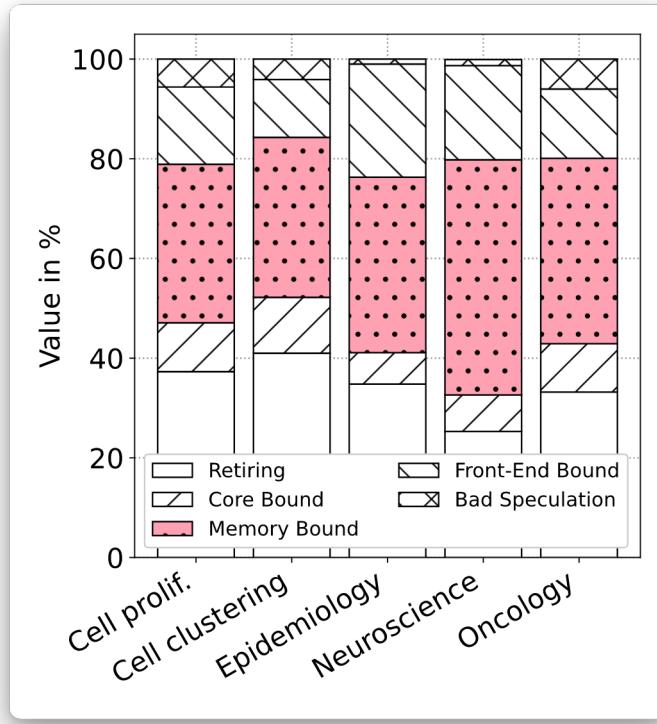
# Key observation: Agent-based simulations are often **memory-bound**

Microarchitecture analysis for five simulations



# Key observation: Agent-based simulations are often **memory-bound**

Microarchitecture analysis for five simulations



# Key challenges and improvements

## Improved fundamental operations:

- Determine neighbors
- Add and remove agents
- Iterate over agents and execute a function
- Iterate over neighbors and execute a function

# Key challenges and improvements



## I: Maximize parallelization

- Optimize radial neighbor search
- Parallelize the addition and removal of agents

## Improved fundamental operations:

- Determine neighbors
- Add and remove agents
- Iterate over agents and execute a function
- Iterate over neighbors and execute a function

# Key challenges and improvements



## I: Maximize parallelization

- Optimize radial neighbor search
- Parallelize the addition and removal of agents



## II: Memory layout

- NUMA-aware iteration
- Agent sorting and balancing
- Pool-based memory allocator

### Improved fundamental operations:

- Determine neighbors
- Add and remove agents
- Iterate over agents and execute a function
- Iterate over neighbors and execute a function

# Key challenges and improvements



## I: Maximize parallelization

- Optimize radial neighbor search
- Parallelize the addition and removal of agents



## II: Memory layout

- NUMA-aware iteration
- Agent sorting and balancing
- Pool-based memory allocator



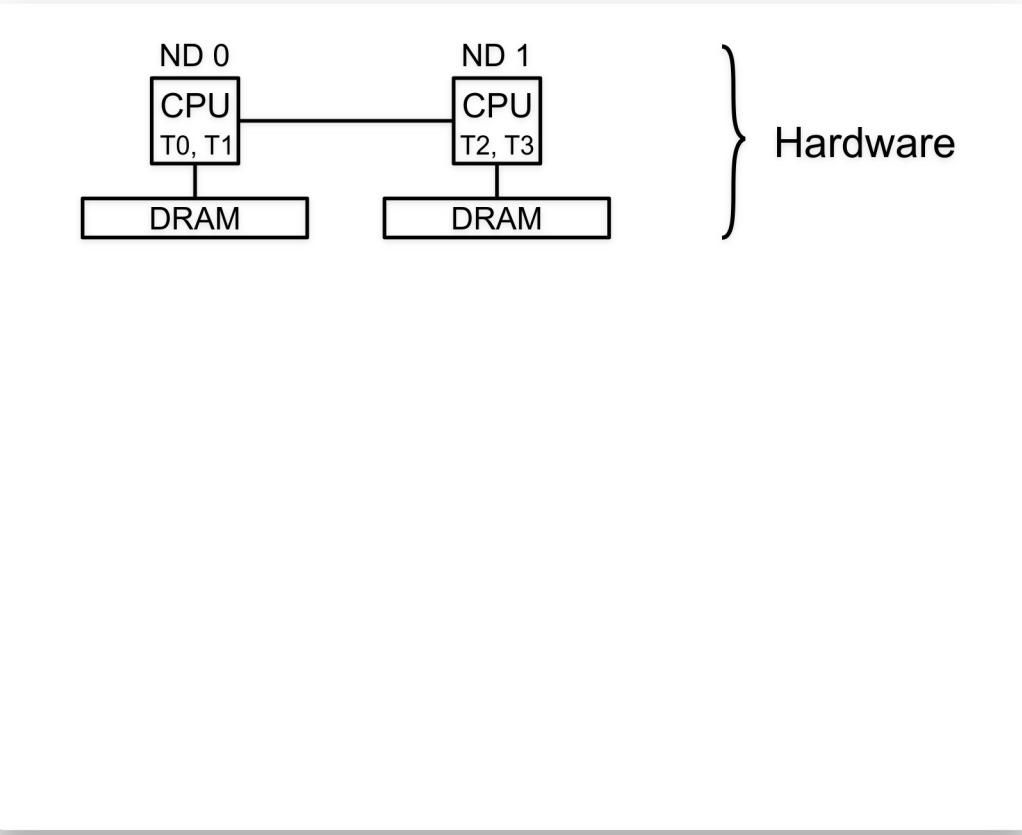
## III: Avoid unnecessary work

- Pair-wise force calculation for static regions

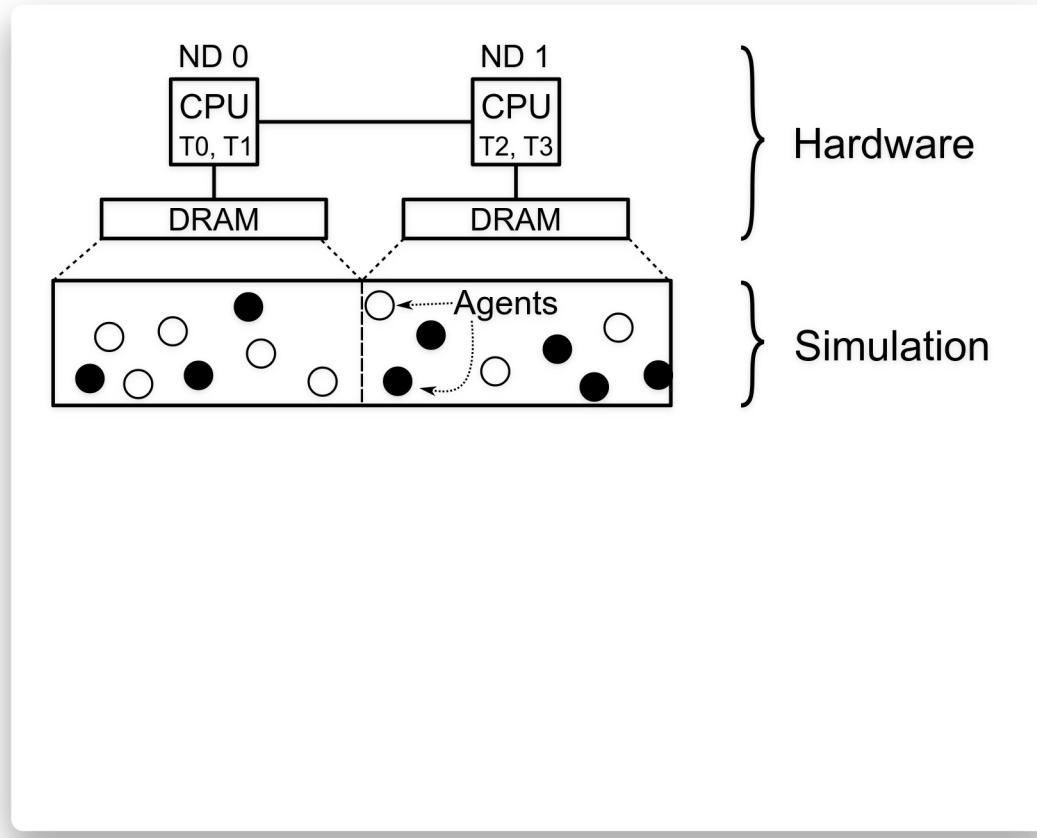
### Improved fundamental operations:

- Determine neighbors
- Add and remove agents
- Iterate over agents and execute a function
- Iterate over neighbors and execute a function

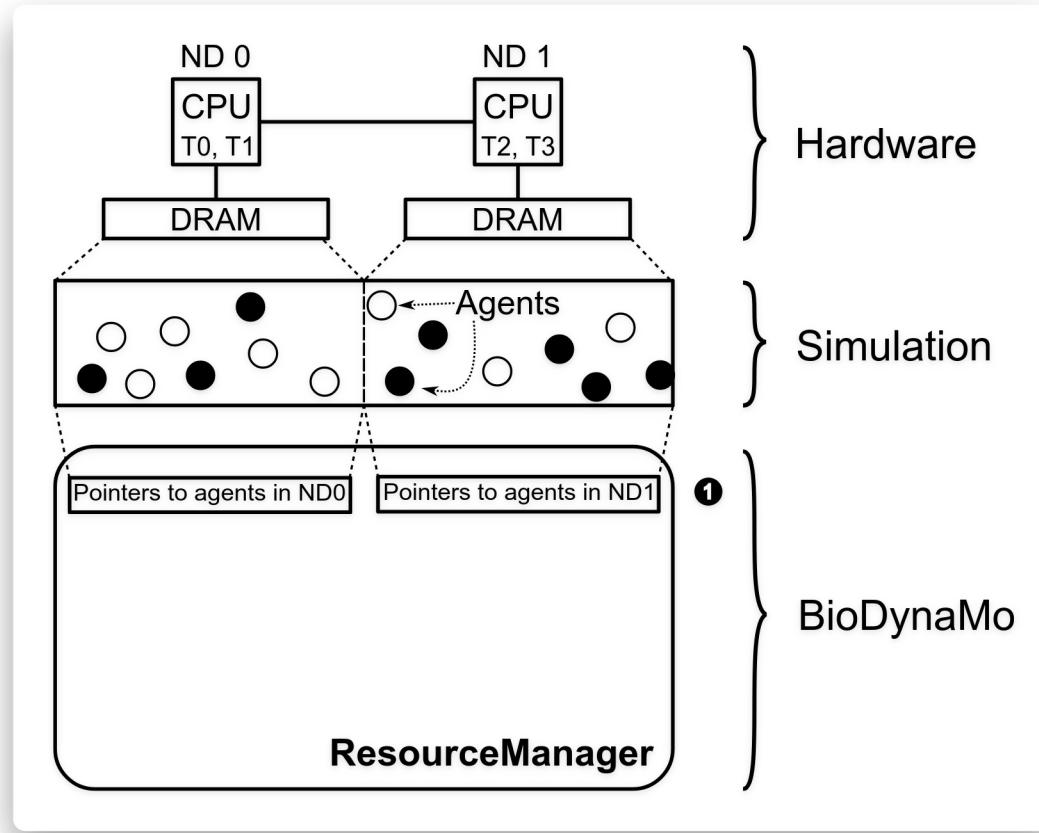
# NUMA-aware iteration



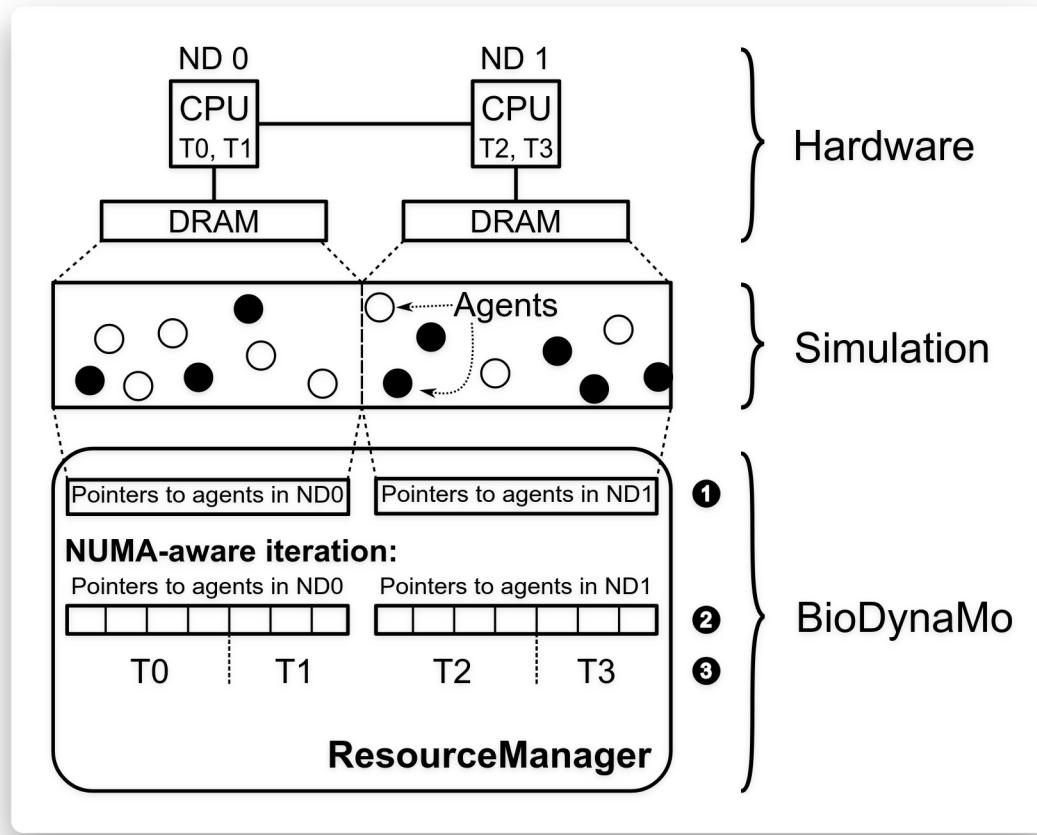
# NUMA-aware iteration



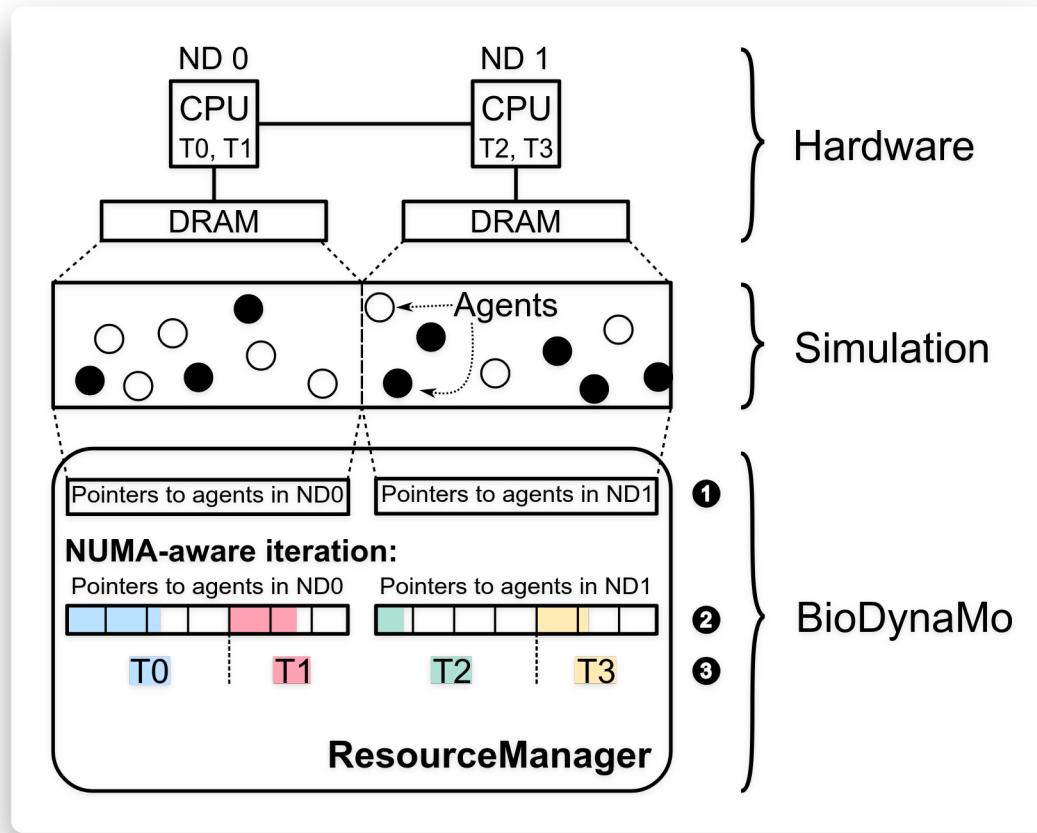
# NUMA-aware iteration



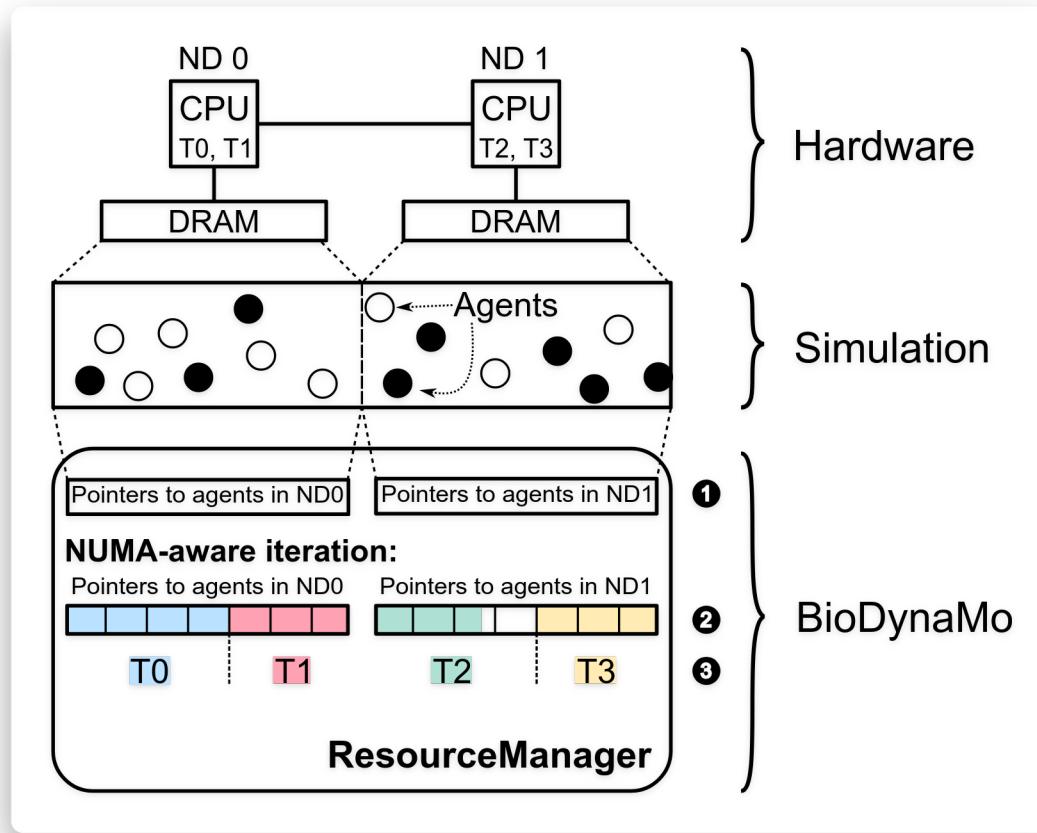
# NUMA-aware iteration



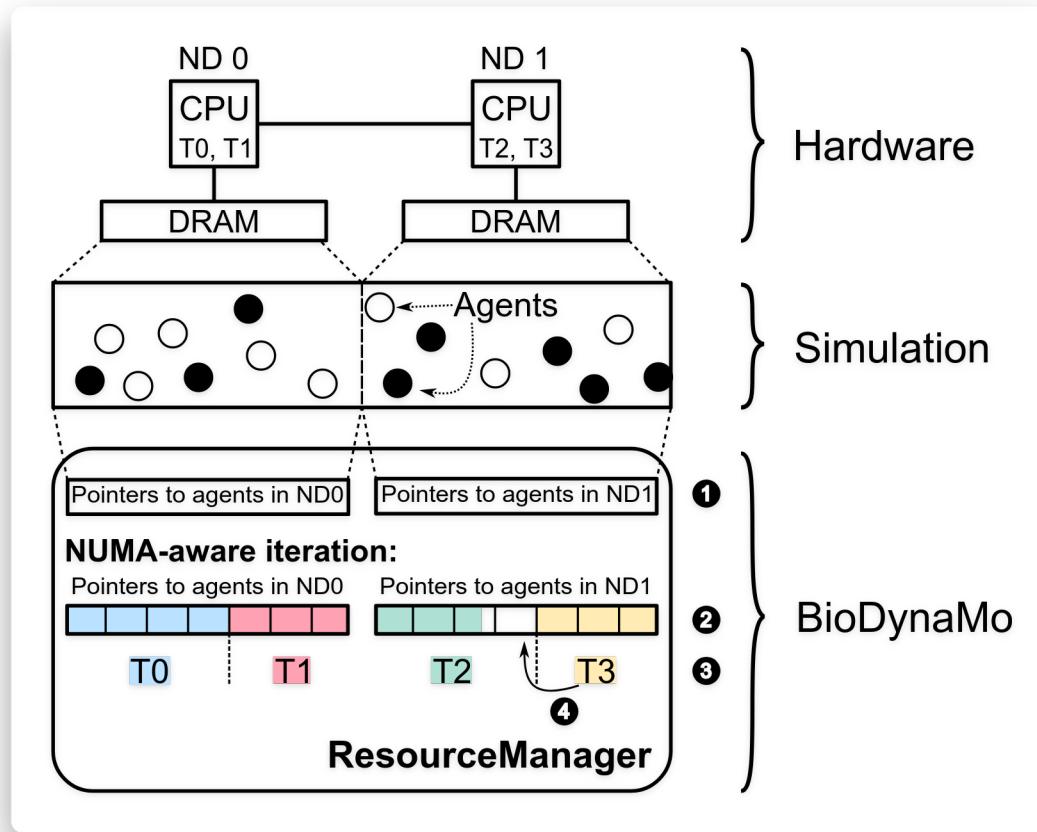
# NUMA-aware iteration



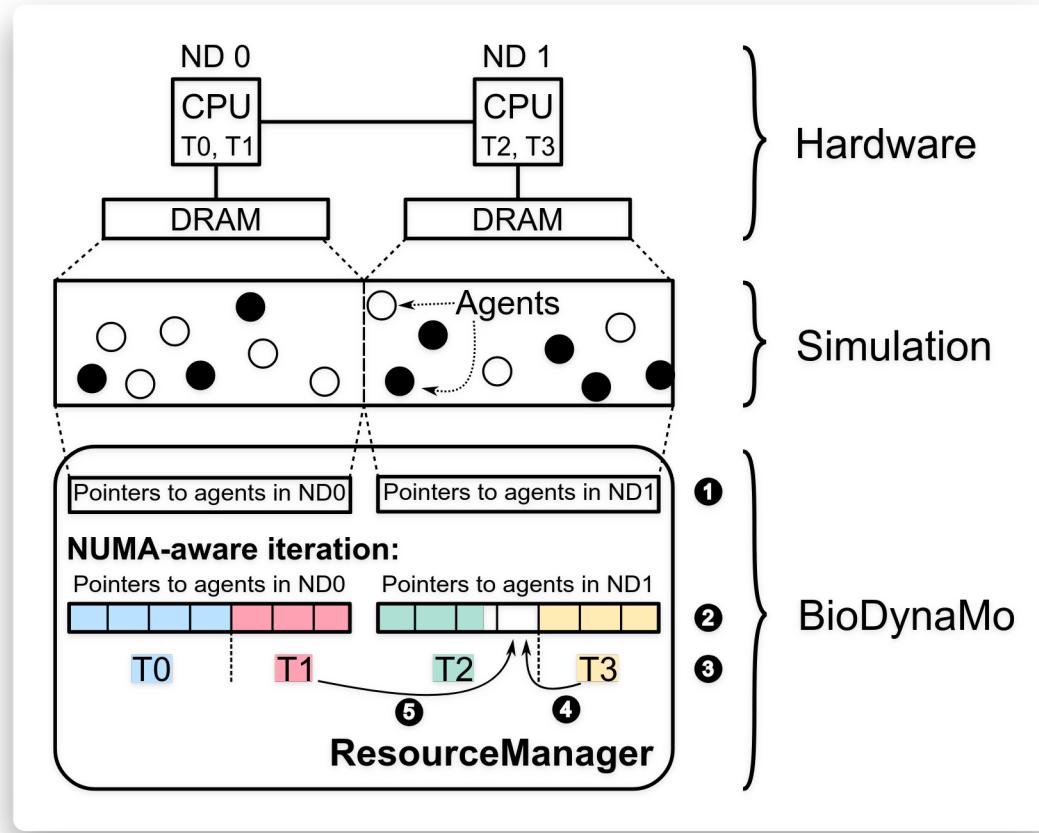
# NUMA-aware iteration



# NUMA-aware iteration



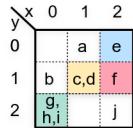
# NUMA-aware iteration



# NUMA-aware iteration

# Agent sorting and balancing

**A** Agents in 3x3 grid



# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g, h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

x	0	1	2	3
0	0	1	2	3
1	z	3	4	5
2	8	9	12	13
3	10	11	14	15

NUMA domain 0  $\leftrightarrow$  NUMA domain 1



# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

x	0	1	2	3
0	0	1	2	3
1	3	4	5	6
2	8	9	12	13
3	10	11	14	15

NUMA domain 0  $\leftrightarrow$  NUMA domain 1



# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

x	0	1	2	3
0	0	1		
1	z	3	6	7
2	8	9	12	13
3	10	11	14	15

NUMA domain 0  $\leftrightarrow$  NUMA domain 1



# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

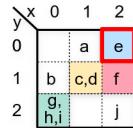
x	0	1	2	3
0	0	1		
1	2	3	4	5
2	6	7	8	9
3	10	11	12	13

NUMA domain 0  $\leftrightarrow$  NUMA domain 1

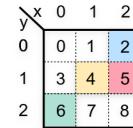


# Agent sorting and balancing

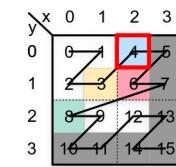
**A** Agents in 3x3 grid



**B** Grid box indices



**C** Morton order of 4x4 grid



NUMA domain 0  $\leftrightarrow$  NUMA domain 1



# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

x	0	1	2	3
0	0	1		
1	z	3	6	7
2	8	9	12	13
3	10	11	14	15

NUMA domain 0  $\leftrightarrow$  NUMA domain 1



# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

x	0	1	2	3
0	0	1		
1	2	3	4	5
2	6	7	8	9
3	10	11	12	13

NUMA domain 0  $\leftrightarrow$  NUMA domain 1



# Agent sorting and balancing

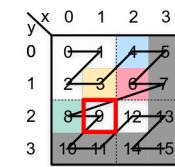
**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid



NUMA domain 0  $\leftrightarrow$  NUMA domain 1



# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

x	0	1	2	3
0	0	1		
1	z	3	6	
2	8	9	12	13
3	10	11	14	15

NUMA domain 0  $\leftrightarrow$  NUMA domain 1

a	b	c	d	e	f	g	h	i	j
---	---	---	---	---	---	---	---	---	---

# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

NUMA domain 0  $\leftrightarrow$  NUMA domain 1



# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

x	0	1	2	3
0	0	1		
1	z	3	6	
2	8	9	12	13
3	10	11	14	15

NUMA domain 0  $\leftrightarrow$  NUMA domain 1



# Agent sorting and balancing

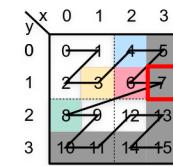
**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid



NUMA domain 0  $\leftrightarrow$  NUMA domain 1



# Agent sorting and balancing

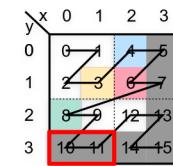
**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

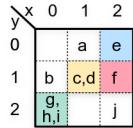


NUMA domain 0  $\leftrightarrow$  NUMA domain 1

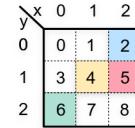


# Agent sorting and balancing

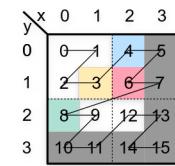
A Agents in 3x3 grid



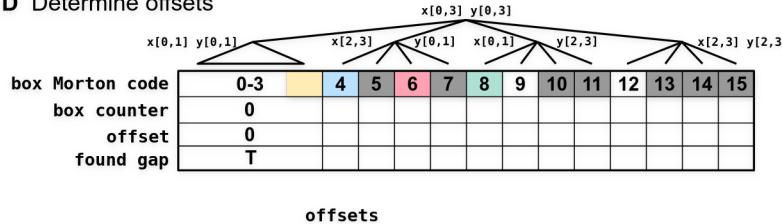
B Grid box indices



C Morton order of 4x4 grid



D Determine offsets



# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g		j

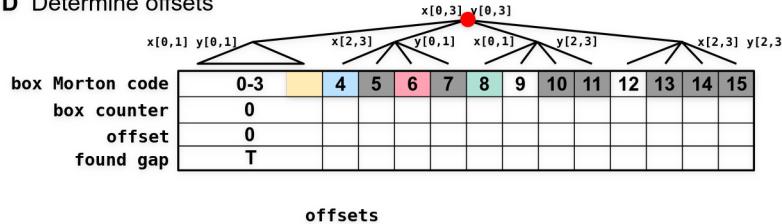
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

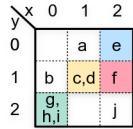
x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**

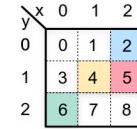


# Agent sorting and balancing

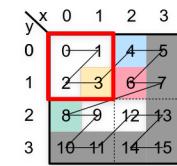
**A Agents in 3x3 grid**



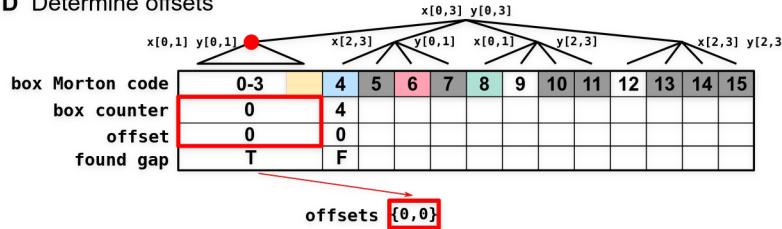
**B Grid box indices**



**C Morton order of 4x4 grid**

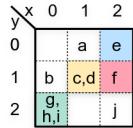


**D Determine offsets**

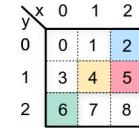


# Agent sorting and balancing

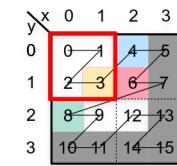
**A Agents in 3x3 grid**



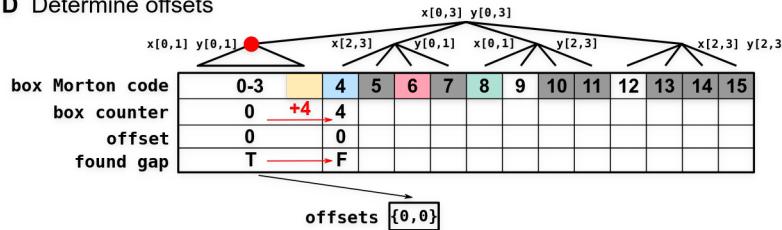
**B Grid box indices**



**C Morton order of 4x4 grid**



**D Determine offsets**



# Agent sorting and balancing

**A** Agents in 3x3 grid

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

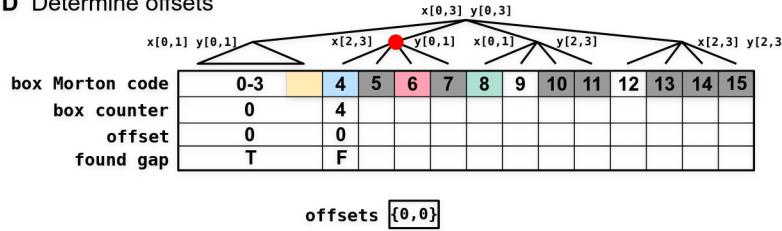
**B** Grid box indices

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C** Morton order of 4x4 grid

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D** Determine offsets



# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g		j

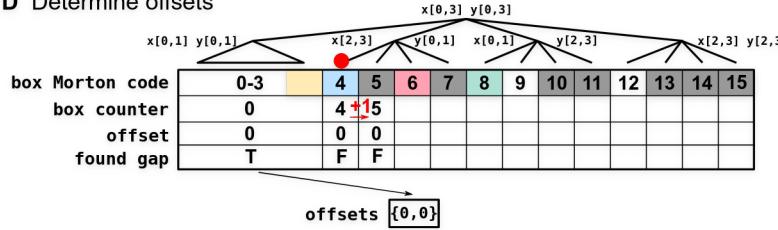
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

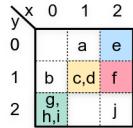
x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**

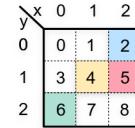


# Agent sorting and balancing

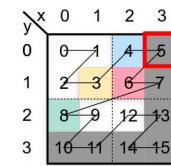
**A Agents in 3x3 grid**



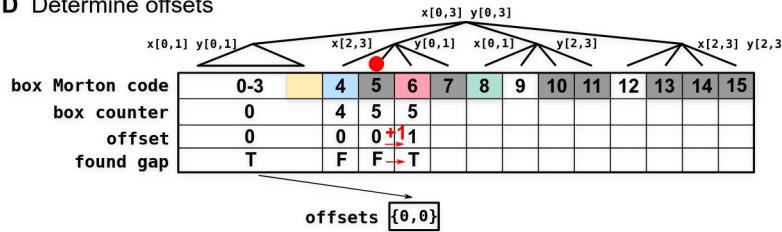
**B Grid box indices**



**C Morton order of 4x4 grid**

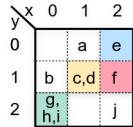


**D Determine offsets**

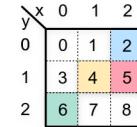


# Agent sorting and balancing

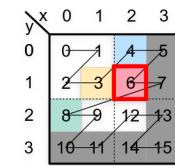
**A Agents in 3x3 grid**



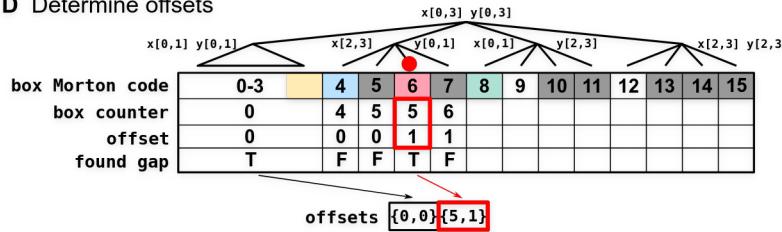
**B Grid box indices**



**C Morton order of 4x4 grid**



**D Determine offsets**



# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g		j

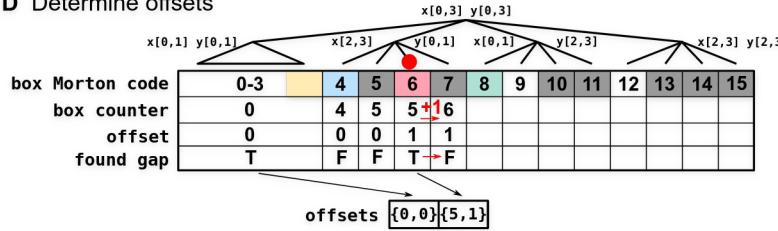
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

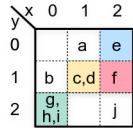
x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**

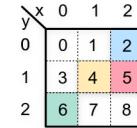


# Agent sorting and balancing

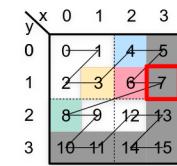
**A Agents in 3x3 grid**



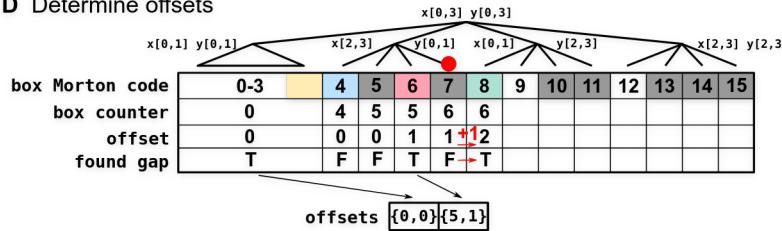
**B Grid box indices**



**C Morton order of 4x4 grid**

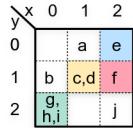


**D Determine offsets**

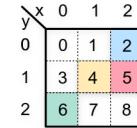


# Agent sorting and balancing

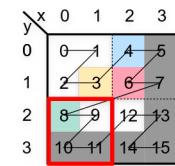
**A Agents in 3x3 grid**



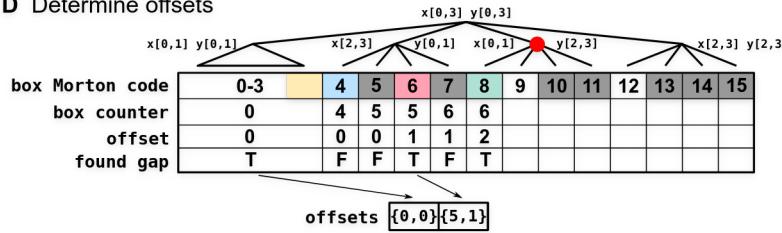
**B Grid box indices**



**C Morton order of 4x4 grid**

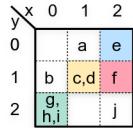


**D Determine offsets**

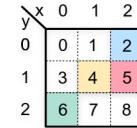


# Agent sorting and balancing

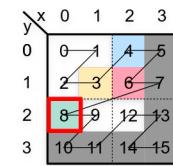
**A Agents in 3x3 grid**



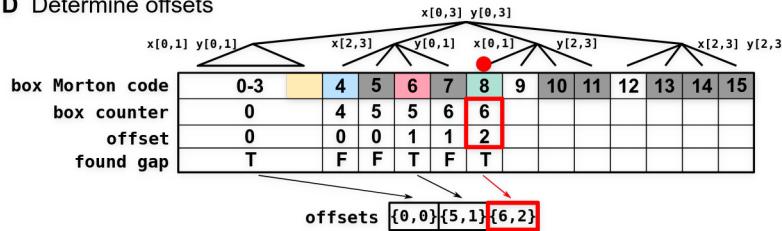
**B Grid box indices**



**C Morton order of 4x4 grid**

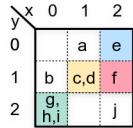


**D Determine offsets**

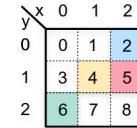


# Agent sorting and balancing

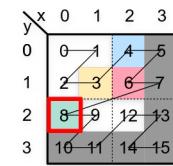
**A Agents in 3x3 grid**



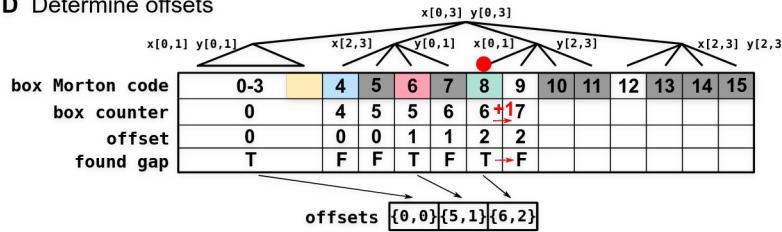
**B Grid box indices**



**C Morton order of 4x4 grid**

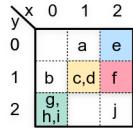


**D Determine offsets**

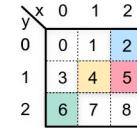


# Agent sorting and balancing

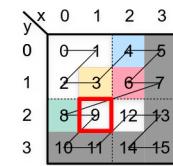
**A Agents in 3x3 grid**



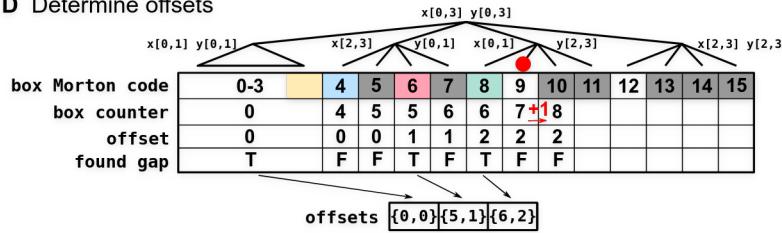
**B Grid box indices**



**C Morton order of 4x4 grid**

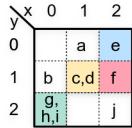


**D Determine offsets**

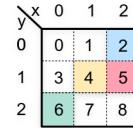


# Agent sorting and balancing

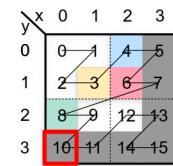
## A Agents in 3x3 grid



## B Grid box indices



### C Morton order of 4x4 grid



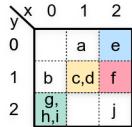
## D Determine offsets

D Determine offsets

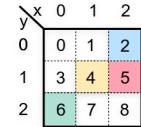
	x[0..3]	y[0..3]
box Morton code	0-3	4 5 6 7 8 9 10 11 12 13 14 15
box counter	0	4 5 5 6 6 6 7 8 8
offset	0	0 0 1 1 2 2 2+13
found gap	T	F F T F T F F -T
		offsets {0,0} {5,1} {6,2}

# Agent sorting and balancing

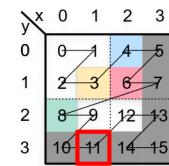
## A Agents in 3x3 grid



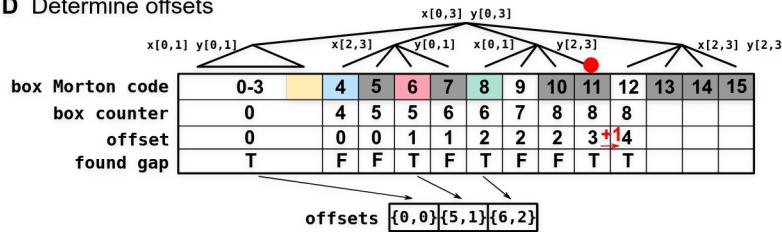
## B Grid box indices



### C Morton order of 4x4 grid

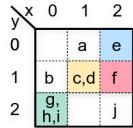


## D Determine offsets

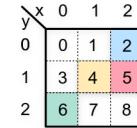


# Agent sorting and balancing

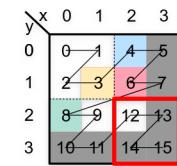
**A Agents in 3x3 grid**



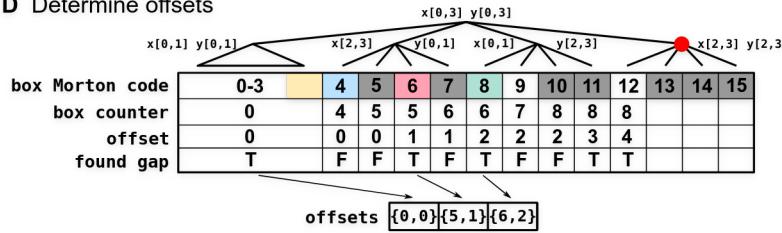
**B Grid box indices**



**C Morton order of 4x4 grid**



**D Determine offsets**



# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g		j

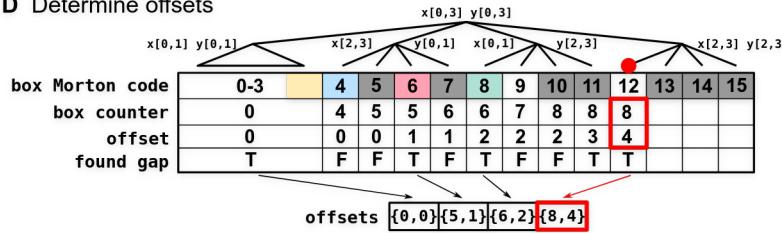
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**



# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g		j

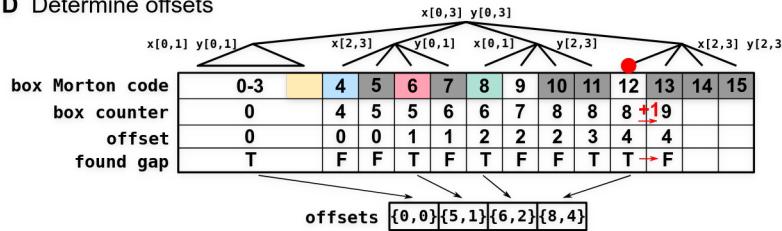
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**



# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

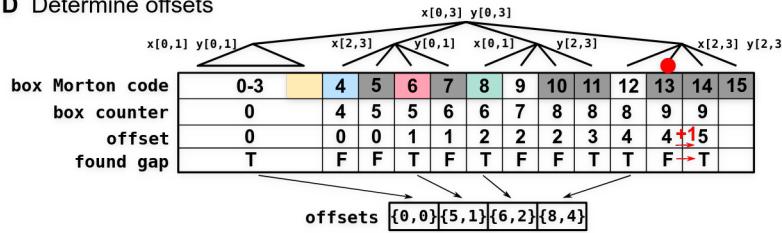
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

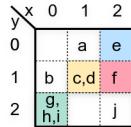
x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**

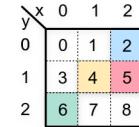


# Agent sorting and balancing

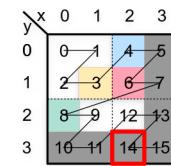
**A Agents in 3x3 grid**



**B Grid box indices**



**C Morton order of 4x4 grid**



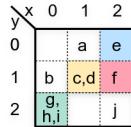
**D Determine offsets**

	x[0,3] y[0,3]												
	x[0,1]	y[0,1]	x[2,3]	y[0,1]	x[0,1]	y[2,3]	x[2,3]	y[2,3]					
box Morton code	0-3		4	5	6	7	8	9	10	11	12	13	14
box counter	0		4	5	5	6	6	7	8	8	8	9	9
offset	0		0	0	1	1	2	2	2	3	4	4	5+16
found gap	T		F	F	T	F	T	F	T	T	F	T	T

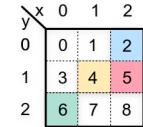
offsets {0,0}{5,1}{6,2}{8,4}

# Agent sorting and balancing

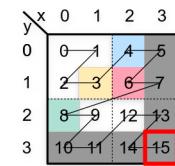
**A Agents in 3x3 grid**



**B Grid box indices**



**C Morton order of 4x4 grid**



**D Determine offsets**

	x[0,1] y[0,1]		x[2,3] y[0,1]		y[0,1] x[0,1]		y[2,3] x[2,3] y[2,3]	
box Morton code	0-3	4	5	6	7	8	9	10-15
box counter	0	4	5	5	6	6	7	8
offset	0	0	0	1	1	2	2	3
found gap	T	F	F	T	F	T	T	T

offsets {0,0}{5,1}{6,2}{8,4}

# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

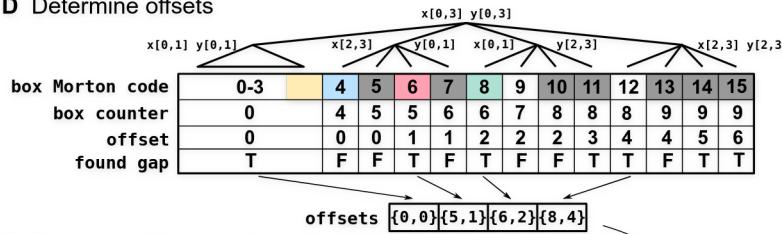
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**



**E Determine Morton order**

index	0	1	2	3	4	5	6	7	8
+ offsets				0		1	2	4	
= Morton order	0	1	2	3	4	6	8	9	12

# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

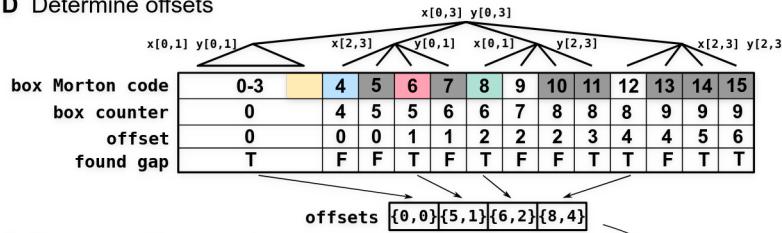
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**

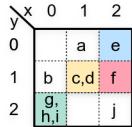


**E Determine Morton order**

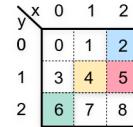
index	0	1	2	3	4	5	6	7	8
+ offsets					0		1	2	4
$= \text{Morton order}$									
0 1 2 3 4 6 8 9 12									

# Agent sorting and balancing

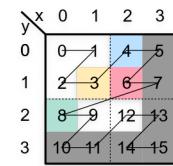
**A Agents in 3x3 grid**



**B Grid box indices**



**C Morton order of 4x4 grid**



**D Determine offsets**

		x[0,3] y[0,3]												
		x[0,1]	y[0,1]	x[2,3]	y[0,1]	x[0,1]	y[2,3]	x[2,3]	y[2,3]					
box	Morton code	0-3	4	5	6	7	8	9	10	11	12	13	14	15
box	counter	0	4	5	5	6	6	7	8	8	8	9	9	9
	offset	0	0	0	1	1	2	2	2	3	4	4	5	6
	found gap	T	F	F	T	F	T	F	T	T	F	T	T	

offsets {0,0}{5,1}{6,2}{8,4}

**E Determine Morton order**

index	0	1	2	3	4	5	6	7	8
+ offsets				0		1	2	4	
<b>= Morton order</b>									
0 1 2 3 4 6 8 9 12									

# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g		j

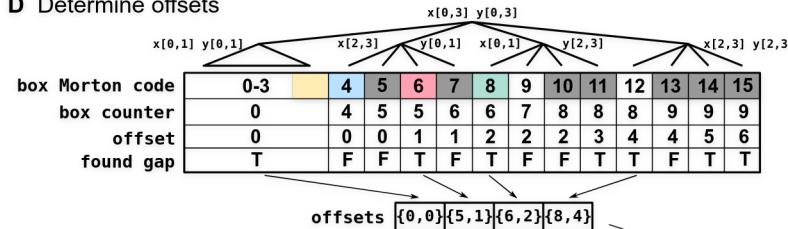
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**



**E Determine Morton order**

index	0	1	2	3	4	5	6	7	8
+ offsets				0		1	2	4	
<b>= Morton order</b>									
0 1 2 3 4 6 8 9 12									

# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g		j

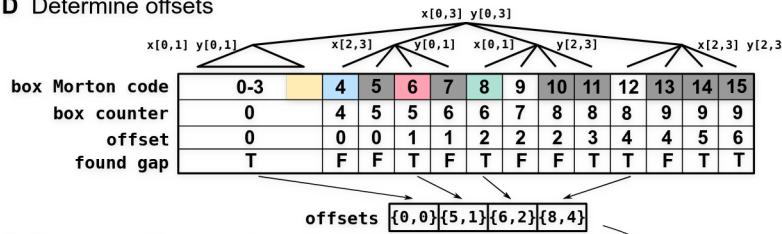
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**



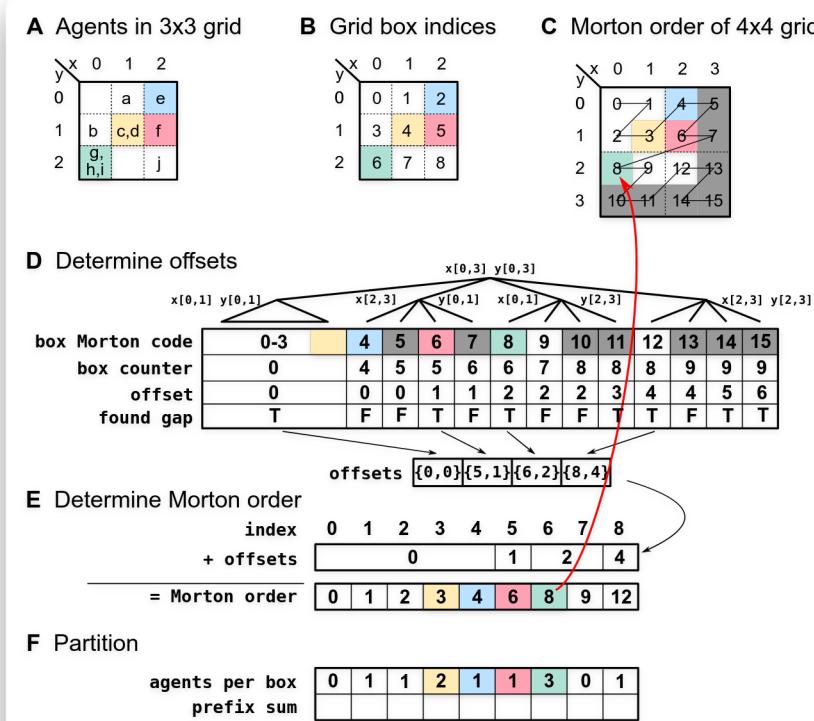
**E Determine Morton order**

index	0	1	2	3	4	5	6	7	8
+ offsets				0		1	2	4	
= Morton order	0	1	2	3	4	6	8	9	12

**F Partition**

agents per box	0	1	1	2	1	1	3	0	1
prefix sum									

# Agent sorting and balancing



# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g		j

**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**

	x[0,3] y[0,3]						
	x[0,1]	y[0,1]	x[2,3]	y[0,1]	x[0,1]	y[2,3]	
box Morton code	0-3	4	5	6	7	8	9 10 11 12 13 14 15
box counter	0	4	5	5	6	6	7 8 8 8 9 9 9
offset	0	0	0	1	1	2	2 2 3 4 4 4 5 6
found gap	T	F	F	T	F	T	T F T T T T

offsets {0,0}{5,1}{6,2}{8,4}

**E Determine Morton order**

index	0	1	2	3	4	5	6	7	8
+ offsets				0		1	2	4	
= Morton order	0	1	2	3	4	6	8	9	12

**F Partition**

agents per box	0	1	1	2	1	1	3	0	1
prefix sum									

# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,i		j

**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**

	x[0,3]	y[0,3]							
x[0,1]	0-3		x[2,3]	y[0,1]	x[0,1]	y[2,3]			
box Morton code	0-3	4	5	6	7	8	9	10	11
box counter	0	4	5	5	6	6	7	8	8
offset	0	0	0	1	1	2	2	2	3
found gap	T	F	F	T	F	T	F	T	T

offsets {0,0}{5,1}{6,2}{8,4}

**E Determine Morton order**

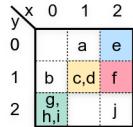
index	0	1	2	3	4	5	6	7	8
+ offsets	0		1	2	4				
= Morton order	0	1	2	3	4	6	8	9	12

**F Partition**

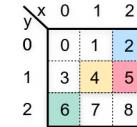
agents per box	0	1	1	2	1	1	3	0	1
prefix sum									

# Agent sorting and balancing

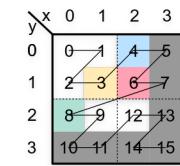
**A Agents in 3x3 grid**



**B Grid box indices**



**C Morton order of 4x4 grid**



**D Determine offsets**

		x[0,3] y[0,3]												
		x[0,1] y[0,1]	x[2,3]	y[0,1]	x[0,1]	y[2,3]	x[2,3]	y[2,3]	x[2,3]	y[0,3]				
box	Morton code	0-3	4	5	6	7	8	9	10	11	12	13	14	15
box	counter	0	4	5	5	6	6	7	8	8	8	9	9	9
offset	0	0	0	1	1	2	2	2	3	4	4	5	6	
found gap	T	F	F	T	F	T	F	F	T	T	F	T	T	

→ offsets {0,0}{5,1}{6,2}{8,4}

**E Determine Morton order**

index	0	1	2	3	4	5	6	7	8
+ offsets					0	1	2	4	
$= \text{Morton order}$									
0 1 2 3 4 6 8 9 12									

**F Partition**

agents per box	0	1	1	2	1	1	3	0	1
prefix sum	0	1	2	4	5	6	9	9	10

# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g		j

**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**

		x[0,3] y[0,3]							
		x[0,1] y[0,1]	x[2,3]	y[0,1]	x[0,1]	y[2,3]	x[2,3]	y[2,3]	
box	Morton code	0-3	4	5	6	7	8	9	10-15
box	counter	0	4	5	5	6	6	7	8
offset		0	0	0	1	1	2	2	2
found gap		T	F	F	T	F	T	T	T

offsets {0,0}{5,1}{6,2}{8,4}

**E Determine Morton order**

index	0	1	2	3	4	5	6	7	8
+ offsets				0		1	2	4	
= Morton order	0	1	2	3	4	5	6	8	9 12

**F Partition**

agents per box	0	1	1	2	1	1	3	0	1
prefix sum	0	1	2	4	5	6	9	9	10

NUMA domain 0 ←→ NUMA domain 1

# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g,h,i		j

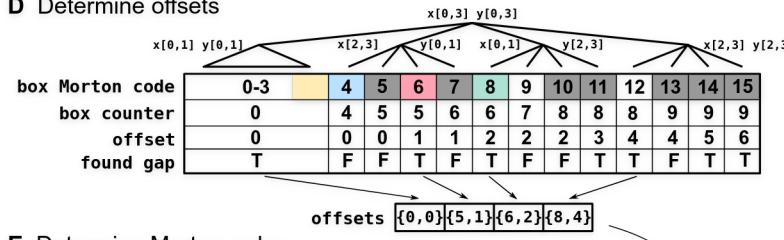
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**



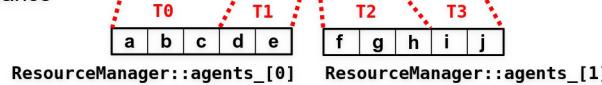
**E Determine Morton order**

index	0	1	2	3	4	5	6	7	8
+ offsets					0	1	2	4	
= Morton order	0	1	2	3	4	5	6	8	9 12

**F Partition**

agents per box	0	1	1	2	1	1	3	0	1
prefix sum	0	1	2	4	5	6	9	9	10

**G Sort and balance**



# Agent sorting and balancing

**A Agents in 3x3 grid**

x	0	1	2
0	a	e	
1	b	c,d	f
2	g		j

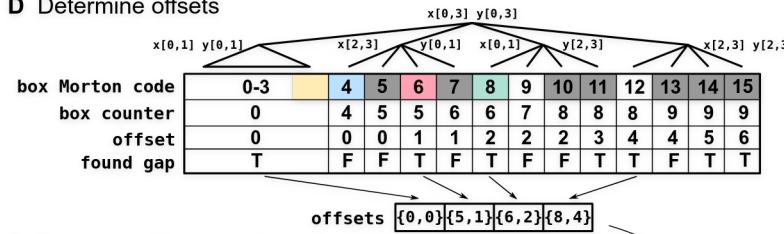
**B Grid box indices**

x	0	1	2
0	0	1	2
1	3	4	5
2	6	7	8

**C Morton order of 4x4 grid**

x	0	1	2	3
0	0	1	4	5
1	2	3	6	7
2	8	9	12	13
3	10	11	14	15

**D Determine offsets**



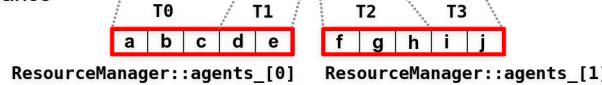
**E Determine Morton order**

index	0	1	2	3	4	5	6	7	8
+ offsets					0	1	2	4	
= Morton order	0	1	2	3	4	5	6	8	9 12

**F Partition**

agents per box	0	1	1	2	1	1	3	0	1
prefix sum	0	1	2	4	5	6	9	9	10

**G Sort and balance**



---

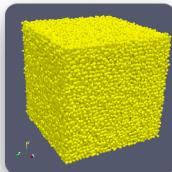
# Evaluation

# Benchmark hardware

System	Memory	CPU	OS
A	504 GB	Four Intel(R) Xeon(R) E7-8890 v3 CPUs @ 2.50GHz with a total of 72 physical cores, two threads per core and four NUMA domains.	CentOS
B	1008 GB		7.9.2009
C	62 GB	Two Intel(R) Xeon(R) E5-2683 v3 CPUs @ 2.00GHz with a total of 28 physical cores, two threads per core and two NUMA domains.	CentOS Stream 8

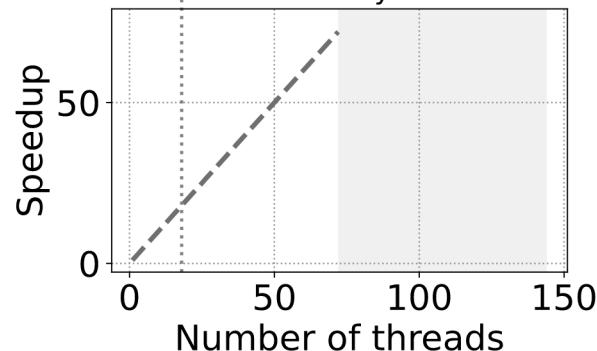
# BioDynaMo scales well across NUMA nodes & large CPU core counts

Cell proliferation simulation

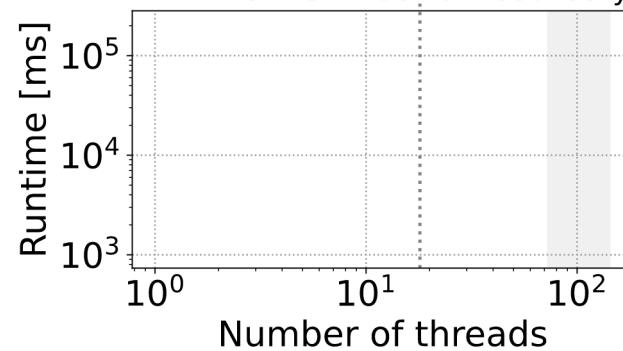


— Ideal speedup

First NUMA domain boundary

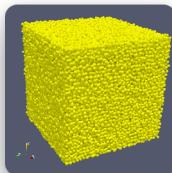


First NUMA domain boundary



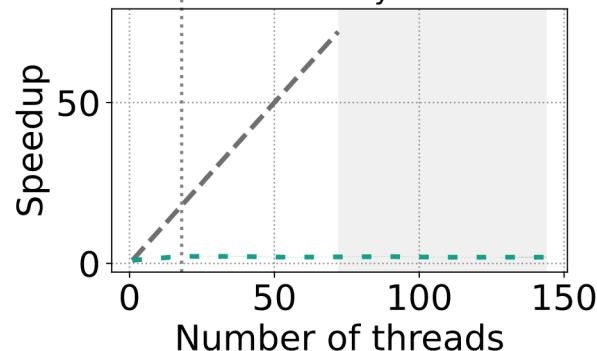
# BioDynaMo scales well across NUMA nodes & large CPU core counts

Cell proliferation simulation

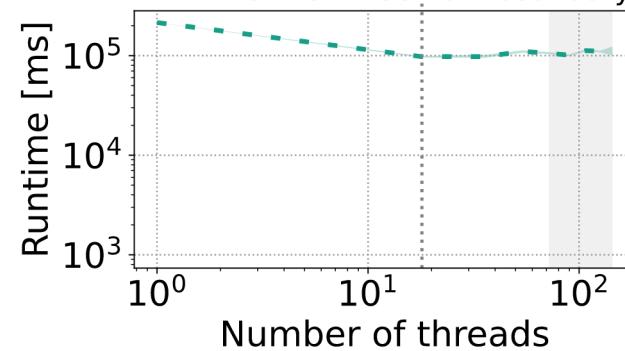


- Ideal speedup
- - BDM standard implementation

First NUMA domain boundary

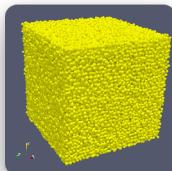


First NUMA domain boundary



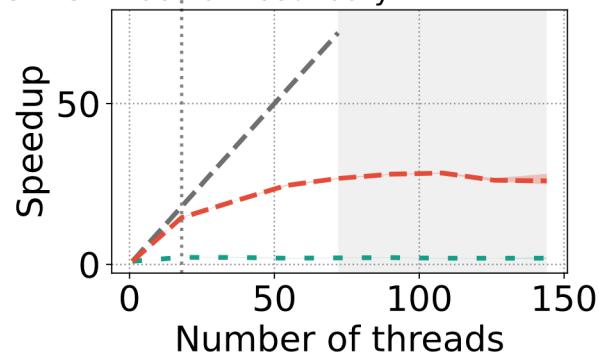
# BioDynaMo scales well across NUMA nodes & large CPU core counts

Cell proliferation simulation

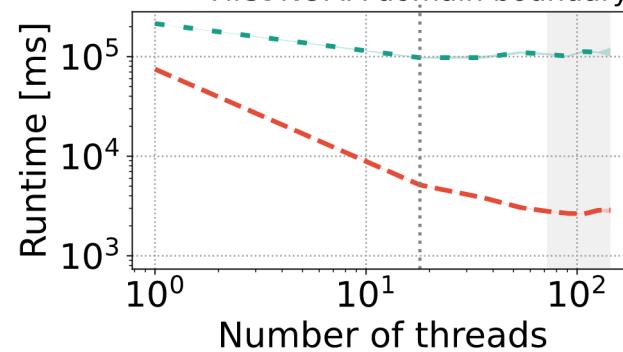


- Ideal speedup
- - BDM standard implementation
- - Plus BDM uniform grid

First NUMA domain boundary

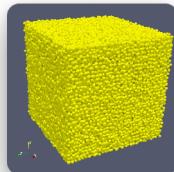


First NUMA domain boundary



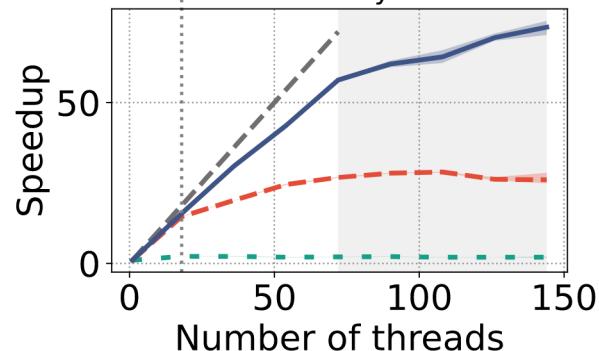
# BioDynaMo scales well across NUMA nodes & large CPU core counts

Cell proliferation simulation

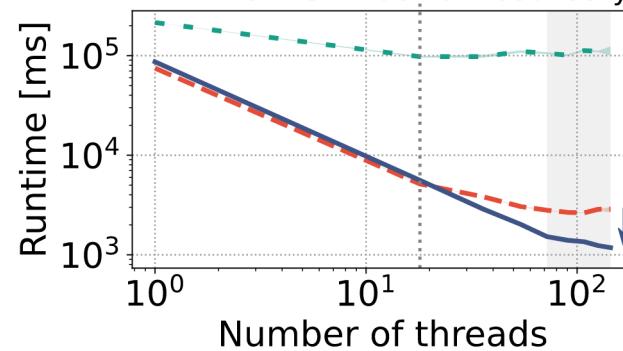


- Ideal speedup
- - BDM standard implementation
- - - Plus BDM uniform grid
- Plus memory improvements

First NUMA domain boundary

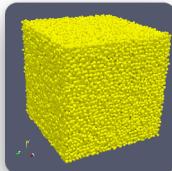


First NUMA domain boundary



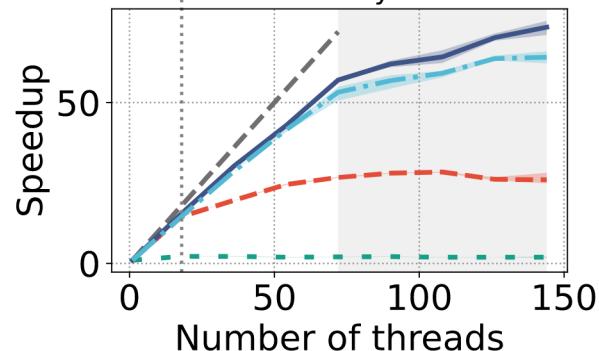
# BioDynaMo scales well across NUMA nodes & large CPU core counts

Cell proliferation simulation

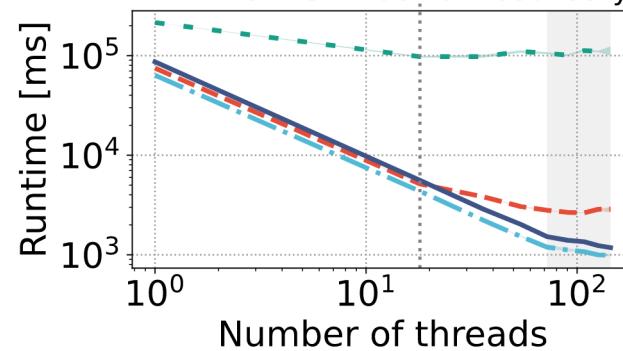


- Ideal speedup
- - BDM standard implementation
- - Plus BDM uniform grid
- Plus memory improvements
- - Plus extra memory

First NUMA domain boundary

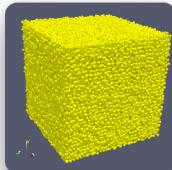


First NUMA domain boundary



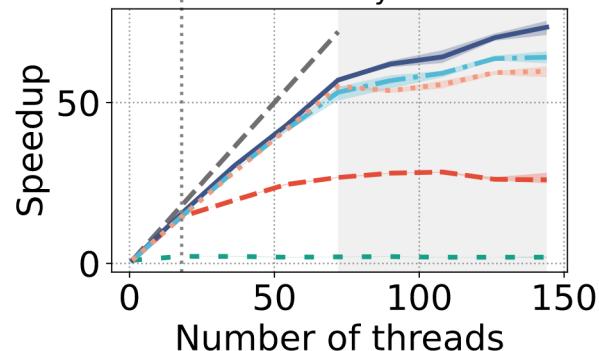
# BioDynaMo scales well across NUMA nodes & large CPU core counts

Cell proliferation simulation

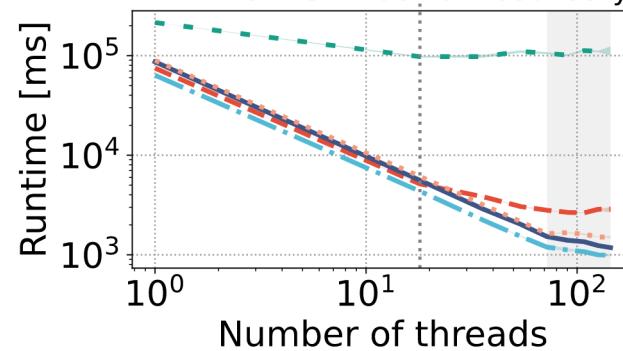


- Ideal speedup
- - BDM standard implementation
- - Plus BDM uniform grid
- Plus memory improvements
- - Plus extra memory
- - - Plus static agents detection

First NUMA domain boundary

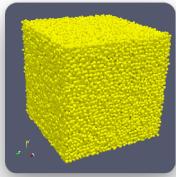


First NUMA domain boundary

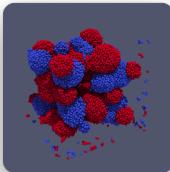


# BioDynaMo scales well across NUMA nodes & large CPU core counts

Cell proliferation simulation



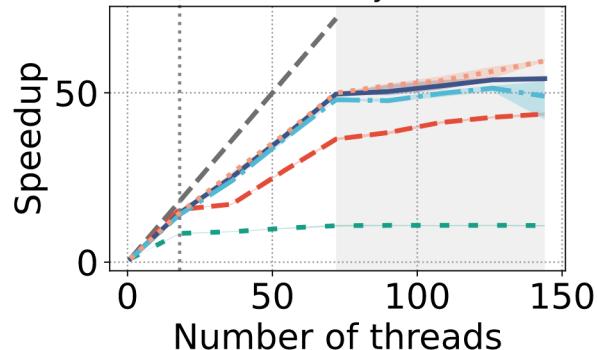
# Cell clustering benefits from BioDynaMo's memory optimizations for any number of CPU cores



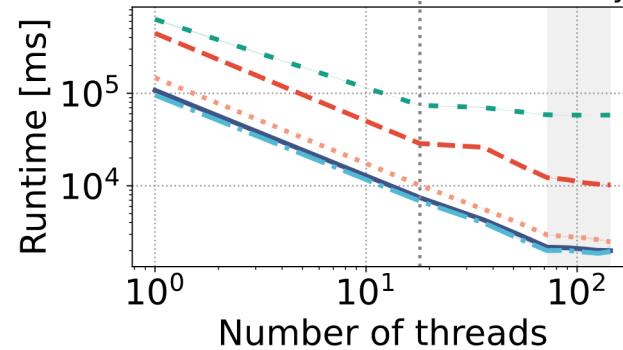
— Ideal speedup  
- - BDM standard implementation  
- - Plus BDM uniform grid

— Plus memory improvements  
— Plus extra memory  
- - Plus static agents detection

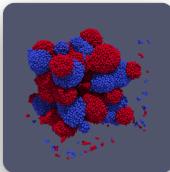
First NUMA domain boundary



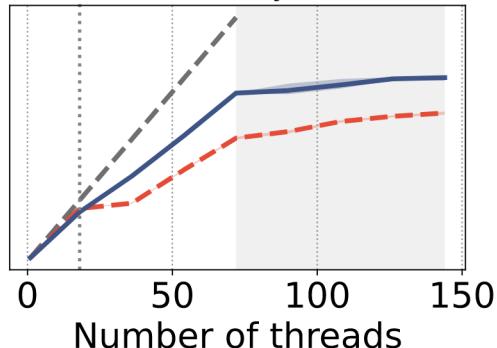
First NUMA domain boundary



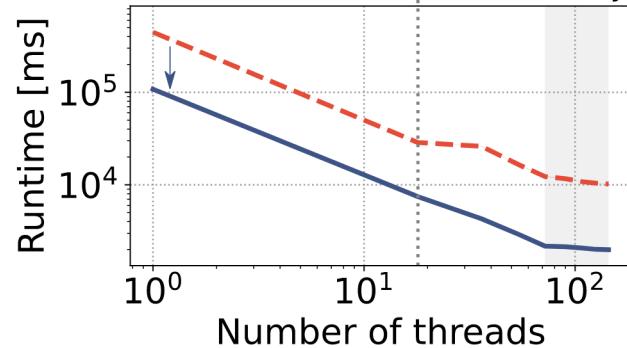
# Cell clustering benefits from BioDynaMo's memory optimizations for any number of CPU cores



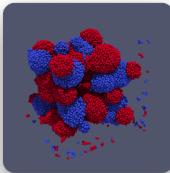
First NUMA domain boundary



First NUMA domain boundary

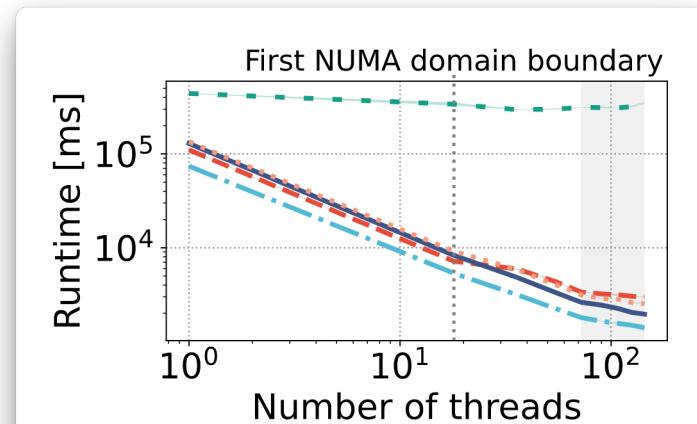
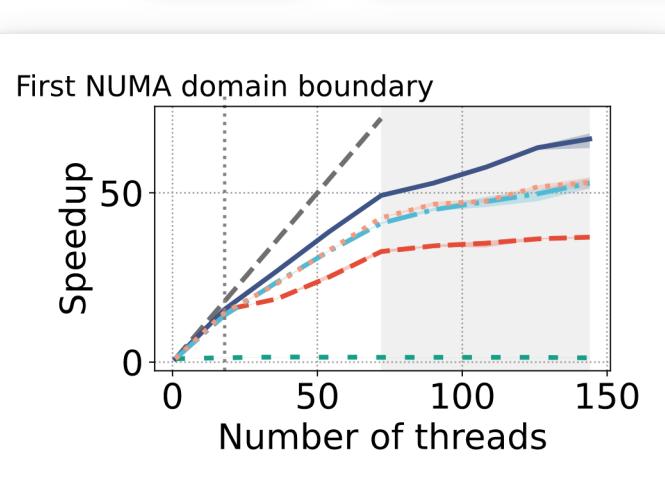
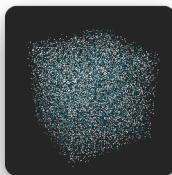


# Cell clustering benefits from BioDynaMo's memory optimizations for any number of CPU cores

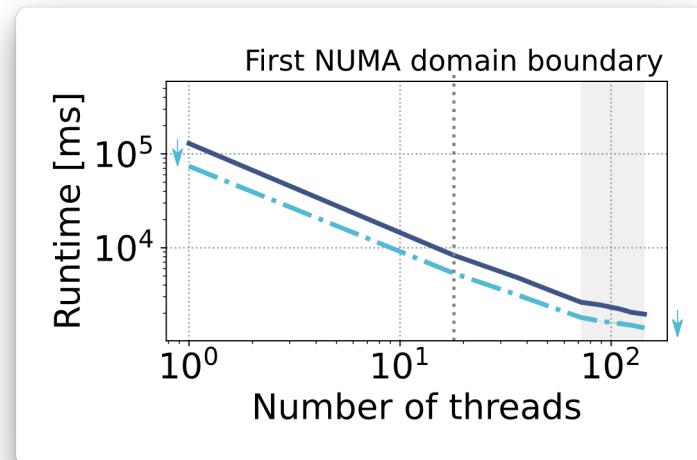
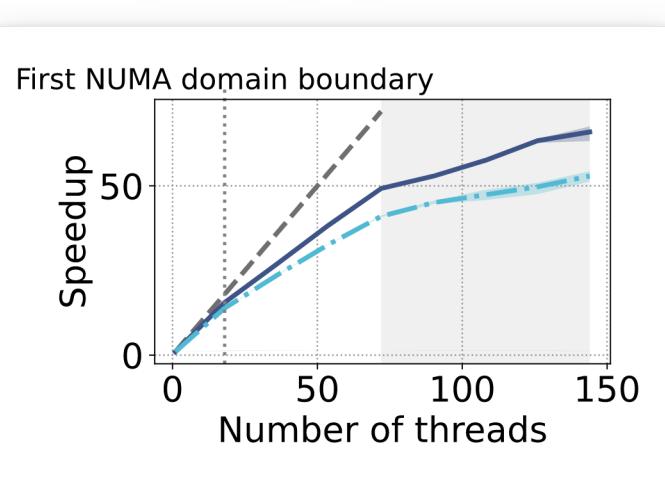


- Ideal speedup
- - BDM standard implementation
- - Plus BDM uniform grid
- Plus memory improvements
- Plus extra memory
- Plus static agents detection

# The epidemiology use case benefits from using additional memory



# The epidemiology use case benefits from using additional memory

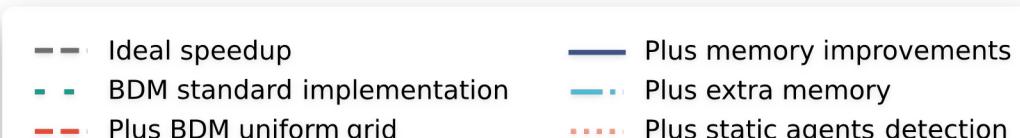


# The epidemiology use case benefits from using additional memory

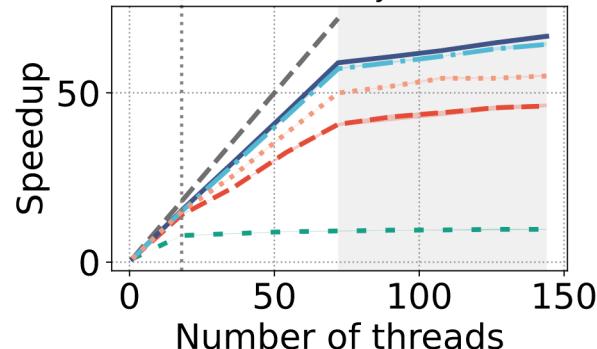


- Ideal speedup
- - BDM standard implementation
- - Plus BDM uniform grid
- Plus memory improvements
- Plus extra memory
- Plus static agents detection

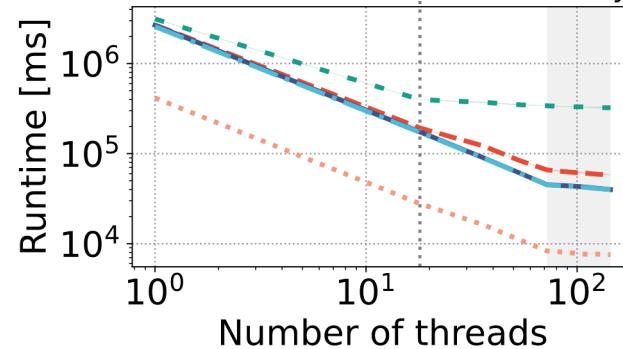
# The neuroscience use case benefits substantially from static region detection



First NUMA domain boundary



First NUMA domain boundary



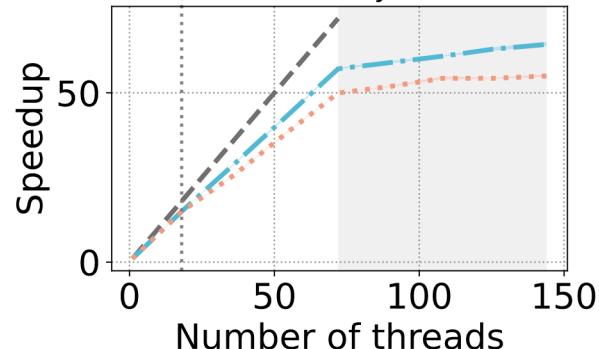
# The neuroscience use case benefits substantially from static region detection



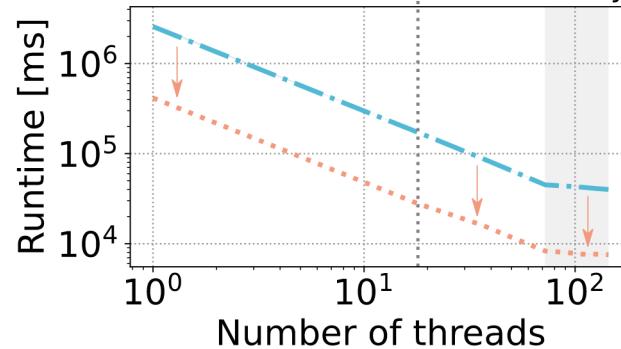
— Ideal speedup  
- - BDM standard implementation  
- - Plus BDM uniform grid

— Plus memory improvements  
- - Plus extra memory  
- - Plus static agents detection

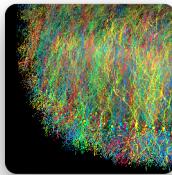
First NUMA domain boundary



First NUMA domain boundary



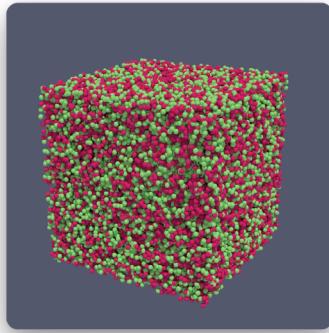
# The neuroscience use case benefits substantially from static region detection



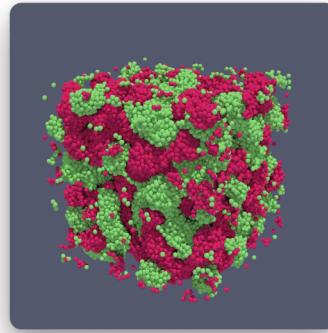
- Ideal speedup
- - BDM standard implementation
- - Plus BDM uniform grid
- Plus memory improvements
- Plus extra memory
- Plus static agents detection

# BioDynaMo is up to $9\times$ more efficient than Biocellion

We implement Biocellions cell clustering simulation in BioDynaMo



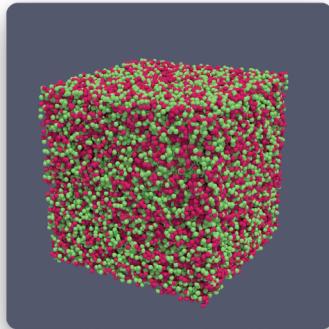
Initial state



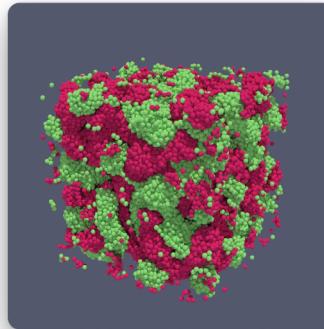
Final state

# BioDynaMo is up to $9\times$ more efficient than Biocellion

We implement Biocellions cell clustering simulation in BioDynaMo



Initial state

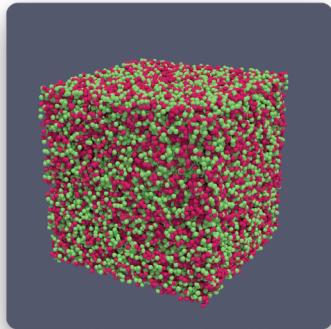


Final state

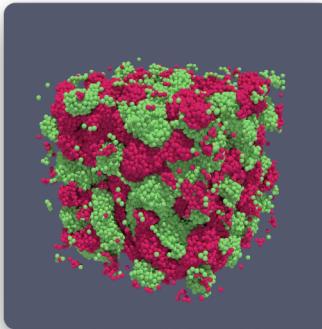
- Small-scale with **26.8 million** cells
  - 16 CPU cores (Biocellion & BioDynaMo)
  - Result: **BioDynaMo is  $4.2\times$  faster**

# BioDynaMo is up to $9\times$ more efficient than Biocellion

We implement Biocellions cell clustering simulation in BioDynaMo



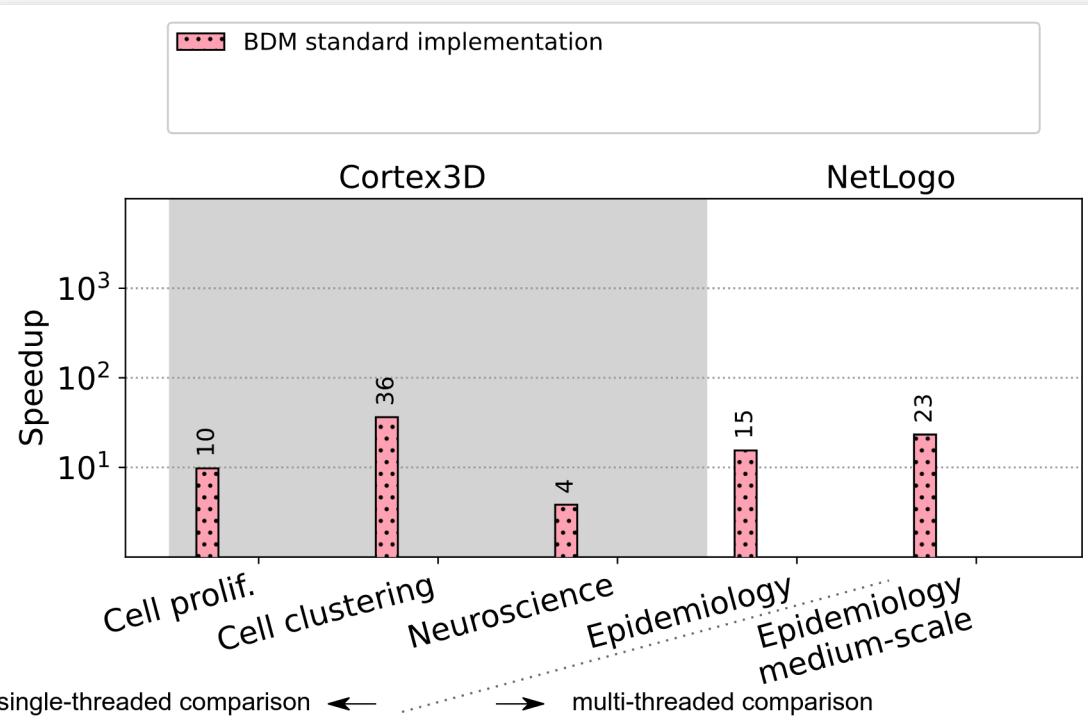
Initial state



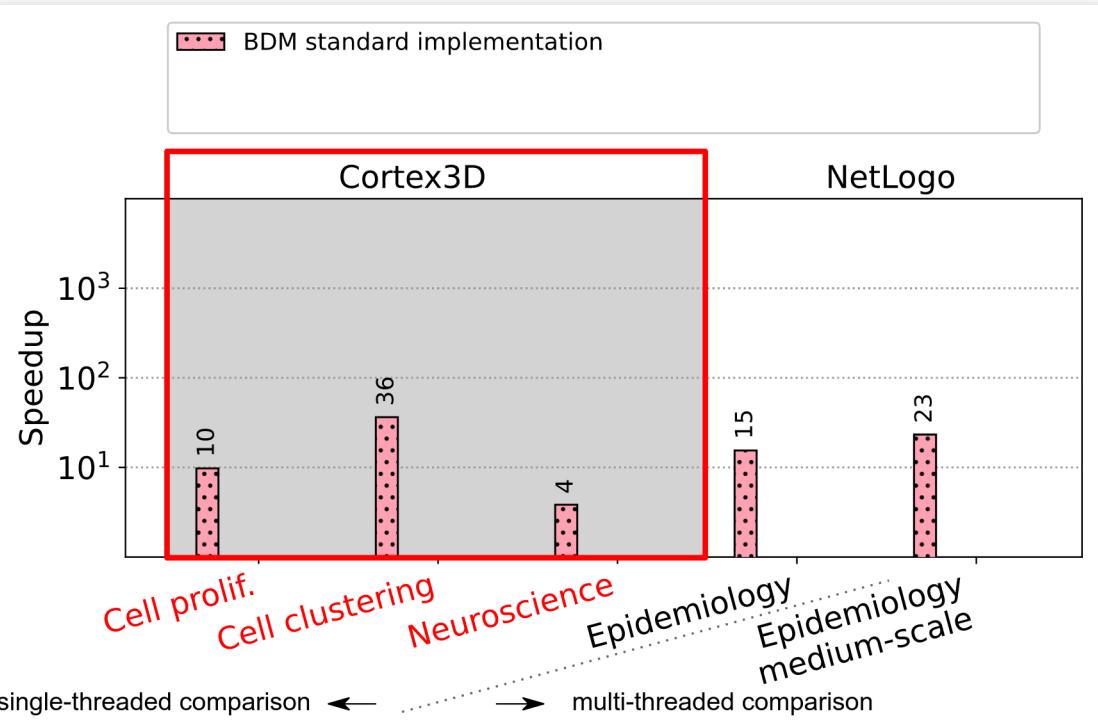
Final state

- Small-scale with **26.8 million cells**
  - 16 CPU cores (Biocellion & BioDynaMo)
  - Result: **BioDynaMo is  $4.2\times$  faster**
- Large-scale with 281 million cells
  - Biocellion: 21 nodes with 672 CPU cores
  - BioDynaMo: 1 node with 72 CPU cores
  - Result: same runtime, but BioDynaMo uses  **$9.3\times$  fewer CPU cores**

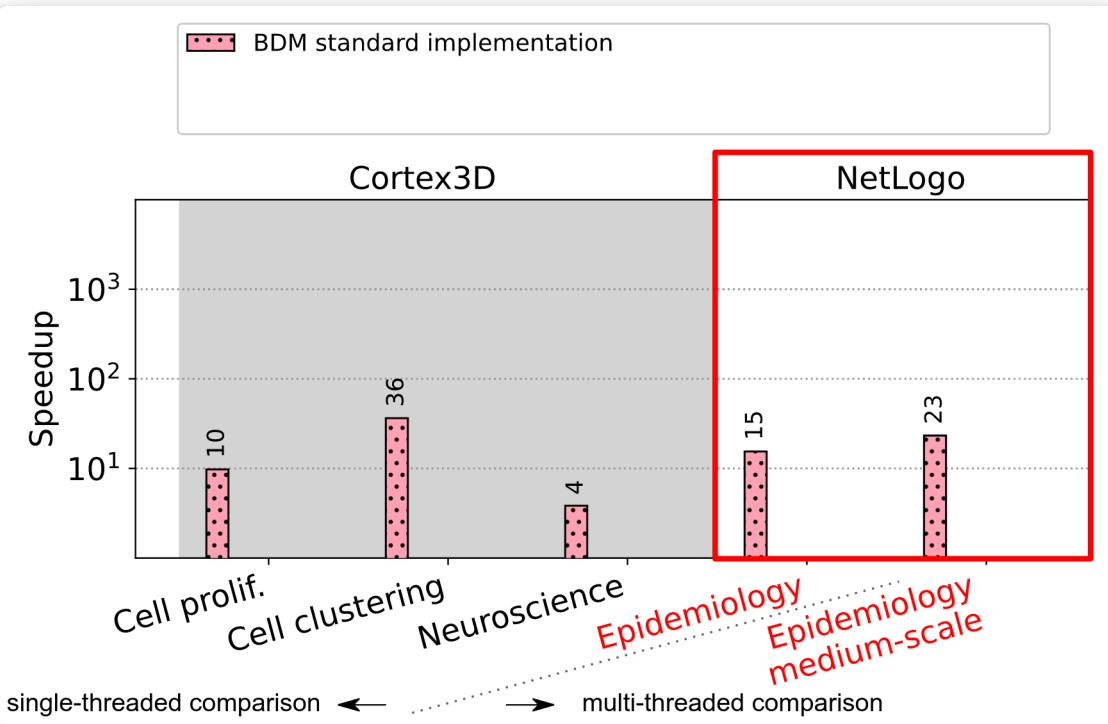
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



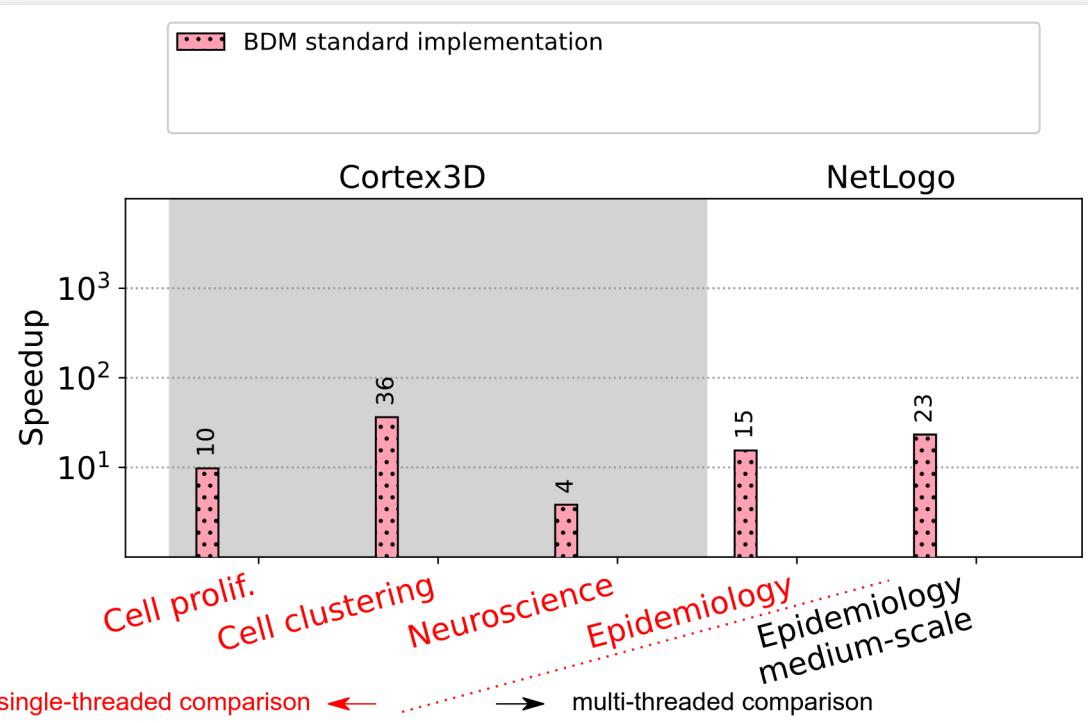
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



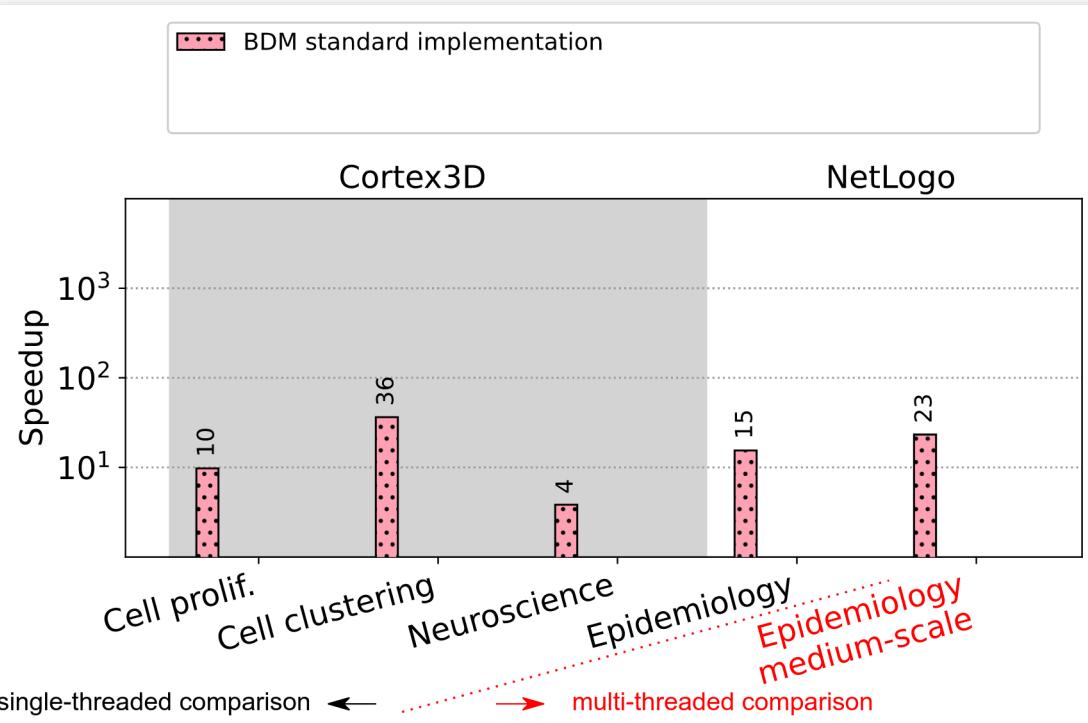
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



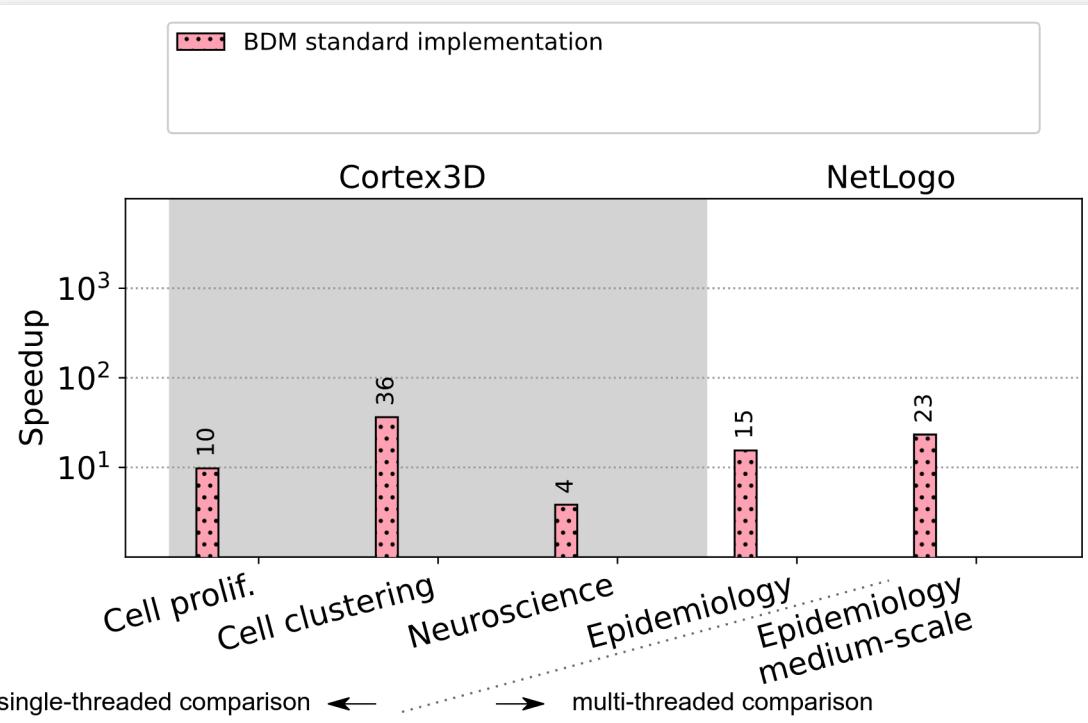
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



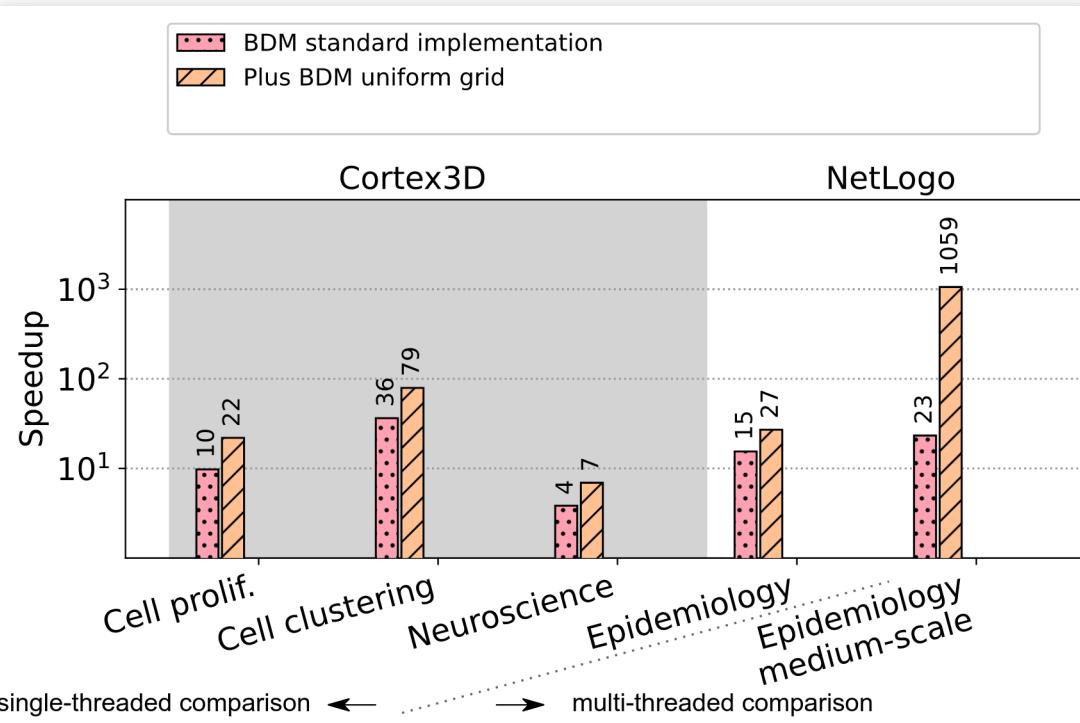
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



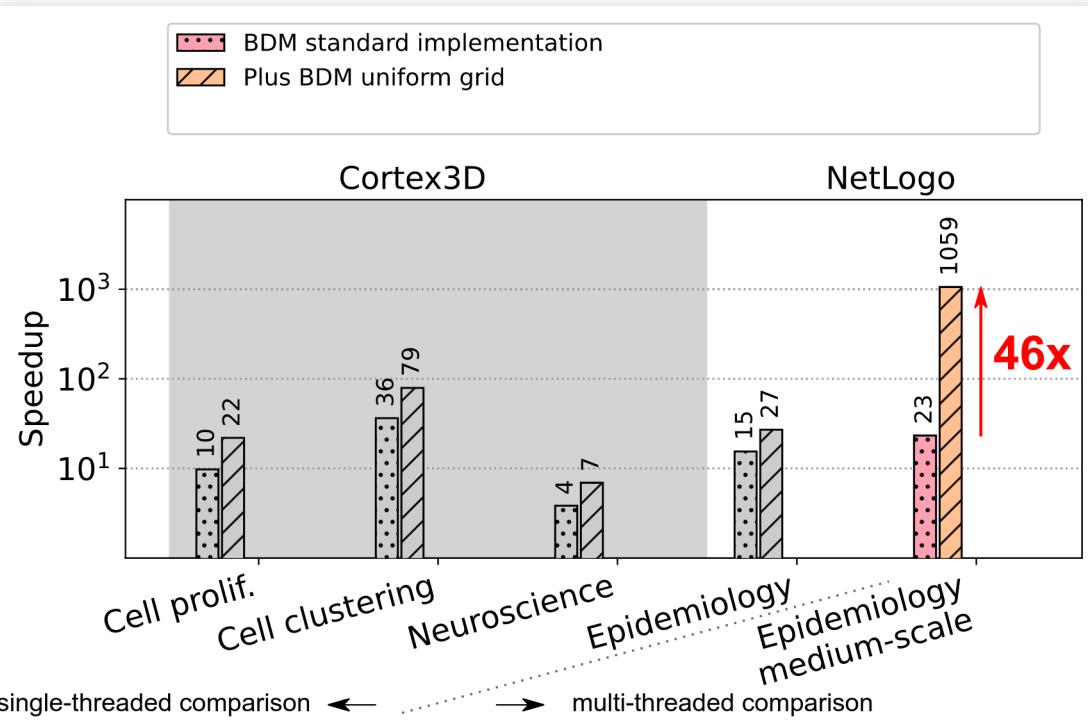
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



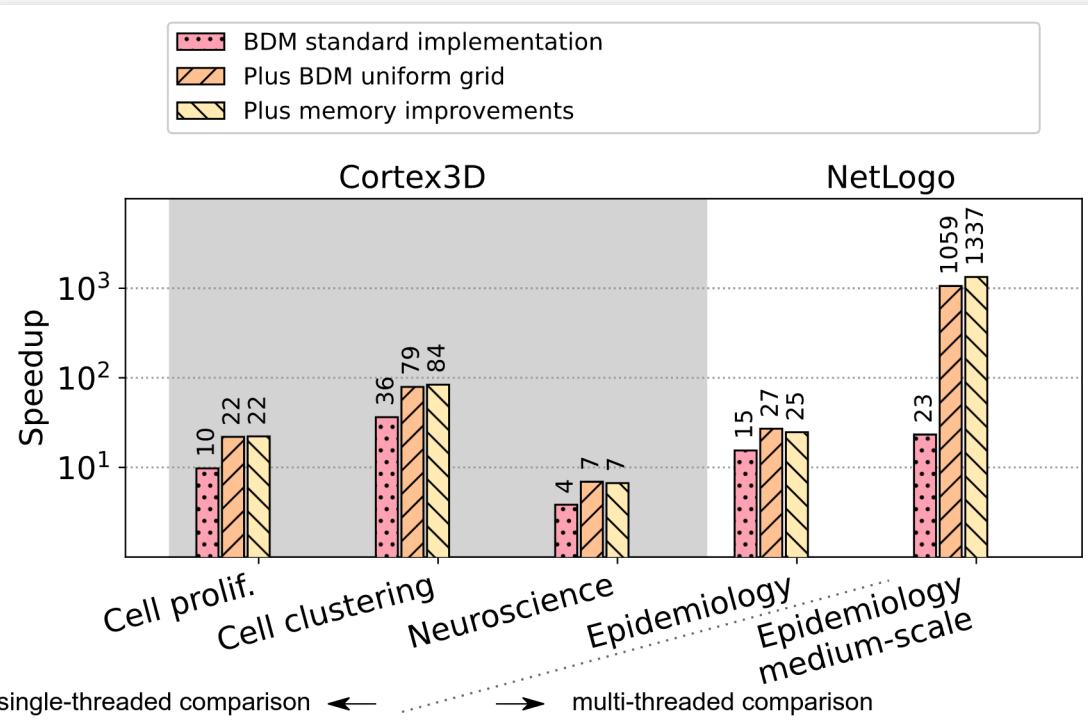
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



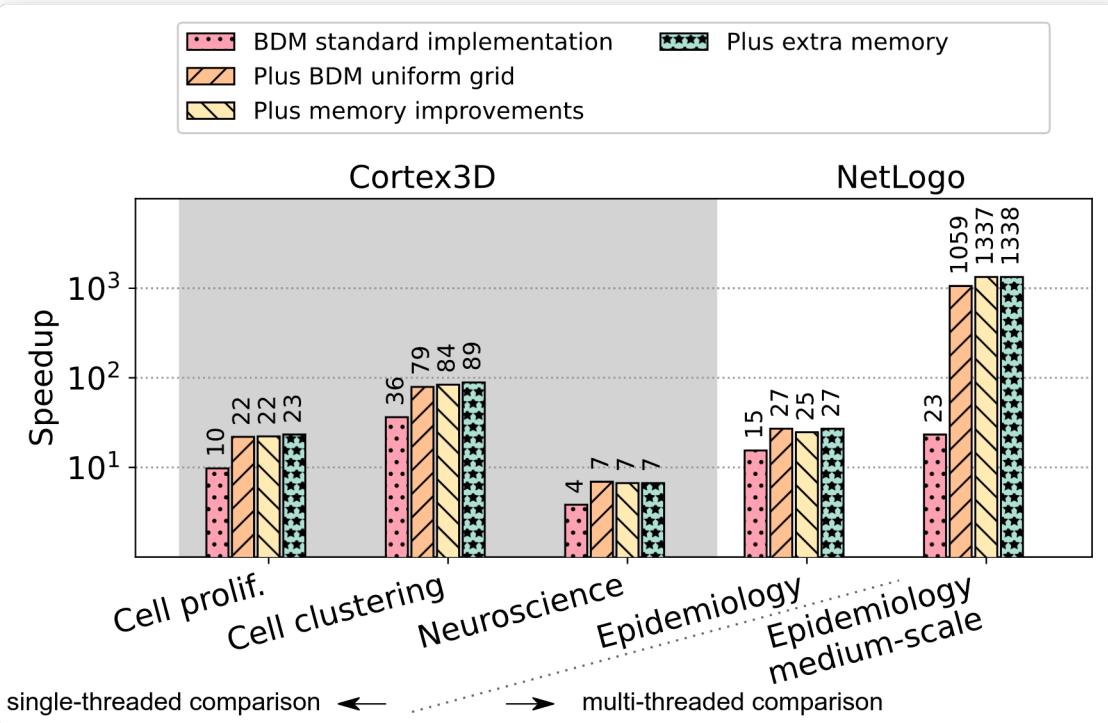
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



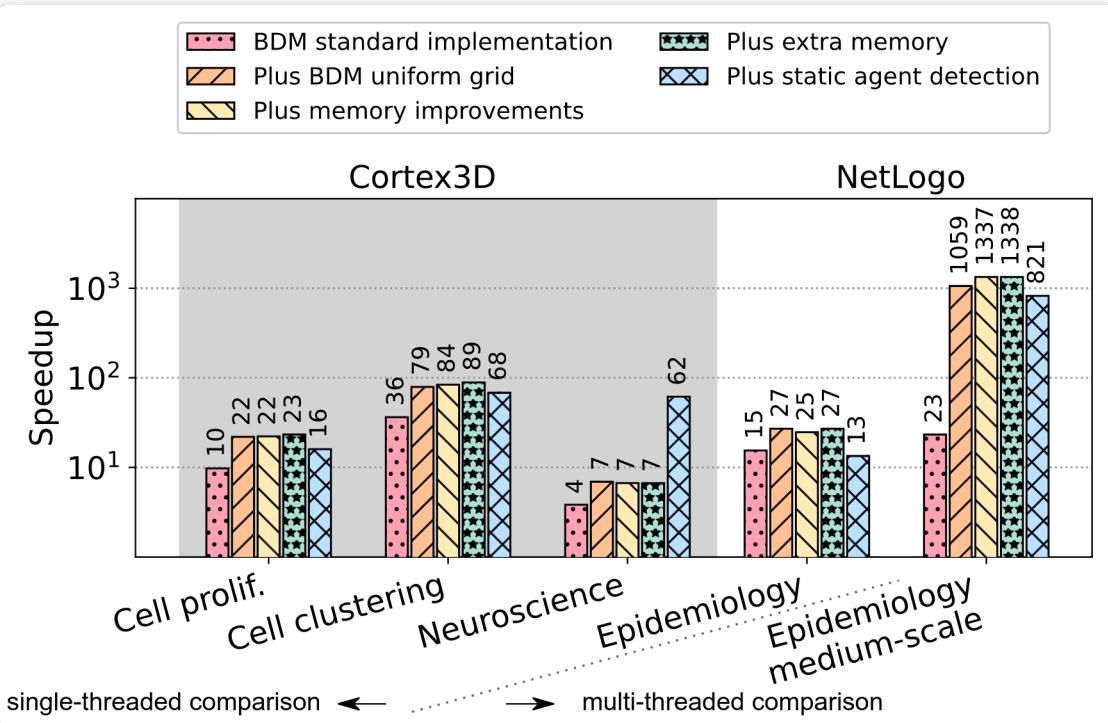
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



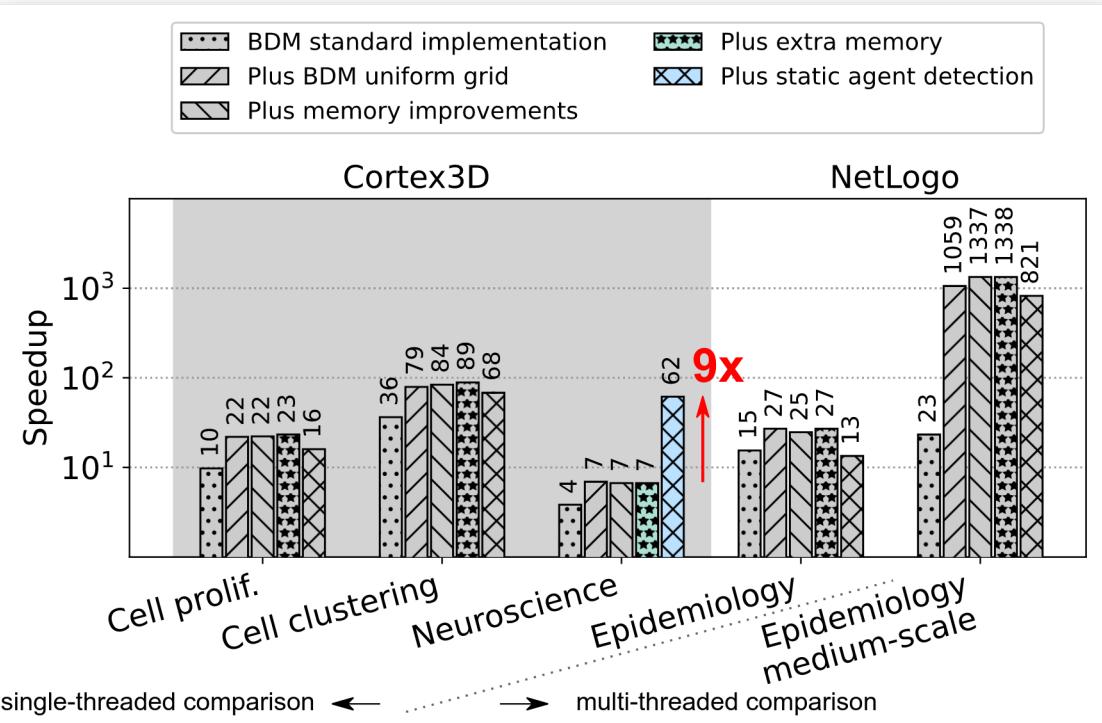
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



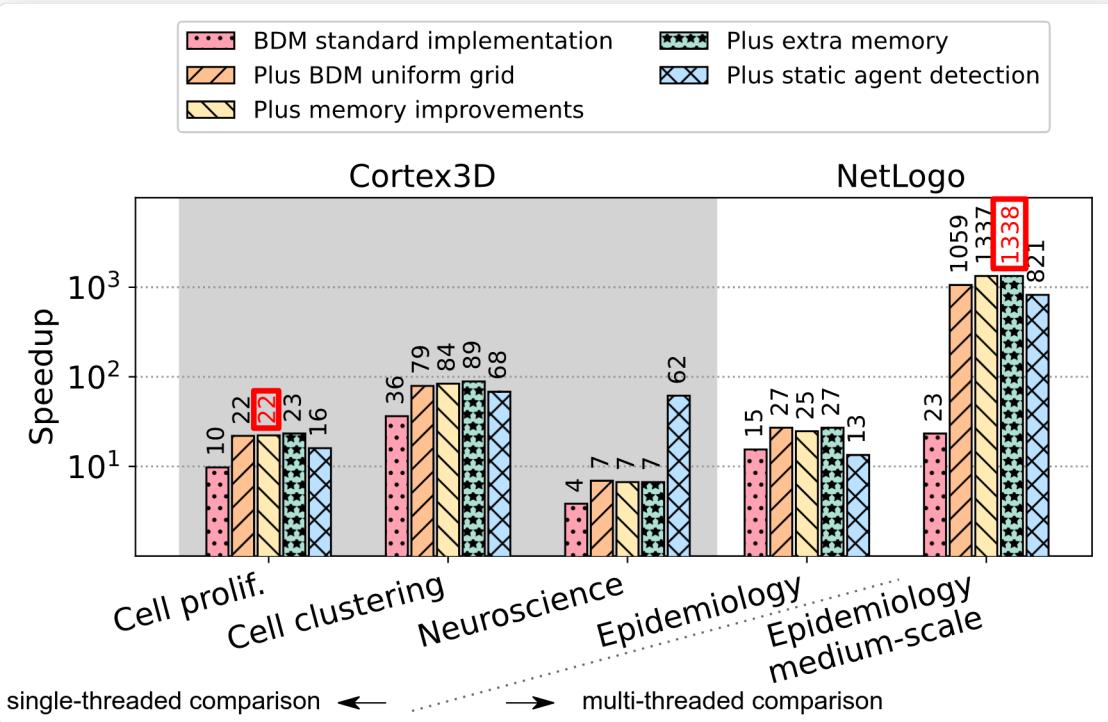
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



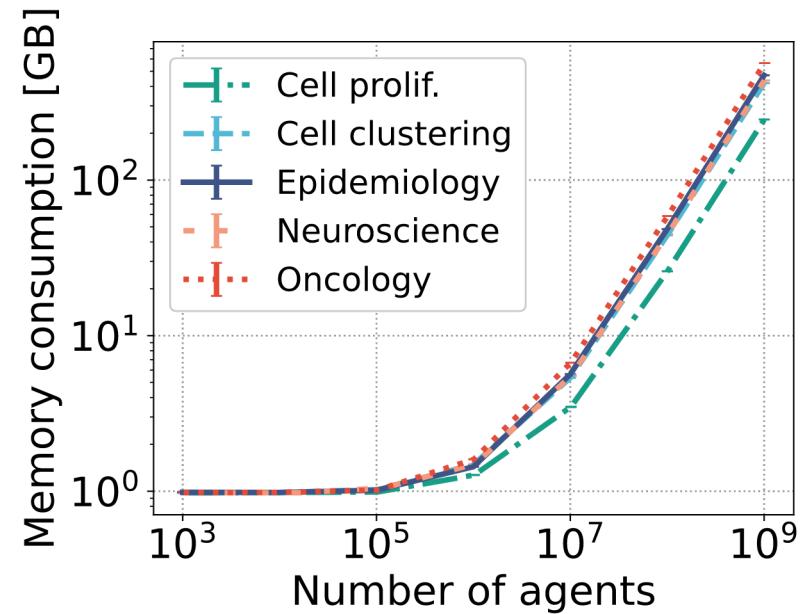
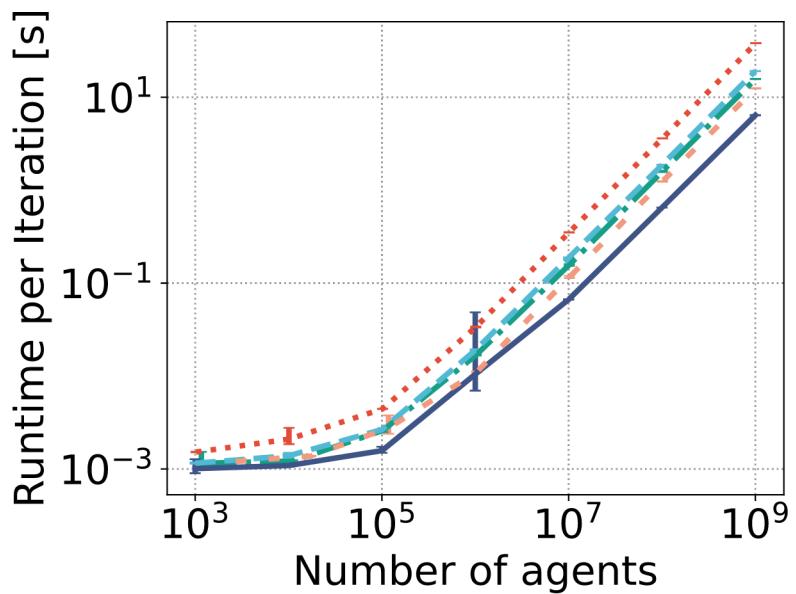
# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



# BioDynaMo is $1000\times$ faster than Cortex3D and NetLogo



# BioDynaMo's runtime and memory consumption increases linearly with model size



# More in the paper

<https://arxiv.org/abs/2301.06984>, <https://doi.org/10.1145/3572848.3577480>



## High-Performance and Scalable Agent-Based Simulation with BioDynaMo

Lukas Breitwieser\*

CERN, Switzerland

ETH Zurich, Switzerland

Ahmad Hesam

Delft University of Technology,

The Netherlands

Fons Rademakers

CERN, Switzerland

Juan Gómez Luna

ETH Zurich, Switzerland

Onur Mutlu†

ETH Zurich, Switzerland

### Abstract

Agent-based modeling plays an essential role in gaining insights into biology, sociology, economics, and other fields. However, many existing agent-based simulation platforms are not suitable for large-scale studies due to the low performance of the underlying simulation engines. To overcome this limitation, we present a novel high-performance simulation engine.

We identify three key challenges for which we present the following solutions. First, to maximize parallelization, we present an optimized grid to search for neighbors and parallelize the merging of thread-local results. Second, we reduce

### 1 Introduction

Agent-based modeling (ABM) allows to simulate complex dynamics in a wide range of research fields. ABM has been used to answer research questions in biology [30, 43, 73], sociology [18], economics [65], technology [50], business [56], and more fields [39]. Agents are individual entities that, among others, can represent subcellular structures to simulate the growth of a neuron, a cell to investigate cancer development, or a person to simulate the spread of infectious diseases [10]. The actions of an agent are defined through instances of class *behavior*. To stay with the examples from before, possible behaviors are neurite bifurcation, uncontrolled cell division, migration, etc.

# Supplementary Materials

Provides additional evaluations and all files required to reproduce the results (  ):

- <https://doi.org/10.5281/zenodo.6463816>
- <https://github.com/CMU-SAFARI/BioDynaMo>

# Supplementary Materials

Provides additional evaluations and all files required to reproduce the results (    ):

- <https://doi.org/10.5281/zenodo.6463816>
- <https://github.com/CMU-SAFARI/BioDynaMo>

```
1 # extract the provided code archive
2 mkdir reproduce
3 tar -xzf <path>/SF2-code.tar.gz -c reproduce
4 cd reproduce/bdm-paper-examples
5
6 # load the provided self-contained docker image
7 docker/load.sh <path>/SF3-bdm-publication-image.tar.gz
8
9 # execute the scripts
10 docker/run.sh ./run-main.sh
```

# Supplementary Materials

Provides additional evaluations and all files required to reproduce the results (    ):

- <https://doi.org/10.5281/zenodo.6463816>
- <https://github.com/CMU-SAFARI/BioDynaMo>

```
1 # extract the provided code archive
2 mkdir reproduce
3 tar -xzf <path>/SF2-code.tar.gz -c reproduce
4 cd reproduce/bdm-paper-examples
5
6 # load the provided self-contained docker image
7 docker/load.sh <path>/SF3-bdm-publication-image.tar.gz
8
9 # execute the scripts
10 docker/run.sh ./run-main.sh
```

# Supplementary Materials

Provides **additional evaluations** and all files required to **reproduce** the results (    ):

- <https://doi.org/10.5281/zenodo.6463816>
- <https://github.com/CMU-SAFARI/BioDynaMo>

```
1 # extract the provided code archive
2 mkdir reproduce
3 tar -xzf <path>/SF2-code.tar.gz -C reproduce
4 cd reproduce/bdm-paper-examples
5
6 # load the provided self-contained docker image
7 docker/load.sh <path>/SF3-bdm-publication-image.tar.gz
8
9 # execute the scripts
10 docker/run.sh ./run-main.sh
```

# Supplementary Materials

Provides additional evaluations and all files required to reproduce the results (    ):

- <https://doi.org/10.5281/zenodo.6463816>
- <https://github.com/CMU-SAFARI/BioDynaMo>

```
1 # extract the provided code archive
2 mkdir reproduce
3 tar -xzf <path>/SF2-code.tar.gz -C reproduce
4 cd reproduce/bdm-paper-examples
5
6 # load the provided self-contained docker image
7 docker/load.sh <path>/SF3-bdm-publication-image.tar.gz
8
9 # execute the scripts
10 docker/run.sh ./run-main.sh
```

# Supplementary Materials

Provides additional evaluations and all files required to reproduce the results (    ):

- <https://doi.org/10.5281/zenodo.6463816>
- <https://github.com/CMU-SAFARI/BioDynaMo>

```
1 # extract the provided code archive
2 mkdir reproduce
3 tar -xzf <path>/SF2-code.tar.gz -C reproduce
4 cd reproduce/bdm-paper-examples
5
6 # load the provided self-contained docker image
7 docker/load.sh <path>/SF3-bdm-publication-image.tar.gz
8
9 # execute the scripts
10 docker/run.sh ./run-main.sh
```

More details in file SF1-readme.pdf →

Instructions to Reproduce the Results in the Paper:  
High-Performance and Scalable Agent-Based Simulation  
with BioDynaMo

Lukas Breitwieser      Ahmad Hesam      Fons Rademakers  
Juan Gómez Luna      Onur Muthu

## Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
<b>2</b>	<b>Getting started</b>	<b>3</b>
2.1	Extract code repositories . . . . .	3
2.2	Install host machine prerequisites . . . . .	3
2.3	Load Docker image . . . . .	4
2.4	Verify successful setup . . . . .	4
<b>3</b>	<b>Documentation</b>	<b>5</b>
3.1	The bdm-paper-examples repository . . . . .	5
3.2	Mapping between simulation names in the paper and bdm-paper-examples . . . . .	5
3.3	Docker image . . . . .	6
3.4	Important information . . . . .	6
3.5	Result directory structure . . . . .	6
3.6	Long execution time . . . . .	7
<b>4</b>	<b>Reproducing results</b>	<b>8</b>
4.1	Main results (Figure 5 (left) and 9–12 in the paper) . . . . .	8
4.2	Comparison with Cortex3D and NetLogo (Figure 8 in the paper) . . . . .	10
4.3	Runtime and space complexity (Figure 6 in the paper) . . . . .	11
4.4	Workload profiling (Figure 5 (right) in the paper) . . . . .	12
4.5	Biocellion comparison small (Figure 7 in the paper) . . . . .	13
4.6	Biocellion comparison large (Figure 7 in the paper) . . . . .	14
<b>5</b>	<b>Reusing and repurposing this artifact</b>	<b>15</b>
5.1	Add additional benchmarks . . . . .	15
5.2	Evaluate the effectiveness of additional optimizations . . . . .	17
5.3	Evaluate BioDynaMo’s performance for additional simulations . . . . .	17
<b>6</b>	<b>Contact</b>	<b>18</b>

# Supplementary Materials

Provides additional evaluations and all files required to reproduce the results (    ):

- <https://doi.org/10.5281/zenodo.6463816>
- <https://github.com/CMU-SAFARI/BioDynaMo>

```
1 # extract the provided code archive
2 mkdir reproduce
3 tar -xzf <path>/SF2-code.tar.gz -C reproduce
4 cd reproduce/bdm-paper-examples
5
6 # load the provided self-contained docker image
7 docker/load.sh <path>/SF3-bdm-publication-image.tar.gz
8
9 # execute the scripts
10 docker/run.sh ./run-main.sh
```

More details in file SF1-readme.pdf →



Instructions to Reproduce the Results in the Paper:  
High-Performance and Scalable Agent-Based Simulation  
with BioDynaMo

Lukas Breitwieser   Ahmad Hesam   Fons Rademakers  
Juan Gómez Luna   Onur Muthu

## Contents

<b>1</b>	<b>Introduction</b>	<b>2</b>
<b>2</b>	<b>Getting started</b>	<b>3</b>
2.1	Extract code repositories . . . . .	3
2.2	Install host machine prerequisites . . . . .	3
2.3	Load Docker image . . . . .	4
2.4	Verify successful setup . . . . .	4
<b>3</b>	<b>Documentation</b>	<b>5</b>
3.1	The bdm-paper-examples repository . . . . .	5
3.2	Mapping between simulation names in the paper and bdm-paper-examples . . . . .	5
3.3	Docker image . . . . .	6
3.4	Important information . . . . .	6
3.5	Result directory structure . . . . .	6
3.6	Long execution time . . . . .	7
<b>4</b>	<b>Reproducing results</b>	<b>8</b>
4.1	Main results (Figure 5 (left) and 9–12 in the paper) . . . . .	8
4.2	Comparison with Cortex3D and NetLogo (Figure 8 in the paper) . . . . .	10
4.3	Runtime and space complexity (Figure 6 in the paper) . . . . .	11
4.4	Workload profiling (Figure 5 (right) in the paper) . . . . .	12
4.5	Biocellion comparison small (Figure 7 in the paper) . . . . .	13
4.6	Biocellion comparison large (Figure 7 in the paper) . . . . .	14
<b>5</b>	<b>Reusing and repurposing this artifact</b>	<b>15</b>
5.1	Add additional benchmarks . . . . .	15
5.2	Evaluate the effectiveness of additional optimizations . . . . .	17
5.3	Evaluate BioDynaMo’s performance for additional simulations . . . . .	17
<b>6</b>	<b>Contact</b>	<b>18</b>

# Summary

Our optimizations to maximize parallelism, improve the memory layout, and avoid unnecessary work are effective and give BioDynaMo the following performance characteristics.

# Summary

Our optimizations to maximize parallelism, improve the memory layout, and avoid unnecessary work are effective and give BioDynaMo the following performance characteristics.

**BioDynaMo scales well** across a large number of CPU cores

# Summary

Our optimizations to maximize parallelism, improve the memory layout, and avoid unnecessary work are effective and give BioDynaMo the following performance characteristics.

BioDynaMo scales well across a large number of CPU cores

Runtime and memory consumption increases linearly with the number of agents

# Summary

Our optimizations to maximize parallelism, improve the memory layout, and avoid unnecessary work are effective and give BioDynaMo the following performance characteristics.

BioDynaMo scales well across a large number of CPU cores

Runtime and memory consumption increases linearly with the number of agents

BioDynaMo is more than  $1000\times$  faster than Cortex3D and NetLogo and up to  $9\times$  more efficient than Biocellion

# Summary

Our optimizations to maximize parallelism, improve the memory layout, and avoid unnecessary work are effective and give BioDynaMo the following performance characteristics.

BioDynaMo scales well across a large number of CPU cores

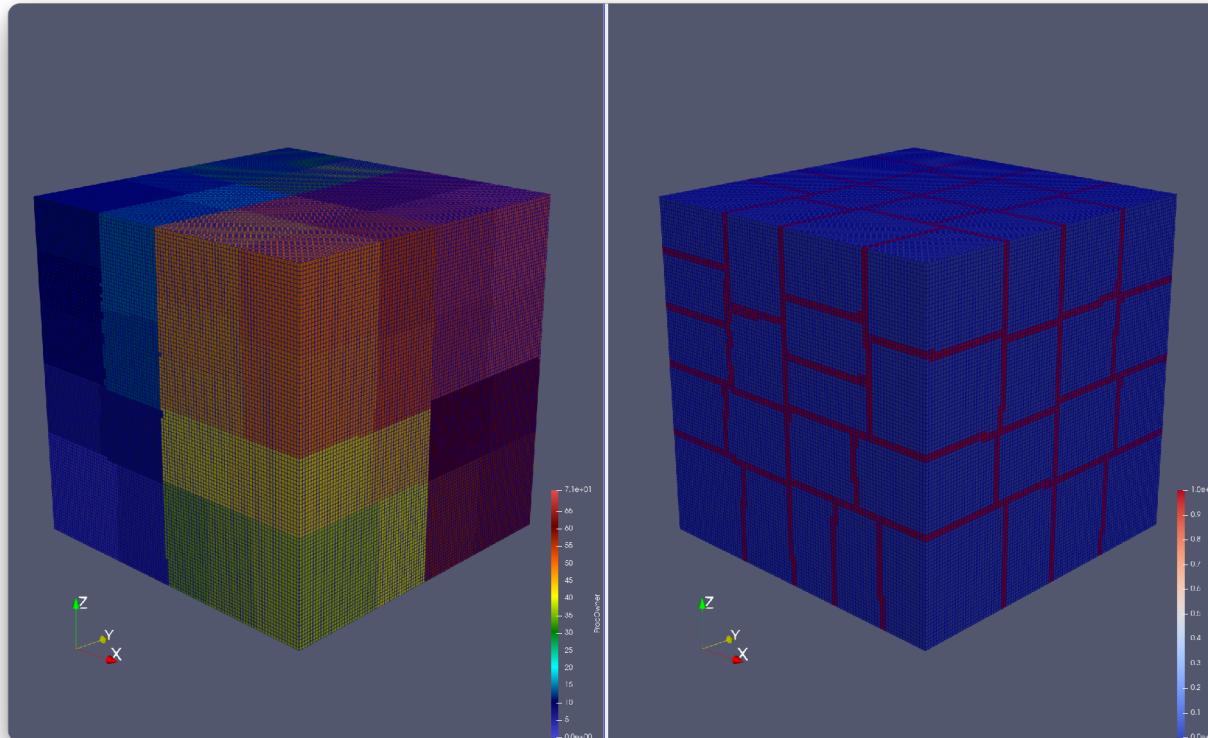
Runtime and memory consumption increases linearly with the number of agents

BioDynaMo is more than  $1000\times$  faster than Cortex3D and NetLogo and up to  $9\times$  more efficient than Biocellion

These performance characteristics enable simulations with billions of agents on a single server.

# Future work

Distributed simulation engine



# BioDynaMo is available under the permissive Apache 2.0 open source license

<https://github.com/BioDynaMo/biodynamo>

The screenshot shows the GitHub repository page for BioDynaMo. The top navigation bar includes 'Code' (selected), 'Issues 8', 'Pull requests 6', 'Discussions', 'Actions', 'Projects', 'Wiki', 'Security', 'Insights', and 'Settings'. Below the navigation is a search bar with dropdowns for 'master', '52 branches', and '8 tags'. Buttons for 'Go to file', 'Add file', and 'Code' are also present. The main content area displays a list of recent commits from TobiasDuswald:

Commit	Message	Date
.github	Introduce libgit2 to track used code for reproducibility (#309)	last month
benchmark	Update Copyright and extend GHA for Copyright	last year
cli	Avoid parsing of bdm.json with bdm test	10 months ago
cmake	Add Paraview sha's for macOS 13.2, also created the links to 13.2 ve...	5 days ago
demo	Replace rm->AddAgent with ctxt->AddAgent in demos (#309)	4 days ago
doc	Replace rm->AddAgent with ctxt->AddAgent in demos (#309)	4 days ago
etc	Pix several issues on macOS and allow building without paraview.	2 years ago
notebook	Make floating-point precision adjustable (#253)	6 months ago
paraview_plugin	Update copyright information	last year
src	Replace rm->AddAgent with ctxt->AddAgent in demos (#309)	4 days ago
test	Add PrintInfo member function to DiffusionGrid (#293)	2 months ago
third_party	Fix optimlib / armadillo dependency (#235)	2 months ago
util	Introduce libgit2 to track used code for reproducibility (#300)	last month
clang-format	Generated new version by clang-format-3.9. Honors Google includ...	6 years ago
clang-tidy	Fix clang-tidy errors	3 years ago
clang-tidy-ignore	Improve automated code checks	5 years ago
editorconfig	Add support for editors supporting <a href="http://editorconfig.org">http://editorconfig.org</a> .	6 years ago
gitignore	Introduce libgit2 to track used code for reproducibility (#300)	last month
.mailmap	Update .mailmap file	4 months ago

To the right of the commit list is the 'About' section, which describes BioDynaMo as a high-performance and modular, agent-based simulation platform. It lists various tags: simulation, cancer, biology, high-performance, neuroscience, epidemiology, agent-based, large-scale, modular-design, agent-based-framework, and agent-based-modelling. Below the 'About' section are links to 'Readme', 'Apache-2.0 license', 'Code of conduct', '61 stars', '10 watching', and '41 forks'. The 'Releases' section shows one release, BioDynaMo 1.04, which was released on Oct 5, 2022. The 'Contributors' section shows 22 contributors, with 11 more listed below.

# Join us in pushing the limits of agent-based modeling

BioDynamo is an open, welcoming, and collaborative project: <https://biodynamo.org>

Besides the organizations behind this paper,



**ETH** zürich

**TU**Delft

BioDynamo is developed by the BioDynamo collaboration,



and further organizations.



# More in the paper

<https://arxiv.org/abs/2301.06984>, <https://doi.org/10.1145/3572848.3577480>



## High-Performance and Scalable Agent-Based Simulation with BioDynaMo

Lukas Breitwieser\*, Ahmad Hesam, Fons Rademakers  
CERN, Switzerland  
Delft University of Technology,  
The Netherlands  
CERN, Switzerland

Juan Gómez Luna, Onur Mutlu†  
ETH Zurich, Switzerland  
ETH Zurich, Switzerland

**Abstract**  
Agent-based modeling plays an essential role in gaining insights into biology, sociology, economics, and other fields. However, many existing agent-based simulation platforms are not suitable for large-scale studies due to the low performance of the underlying simulation engines. To overcome this limitation, we present a novel high-performance simulation engine.  
We identify three key challenges for which we present the following solutions. First, to maximize parallelization, we present an optimized grid to search for neighbors and parallelize the merging of thread-local results. Second, we reduce the memory access latency with a NUMA-aware agent iterator, agent sorting with a space-filling curve, and a custom heap memory allocator. Third, we present a mechanism to omit the collision force calculation under certain conditions.  
Our evaluation shows an order of magnitude improvement over Biocellion, three orders of magnitude speedup over Cortex3D and NetLogo, and the ability to simulate 1.72 billion agents on a single server.  
Supplementary Materials, including instructions to reproduce the results, are available at: <https://doi.org/10.5281/zendodo.6463816>

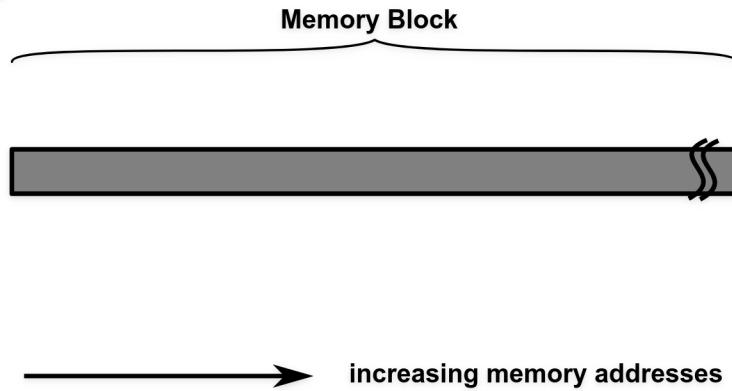


---

# Appendix

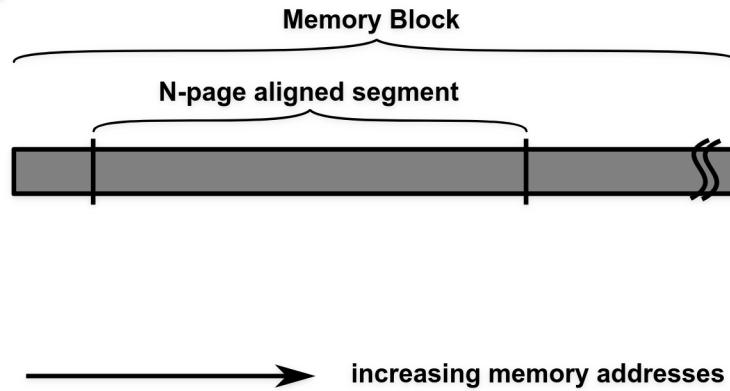
# Memory allocation

## A Layout



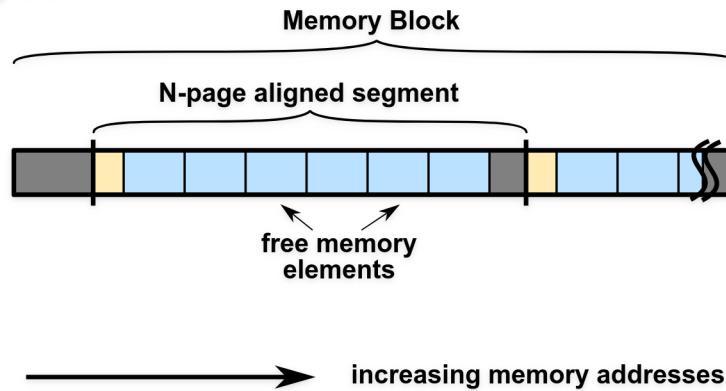
# Memory allocation

## A Layout



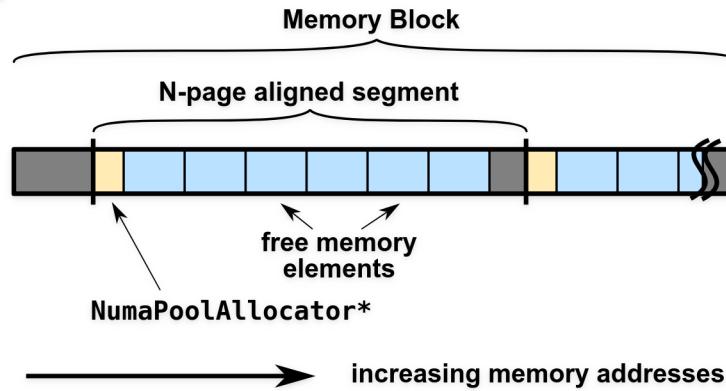
# Memory allocation

## A Layout



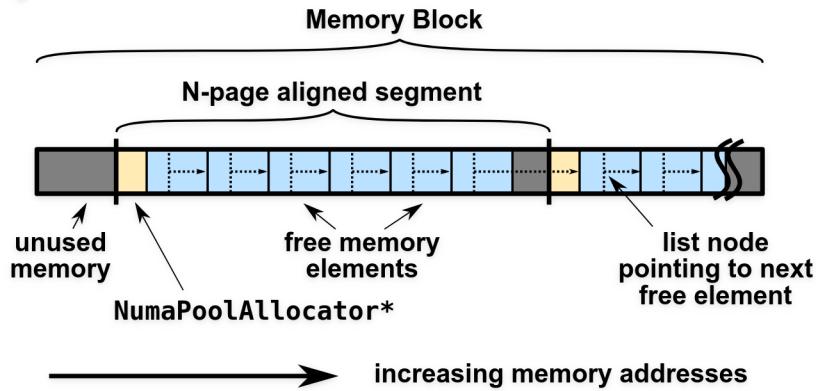
# Memory allocation

## A Layout



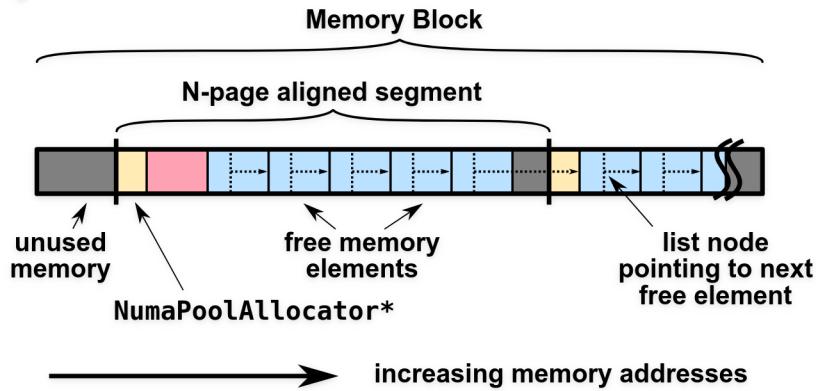
# Memory allocation

## A Layout



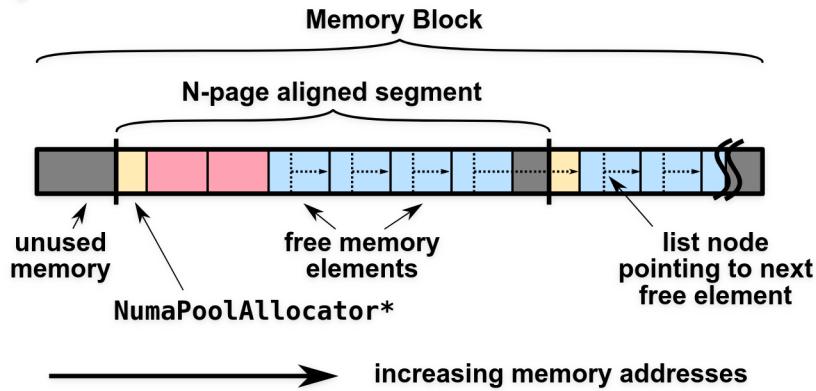
# Memory allocation

## A Layout



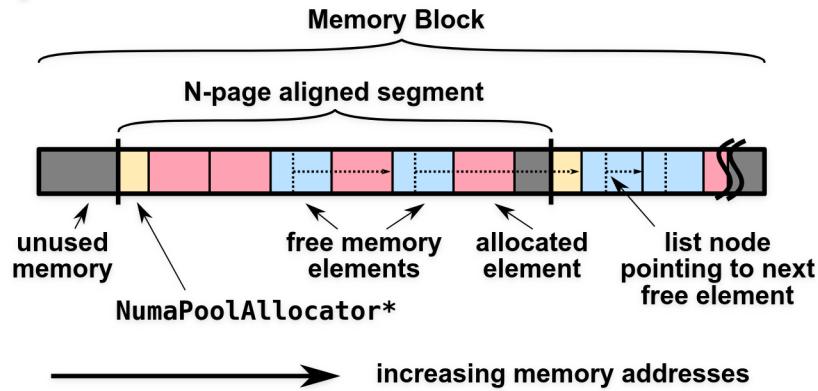
# Memory allocation

## A Layout



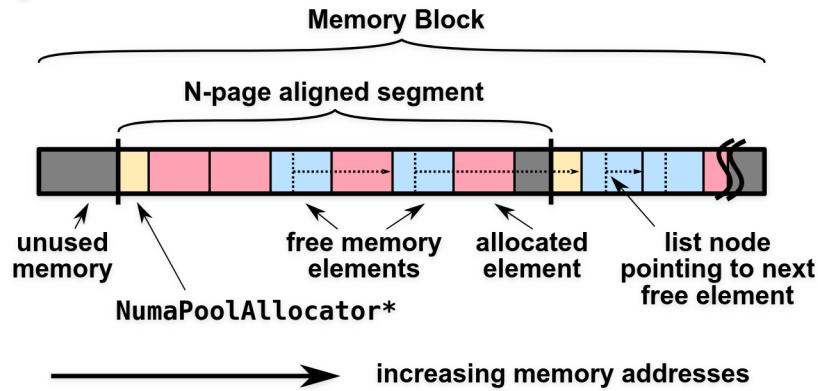
# Memory allocation

## A Layout

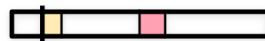


# Memory allocation

## A Layout

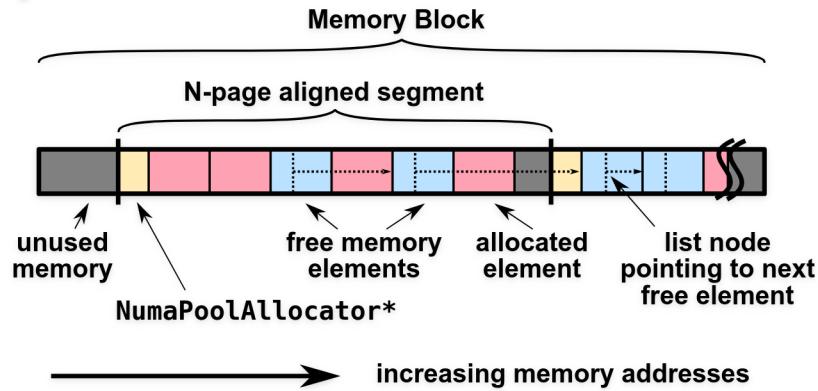


## B Deallocation

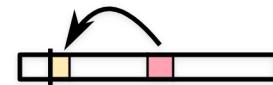


# Memory allocation

## A Layout



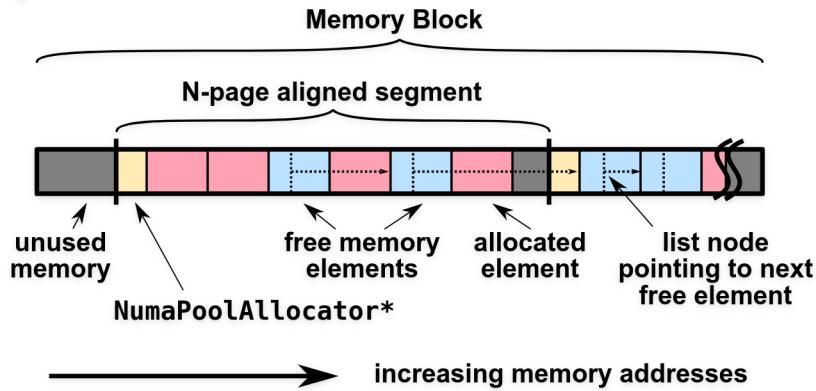
## B Deallocation



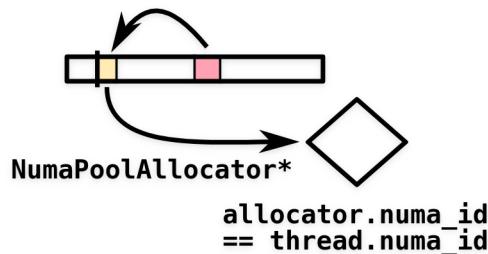
NumaPoolAllocator\*

# Memory allocation

## A Layout

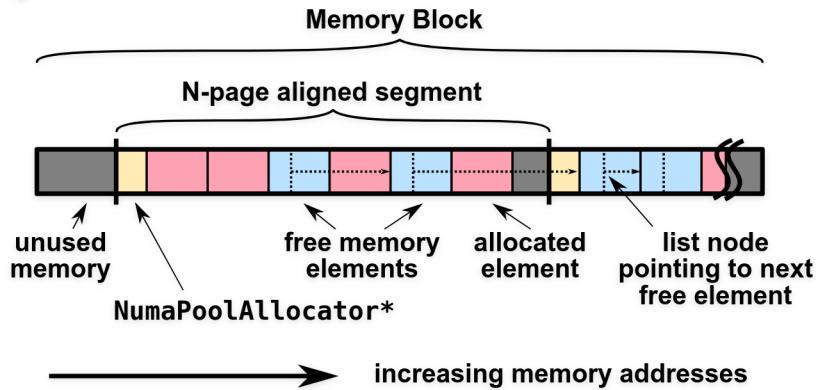


## B Deallocation

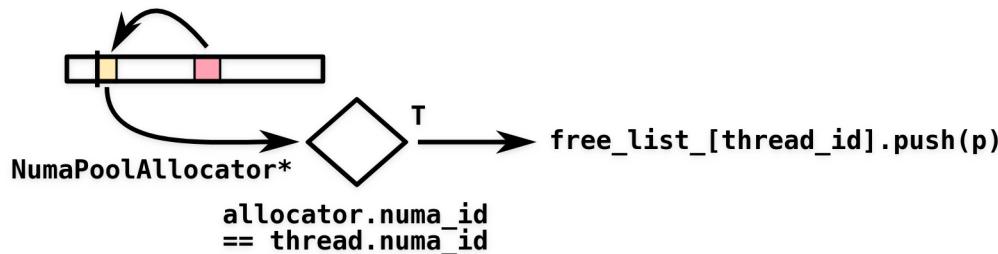


# Memory allocation

## A Layout

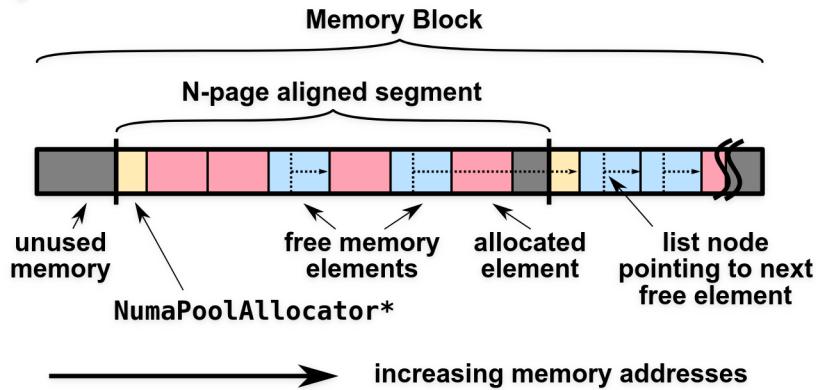


## B Deallocation

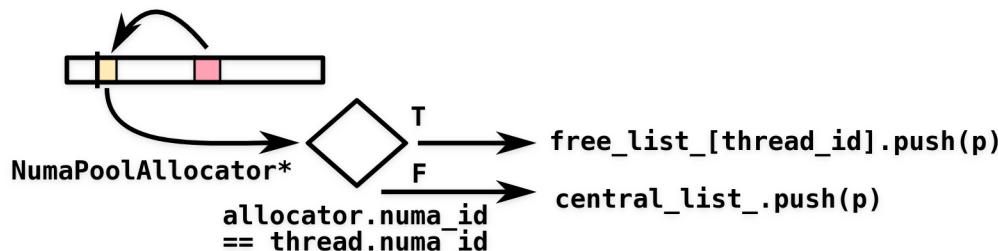


# Memory allocation

## A Layout



## B Deallocation



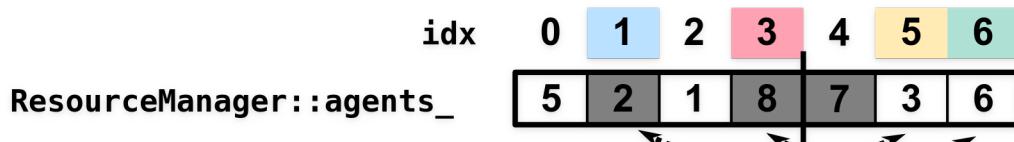
# Memory allocation

# Parallel agent removal

Removed agents:

Thread 0: {2, 8}

Thread 1: {7}



1. Initialize

to_right	<table border="1"><tr><td><math>\infty</math></td><td><math>\infty</math></td><td><math>\infty</math></td></tr></table>	$\infty$	$\infty$	$\infty$	<table border="1"><tr><td>0</td><td>0</td><td>0</td></tr></table>	0	0	0	not_to_left
$\infty$	$\infty$	$\infty$							
0	0	0							

2. Fill

to_right	<table border="1"><tr><td>1</td><td>3</td><td><math>\infty</math></td></tr></table>	1	3	$\infty$	<table border="1"><tr><td>1</td><td>0</td><td>0</td></tr></table>	1	0	0	not_to_left
1	3	$\infty$							
1	0	0							

3. Reorder

to_right	<table border="1"><tr><td>1</td><td>3</td><td><math>\infty</math></td></tr></table>	1	3	$\infty$	<table border="1"><tr><td>5</td><td>0</td><td>6</td></tr></table>	5	0	6	to_left
1	3	$\infty$							
5	0	6							

#swaps

<table border="1"><tr><td>2</td><td>0</td></tr></table>	2	0	<table border="1"><tr><td>1</td><td>1</td></tr></table>	1	1
2	0				
1	1				

4. Swap

to_right	<table border="1"><tr><td>1</td><td>3</td><td><math>\infty</math></td></tr></table>	1	3	$\infty$	<table border="1"><tr><td>5</td><td>0</td><td>6</td></tr></table>	5	0	6	to_left
1	3	$\infty$							
5	0	6							

Thread 0

Thread 1

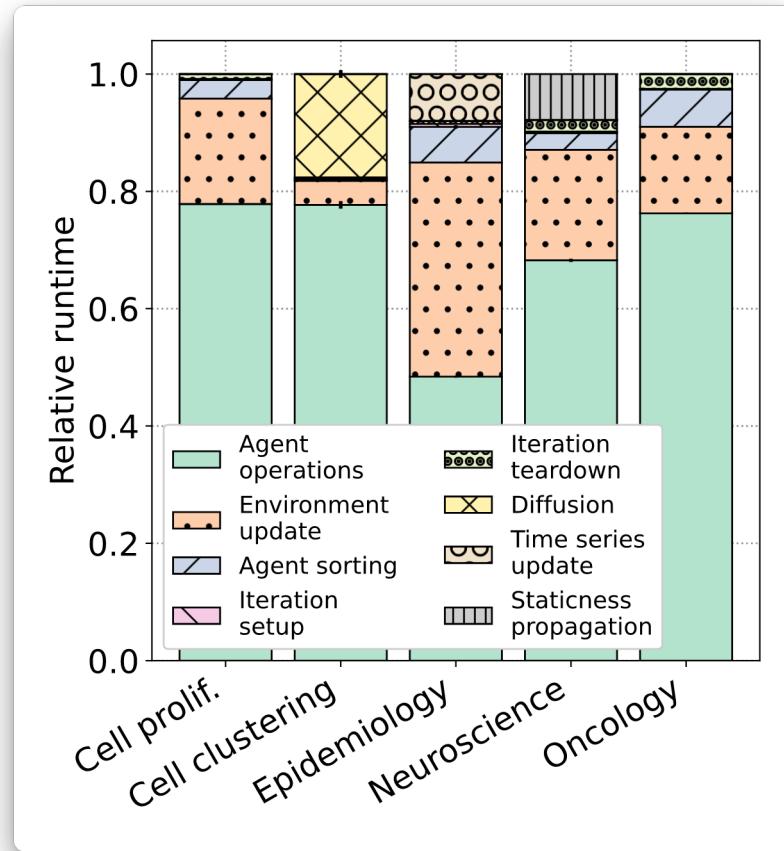
5. Resize

5	3	1	6
---	---	---	---

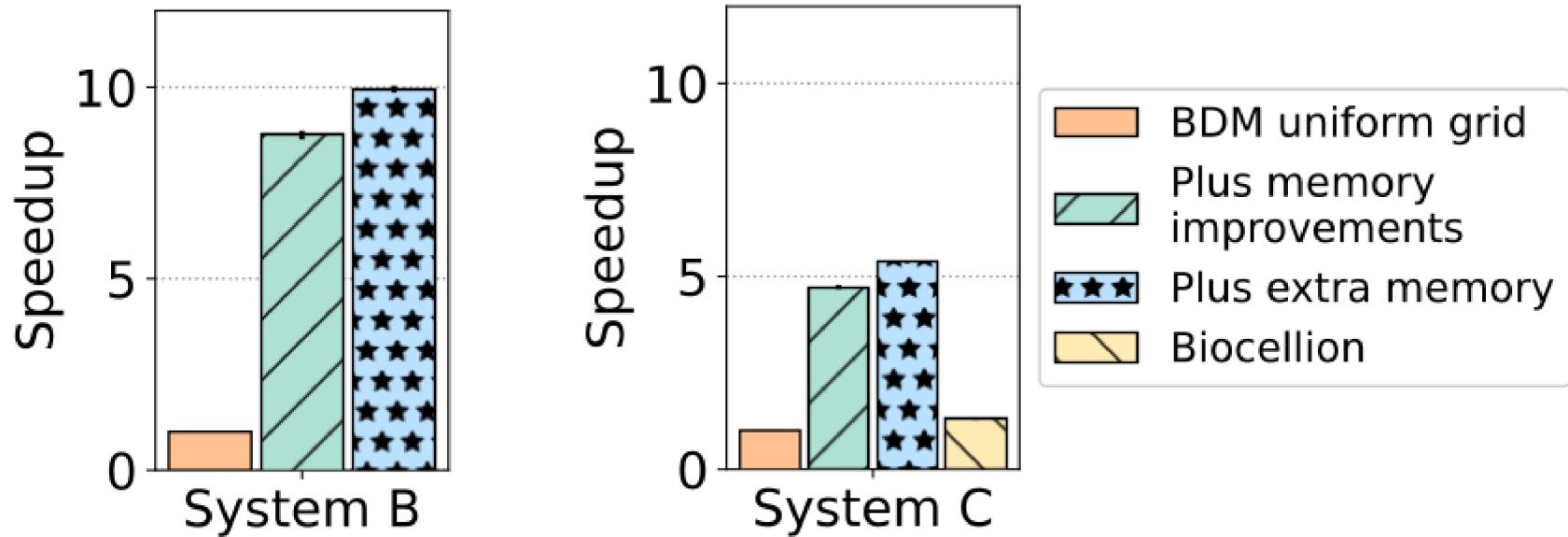
# Performance-related simulation characteristics

Characteristic	Cell proliferation	Cell clustering	Epidemiology	Neuroscience	Oncology
Create new agents during simulation	x			x	x
Delete agents during simulation					x
Agents modify neighbors			x	x	x
Load imbalance			x	x	
Agents move randomly			x		x
Simulation uses diffusion	x		x		
Simulation has static regions			x		
Number of iterations	500	1000	1000	500	288
Number of agents (in millions)	12.6	2	10	9	10
Number of diffusion volumes	0	54m	0	65k	0

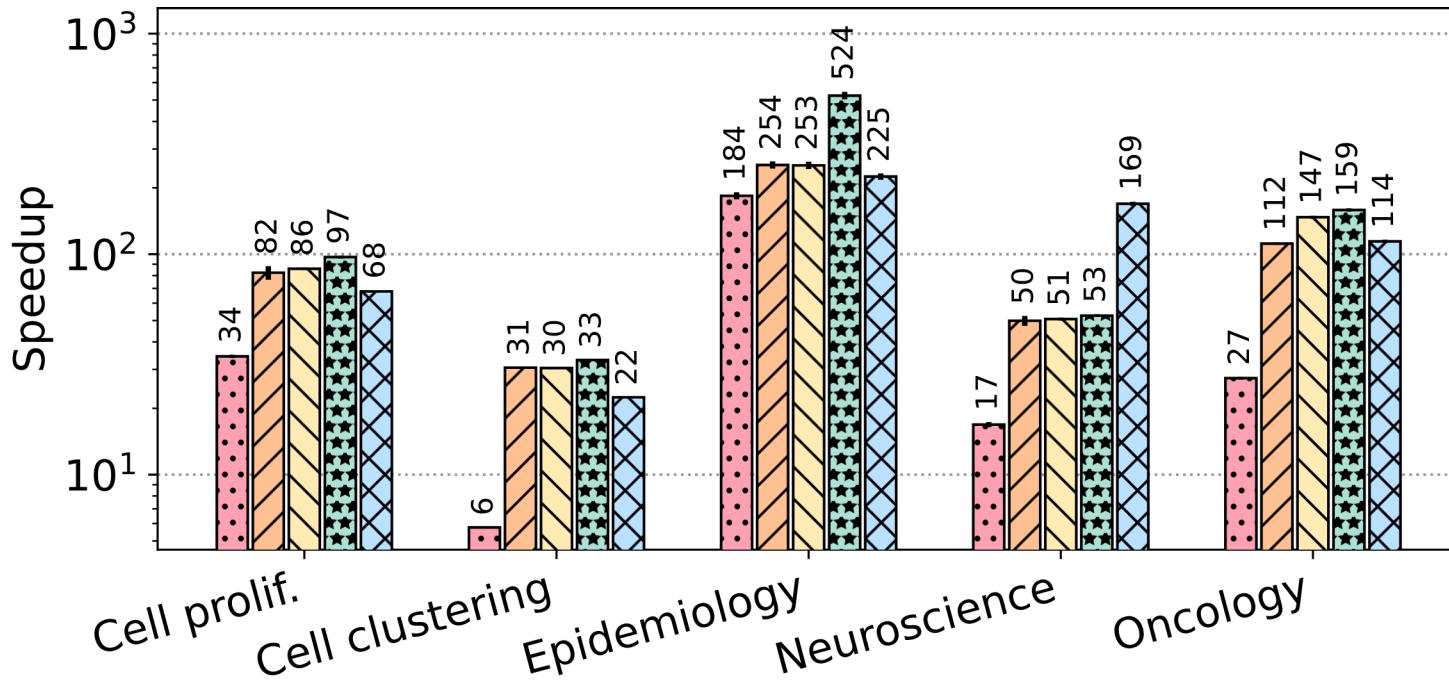
# Operation runtime breakdown



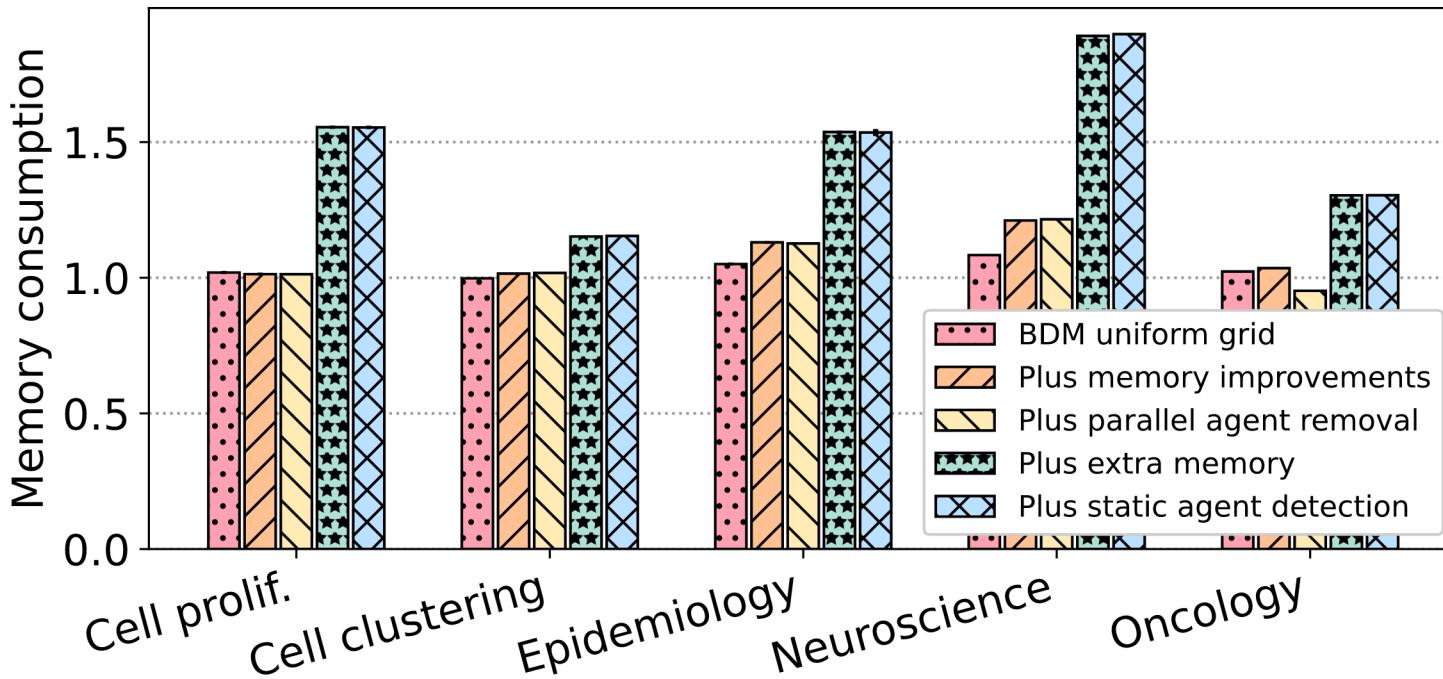
# BioDynaMo / Biocellion comparison analysis



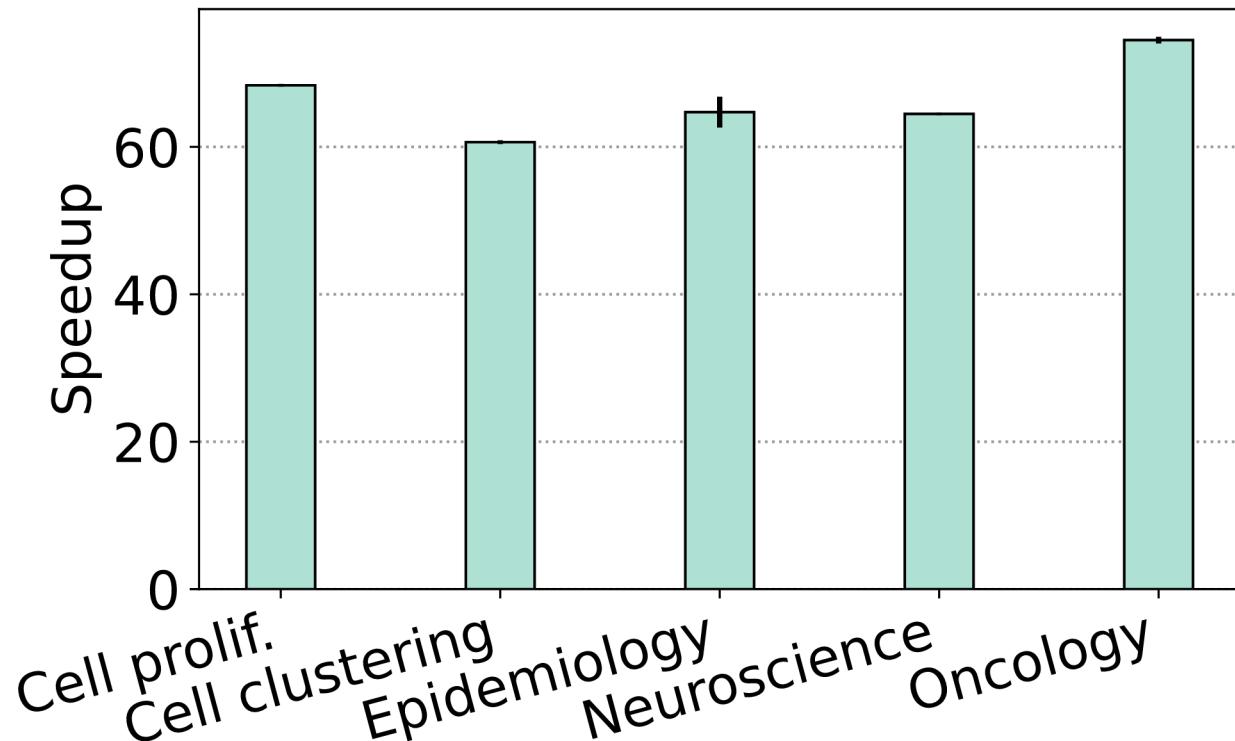
# Optimization overview for larger scale simulations



# Optimization overview for larger scale simulations

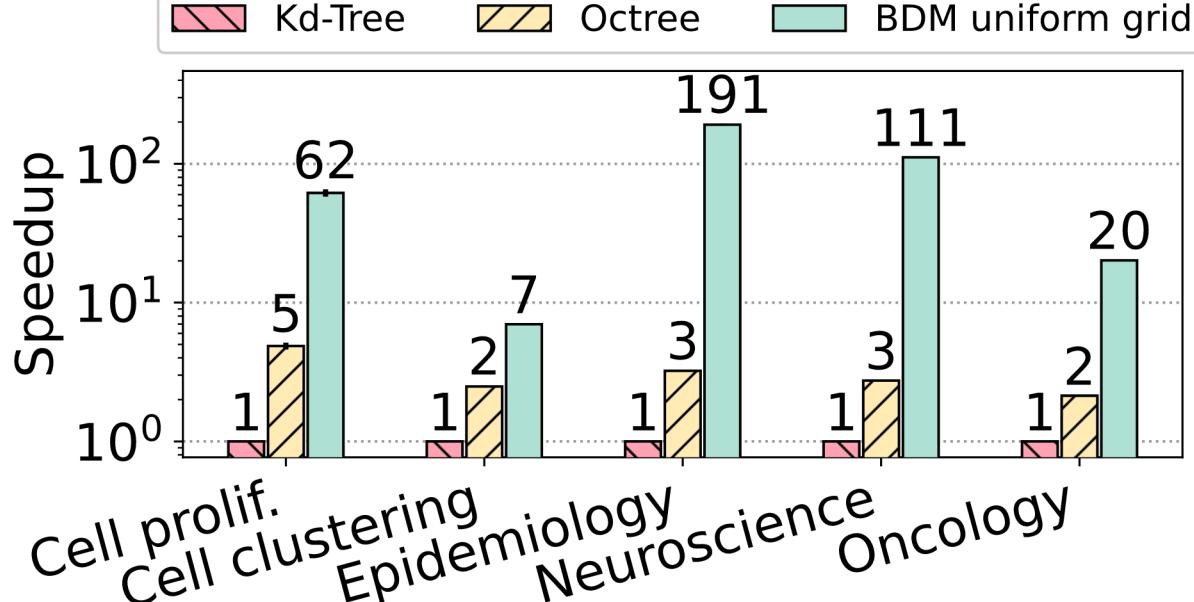


# Full simulation scalability



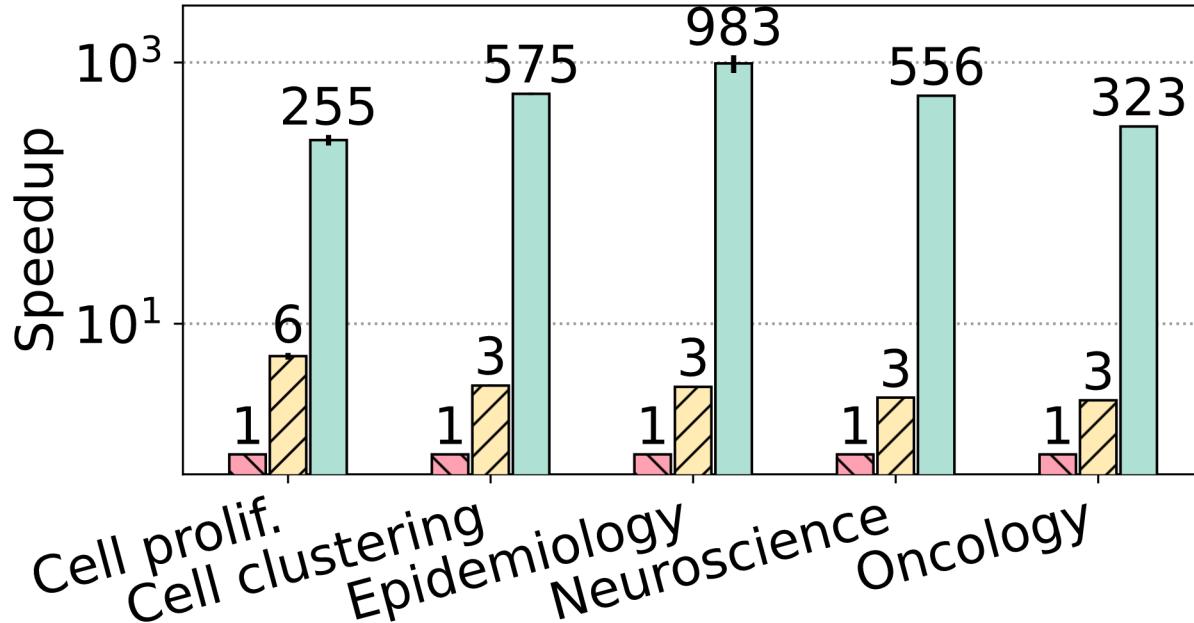
# Radial neighbor search comparison

Whole simulation (144 threads and 4 NUMA domains)



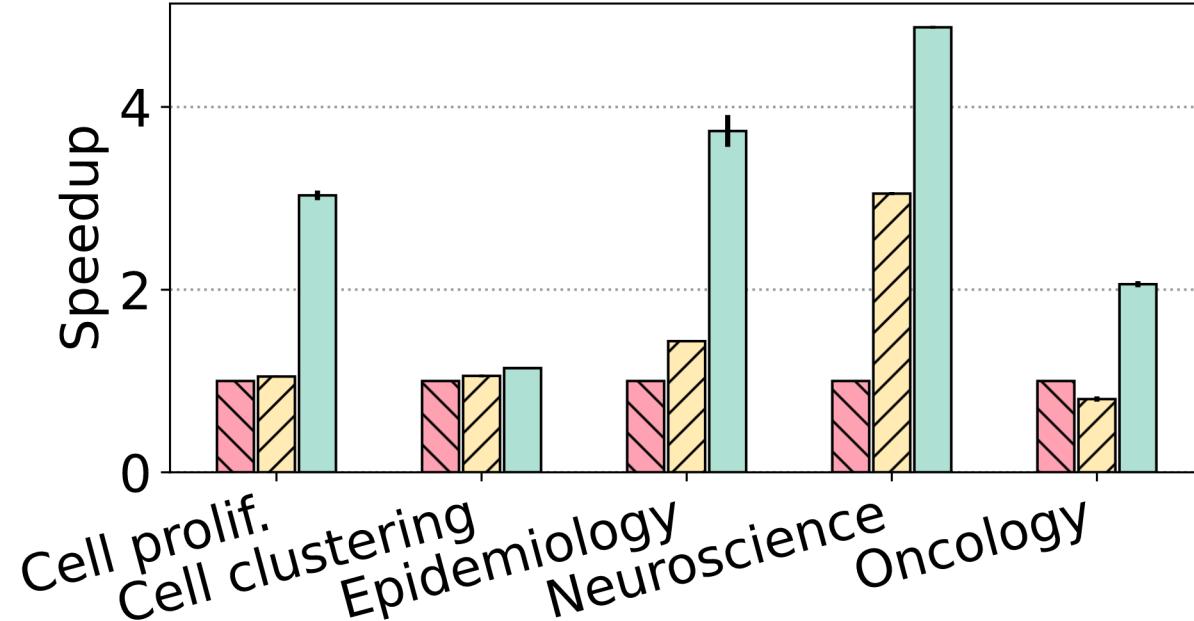
# Radial neighbor search comparison

Build time (144 threads and 4 NUMA domains)



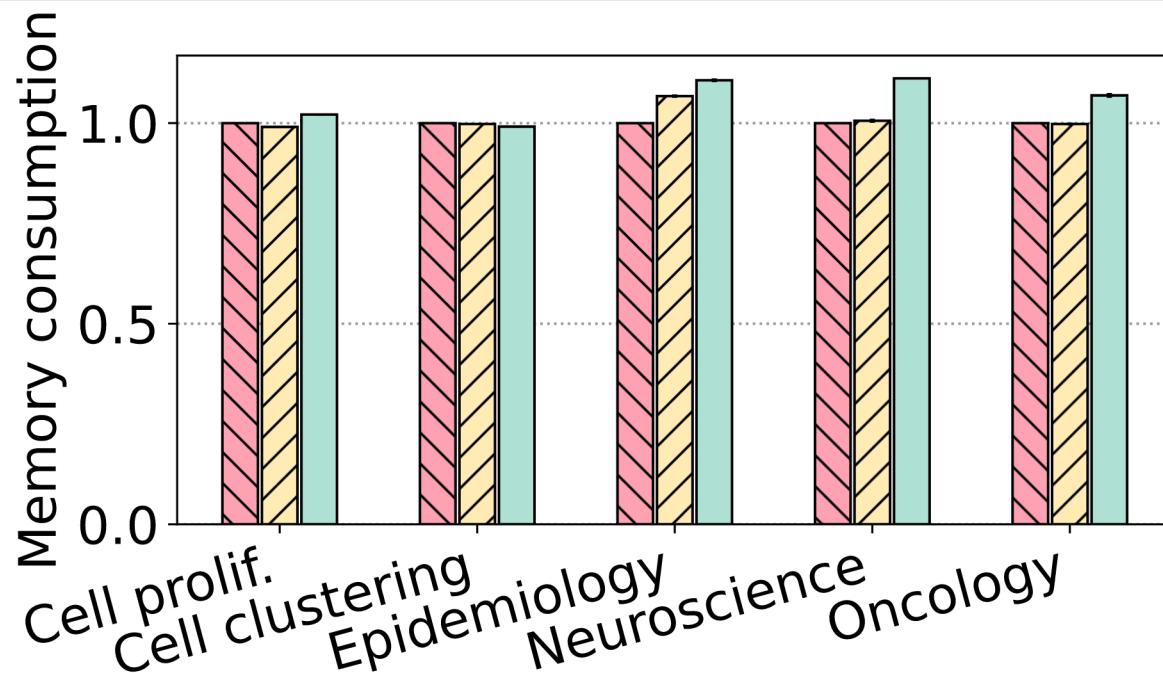
# Radial neighbor search comparison

Search time indirect (144 threads and 4 NUMA domains)



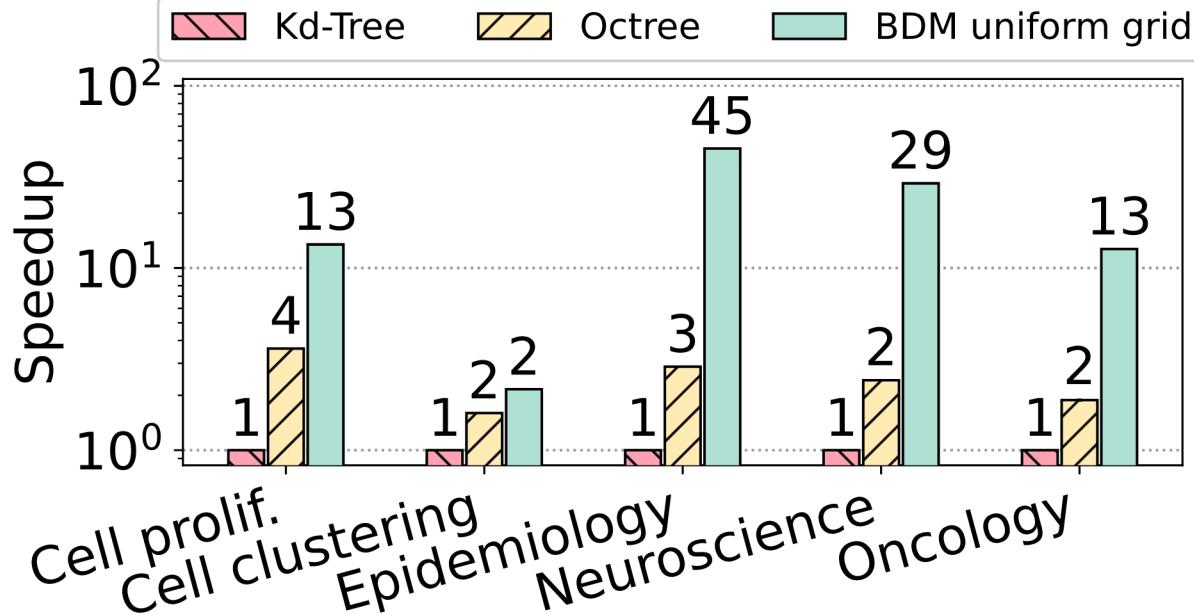
# Radial neighbor search comparison

Memory consumption (144 threads and 4 NUMA domains)



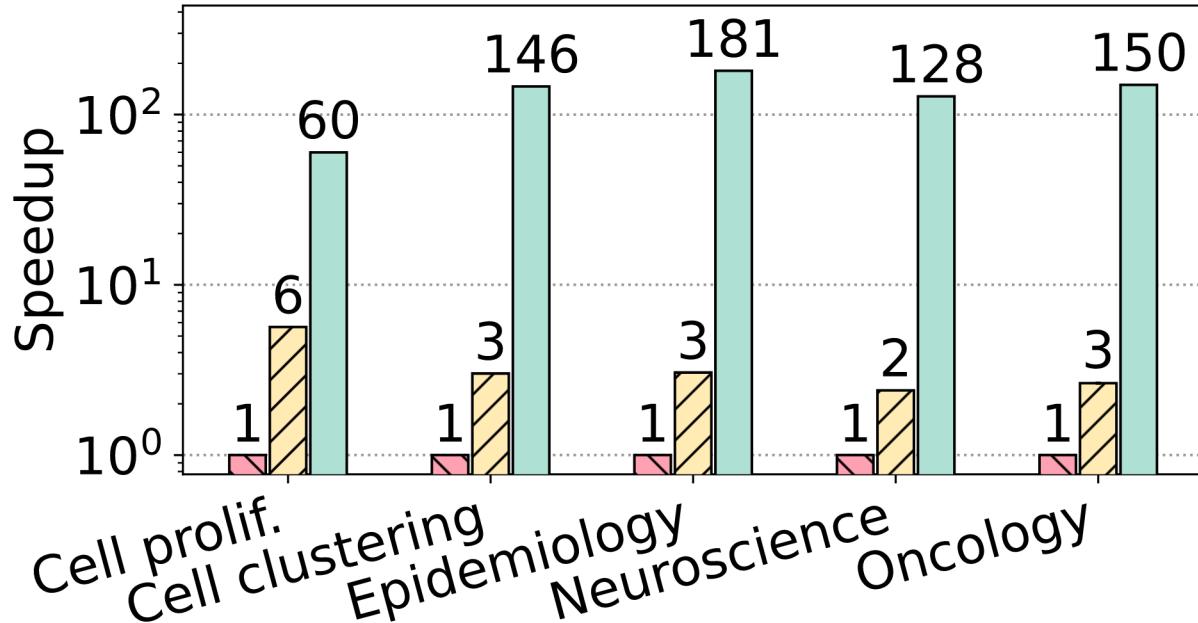
# Radial neighbor search comparison

Whole simulation (18 threads and one NUMA domain)



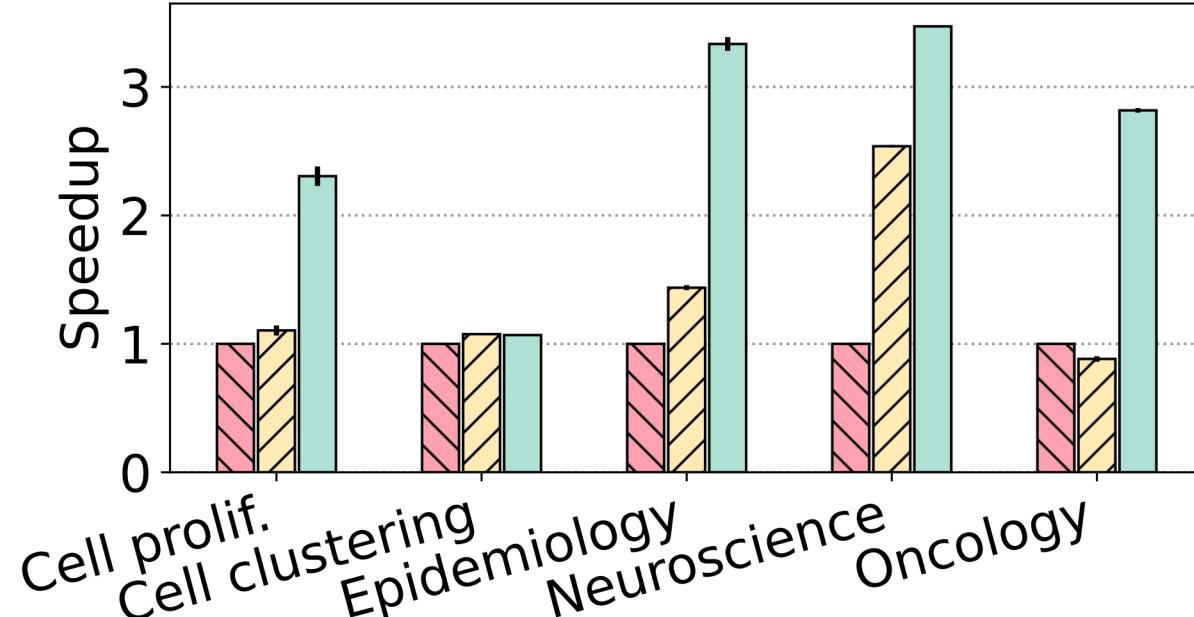
# Radial neighbor search comparison

Build time (18 threads and one NUMA domain)



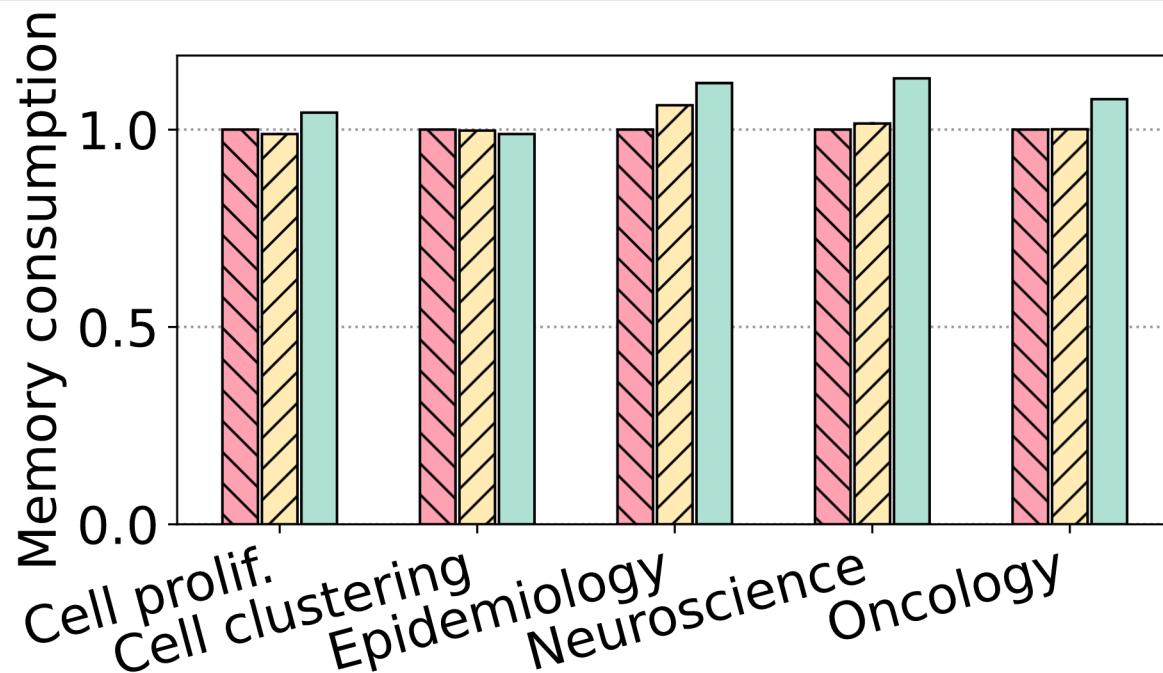
# Radial neighbor search comparison

Search time indirect (18 threads and one NUMA domain)

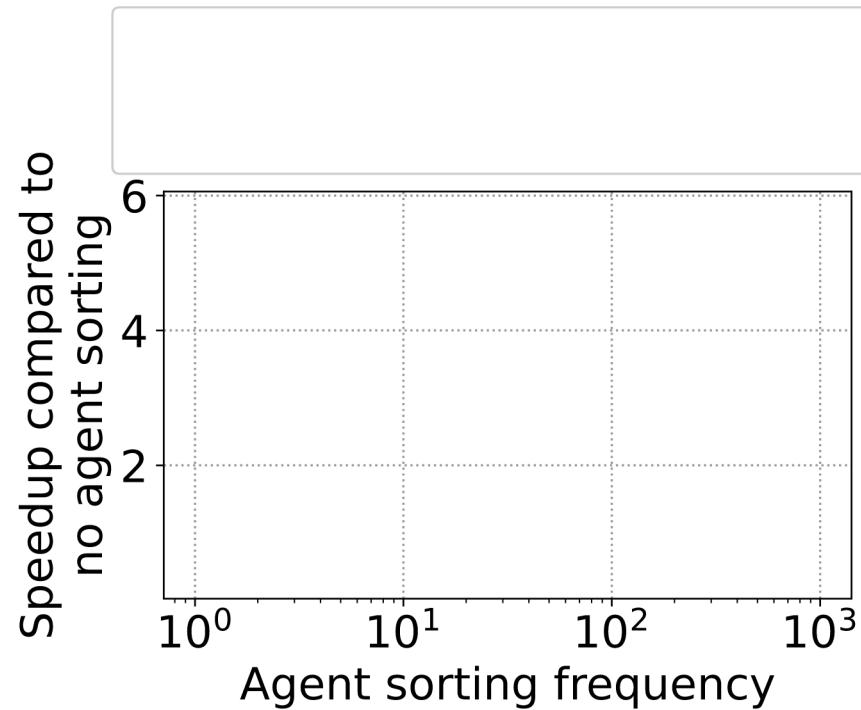


# Radial neighbor search comparison

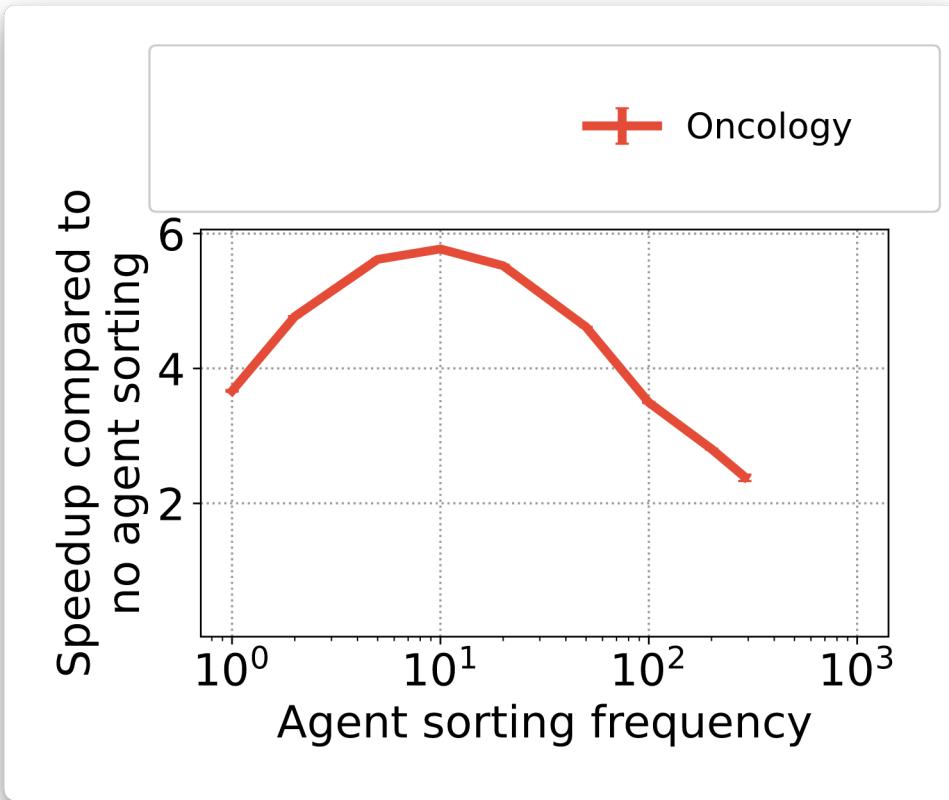
Memory consumption (18 threads and one NUMA domain)



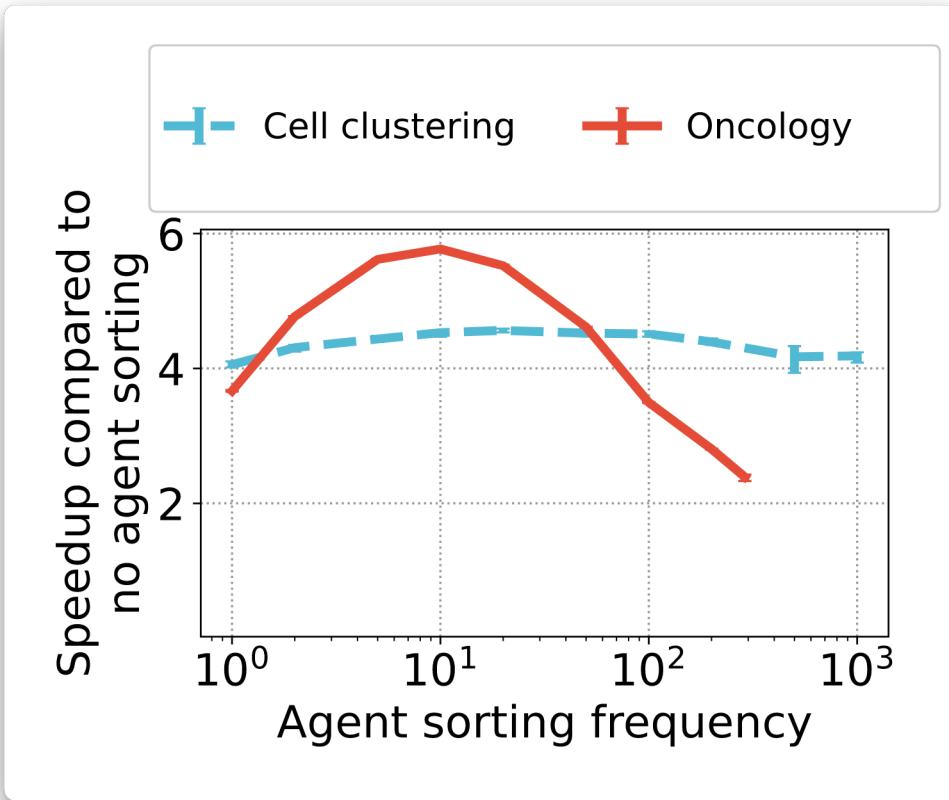
# Agent sorting speeds up simulations up to $6\times$



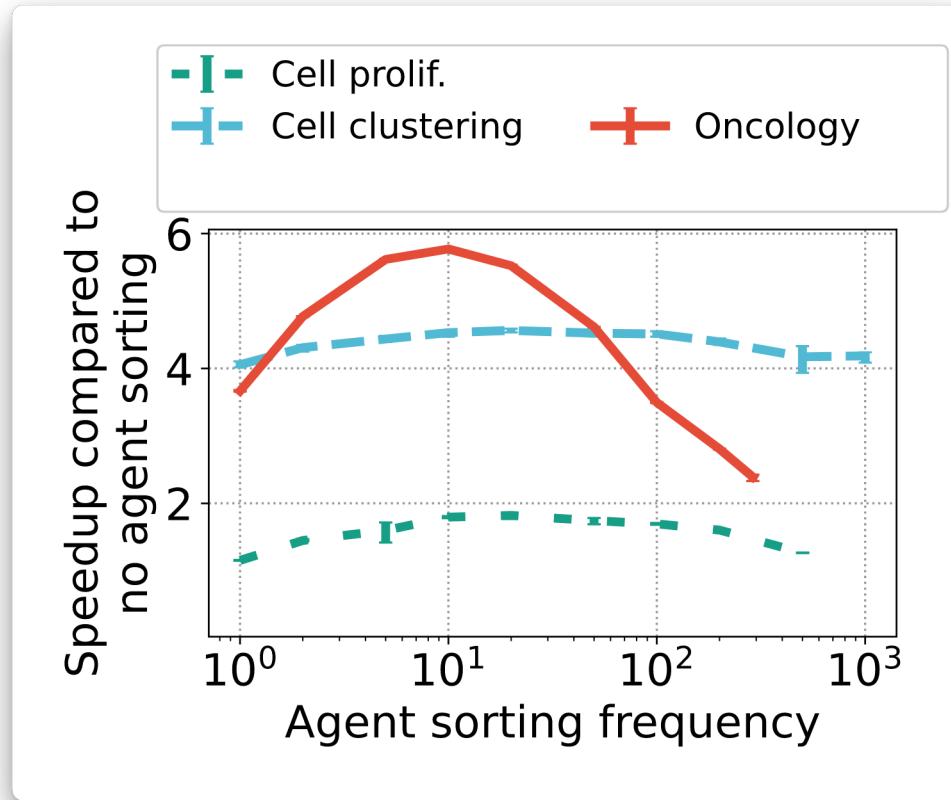
# Agent sorting speeds up simulations up to 6×



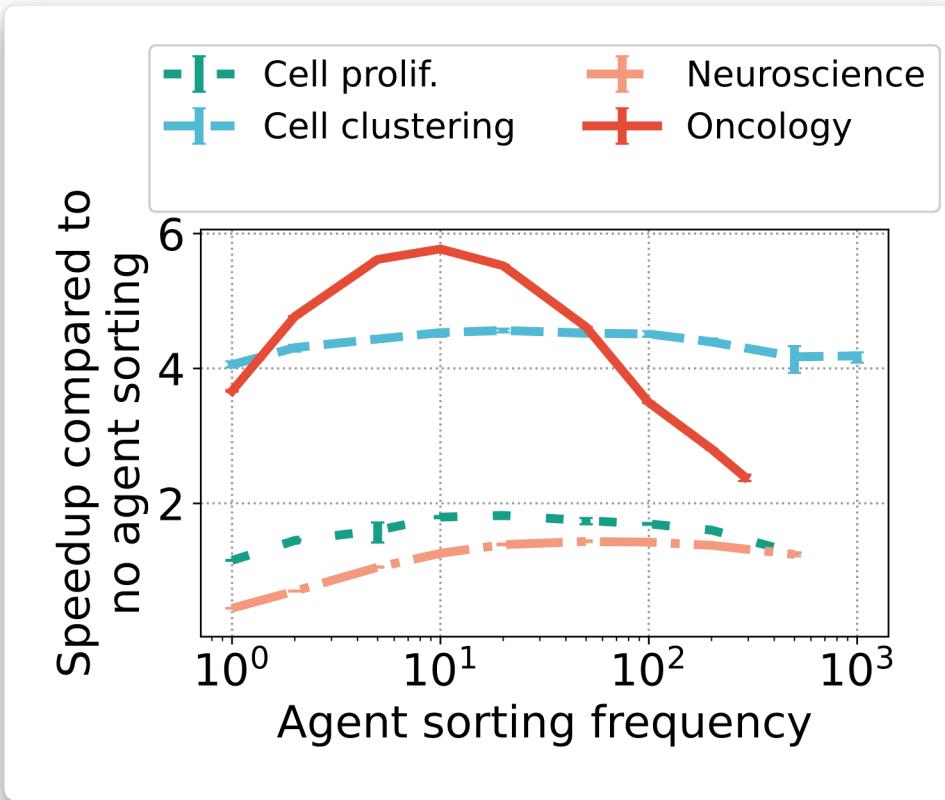
# Agent sorting speeds up simulations up to $6\times$



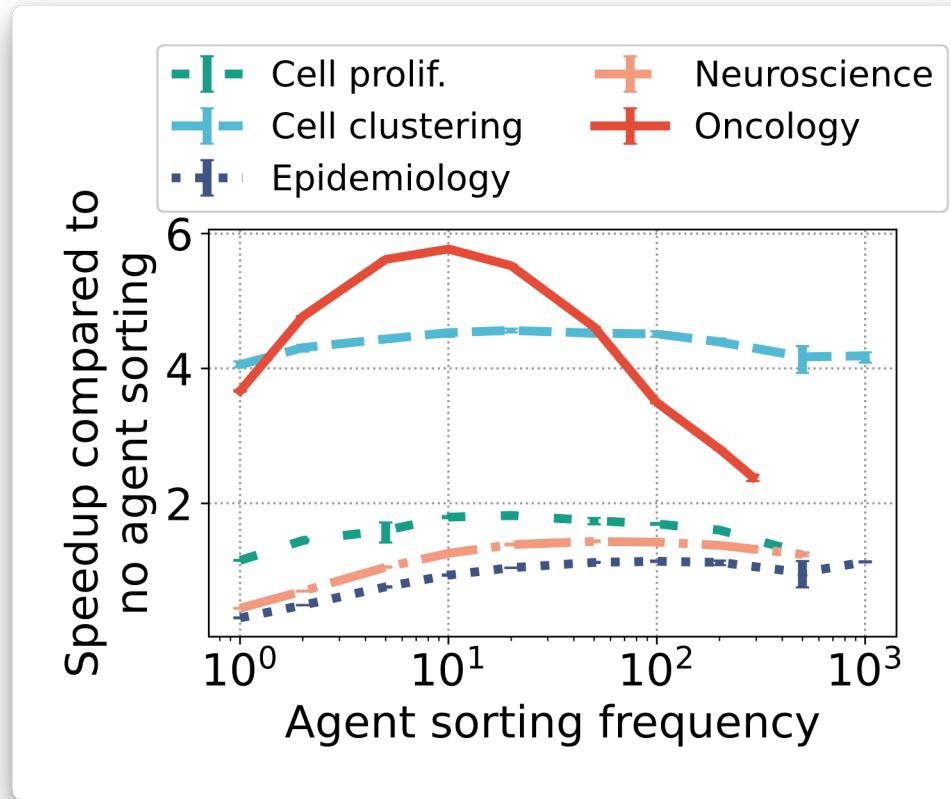
# Agent sorting speeds up simulations up to 6×



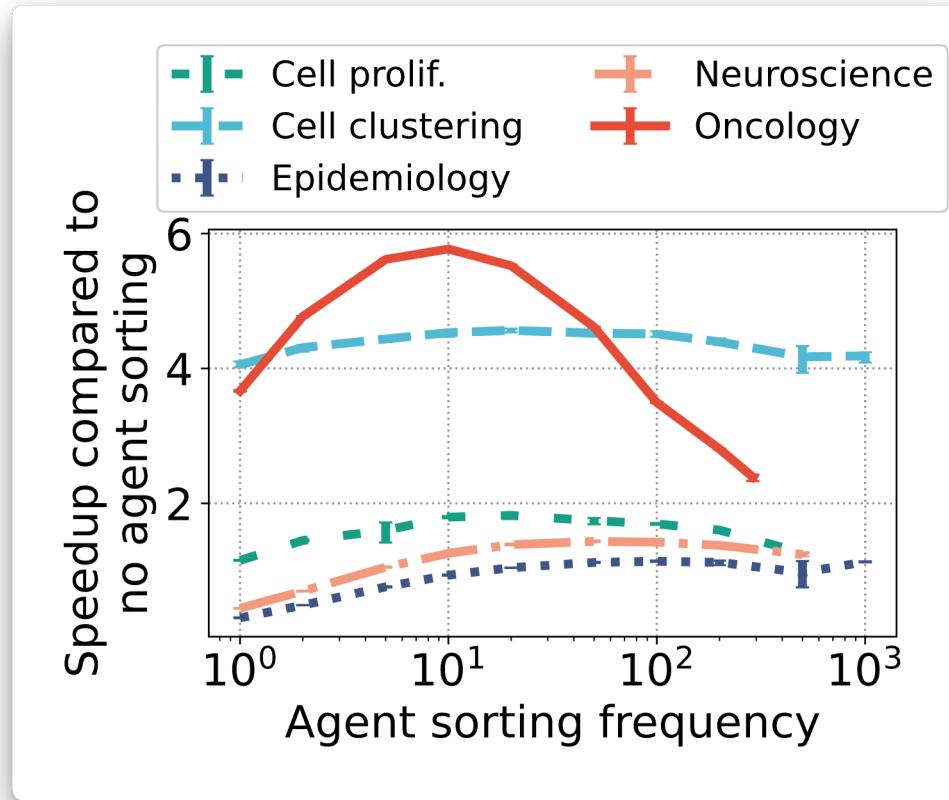
# Agent sorting speeds up simulations up to 6×



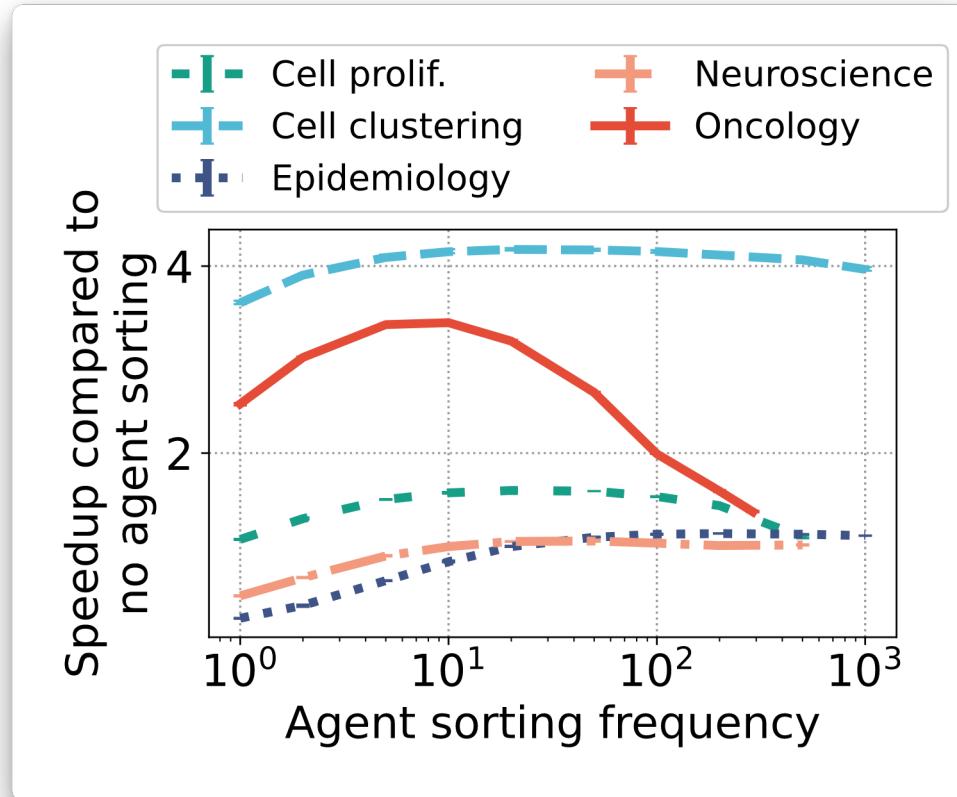
# Agent sorting speeds up simulations up to 6×



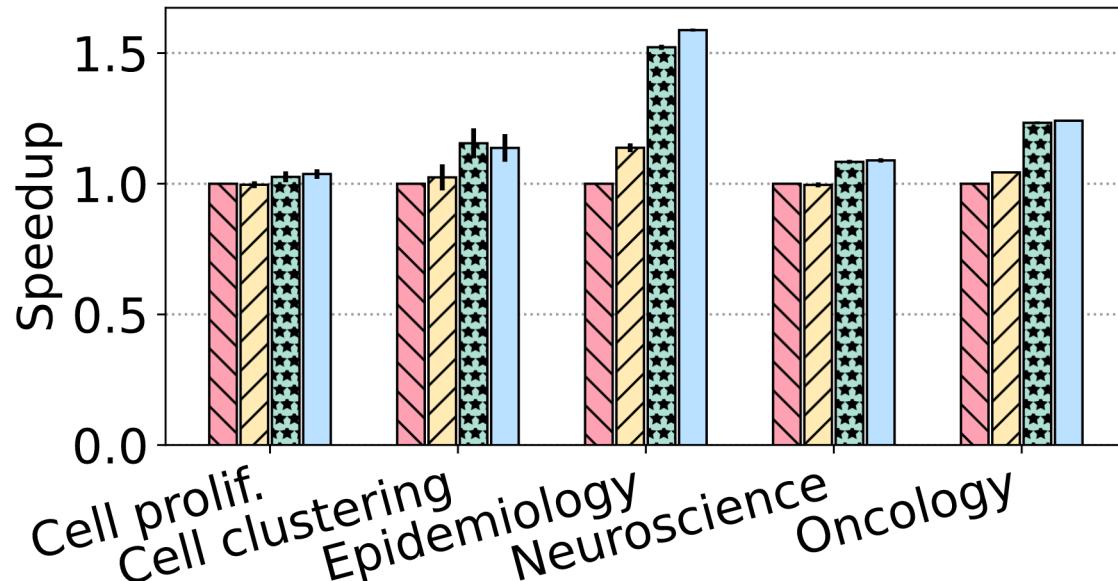
# Agent sorting speeds up simulations up to 6×



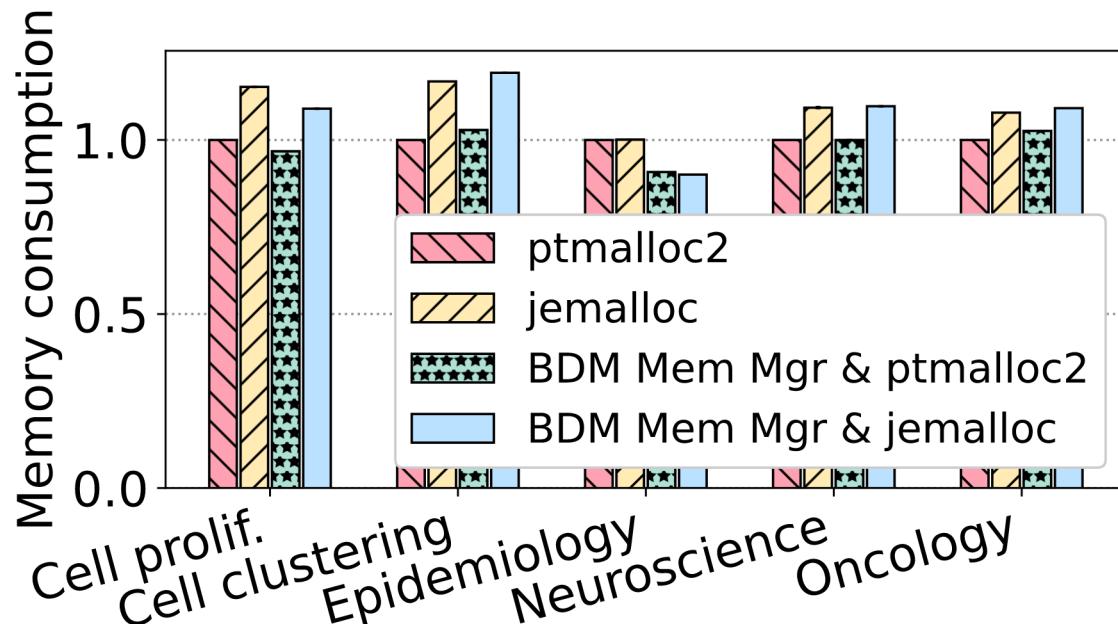
# Agent sorting speedup for one NUMA domain



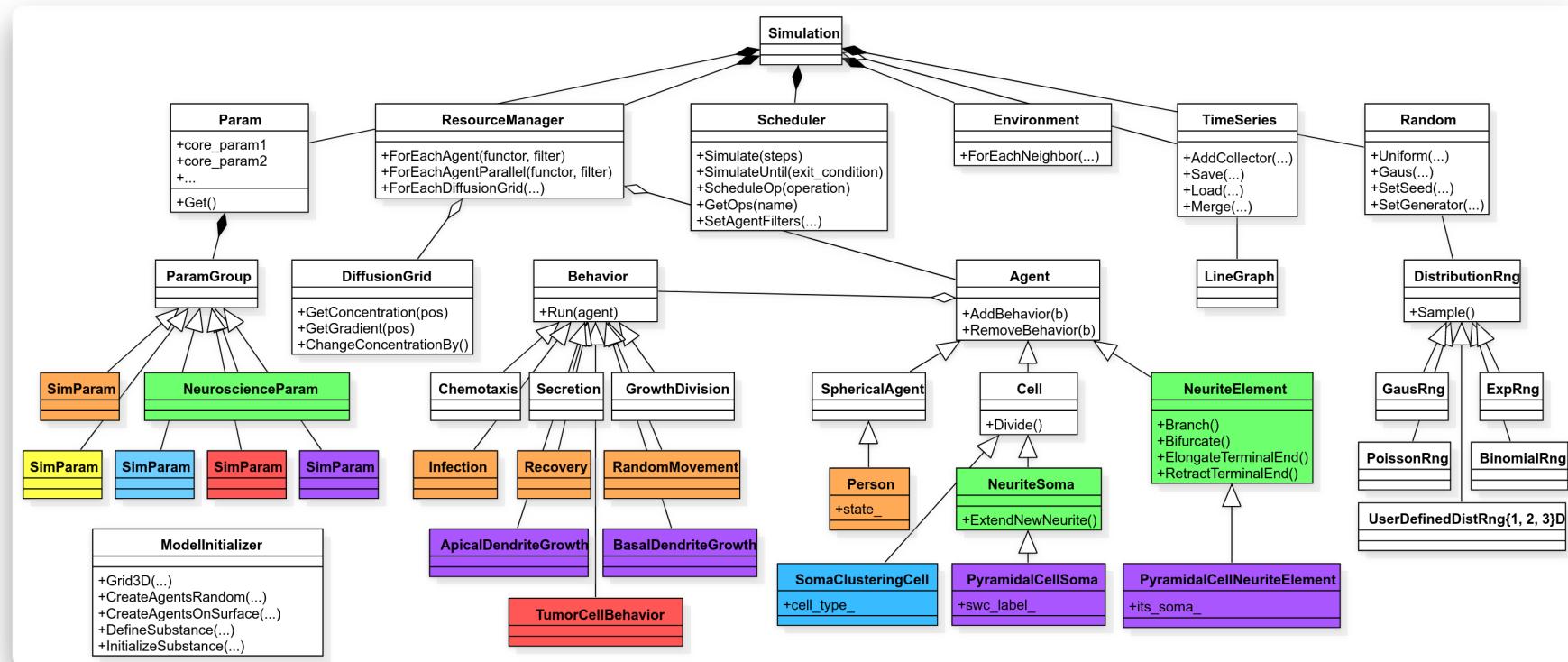
# Memory allocator comparison



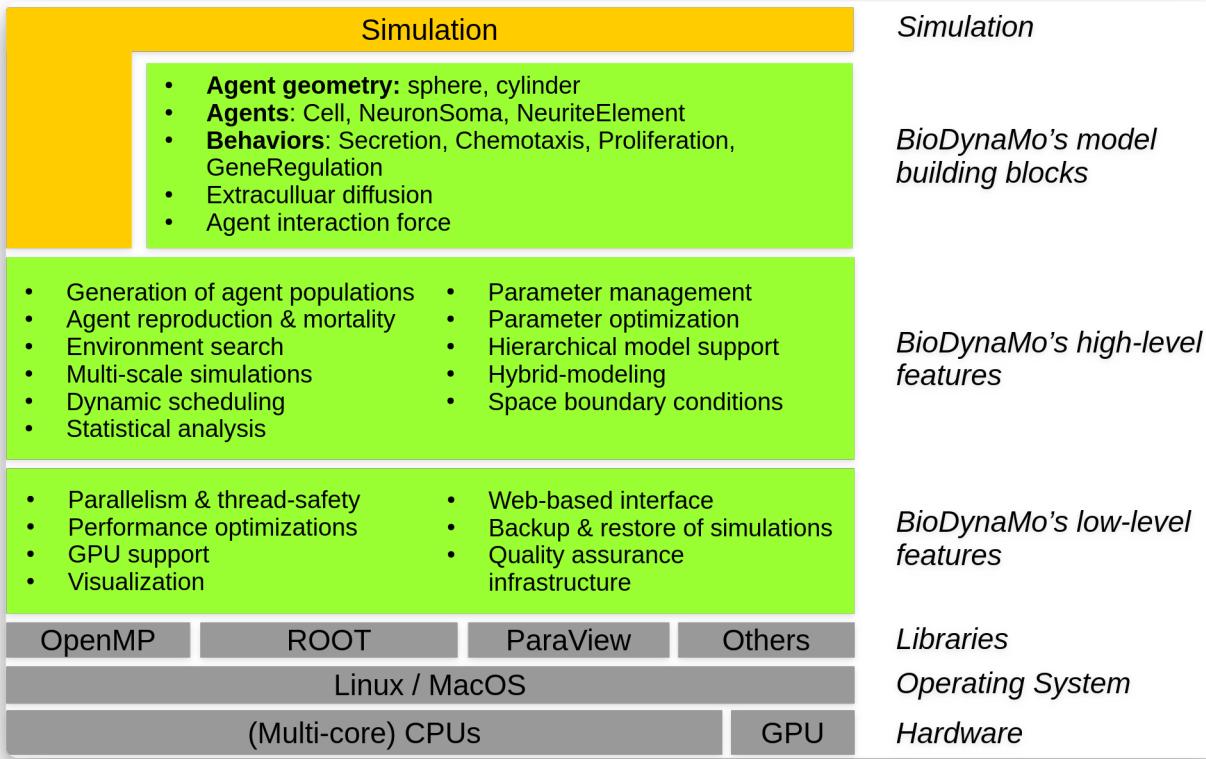
# Memory allocator comparison



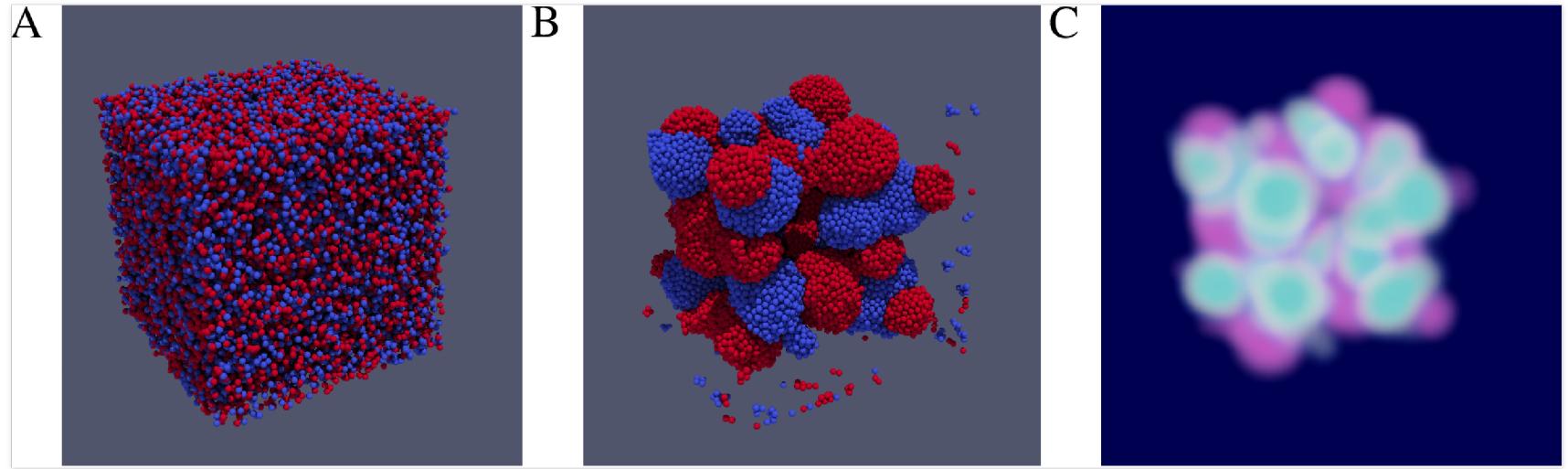
# Modularity



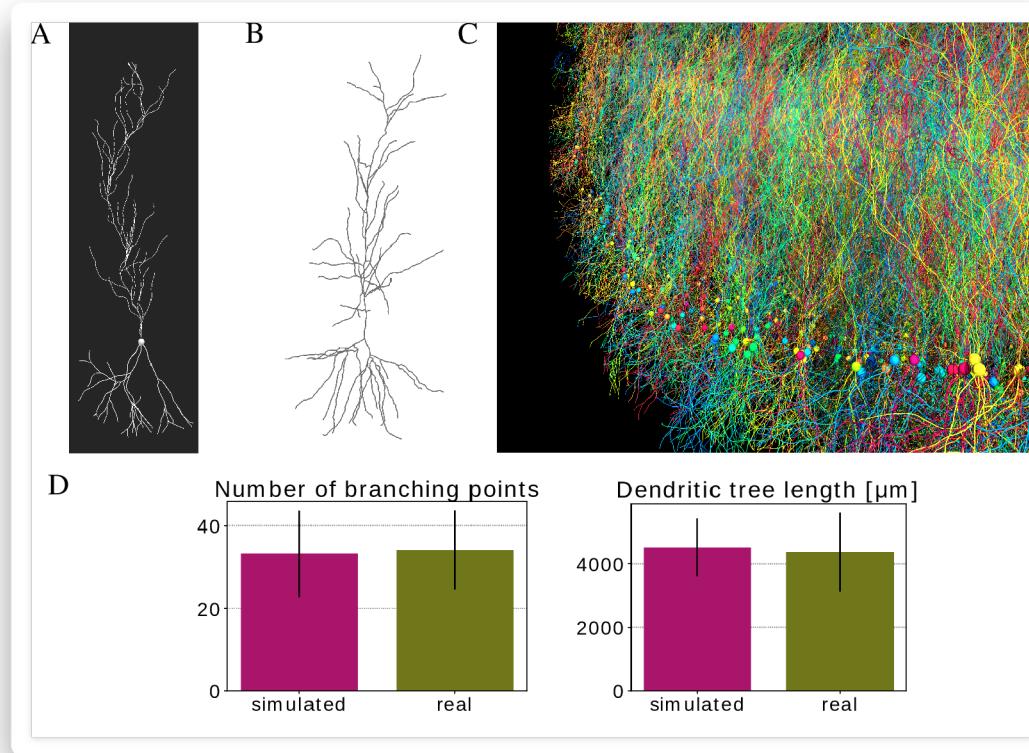
# Abstraction layers and modeling features



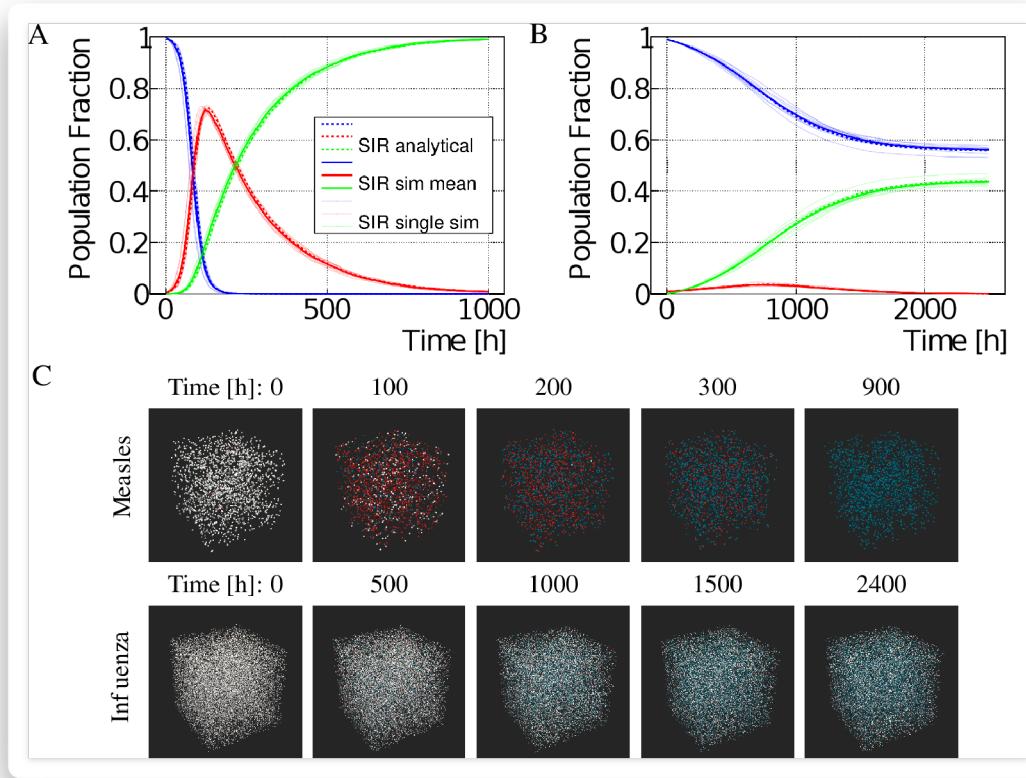
# Cell sorting



# Neuroscience use case

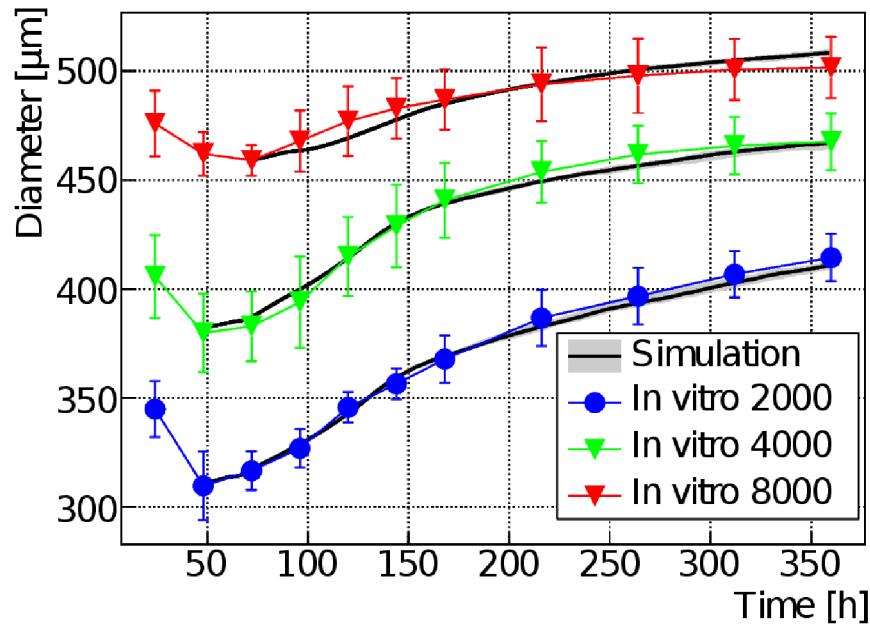


# Epidemiology use case

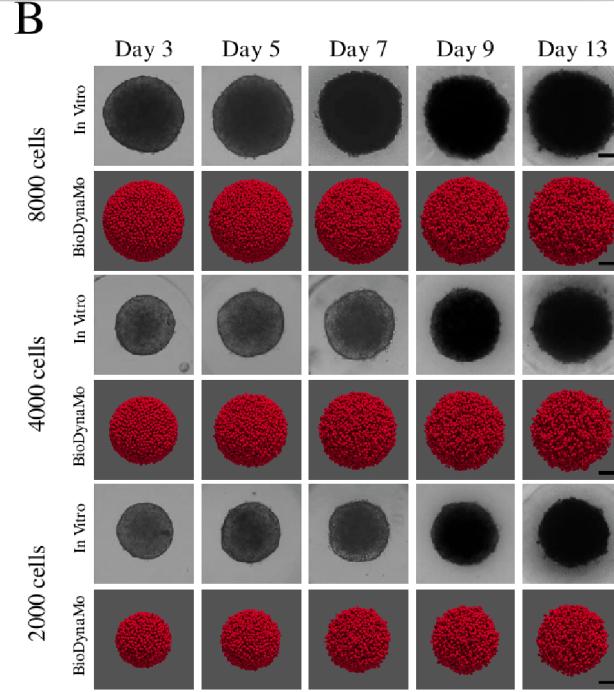


# Oncology use case

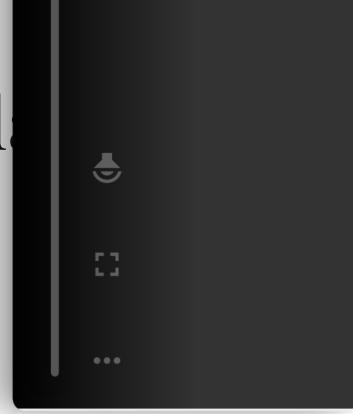
A



B



# Pyramid with video



# Performance data table

**Table 6. Performance data.** The values in column “Agents” and “Diffusion volumes” are taken from the end of the simulation. Runtime measures the wall-clock time to simulate the number of iterations. It excludes the time for simulation setup and visualization.

Simulation	Agents	Diffusion volumes	Iterations	System (Table 5)	Physical CPUs	Runtime	Memory
Neuroscience use case							
Single (Figure 4A in the main manuscript)	1 494	250	500	A	1	0.16 s	382 MB
				D	1	0.12 s	479 MB
Large-scale (Figure 4C in the main manuscript)	9 036 986	65 536	500	A	72	35 s	6.47 GB
				D	2	11 min 28 s	5.37 GB
Very-large-scale	1 018 644 154	5 606 442	500	B	72	1 h 24 min	438 GB
Oncology use case (Figure 5 in the main manuscript)							
2000 initial cells	4 177	0	312	A	1	1.05 s	382 MB
				D	1	0.832 s	480 MB
4000 initial cells	5 341	0	312	A	1	1.76 s	382 MB
				D	1	1.34 s	480 MB
8000 initial cells	7 861	0	288	A	1	3.27 s	384 MB
				D	1	2.60 s	482 MB
Large-scale	1 000 3925	0	288	A	72	1 min 42 s	7.42 GB
				D	2	43 min 56 s	5.84 GB
Very-large-scale	986 054 868	0	288	B	72	6 h 21 min	604 GB
Epidemiology use case (Figure 6C in the main manuscript)							
Measles	2 010	0	1000	A	1	0.53 s	381 MB
				D	1	0.42 s	479 MB
Seasonal Influenza	20 200	0	2500	A	1	16.41 s	383 MB
				D	1	16.40 s	479 GB
Medium-scale (measles)	100 500	0	1000	A	72	1.36 s	1 GB
Large-scale (measles)	10 050 000	0	1000	A	72	59.19 s	5.87 GB
				D	2	19 min 18 s	5.41 GB
Very-large-scale (measles)	1 005 000 000	0	1000	B	72	2 h 0 min	495 GB
Soma clustering (Figure 2)	32 000	1 240 000	6 000	A	72	12.91 s	1.02 GB
				D	2	2 min 7 s	522 MB

# BioDynaMo's GPU offloading capabilities

*Bioinformatics*, 38(2), 2022, 453–460  
doi: 10.1093/bioinformatics/btab649  
Advance Access Publication Date: 16 September 2021  
Original Paper

**OXFORD**

---

**Systems biology**  
**BioDynaMo: a modular platform for high-performance agent-based simulation**

Lukas Breitwieser  <sup>1,2,\*</sup>, Ahmad Hesam <sup>1,3,\*</sup>, Jean de Montigny<sup>1</sup>, Vasileios Vavourakis<sup>4,5</sup>, Alexandros Iosif<sup>4</sup>, Jack Jennings<sup>6</sup>, Marcus Kaiser<sup>6,7,8</sup>, Marco Manca  <sup>9</sup>, Alberto Di Meglio<sup>1</sup>, Zaid Al-Ars<sup>3</sup>, Fons Rademakers<sup>1</sup>, Onur Mutlu<sup>2,10,\*</sup> and Roman Bauer<sup>11,\*</sup>

<sup>1</sup>CERN openlab, IT Department, CERN, Geneva 1211, Switzerland, <sup>2</sup>Department of Computer Science, ETH Zurich, Zurich 8092, Switzerland, <sup>3</sup>Department of Quantum & Computer Engineering, Delft University of Technology, Delft 2628CD, The Netherlands, <sup>4</sup>Department of Mechanical & Manufacturing Engineering, University of Cyprus, Nicosia 2109, Cyprus, <sup>5</sup>Department of Medical Physics & Biomedical Engineering, University College London, London WC1E 6BT, UK, <sup>6</sup>School of Computing, Newcastle University, Newcastle upon Tyne NE4 5TG, UK, <sup>7</sup>Department of Functional Neurosurgery, Ruijin Hospital, Shanghai Jiao Tong University School of Medicine, Shanghai 200025, China, <sup>8</sup>Precision Imaging Beacon, School of Medicine, University of Nottingham, Nottingham NG7 2UH, UK, <sup>9</sup>ScimPulse Foundation, Geleen 6162 BC, The Netherlands, <sup>10</sup>Department of Information Technology and Electrical Engineering, ETH Zurich, Zurich 8092, Switzerland and <sup>11</sup>Department of Computer Science, University of Surrey, Guildford GU2 7XH, UK

\*To whom correspondence should be addressed.  
Associate Editor: Jonathan Wren

Received on February 4, 2021; revised on September 2, 2021; editorial decision on September 3, 2021; accepted on September 13, 2021

## GPU Acceleration of 3D Agent-Based Biological Simulations

Ahmad Hesam  
*ABS group*  
*Delft University of Technology*  
Delft, Netherlands  
a.hesam@tudelft.nl

Lukas Breitwieser  
*CERN openlab*  
*CERN*  
Geneva, Switzerland  
lukas.breitwieser@cern.ch

Fons Rademakers  
*CERN openlab*  
*CERN*  
Geneva, Switzerland  
fons.rademakers@cern.ch

Zaid Al-Ars  
*ABS group*  
*Delft University of Technology*  
Delft, Netherlands  
z.al-ars@tudelft.nl

**Abstract**—Researchers in biology are faced with the tough challenge of developing high-performance computer simulations of their increasingly complex agent-based models. BioDynaMo is an open-source agent-based simulation platform that aims to alleviate researchers from the intricacies that go into the development of high-performance computing. Through a high-level interface, researchers can implement their models on top of BioDynaMo's multi-threaded core execution engine to rapidly develop simulations that effectively utilize parallel computing hardware. In biological agent-based modeling, the type of operations that are typically the most compute-intensive are those that involve agents interacting with their local neighborhood. In this work, we investigate the currently implemented method of handling neighborhood interactions of cellular agents in BioDynaMo, and ways to improve the performance to enable large-scale and complex simulations. We propose to replace the kd-tree implementation to find and iterate over the neighborhood of each agent with a uniform grid method that allows us to take advantage of the massively parallel architecture of graphics processing units (GPUs). We implement the uniform grid method in both CUDA and OpenCL to address GPUs from all major vendors and evaluate several techniques to further improve the performance. Furthermore, we analyze the performance of our implementations for models with a varying density of neighboring agents. As a result, the performance of the mechanical interactions method improved by up to two orders of magnitude in comparison to the multithreaded baseline version. The implementations are open-source and publicly available on GitHub.

**Index Terms**—agent-based modeling, simulation, GPU, co-processing, biological models, acceleration

becoming increasingly more parallelized as a result of Dennard scaling [4] and the stagnation of Moore's law [5], as pointed out in [6]. Moreover, general-purpose computing on graphics processing units (GPUs) is an attractive solution to improve the computational efficiency of ABS applications in particular [7], [8], and parallel applications in general [9], [10]. By porting applications to, either fully or partially, run on GPUs it is possible to observe speedups of several orders of magnitude in comparison to the CPU-only execution [11]. Although several ABS frameworks exist that achieve significant speedups using GPUs in the field of ABS, there is still significant room for improvement, which we wish to address in this article.

BioDynaMo [6] is an open-source software platform for life scientists for simulating biological agent-based models. Each agent in BioDynamO is programmed to follow a specified set of rules, imposed by the modeler, that can trigger specified actions affecting itself or other agents. Agents in biological systems often interact with their local environment, and their behavior can be influenced by other agents that reside within a certain range. An example is the mechanical interactions a cellular agent undergoes when it physically collides with another agent. Local interactions are an extremely important concept in biological systems since it is the driving force behind key biological processes, such as tissue development [12].

BioDynaMo is fully parallelized using OpenMP and its

- Lukas Breitwieser et al., 2022, DOI: 10.1093/bioinformatics/btab649
- Ahmad Hesam et al., 2021, DOI: 10.1109/IPDPSW52791.2021.00040