

ACCELERATED KINETIC MONTE CARLO SIMULATIONS OF ATOMISTICALLY- RESOLVED RESISTIVE MEMORY ARRAYS

Manasa Kaniselvan*, **Alexander Maeder***, Marko Mladenović,
Mathieu Luisier, Alexandros Nikolaos Ziogas

Date: Thursday, 21 November

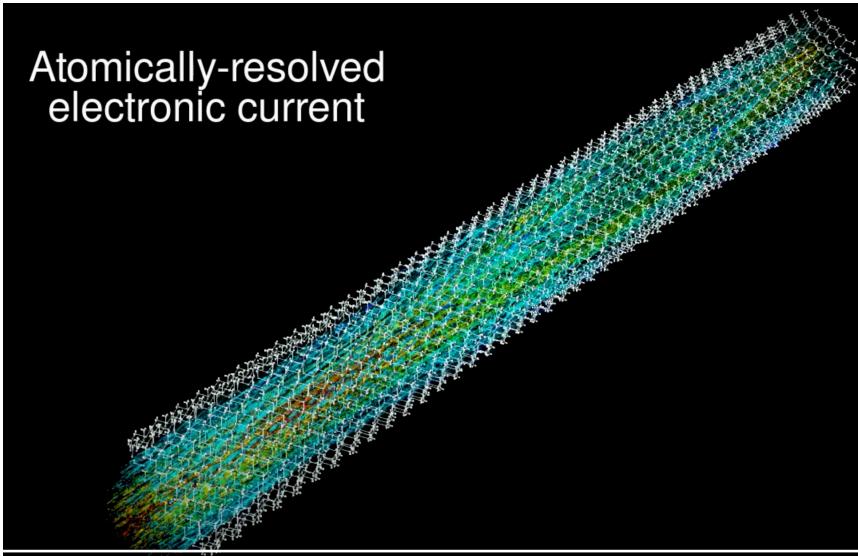
Time: 1:30pm - 2pm EST

Place: Georgia World Congress Centre, room B311

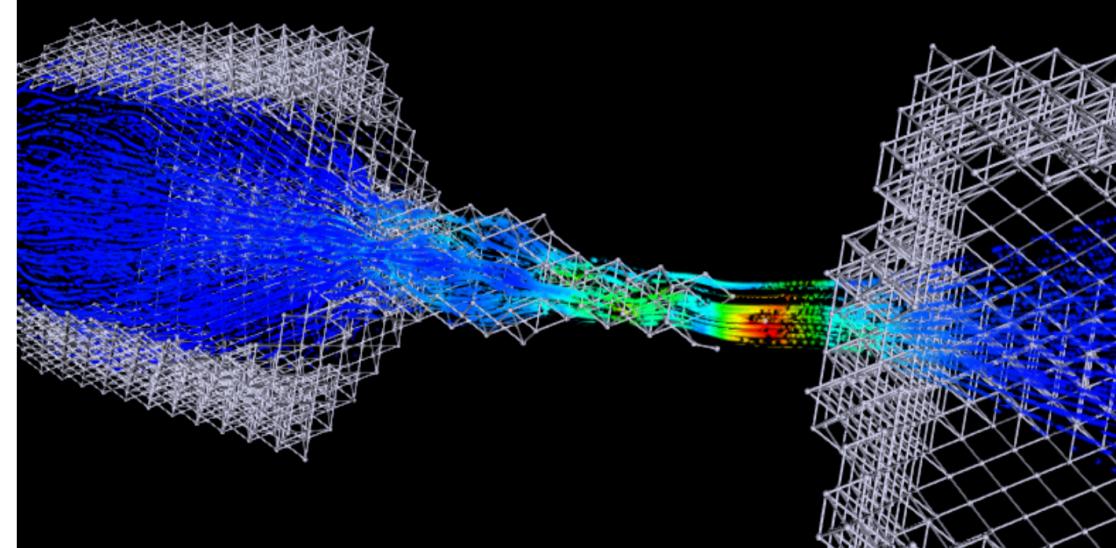


COMPUTATIONAL NANOELECTRONICS

Examples



Current through a nanotube transistor



Current through a conductive bridging RAM cell

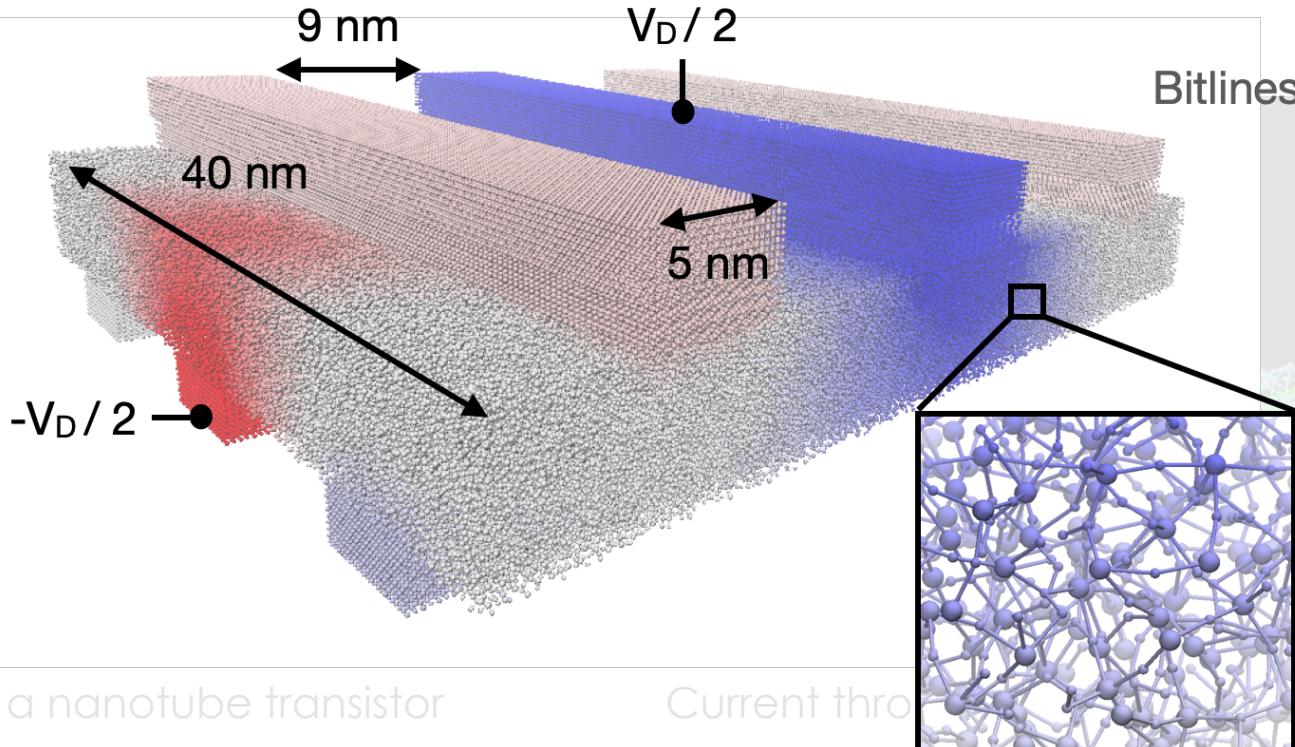
→ Developing specialized simulations for modern semiconductor devices



COMPUTATIONAL NANOELECTRONICS

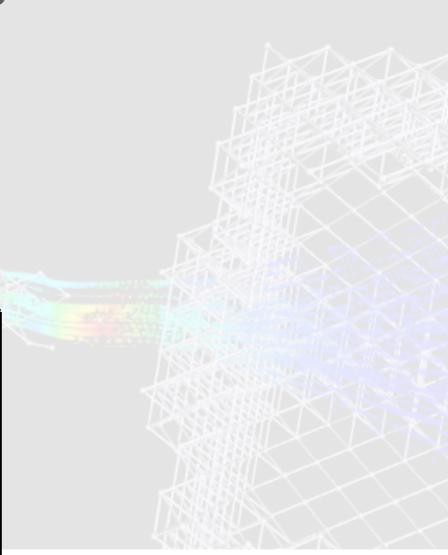
Examples

Atomically-resolved
electronic current



Current through a nanotube transistor

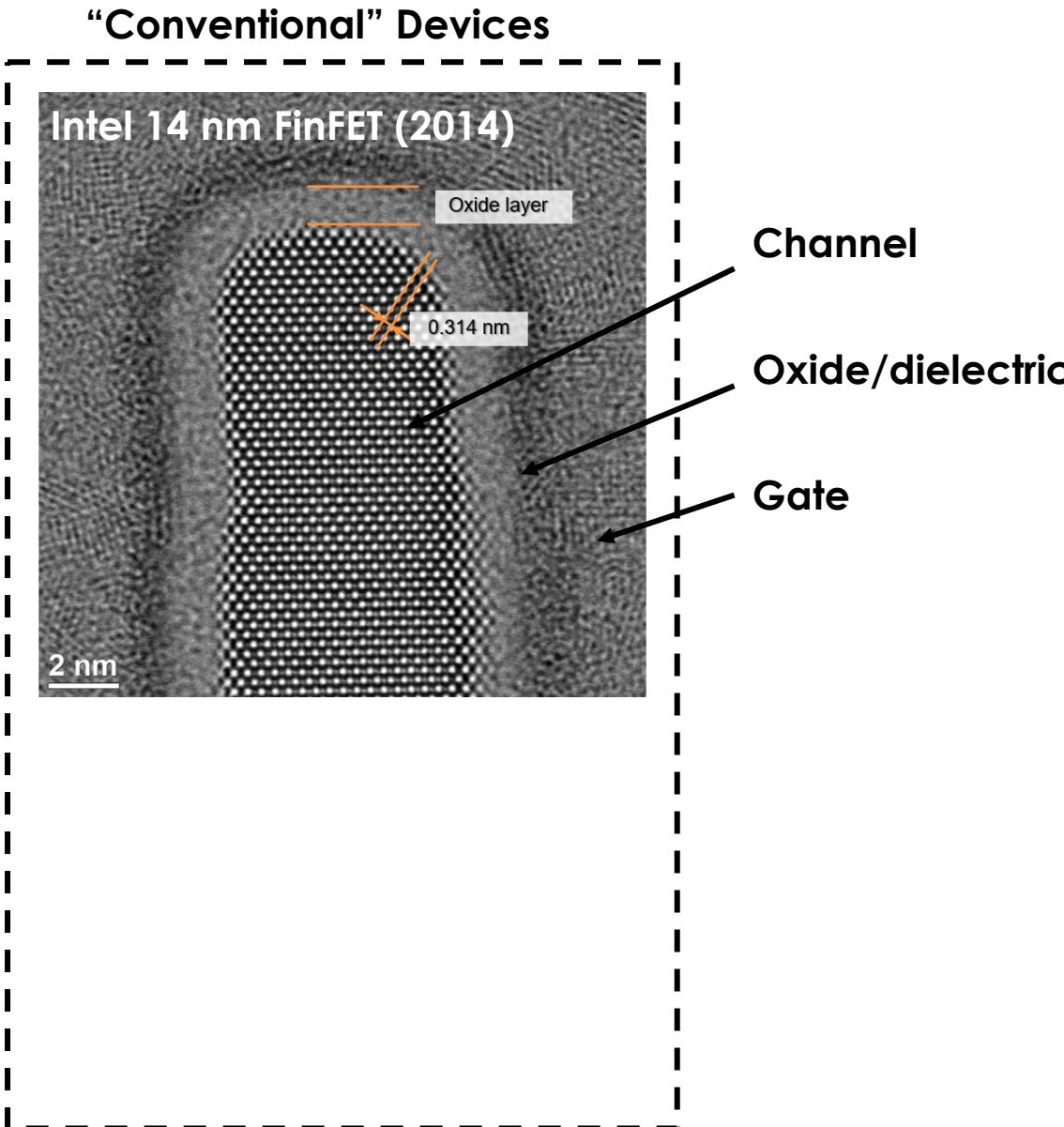
Current through a bridging RAM cell



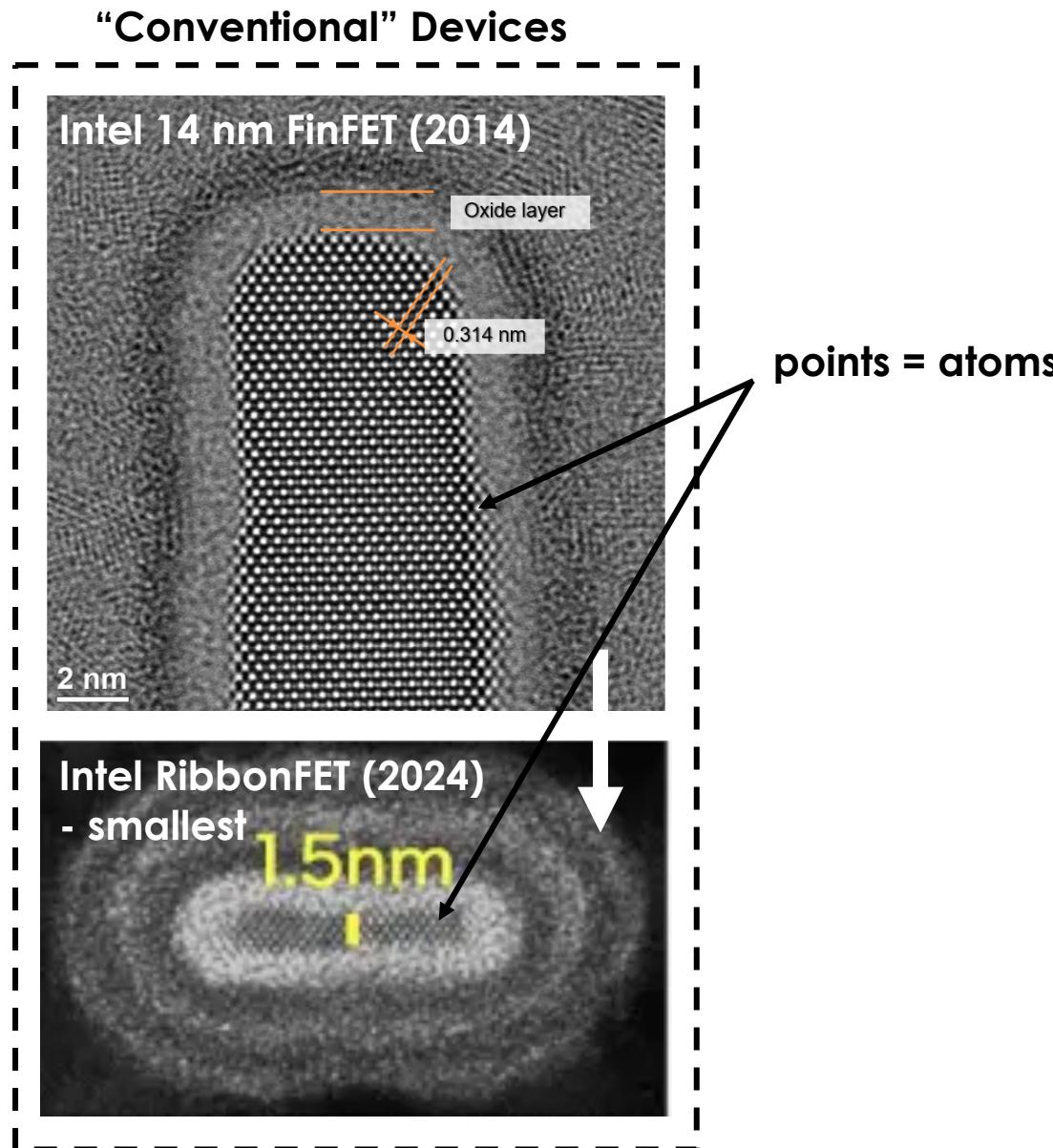
→ Developing specialized simulations for modern semiconductor devices



THE SCALE OF MODERN SEMICONDUCTOR DEVICES

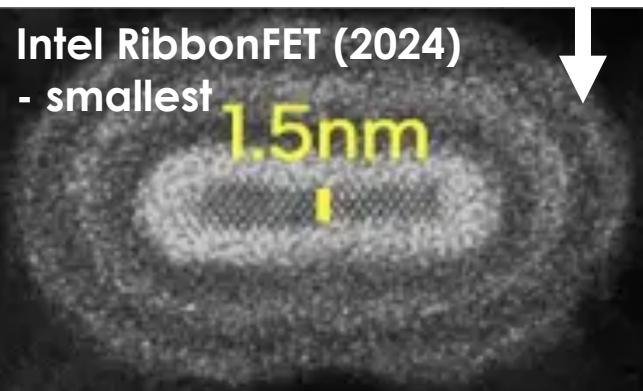
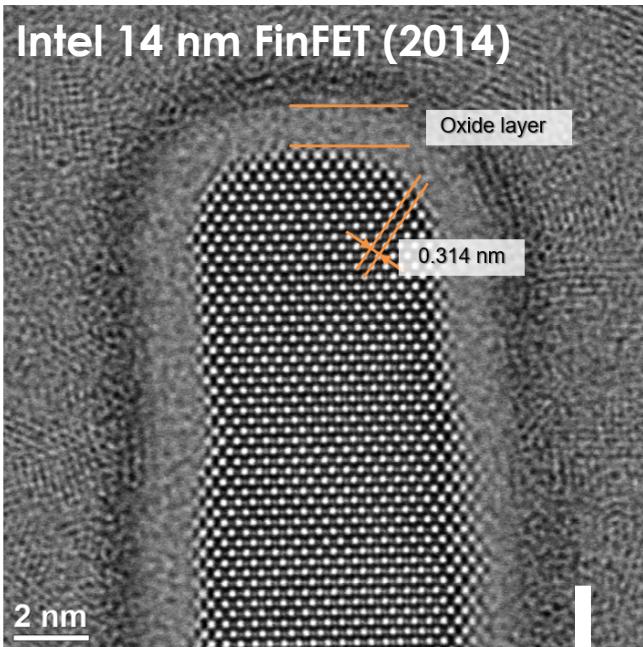


THE SCALE OF MODERN SEMICONDUCTOR DEVICES

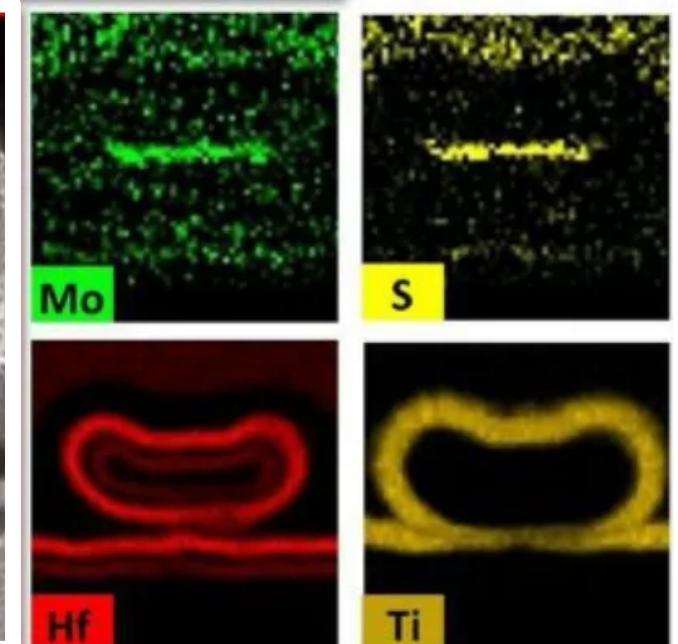
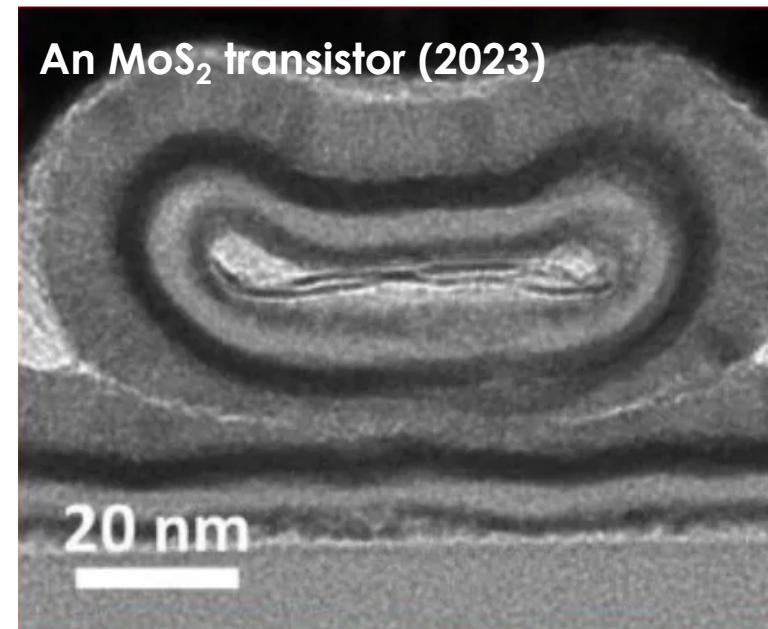


THE SCALE OF MODERN SEMICONDUCTOR DEVICES

“Conventional” Devices

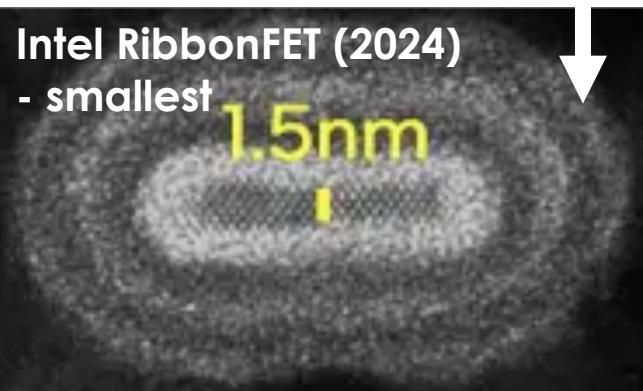
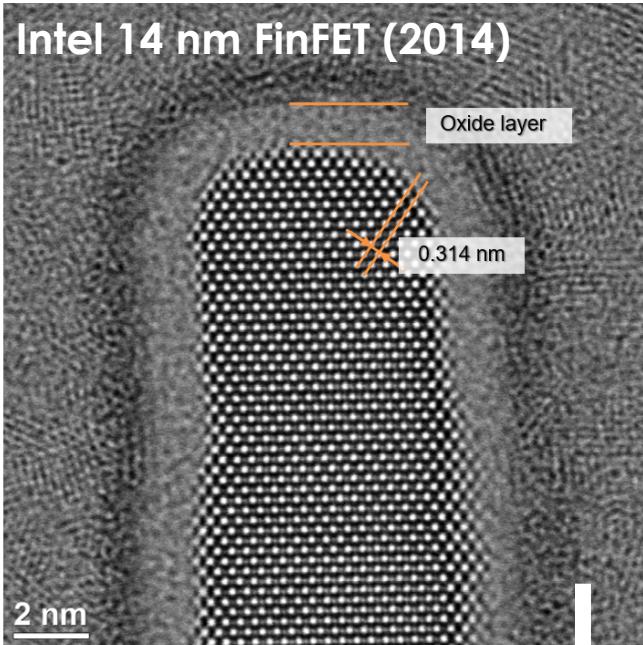


“Emerging” Devices

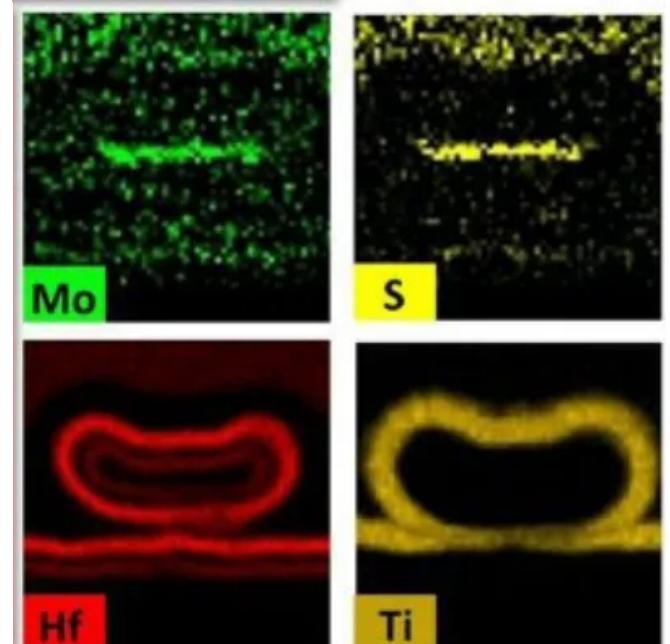
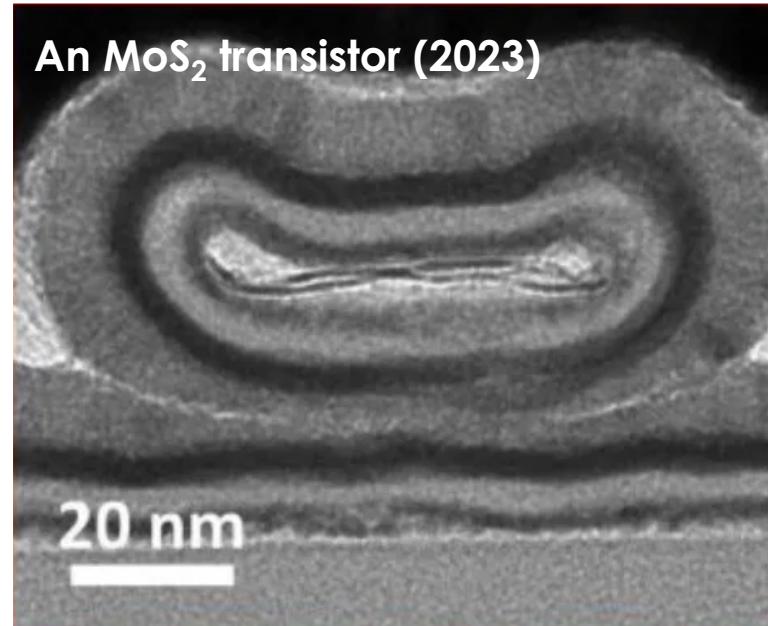


THE SCALE OF MODERN SEMICONDUCTOR DEVICES

“Conventional” Devices



“Emerging” Devices

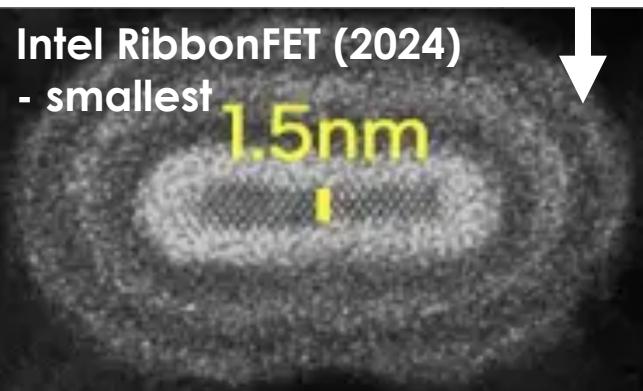
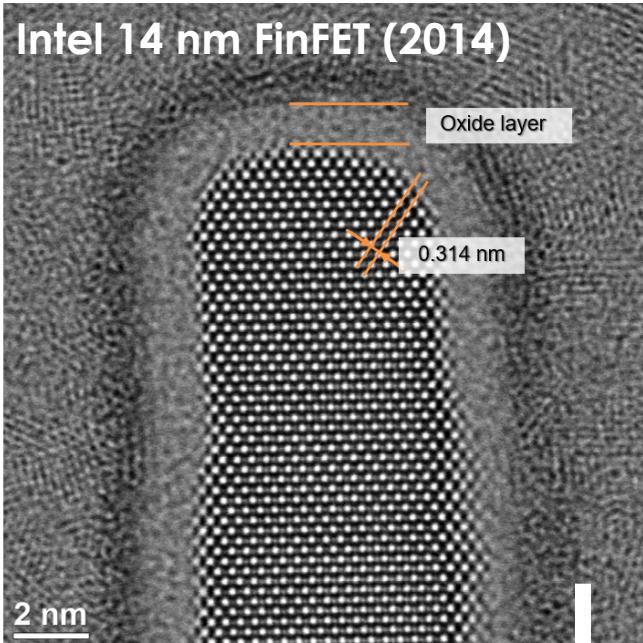


→ Electronic devices can no longer be described using a continuous description of materials

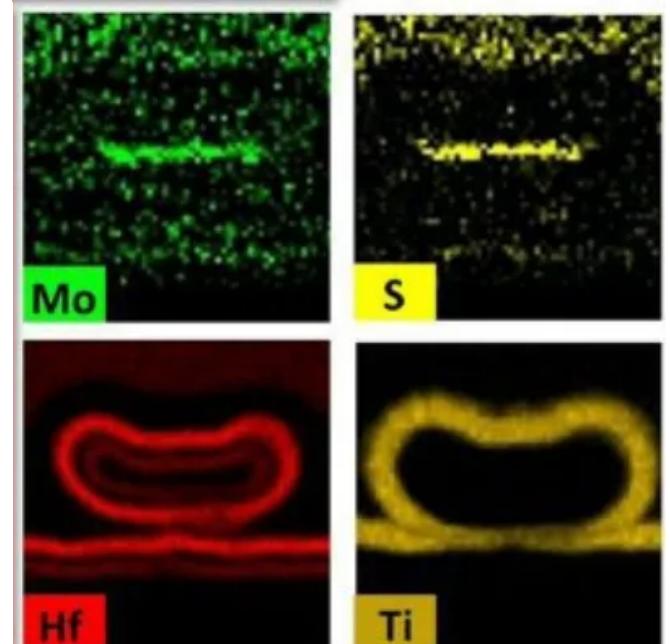
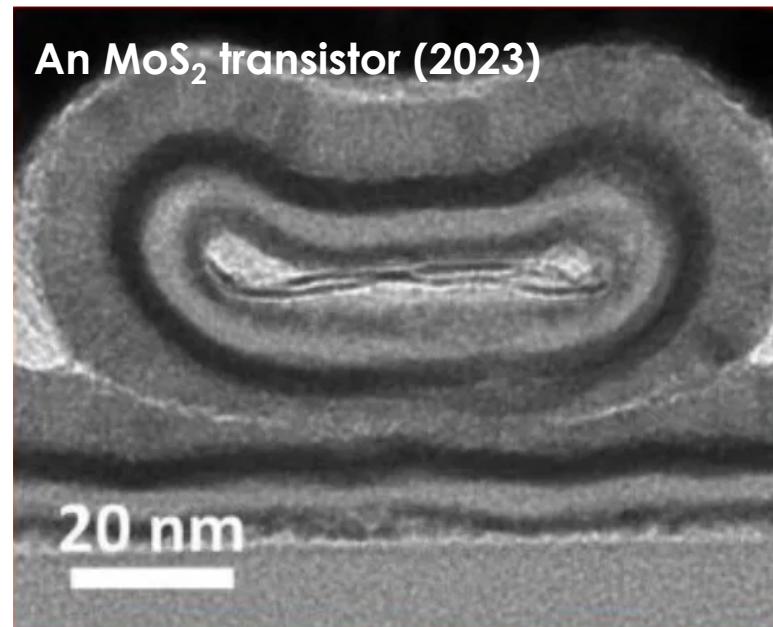


THE SCALE OF MODERN SEMICONDUCTOR DEVICES

"Conventional" Devices



"Emerging" Devices



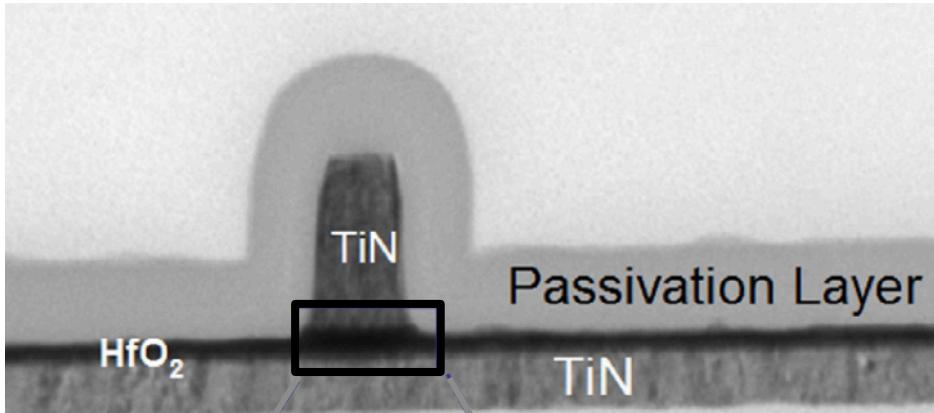
→ Electronic devices can no longer be described using a continuous description of materials

→ The concept of a 'material' with given macroscopic properties no longer holds at these scales



BACKGROUND: NANOIONIC RESISTIVE MEMORY

TiN-HfO₂/Hf-TiN device cross-section

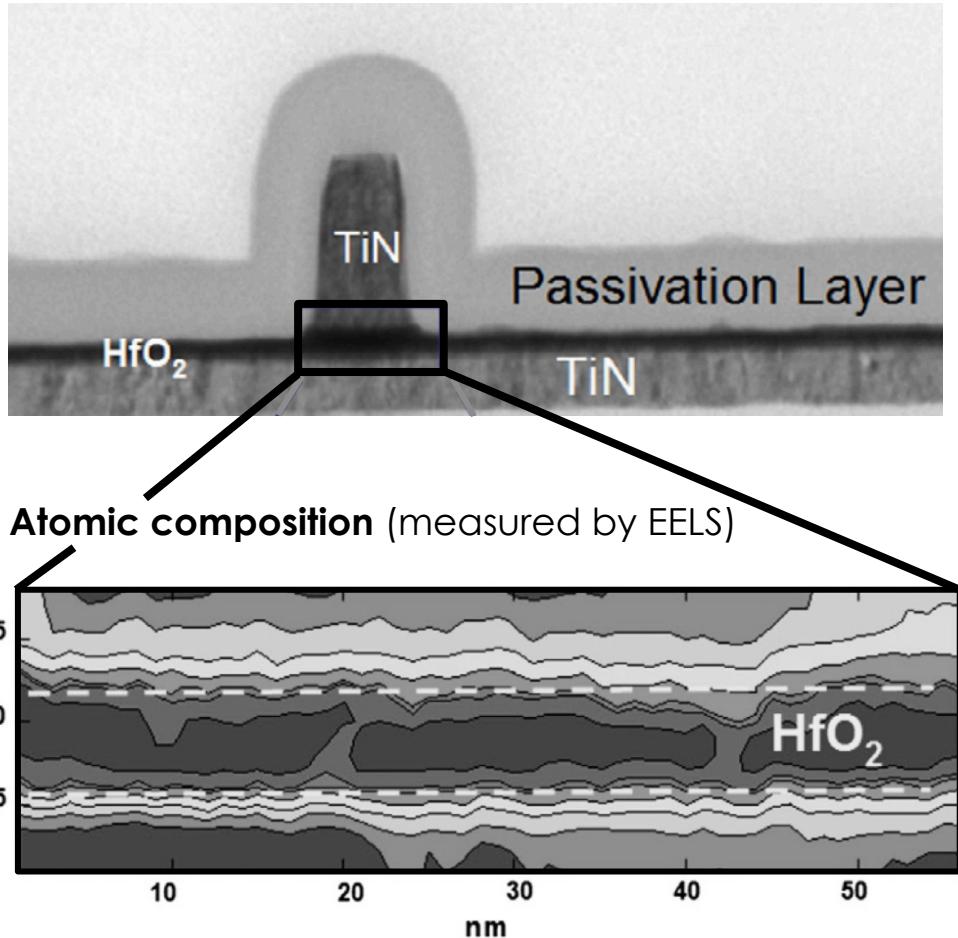


Privitera, S. et. al. (2015) "Conductive filament structure in HfO₂ resistive switching memory devices," Solid State Physics



BACKGROUND: NANOIONIC RESISTIVE MEMORY

TiN-HfO₂/Hf-TiN device cross-section

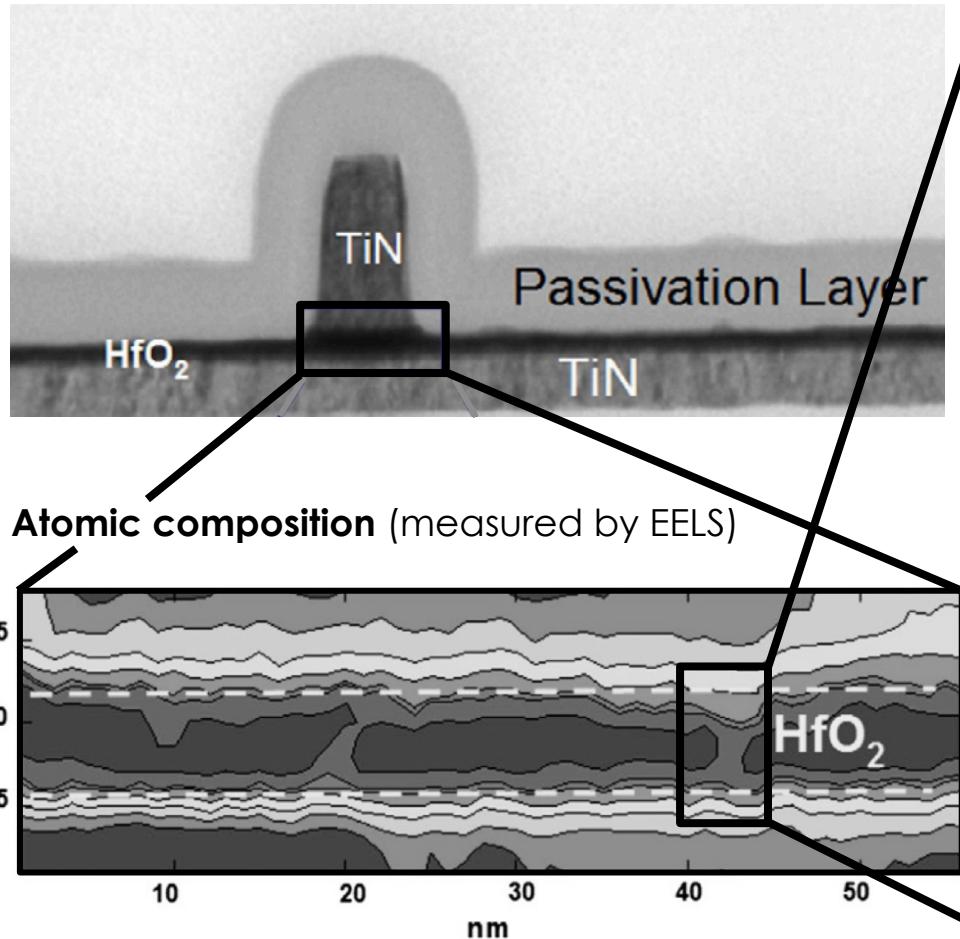


Privitera, S. et. al. (2015) "Conductive filament structure in HfO₂ resistive switching memory devices," *Solid State Physics*

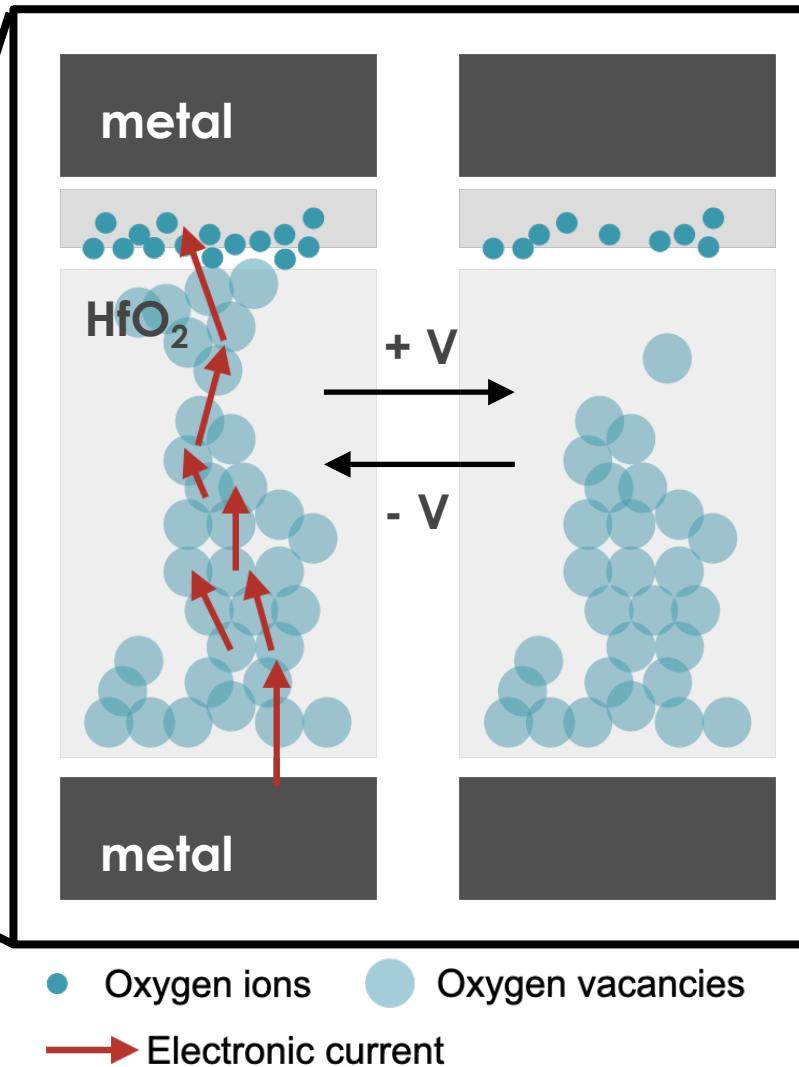


BACKGROUND: NANOIONIC RESISTIVE MEMORY

TiN-HfO₂/Hf-TiN device cross-section



Reversible voltage-controlled resistance

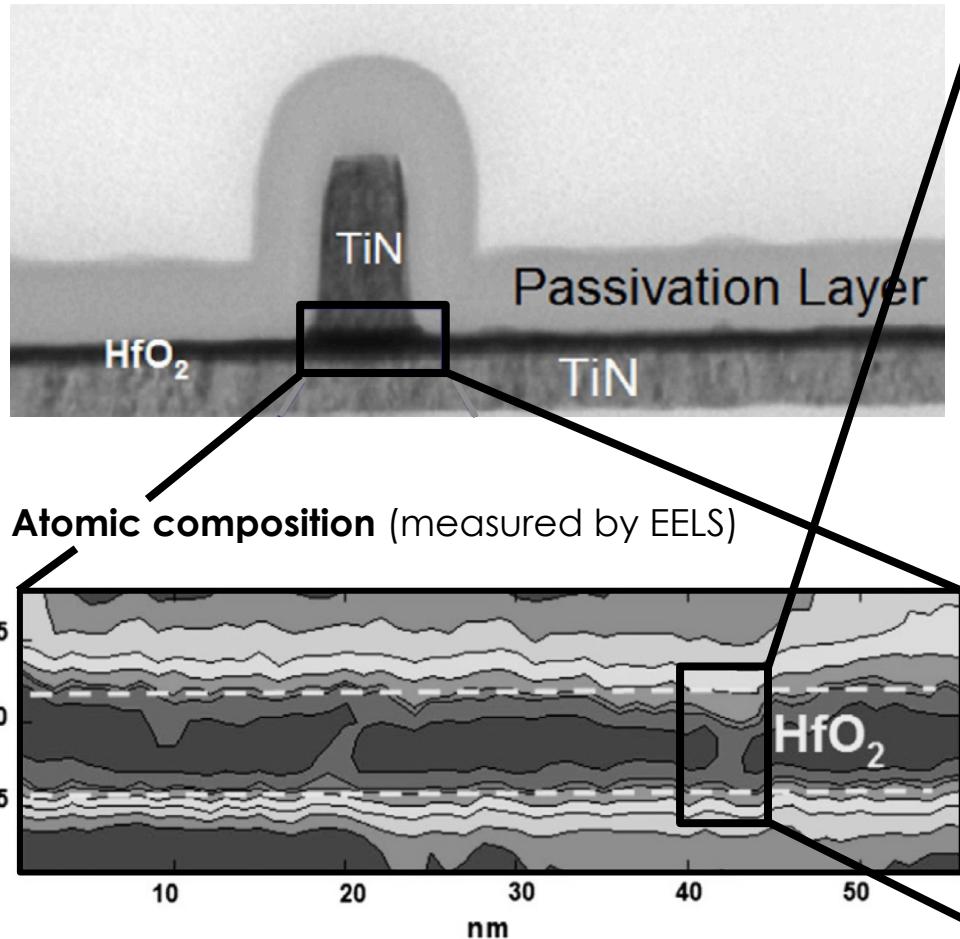


Privitera, S. et. al. (2015) "Conductive filament structure in HfO₂ resistive switching memory devices," *Solid State Physics*

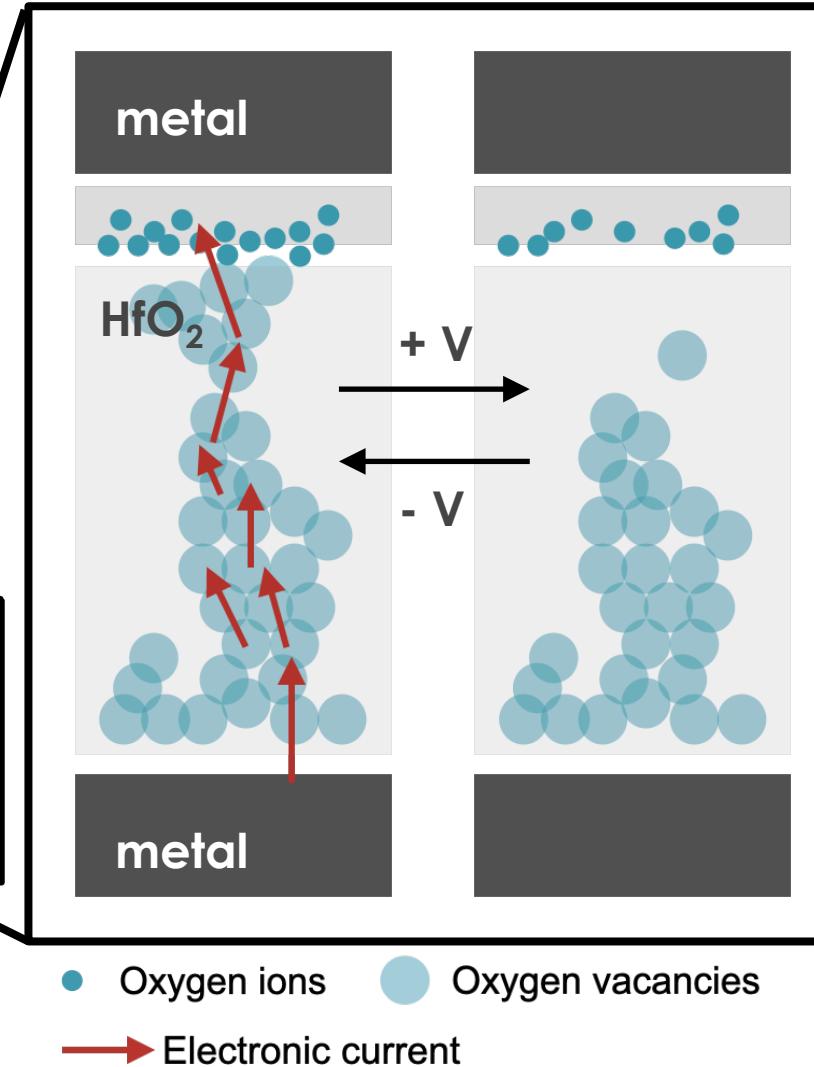


BACKGROUND: NANOIONIC RESISTIVE MEMORY

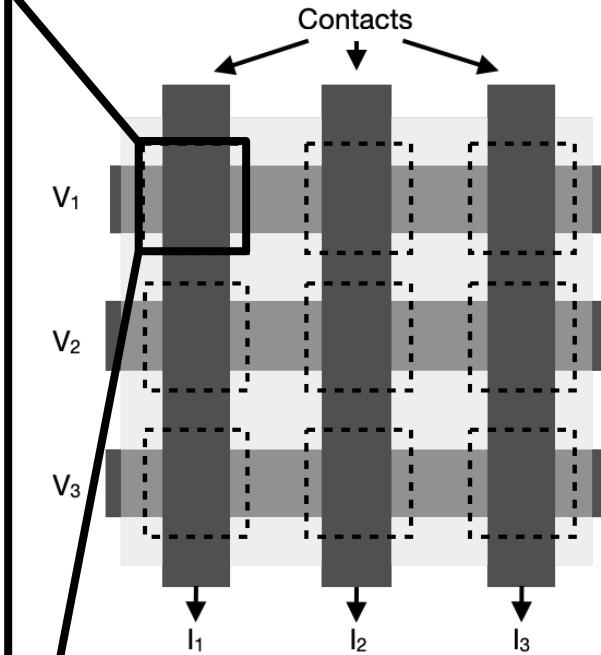
TiN-HfO₂/Hf-TiN device cross-section



Reversible voltage-controlled resistance



Random Access Arrays



Applications in

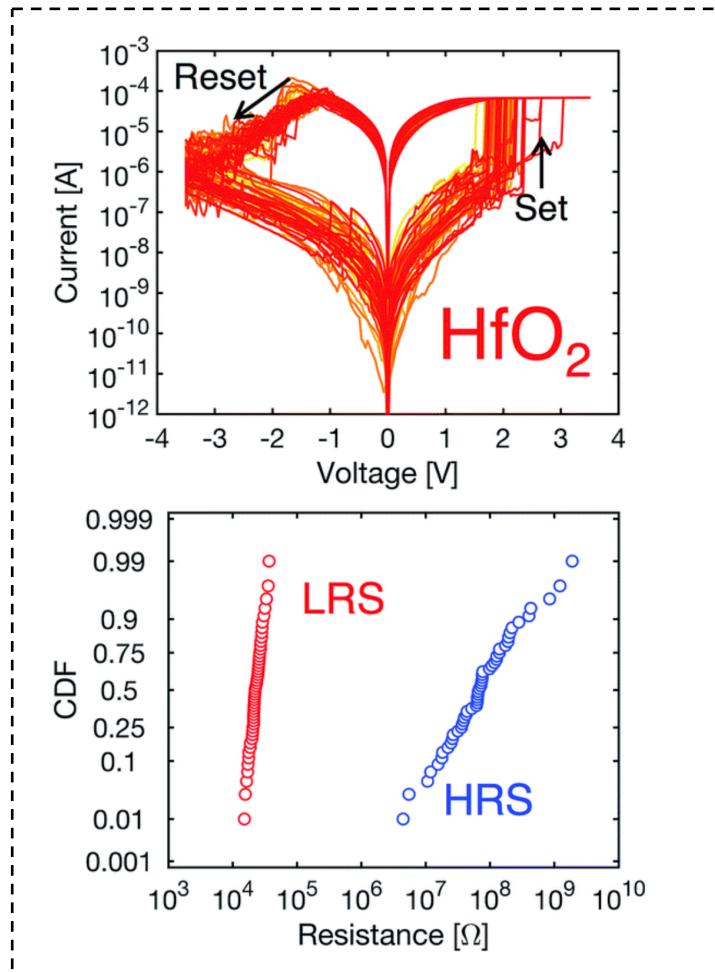
- Compute in memory
- AI hardware accelerators

Privitera, S. et. al. (2015) "Conductive filament structure in HfO₂ resistive switching memory devices," *Solid State Physics*



BACKGROUND: NANOIONIC RESISTIVE MEMORY

Variability

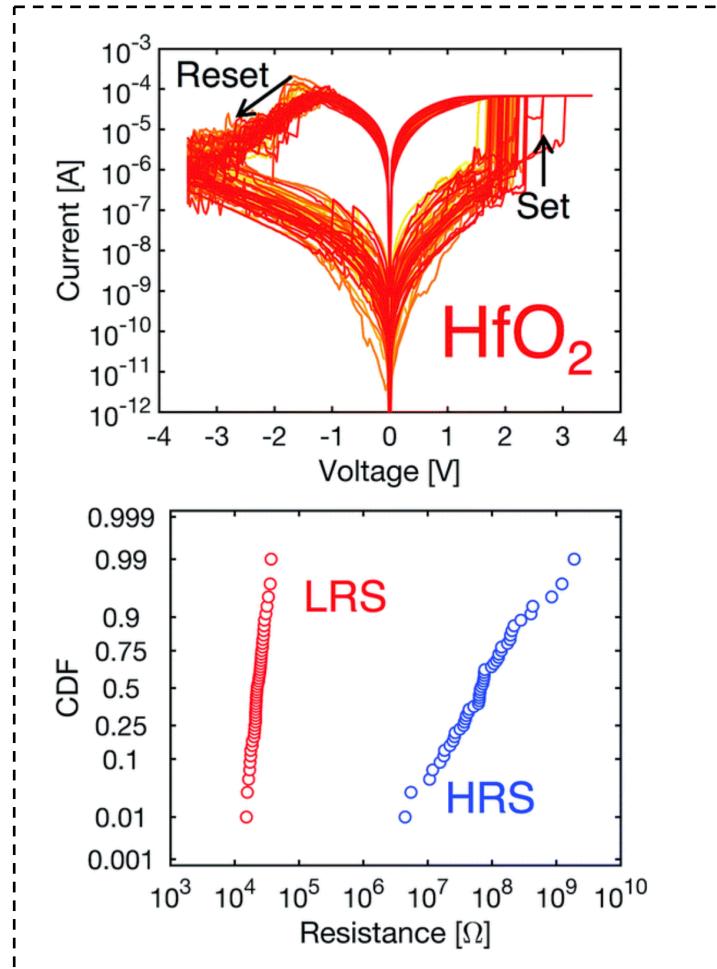


Ambrosi et al, "Impact of oxide and electrode materials on the switching characteristics of oxide ReRAM devices", Faraday Discuss.



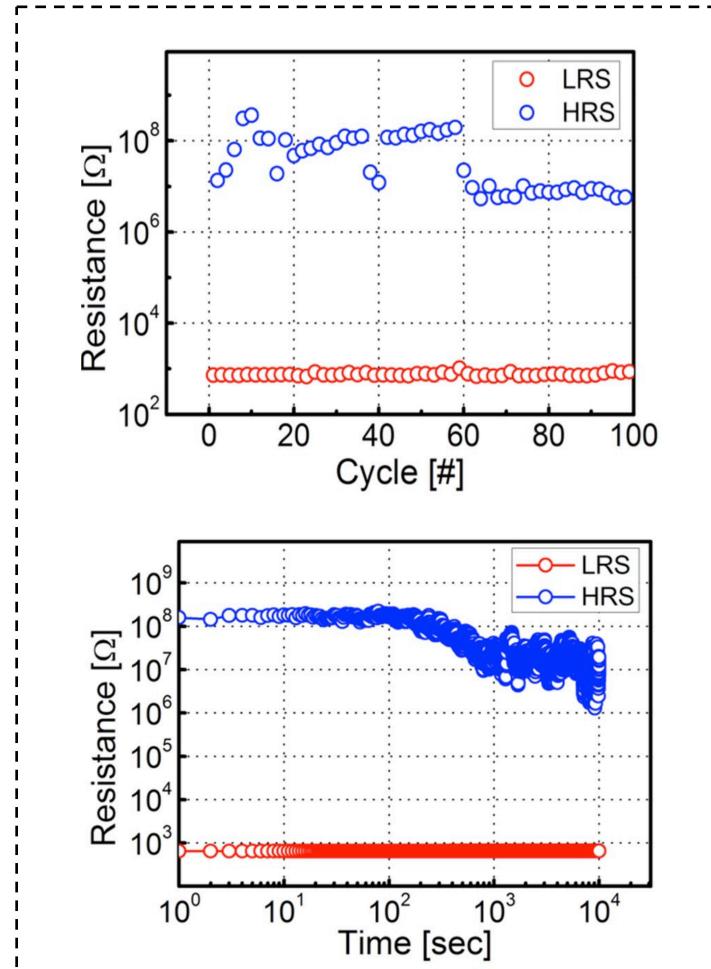
BACKGROUND: NANOIONIC RESISTIVE MEMORY

Variability



Ambrosi et al, "Impact of oxide and electrode materials on the switching characteristics of oxide ReRAM devices", Faraday Discuss.

Retention

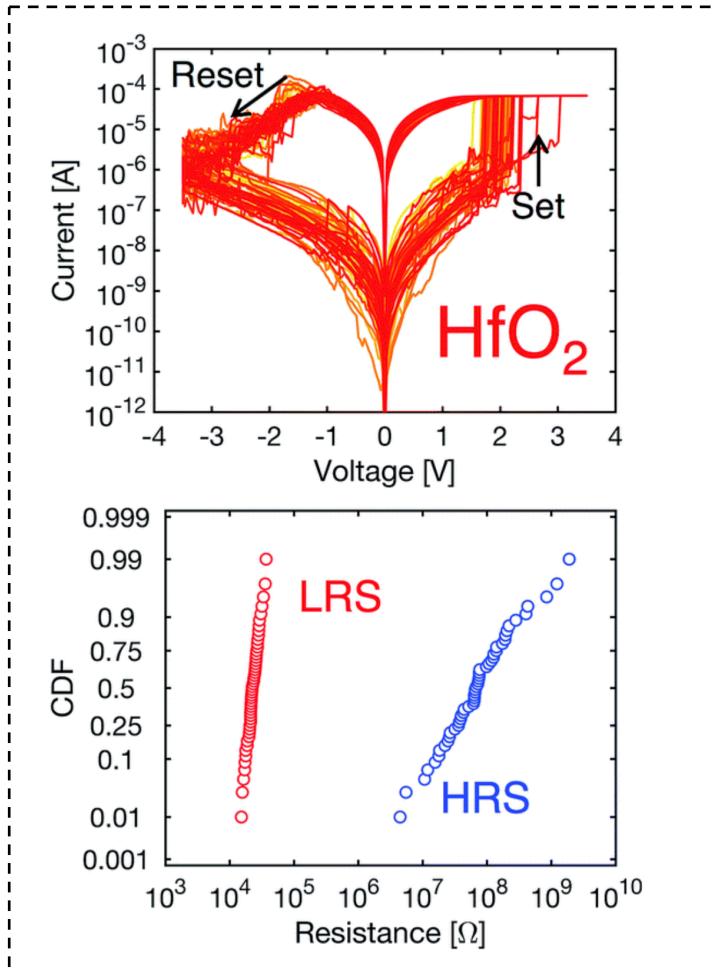


Ha et al, "Effect of Annealing Environment on the Performance of Sol-Gel-Processed ZrO₂ RRAM", Electronics

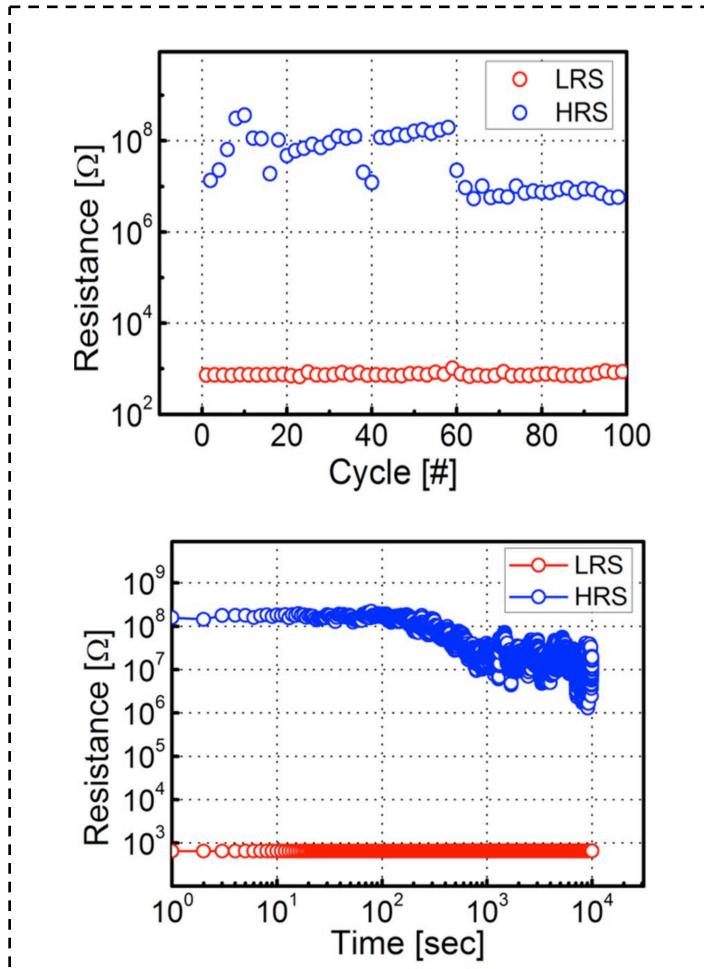


BACKGROUND: NANOIONIC RESISTIVE MEMORY

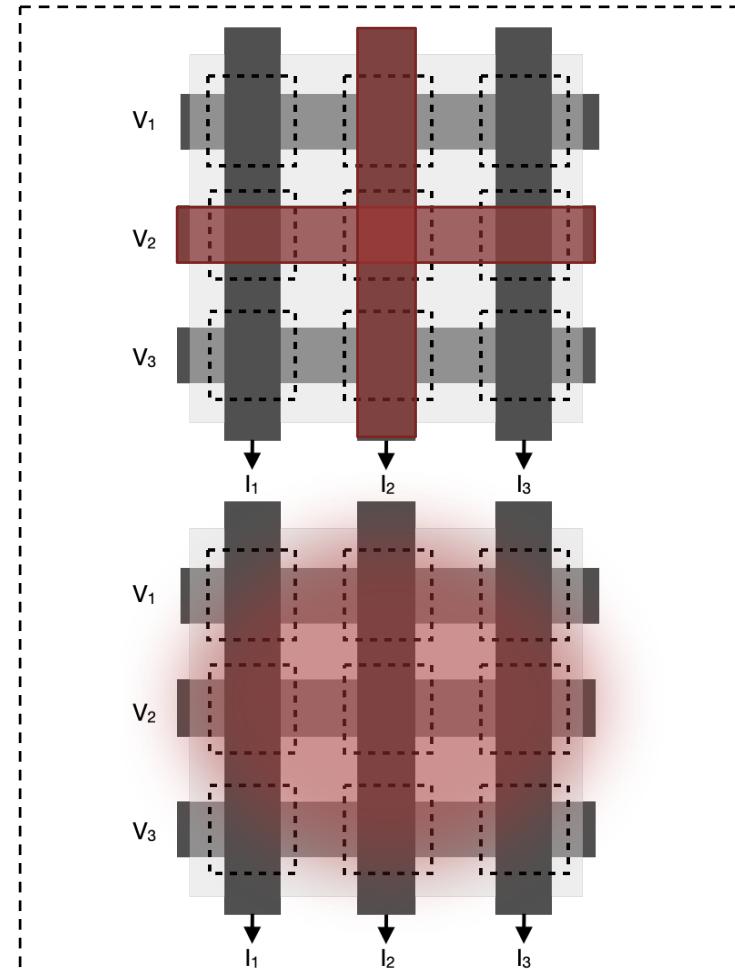
Variability



Retention



Crosstalk

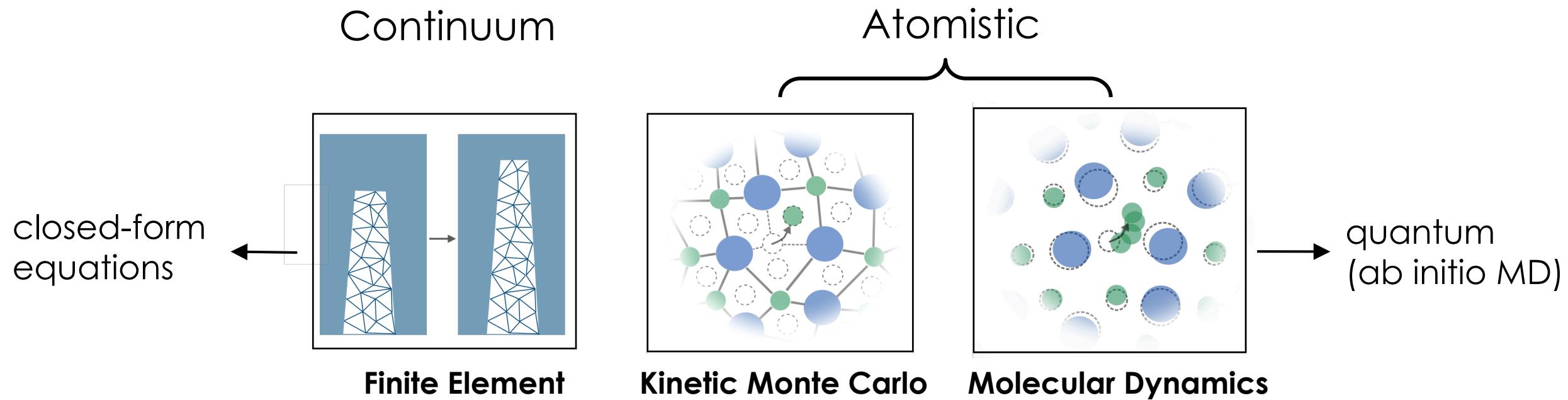


Ambrosi et al, "Impact of oxide and electrode materials on the switching characteristics of oxide ReRAM devices", Faraday Discuss.

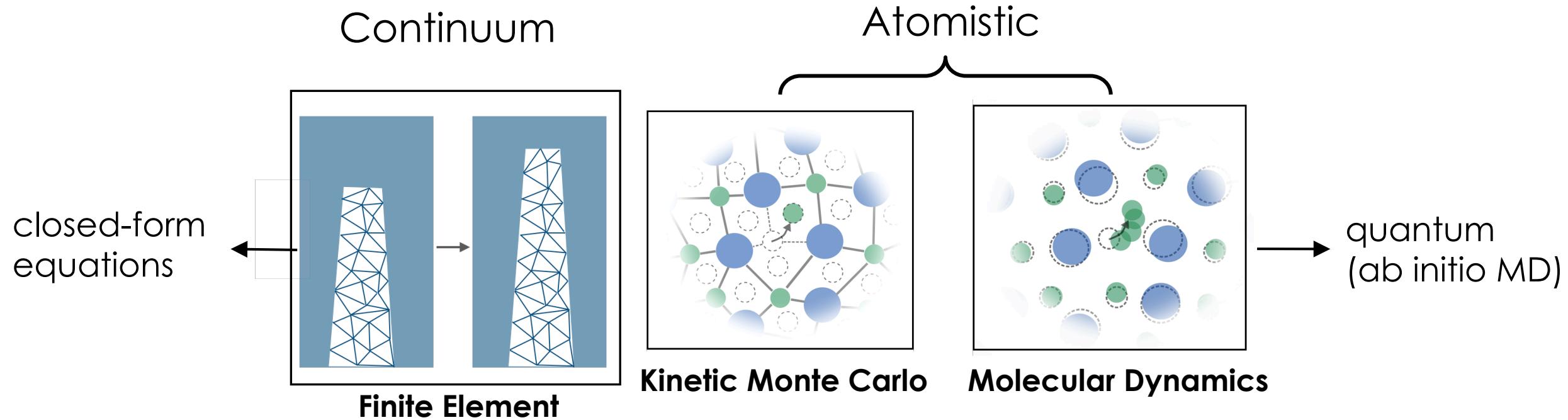
Ha et al, "Effect of Annealing Environment on the Performance of Sol-Gel-Processed ZrO_2 RRAM", Electronics



DEVICE SIMULATIONS: LEVELS OF THEORY



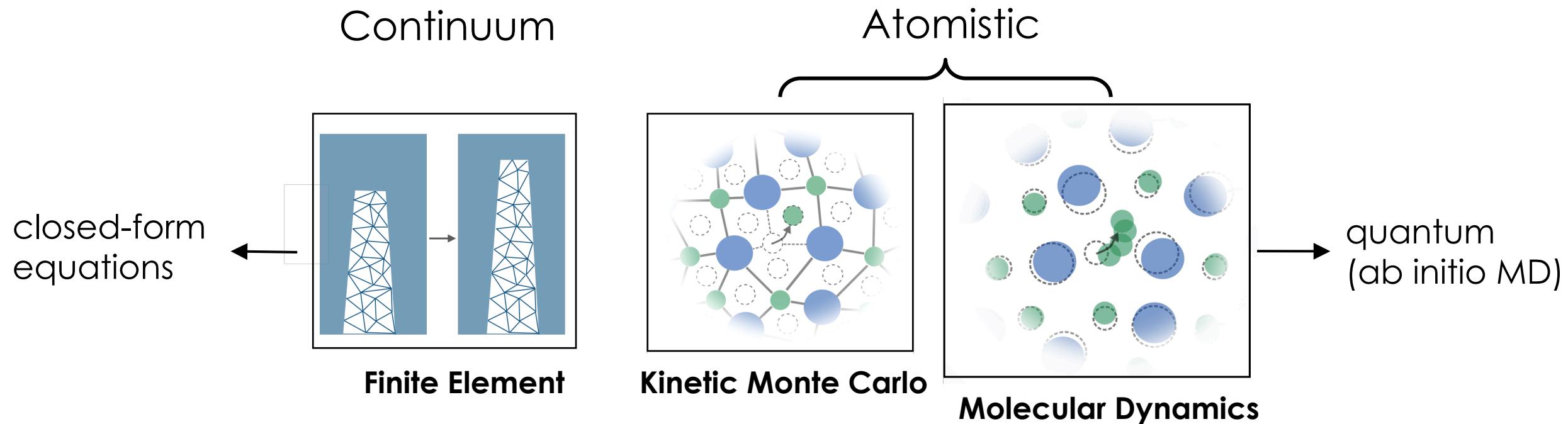
DEVICE SIMULATIONS: LEVELS OF THEORY



- Inaccurate down at the nanoscale



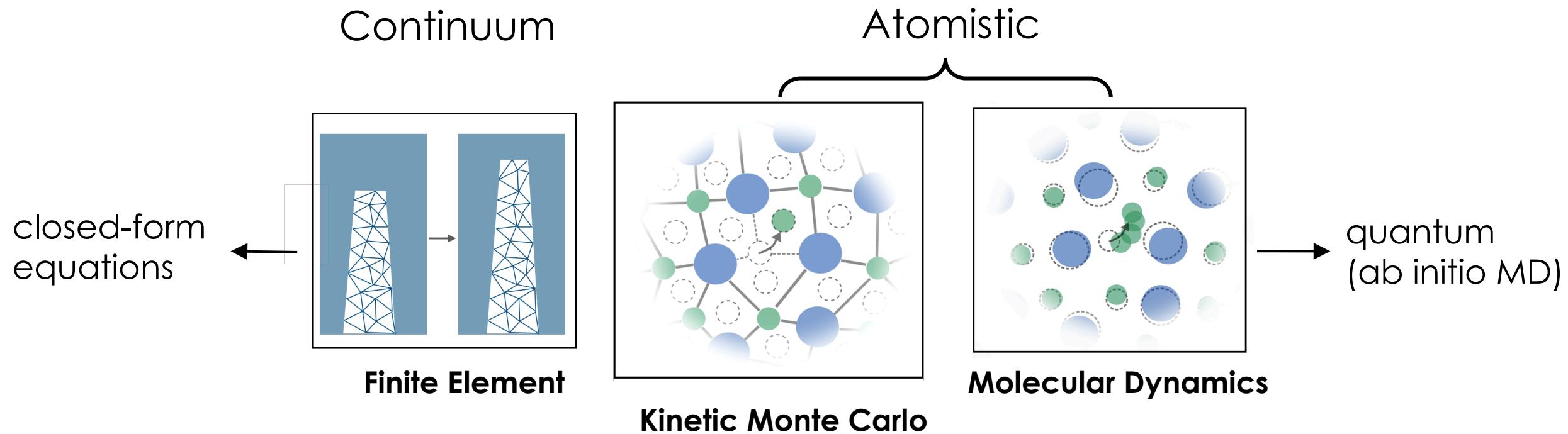
DEVICE SIMULATIONS: LEVELS OF THEORY



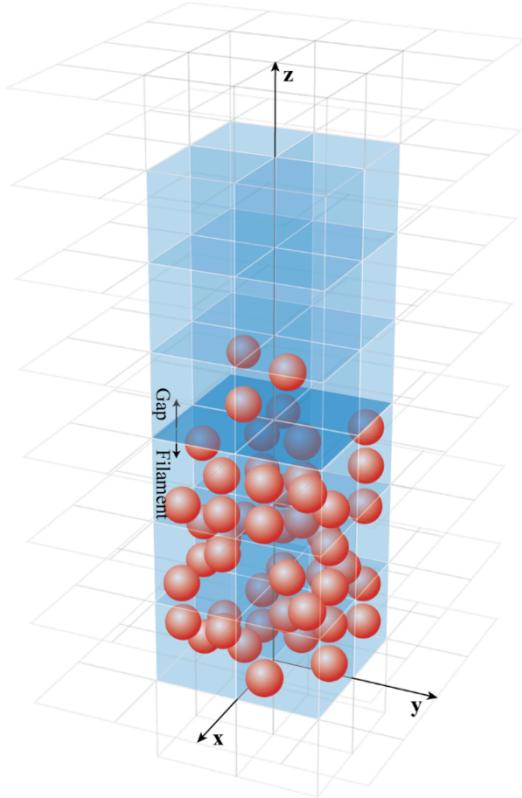
- Unaffordable up to the nanoscale



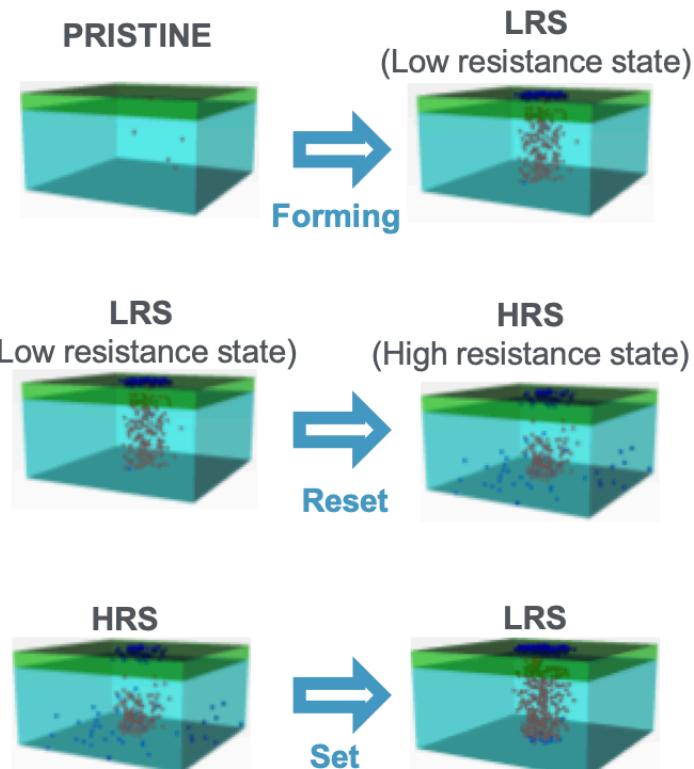
DEVICE SIMULATIONS: LEVELS OF THEORY



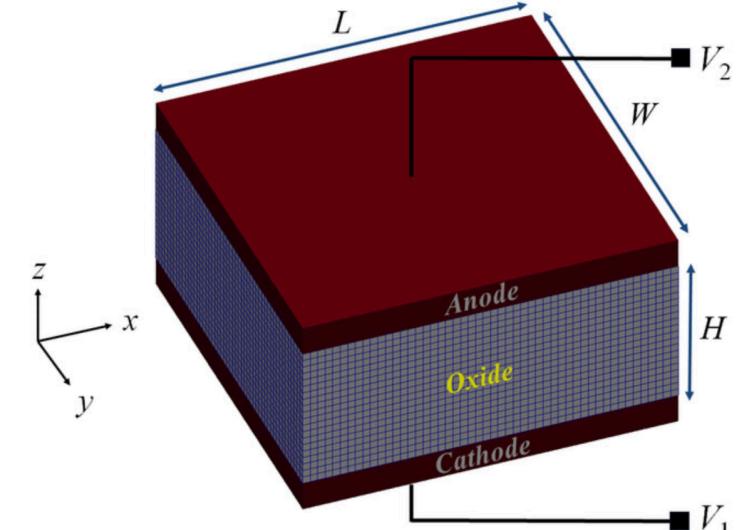
PREVIOUS SMALL-SCALE APPLICATIONS



Retention model for RRAM,
Nils Kopperberg et al



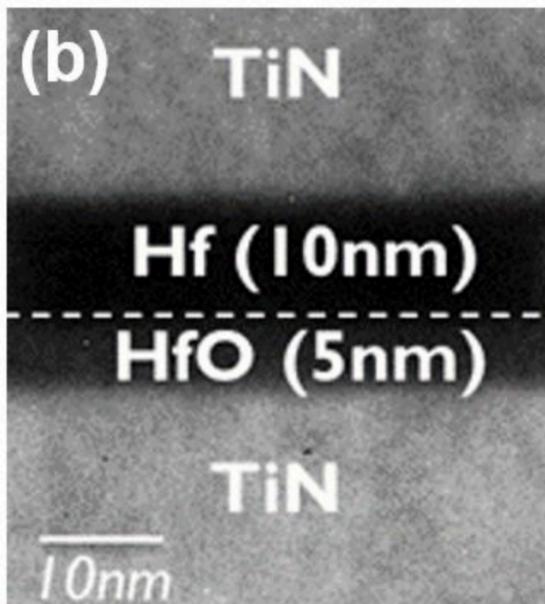
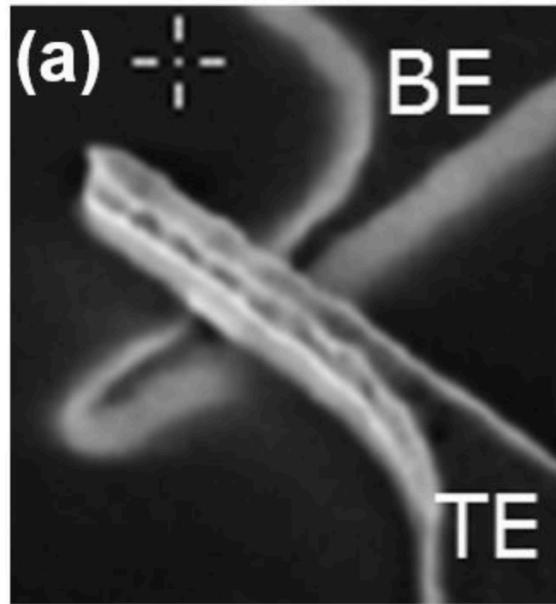
Part of the Ginestra Software Suite,
Applied Materials



Investigation of Resistance Switching in SiO_x RRAM
Cells Using a 3D Multi-Scale Kinetic Monte Carlo
Simulator



DEVICE → ATOMS: RELEVANT DOMAIN SIZES



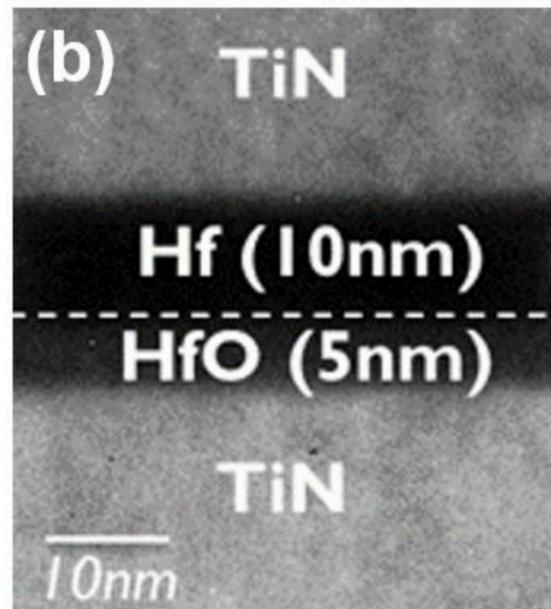
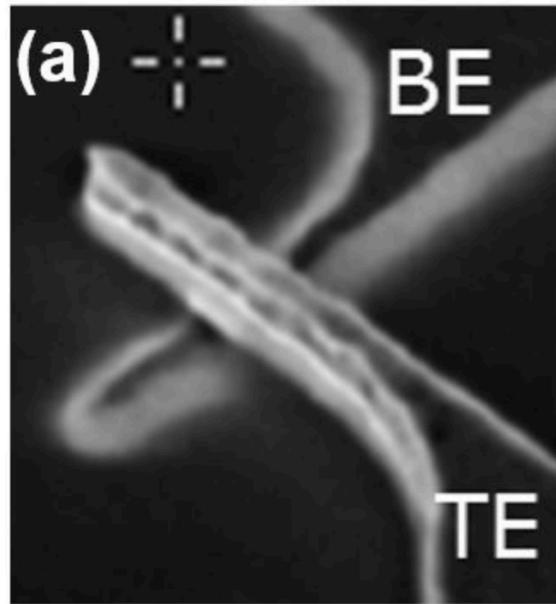
IEDM, 2011

Each device: 10 nm x 10 nm x 5 nm

Govoreanu et al, "10×10nm² Hf/HfOx crossbar resistive RAM with excellent performance, reliability and low-energy operation", IEDM 2011



DEVICE → ATOMS: RELEVANT DOMAIN SIZES



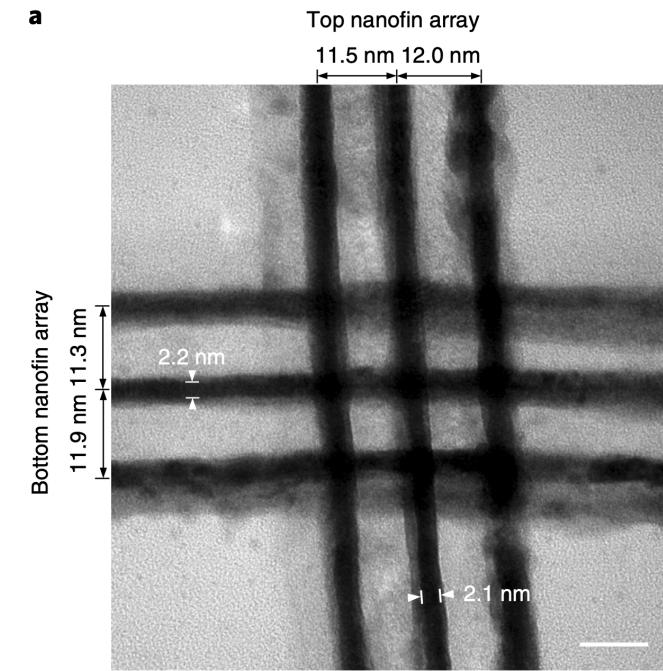
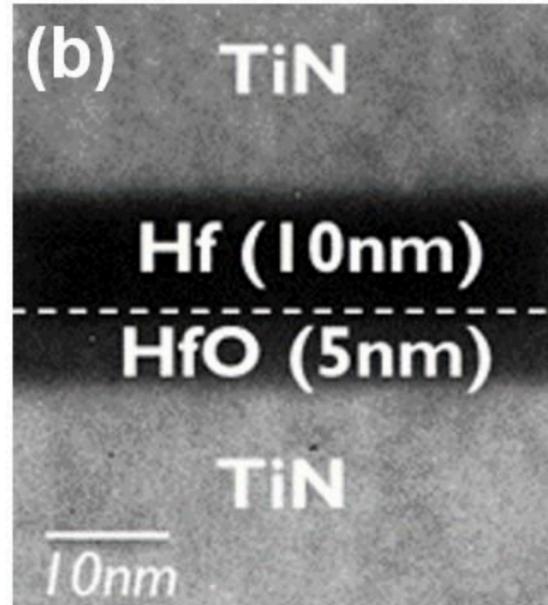
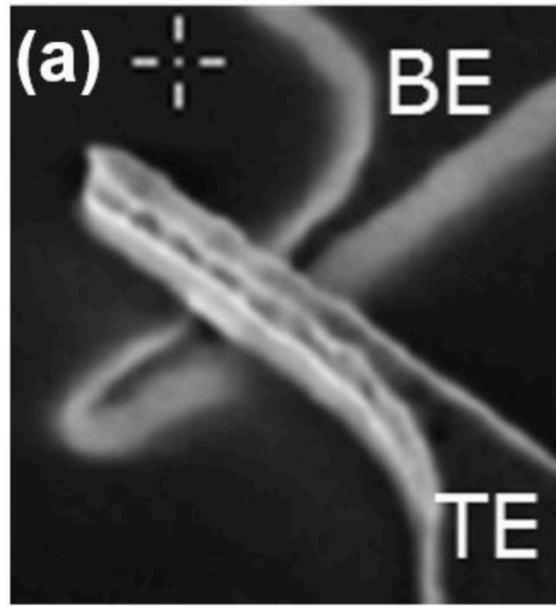
IEDM, 2011

Each device: 10 nm x 10 nm x 5 nm

~100k atoms



DEVICE → ATOMS: RELEVANT DOMAIN SIZES



Each device: ~5K atoms
Entire array: ~1M atoms



→ A driven-KMC approach to simulate the kinetics of resistive memory devices

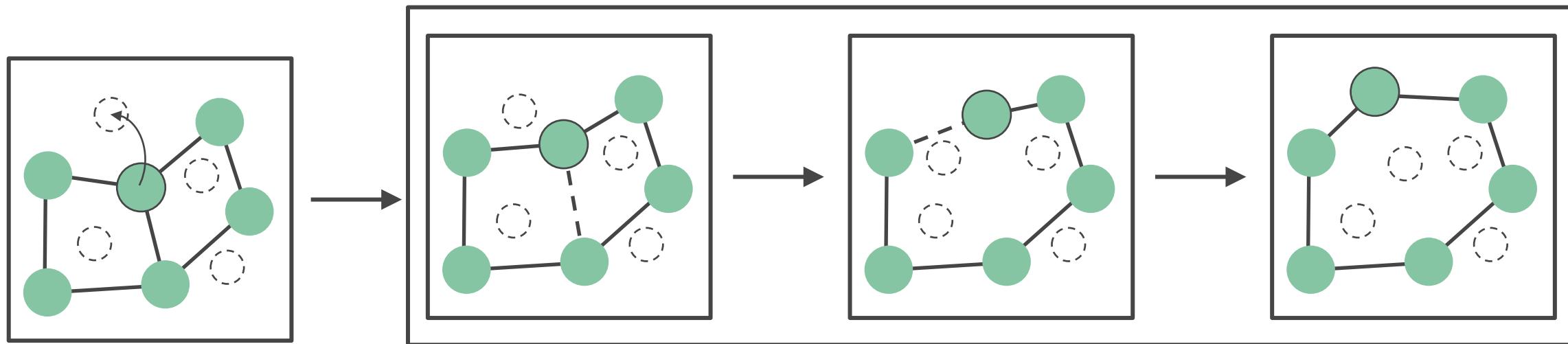
→ Optimizations to enable simulations of experimentally relevant geometries

→ Computational explorations of device operation at the nanoscale



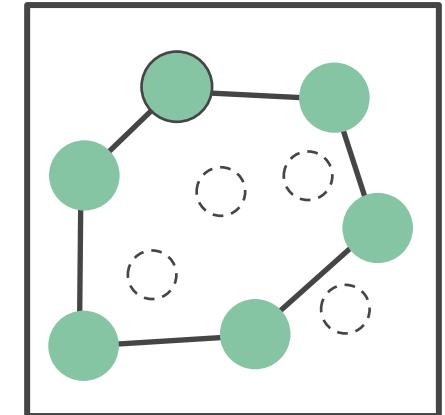
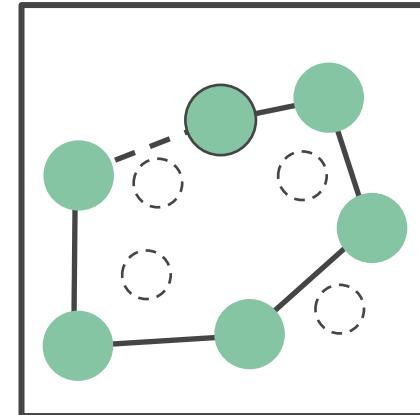
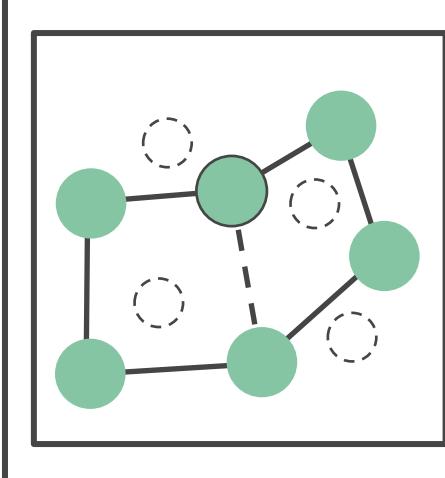
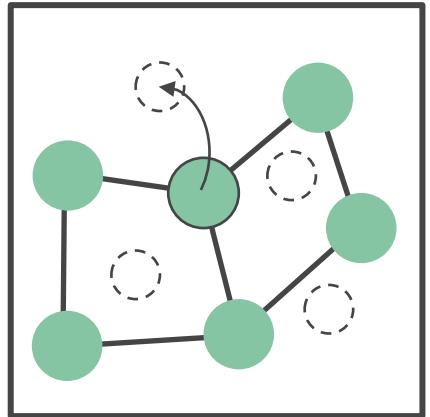
LATTICE KINETIC MONTE CARLO

one possible trajectory

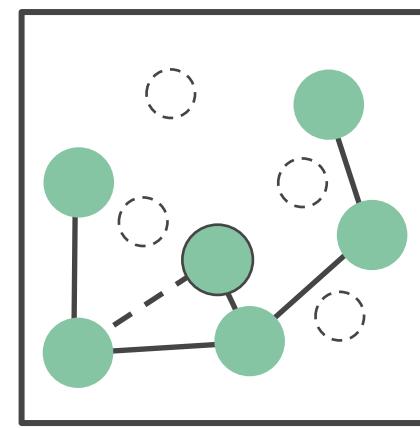
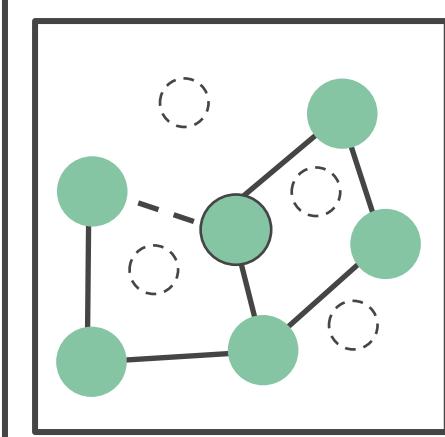
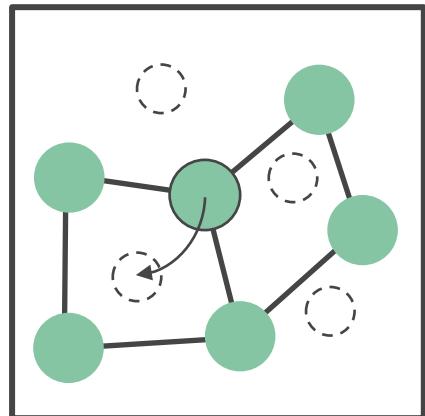


LATTICE KINETIC MONTE CARLO

one possible trajectory

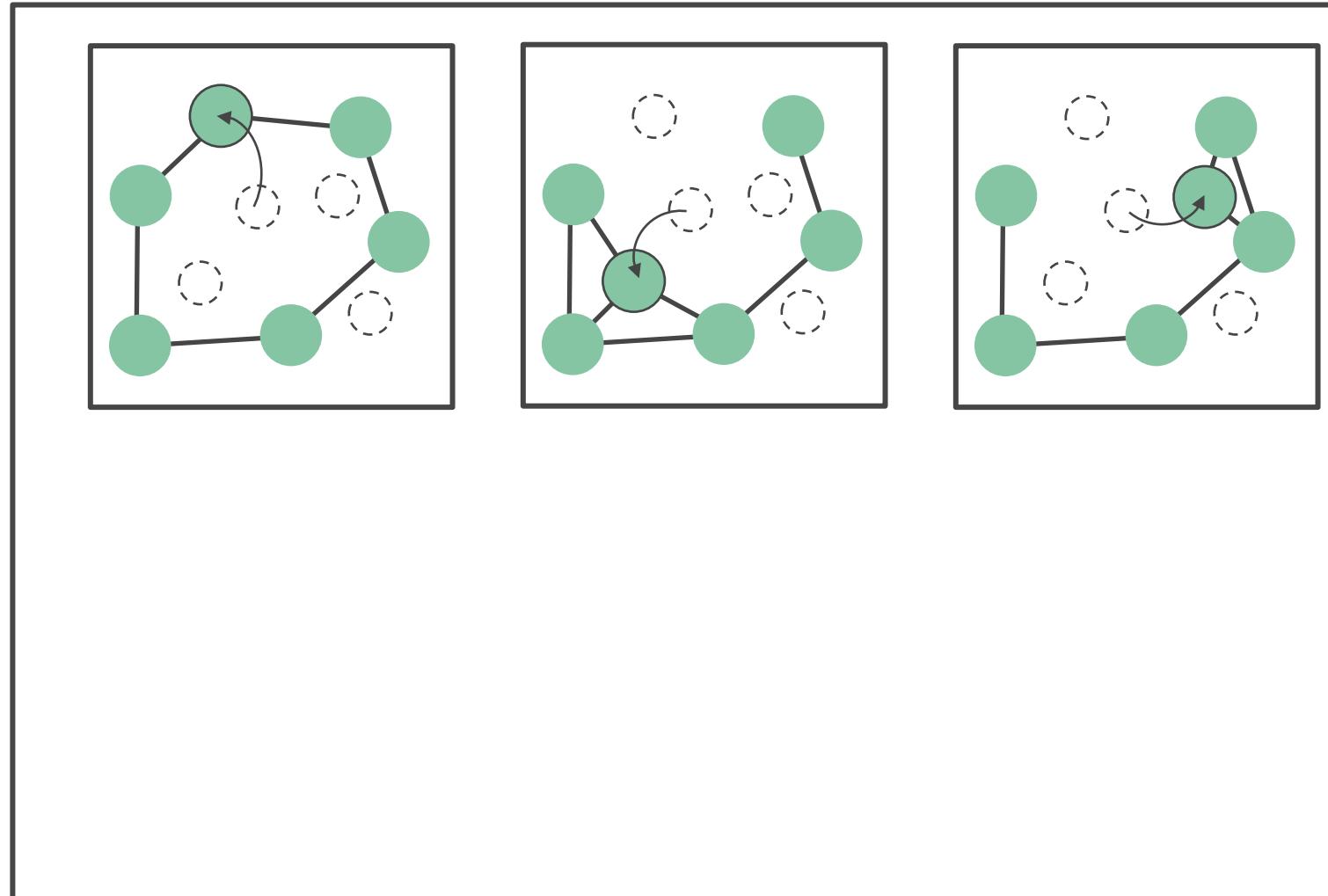
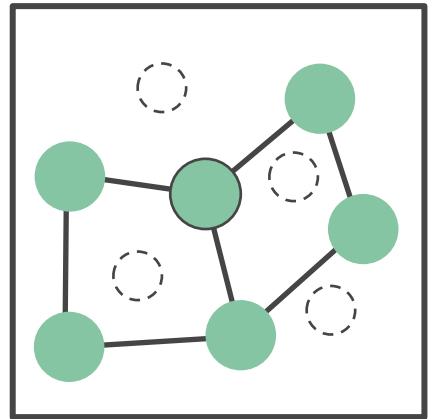


another possible trajectory



CONVENTIONAL KINETIC MONTE CARLO

possible “events”

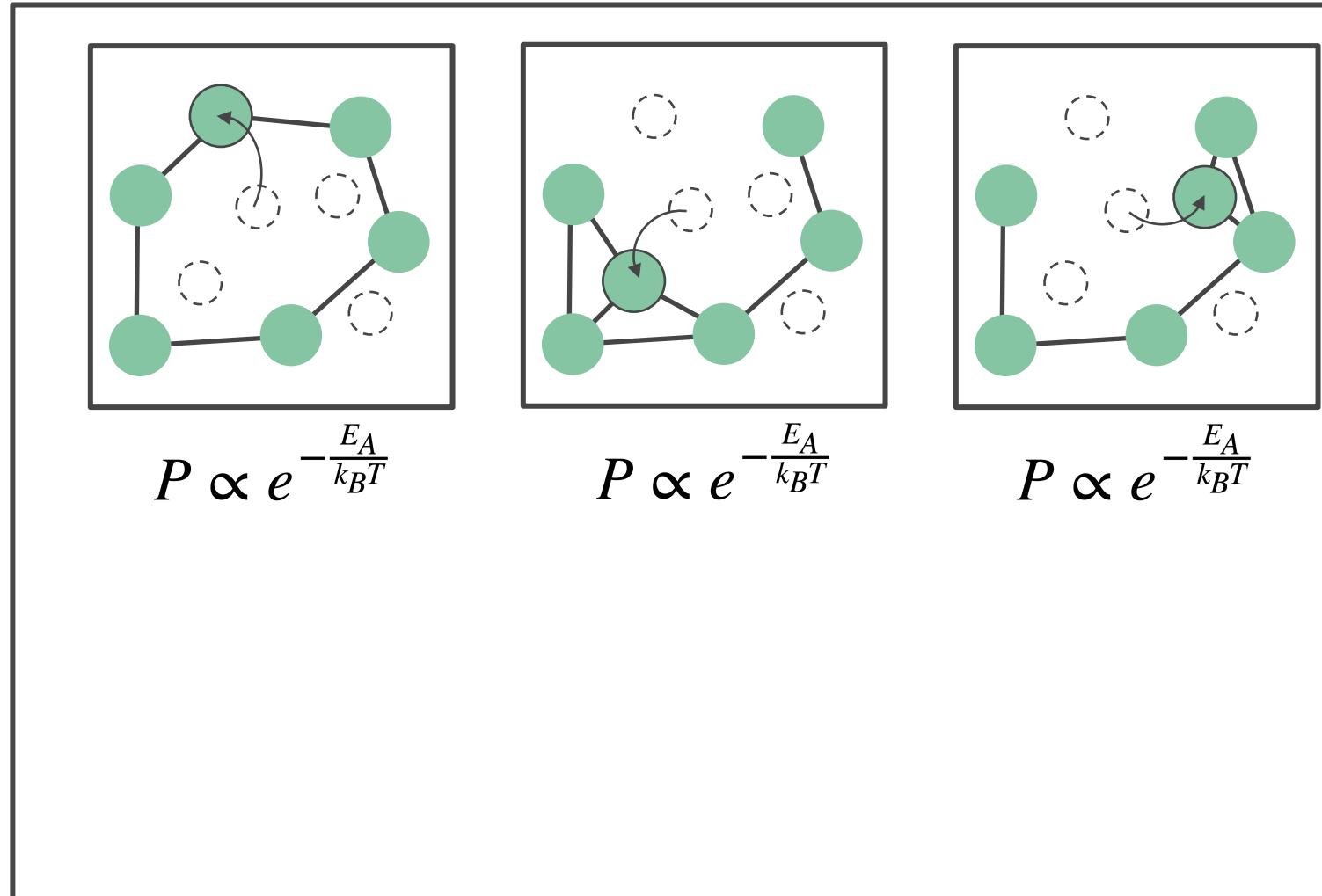
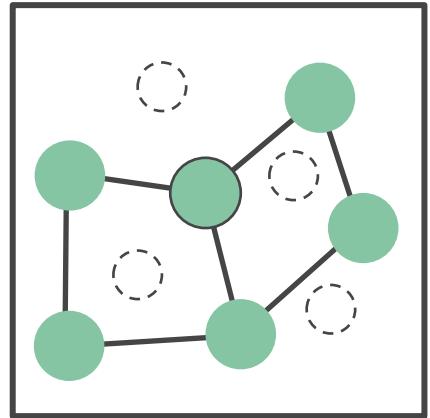


- weighted-stochastic selection of the next ‘event’



CONVENTIONAL KINETIC MONTE CARLO

possible “events”

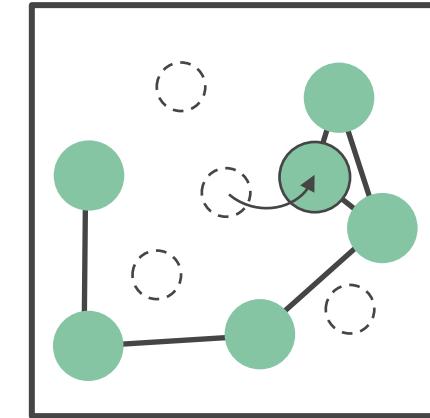
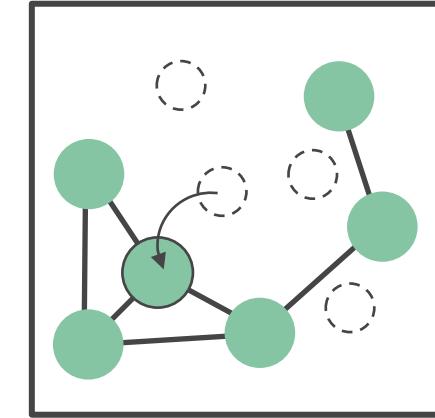
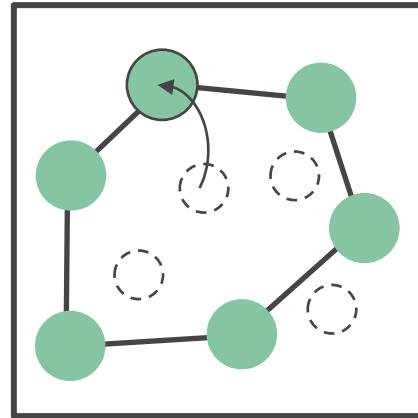
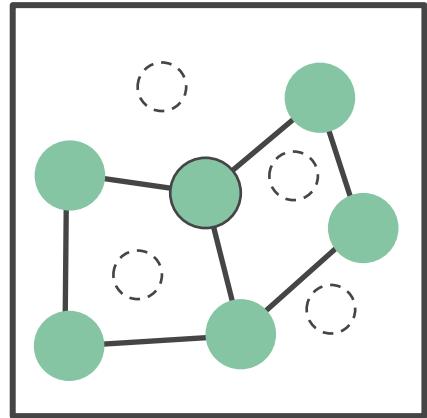


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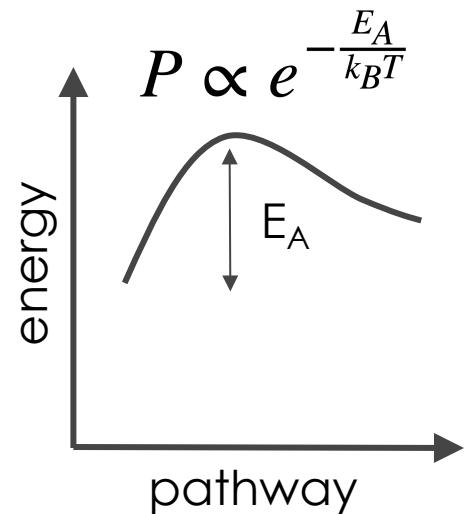
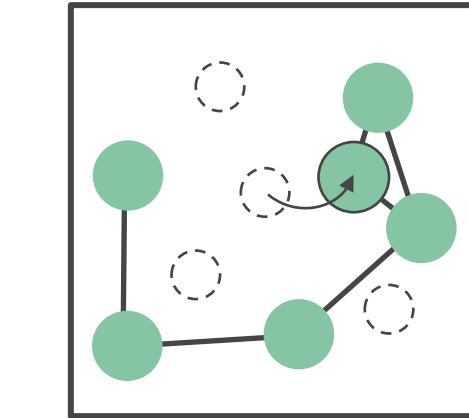
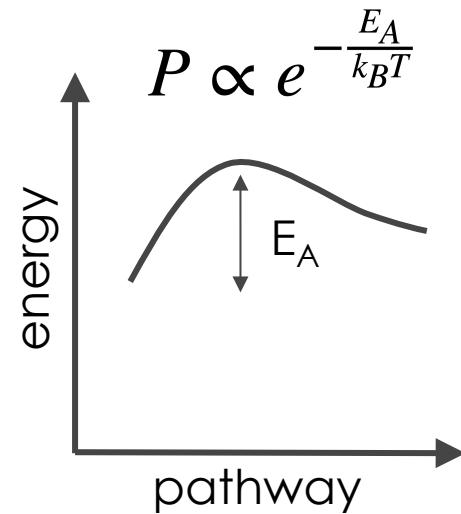
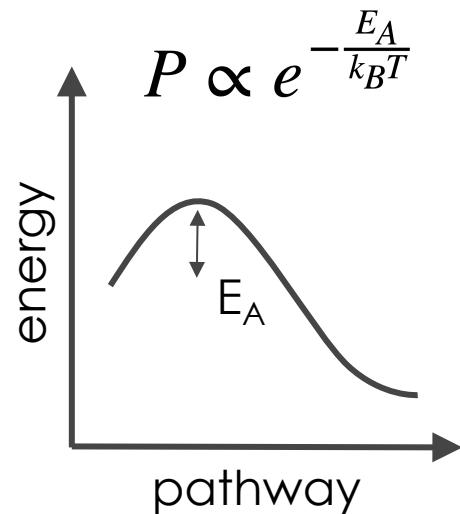


CONVENTIONAL KINETIC MONTE CARLO

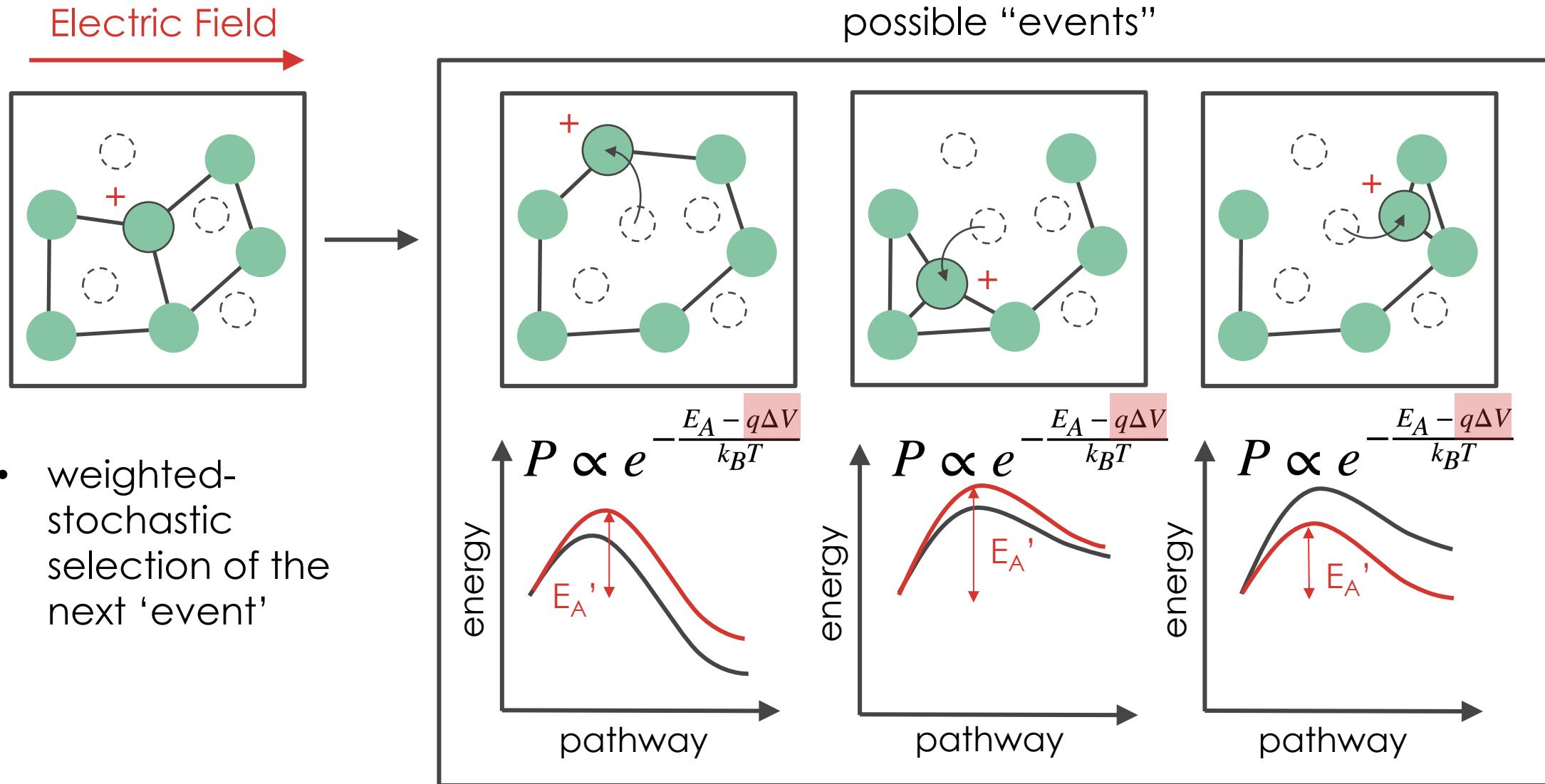
possible “events”



- weighted-stochastic selection of the next ‘event’

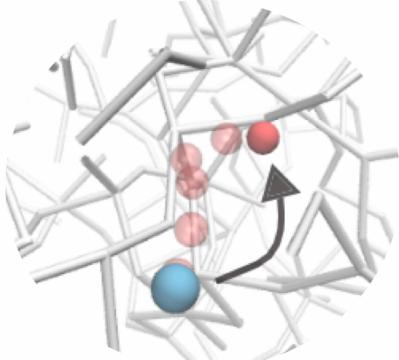


DRIVEN KINETIC MONTE CARLO

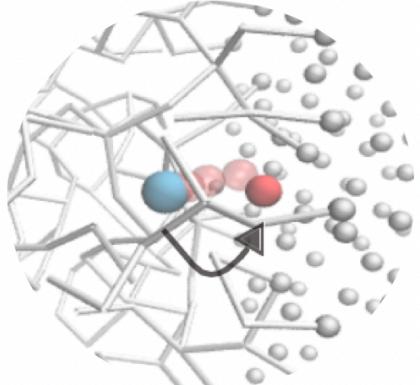


SIMULATING THE INITIAL BREAKDOWN

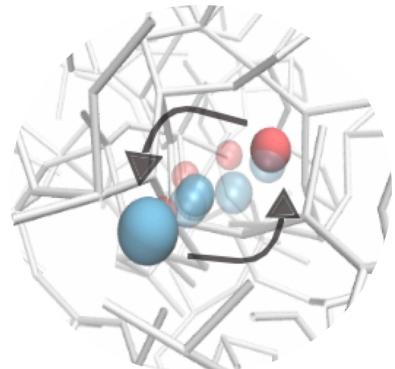
Classes of logged events



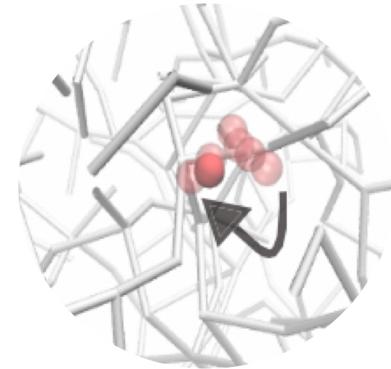
Bulk generation



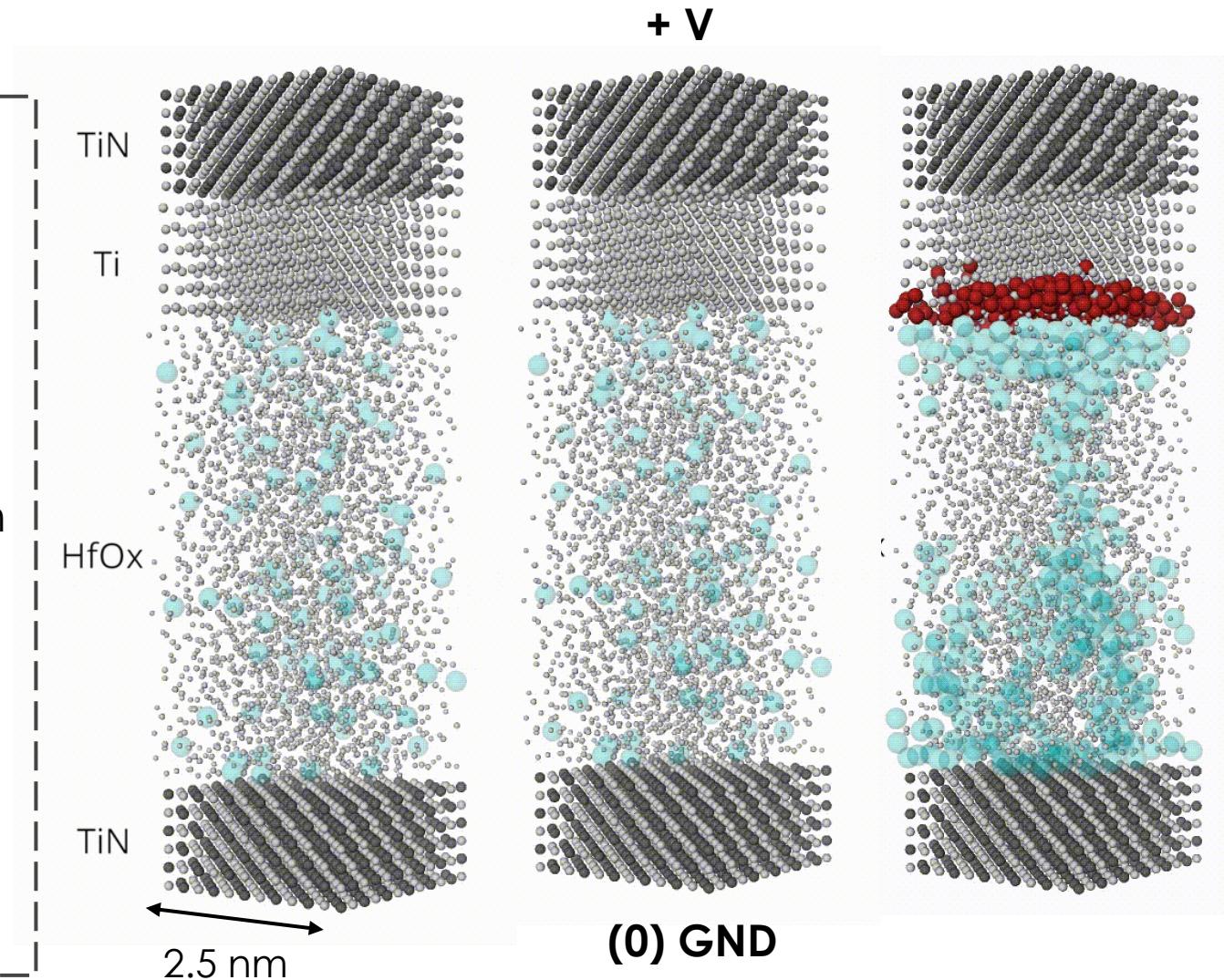
Interface generation



Vacancy Diffusion



Ion Diffusion



Kaniselvan, M. et al. "An Atomistic Model of Field-Induced Resistive Switching in Valence Change Memory", ACS Nano



APPLICATION FLOW

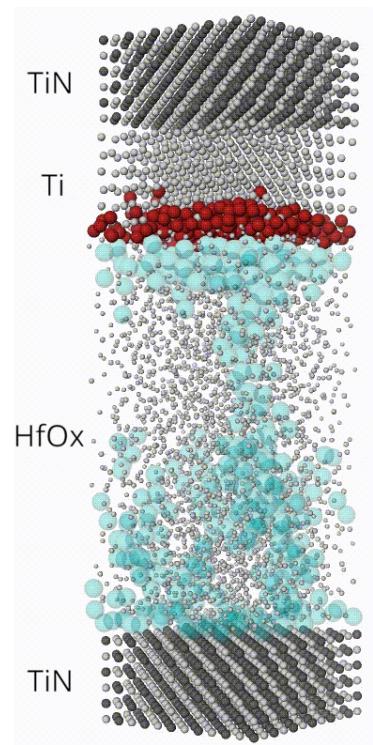
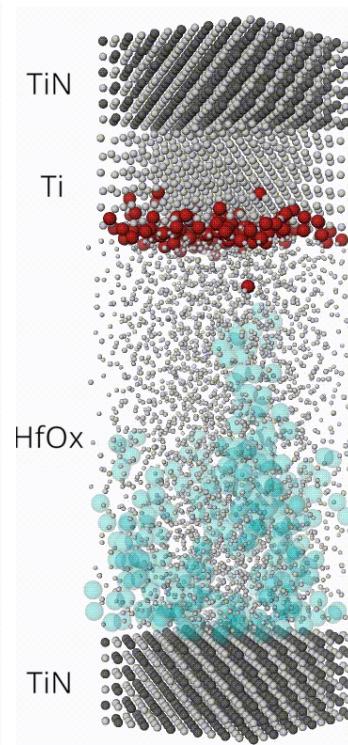
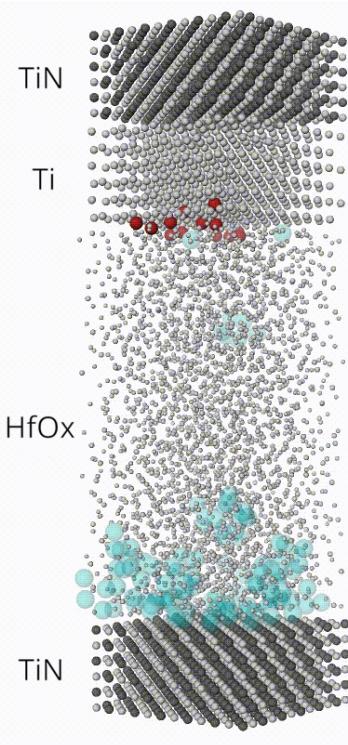
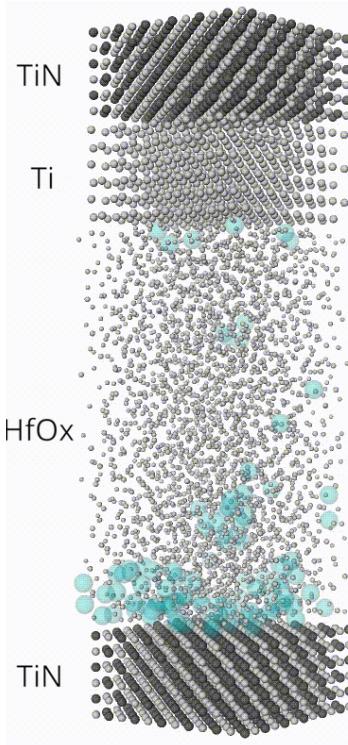
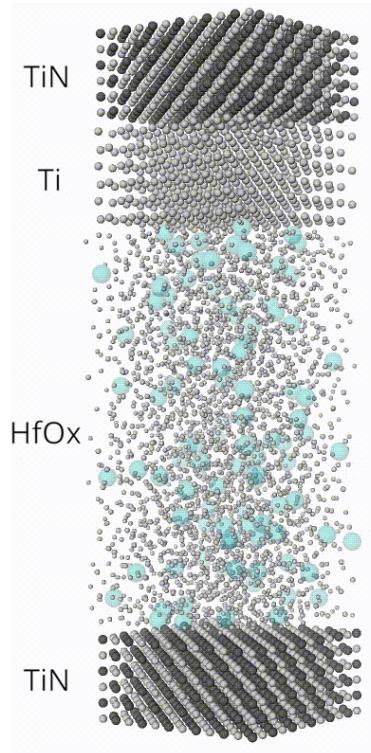
One superstep

Global simulation clock (s)

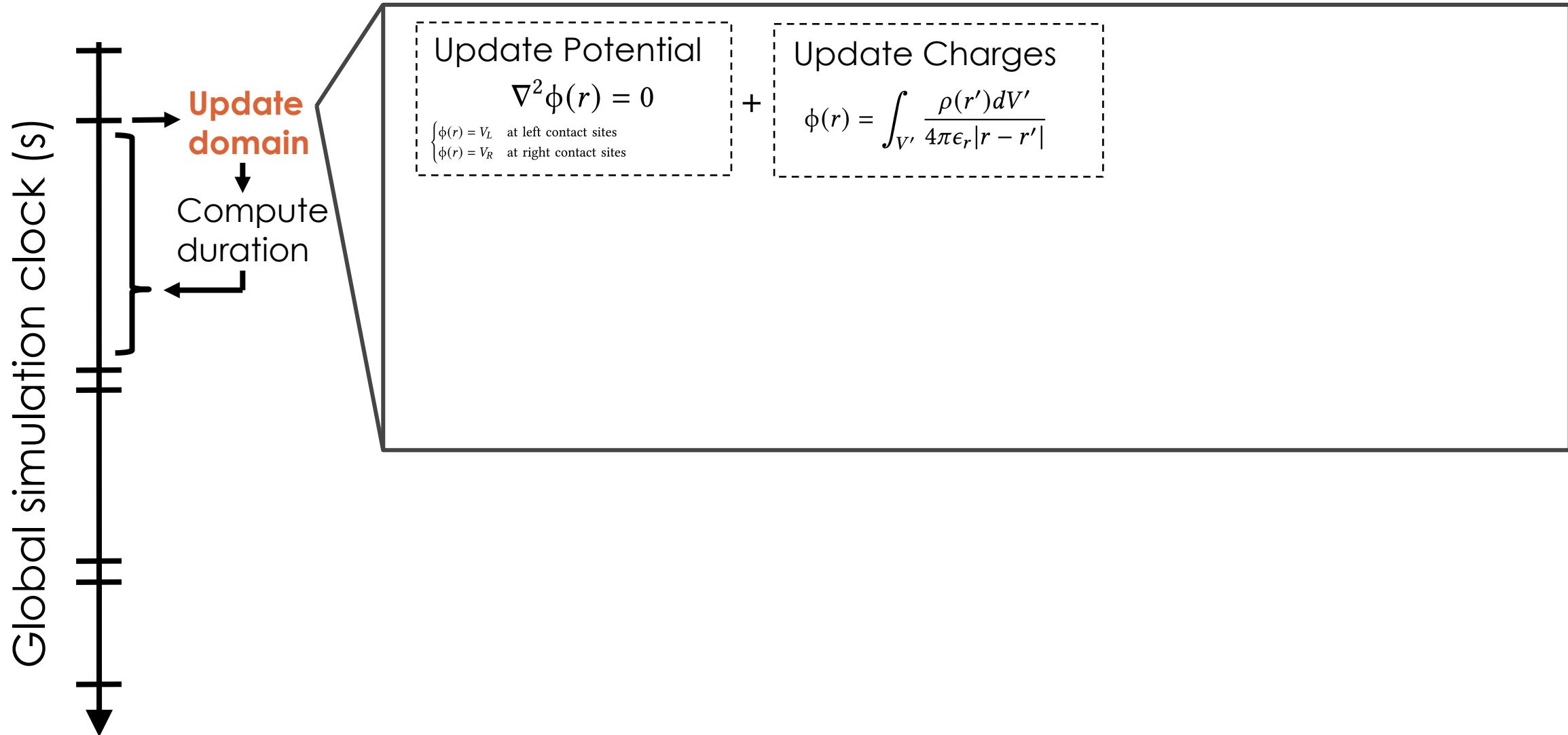
A horizontal number line starting at 0 and ending at 100. Major tick marks are at intervals of 10, labeled 0, 1, 2, ..., 100. Minor tick marks are at intervals of 1. The segment from 0 to 1 is labeled '1'. The segment from 1 to 2 is labeled '2'. The segment from 9 to 10 is labeled '10'.

Update domain

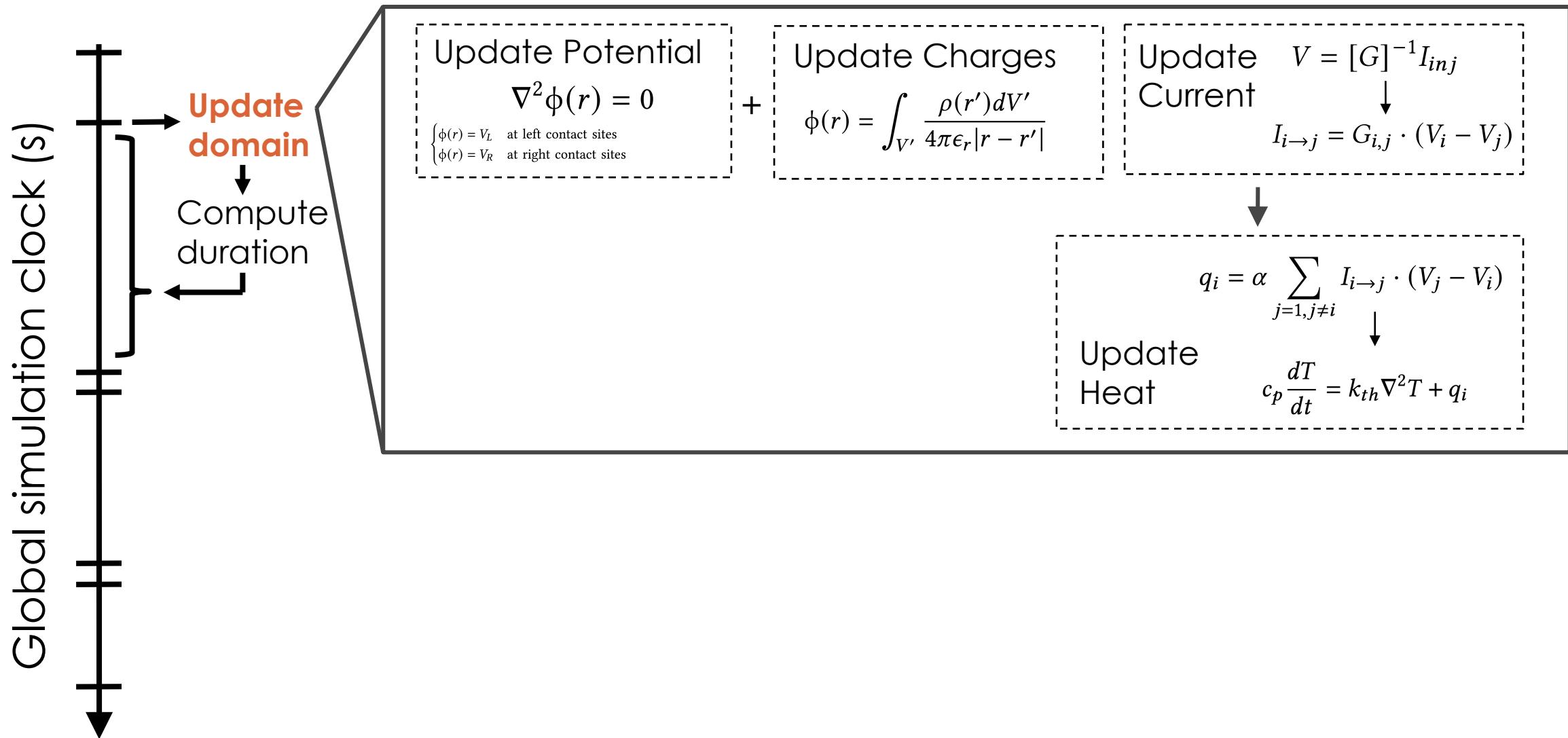
Compute duration



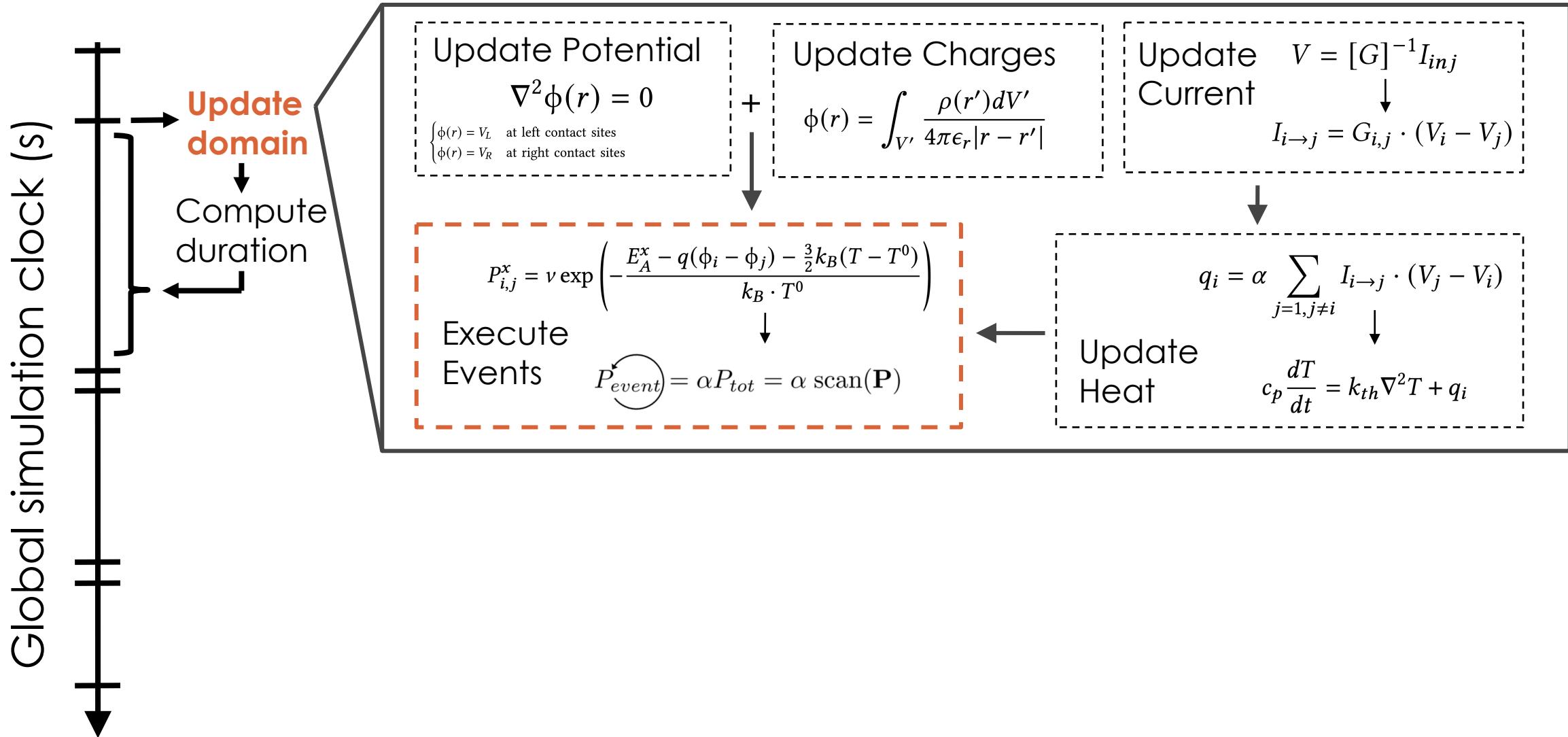
DOMAIN STRUCTURE UPDATES



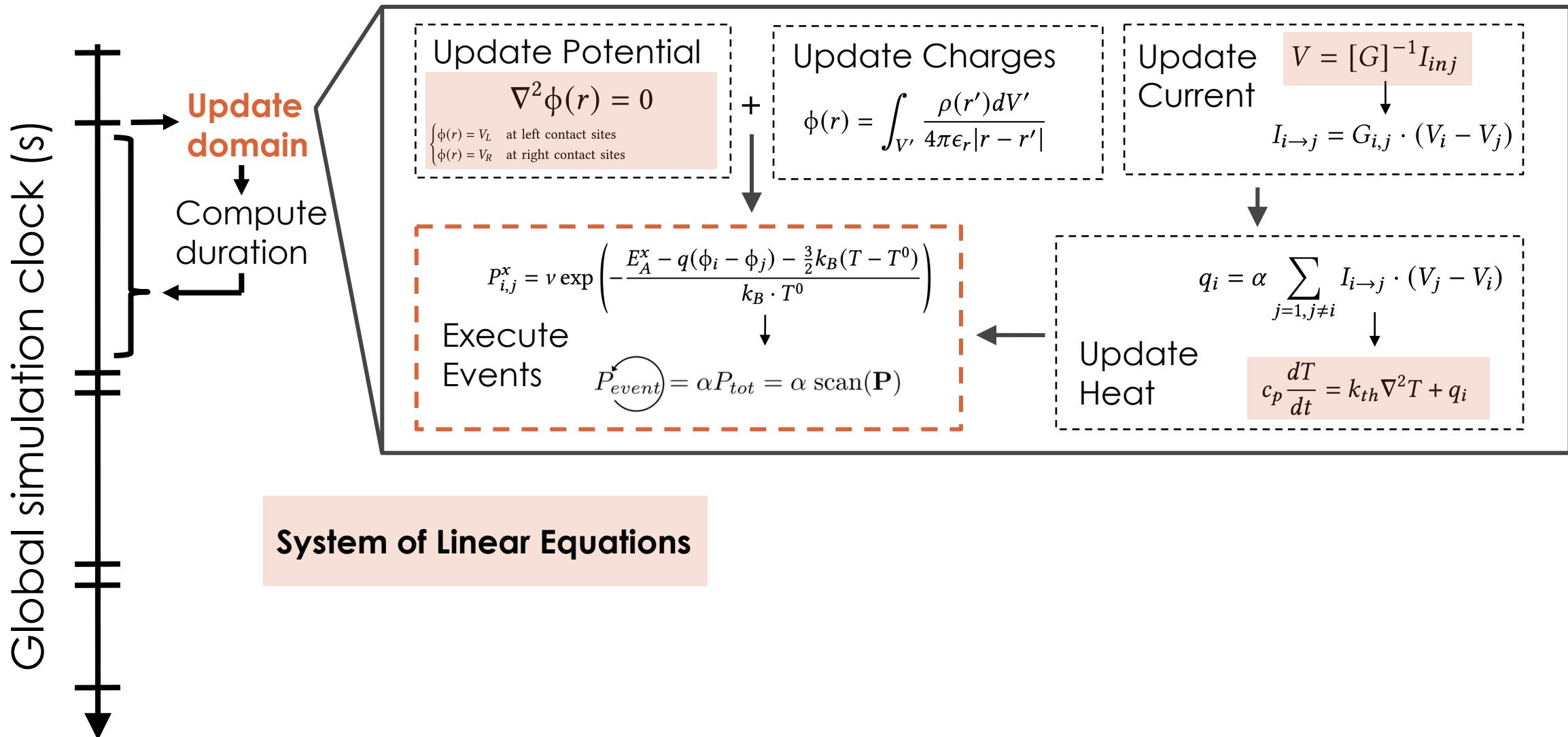
DOMAIN STRUCTURE UPDATES



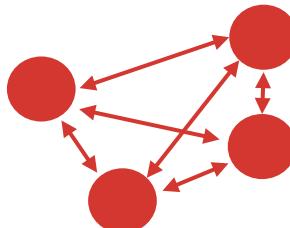
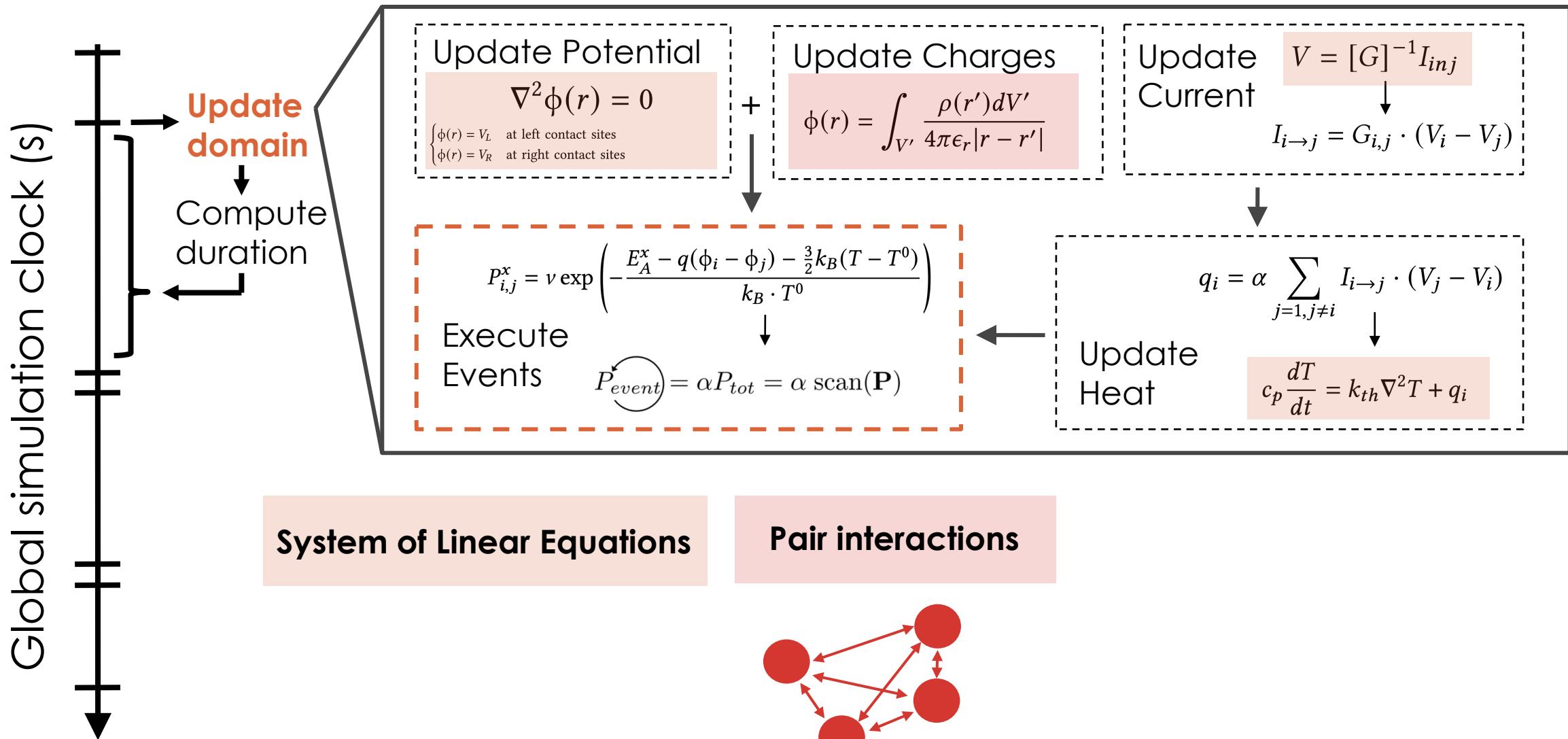
DOMAIN STRUCTURE UPDATES



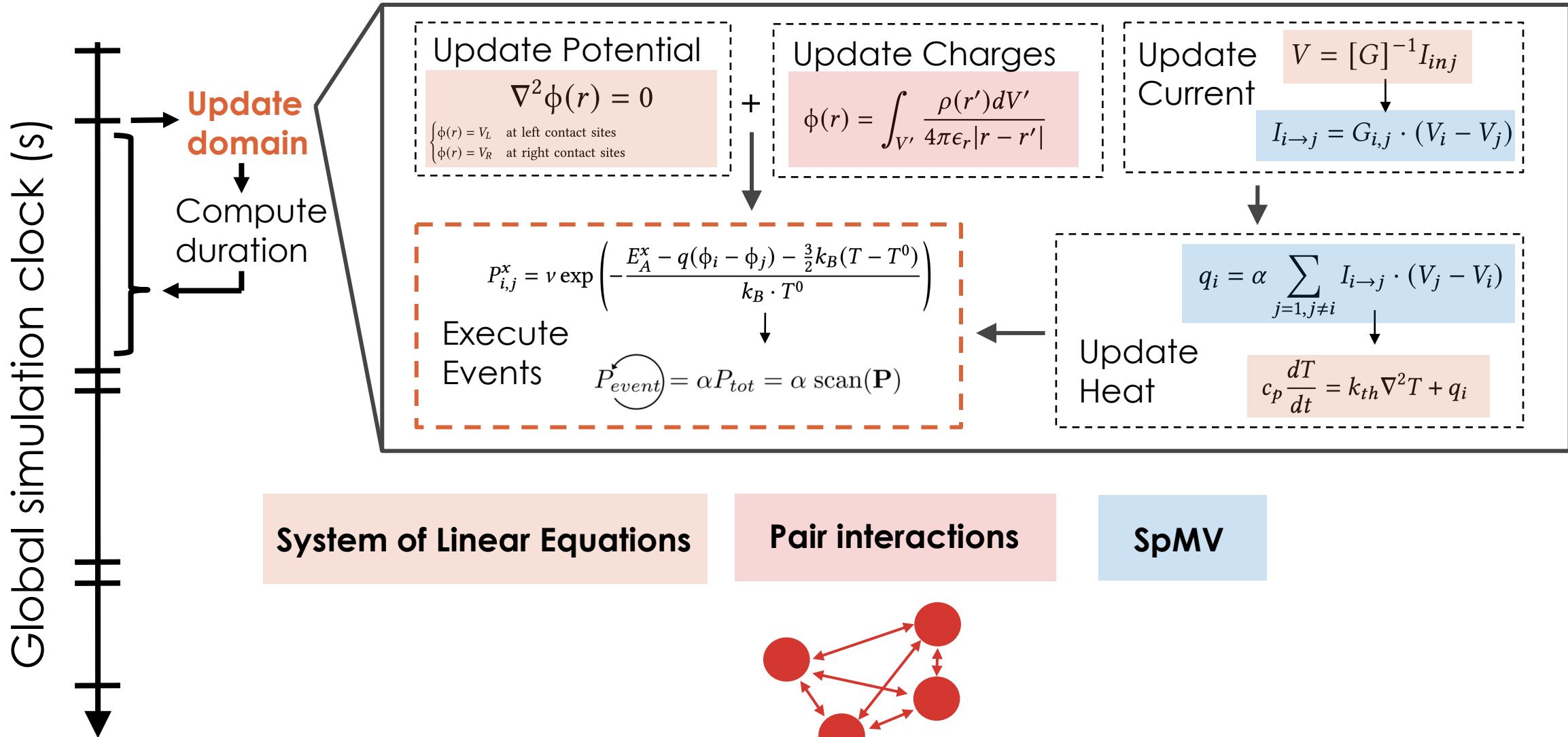
DOMAIN STRUCTURE UPDATES



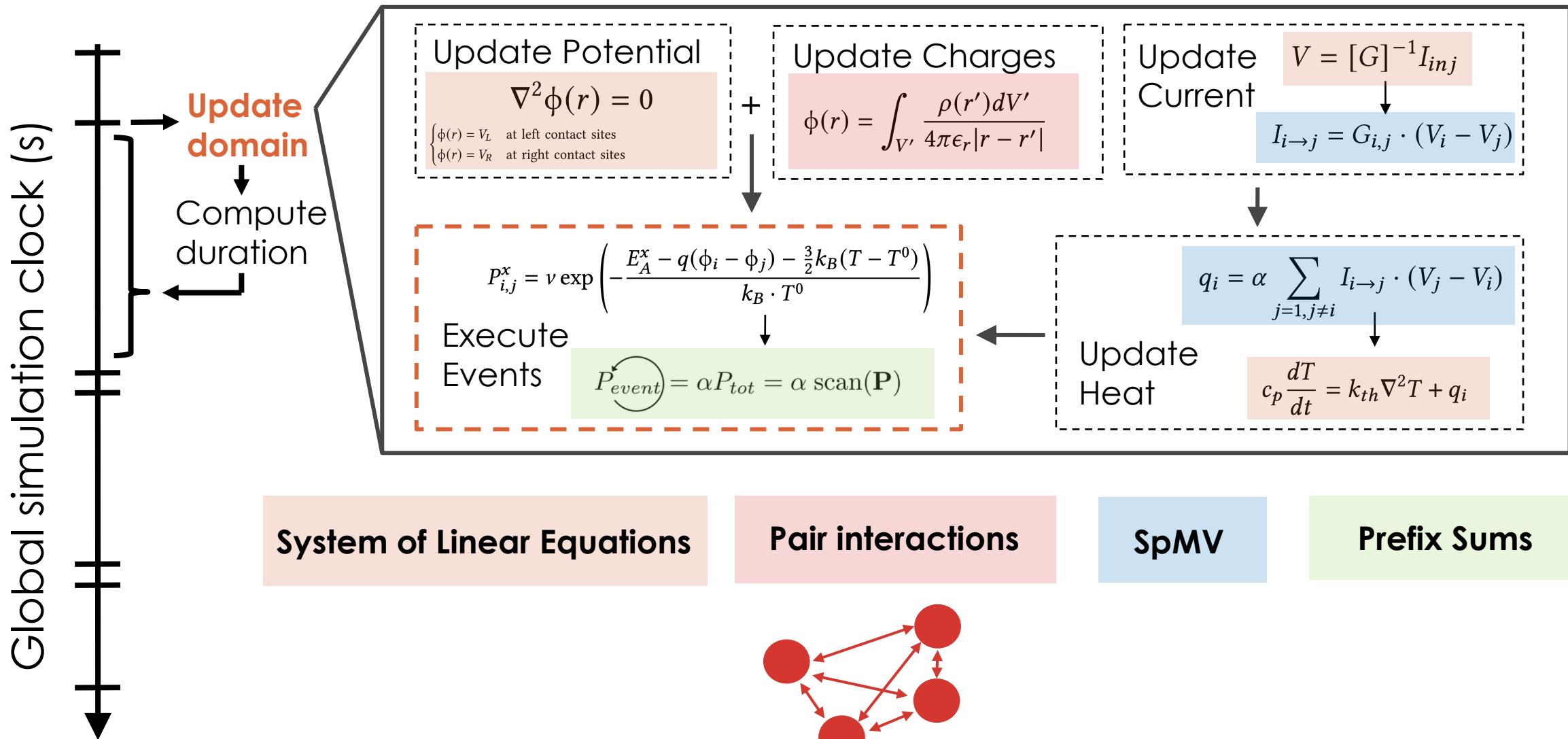
DOMAIN STRUCTURE UPDATES



DOMAIN STRUCTURE UPDATES



DOMAIN STRUCTURE UPDATES



→ Development of an application to simulate the kinetics of RRAM devices

→ Enabling simulations of experimentally relevant geometries

→ Computational explorations of device operation at the nanoscale



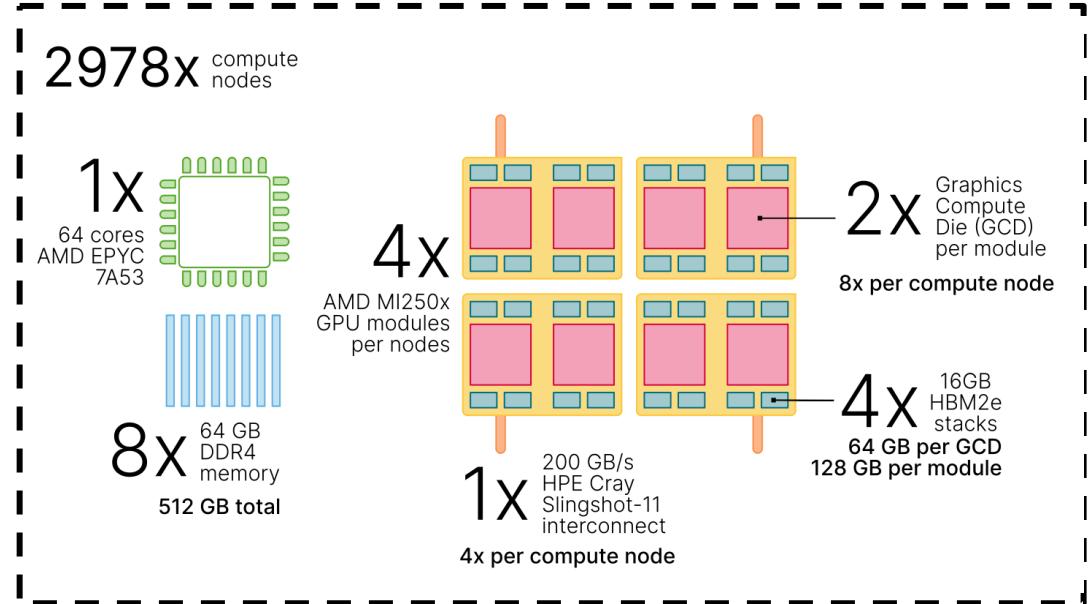
HARDWARE & SOFTWARE

Microbenchmarks: Piz Daint, Switzerland



- **Each node:**
- C++, CUDA
- **GPU-aware MPI:** X

Full application: LUMI, Finland



- **Each node:**
- C++, HIP
- **GPU-aware MPI:**



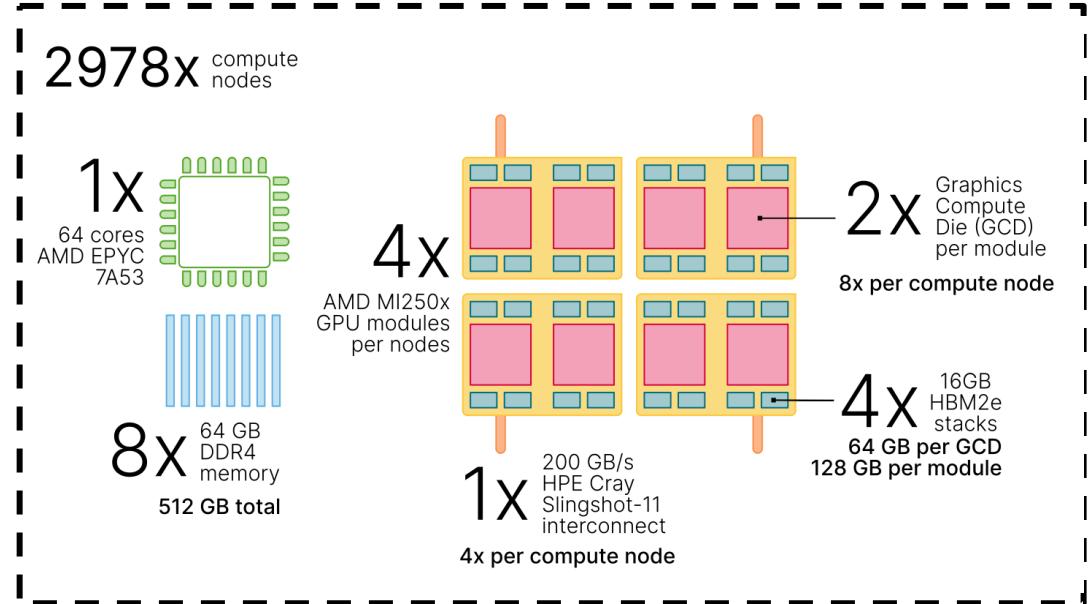
HARDWARE & SOFTWARE

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- **Each node:** NVIDIA P100 GPUs
- C++, CUDA
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Full application: LUMI, Finland



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 - C++, HIP
- **GPU-aware MPI:**



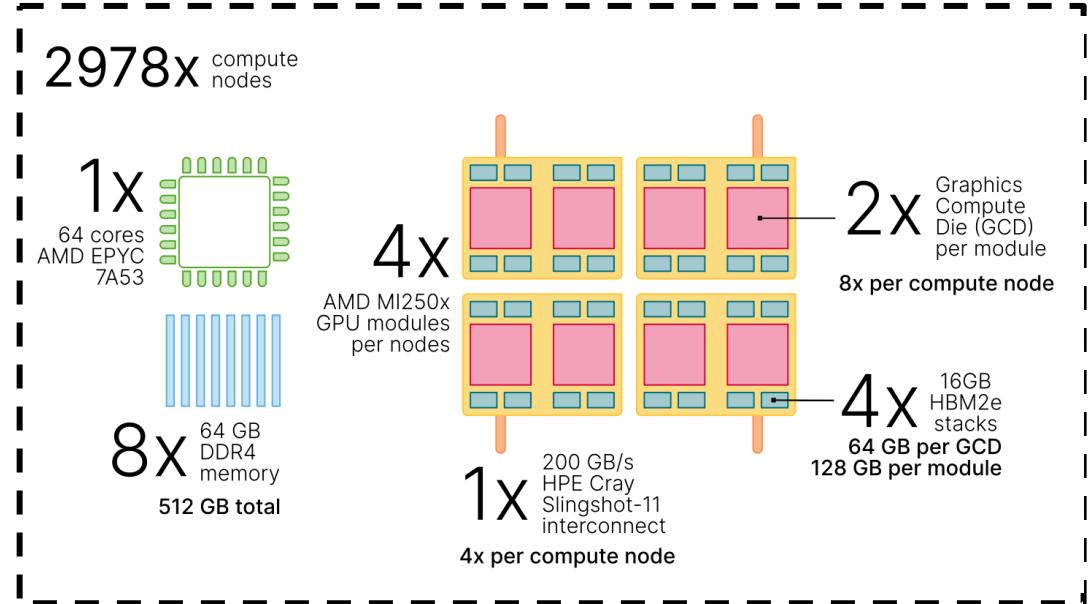
HARDWARE & SOFTWARE

Microbenchmarks: Piz Daint, Switzerland



- **Each node:** NVIDIA P100 GPUs
- C++, CUDA
- **GPU-aware MPI:**

Full application: LUMI, Finland



- **Each node:** 4 AMD MI250X GCDs (8 GPUs programmatically)
- C++, HIP
- **GPU-aware MPI:**



KEY OPTIMIZATION AREAS

Field Updates



Development of a
sparsity-optimized
**distributed Conjugate
Gradient** solver

Event Selection



Distributed Monte Carlo
event **selection** process

Repeat supersteps



Task-based distribution
of application modules



KEY OPTIMIZATION AREAS

Field Updates



Development of a sparsity-optimized
distributed Conjugate Gradient solver

Event Selection



Distributed Monte Carlo
event selection process

Repeat supersteps

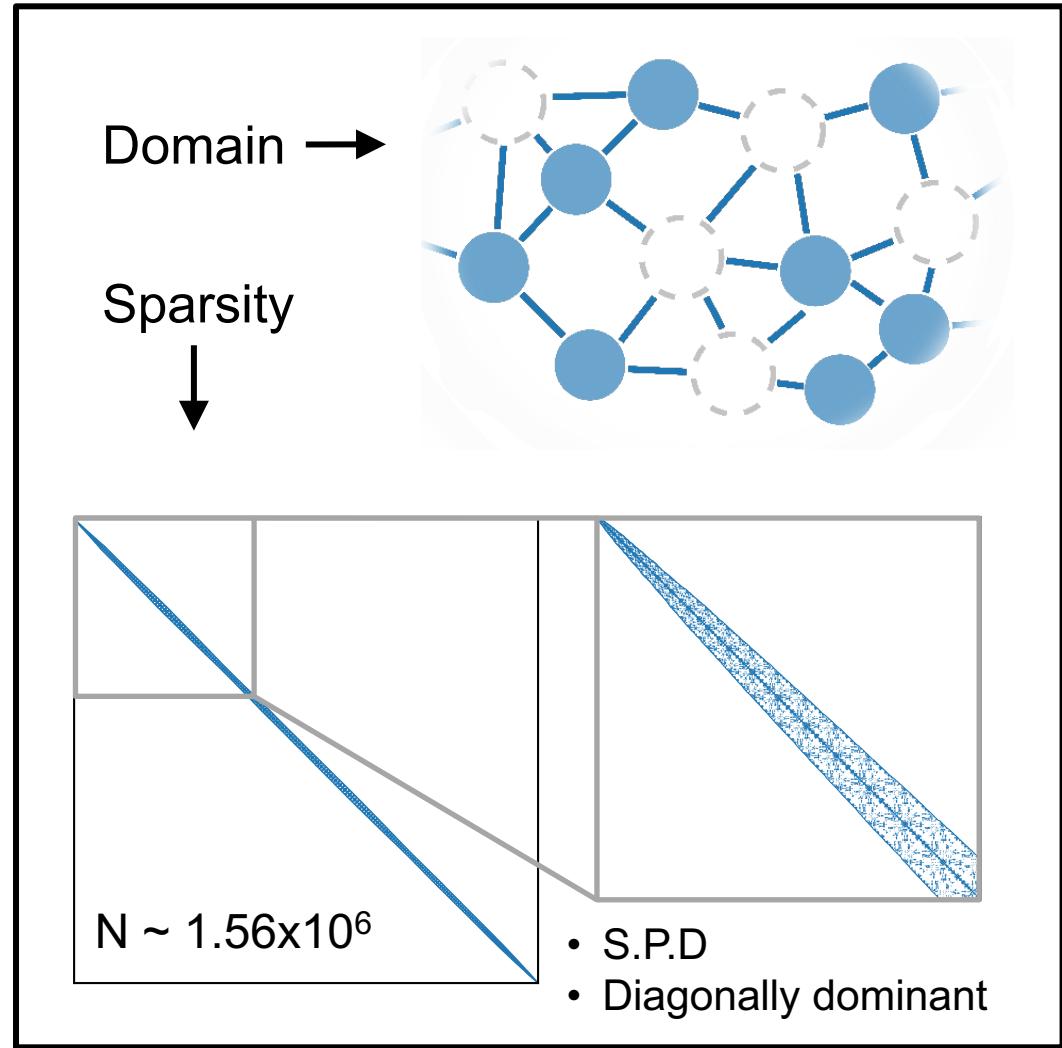


Task-based distribution
of application modules



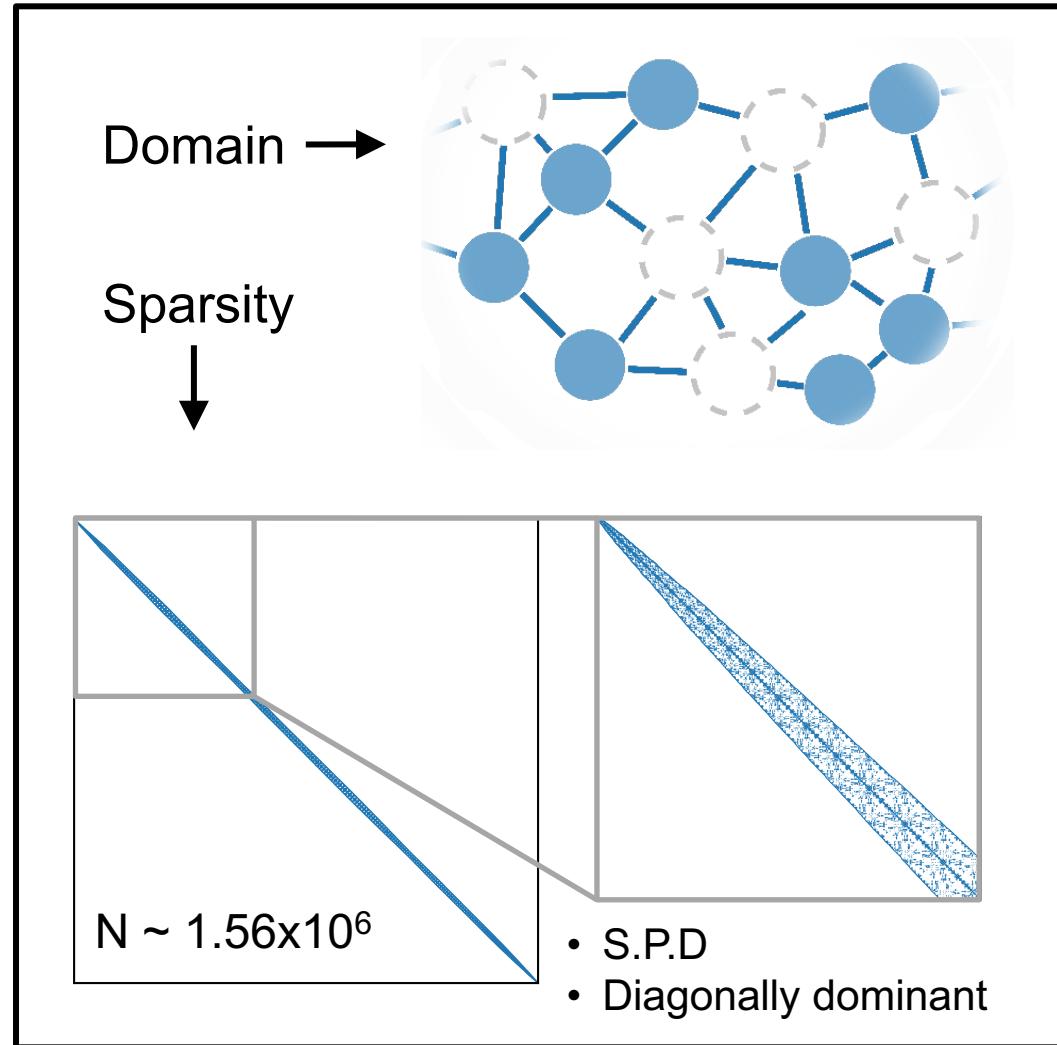
MATRIX SPARSITY STRUCTURE

Potential/Heat solvers

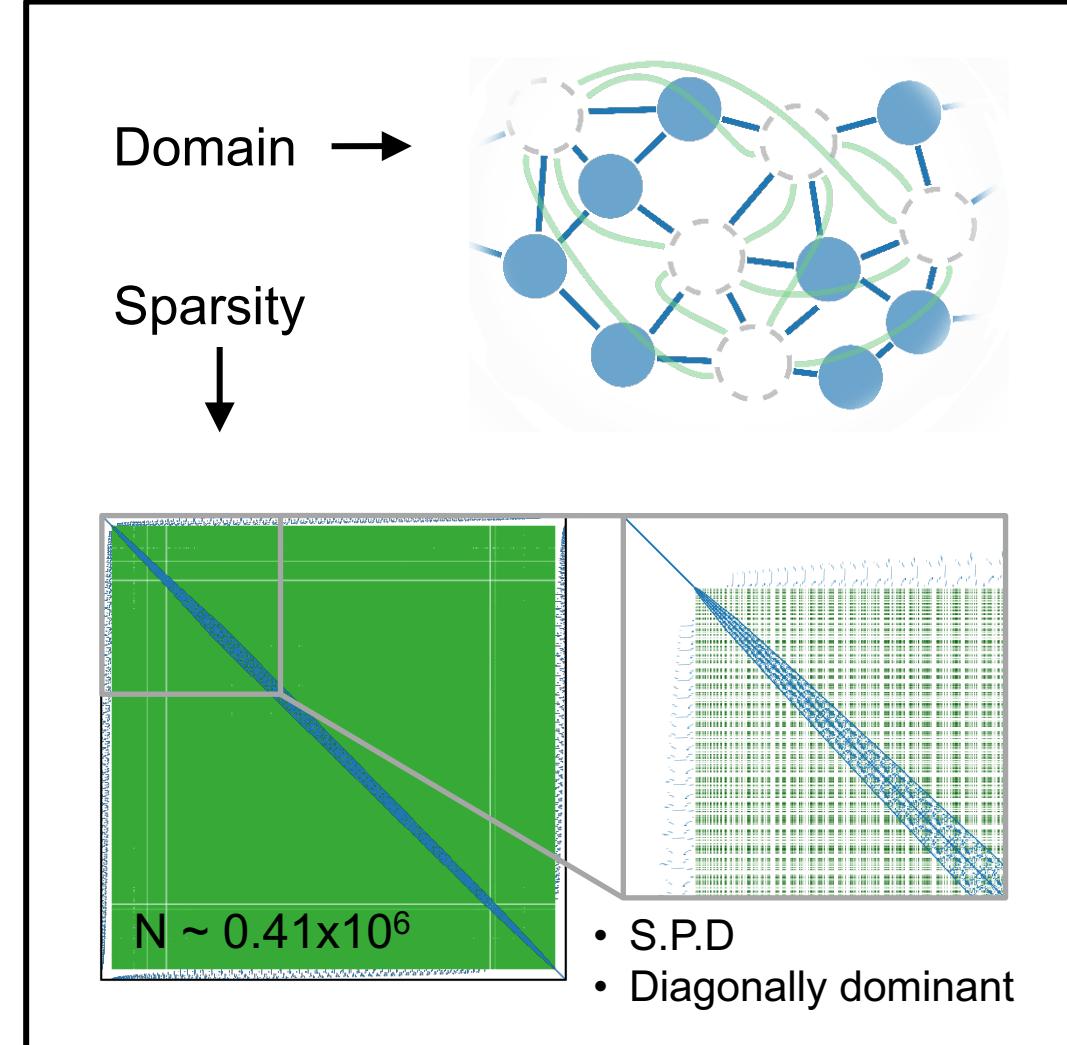


MATRIX SPARSITY STRUCTURE

Potential/Heat solvers



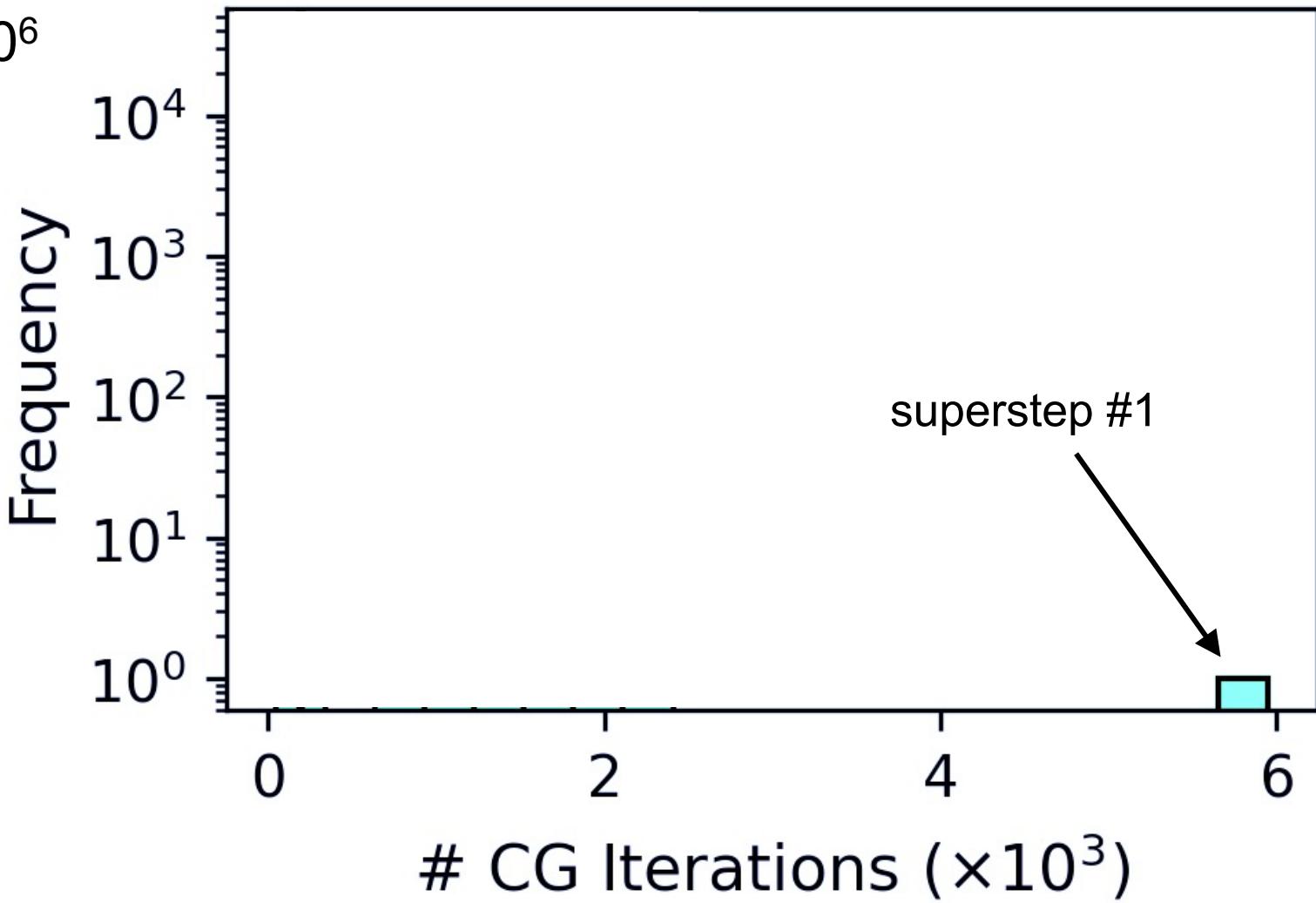
Current solver



USING AN ITERATIVE SOLVER

Matrix Size: $N \sim 1.56 \times 10^6$

Nonzeros: $nnz \sim 40 \times 10^6$

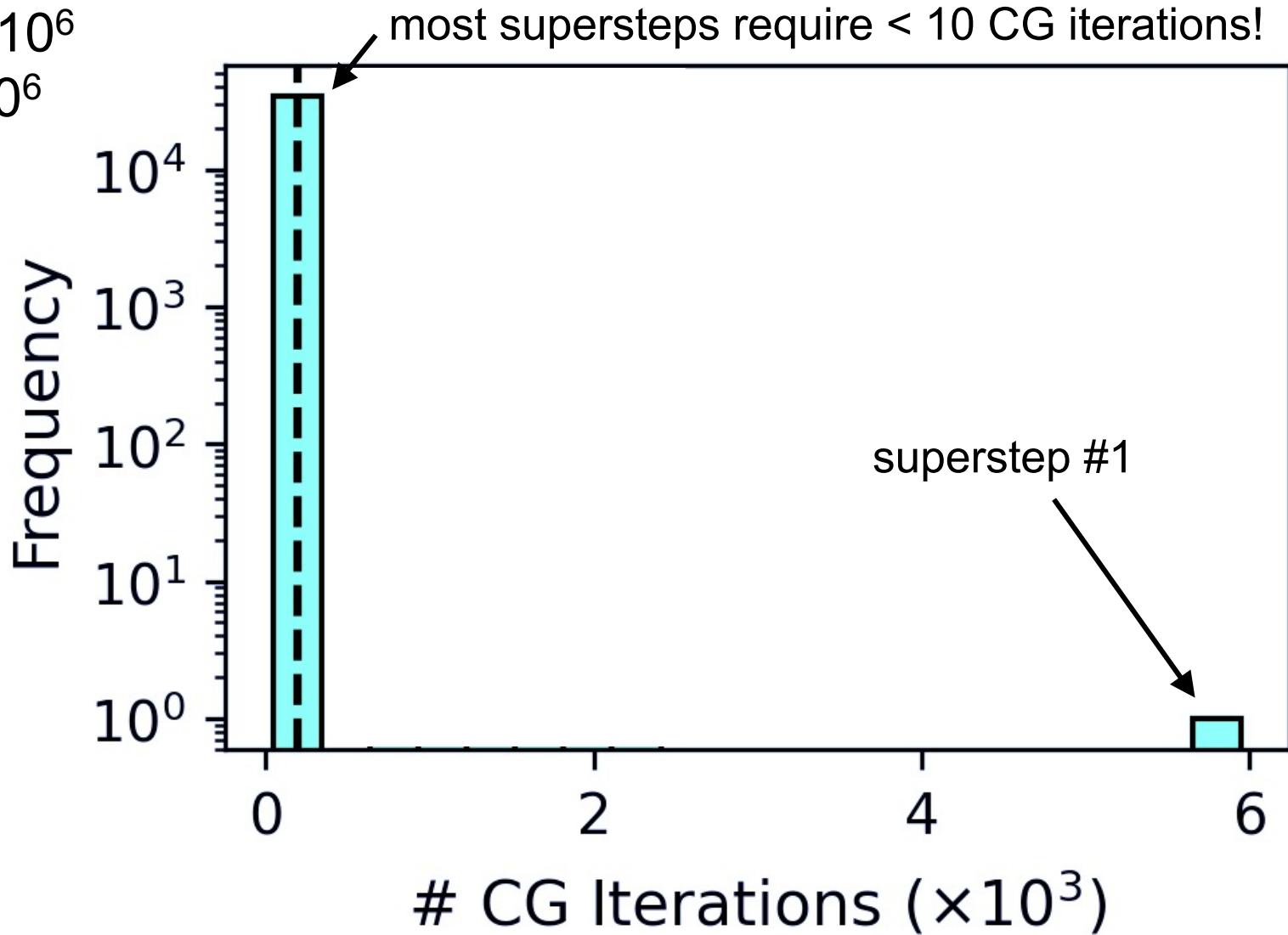


USING AN ITERATIVE SOLVER

Matrix Size: $N \sim 1.56 \times 10^6$

Nonzeros: $nnz \sim 40 \times 10^6$

- Exploiting the gradual variation in the solution vectors

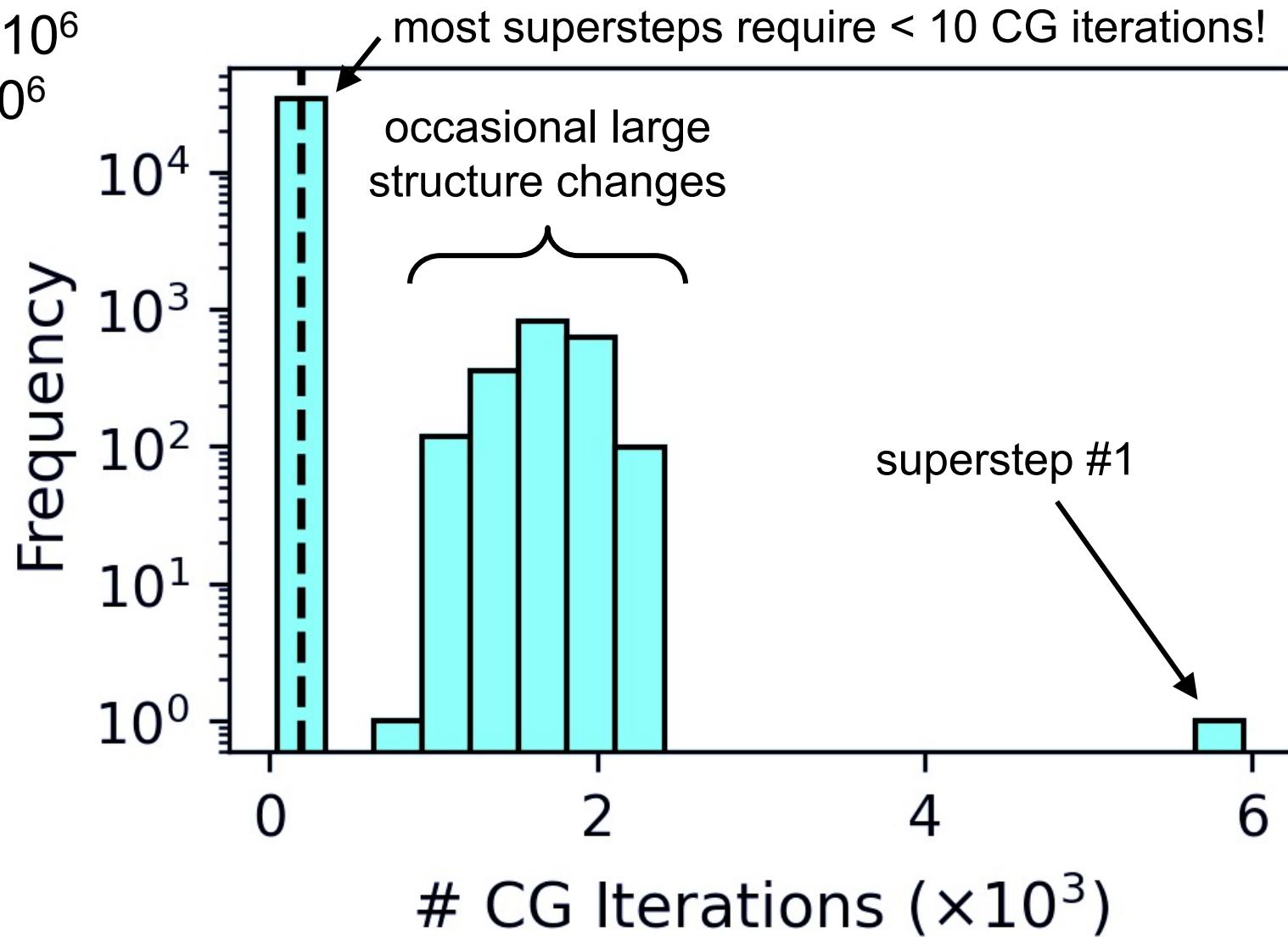


USING AN ITERATIVE SOLVER

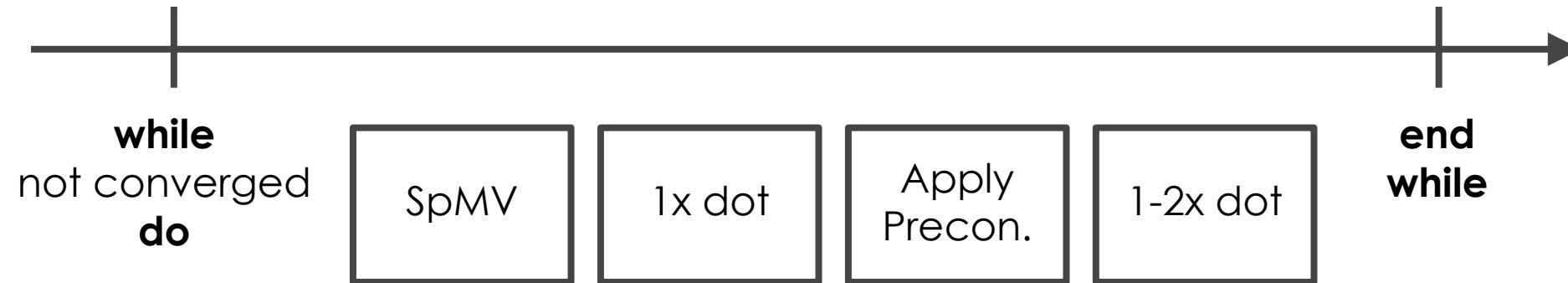
Matrix Size: $N \sim 1.56 \times 10^6$

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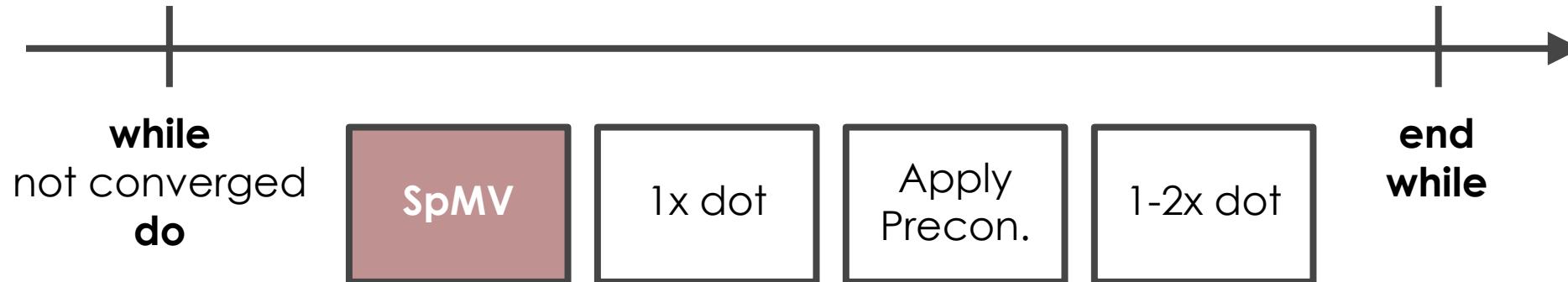
- Exploiting the gradual variation in the solution vectors
- Time spent on larger variations is amortized by time saved on smaller ones



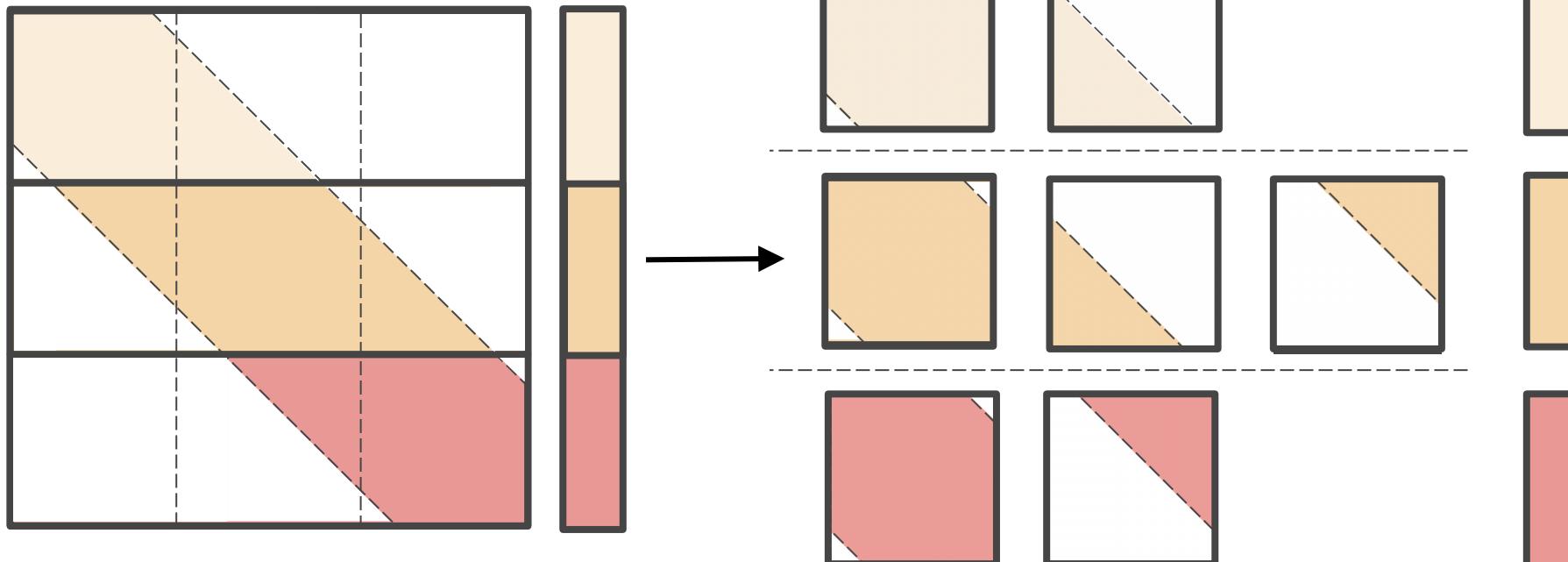
DISTRIBUTED ITERATIVE SOLVER



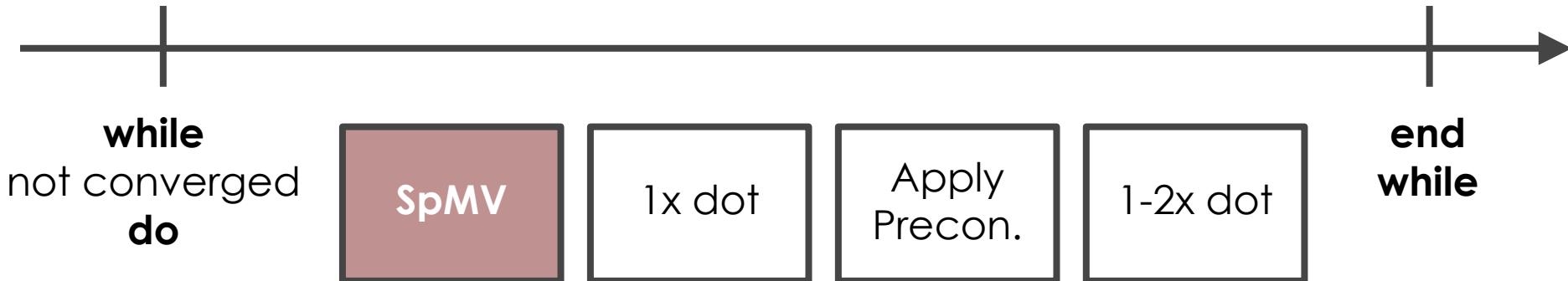
DISTRIBUTED ITERATIVE SOLVER



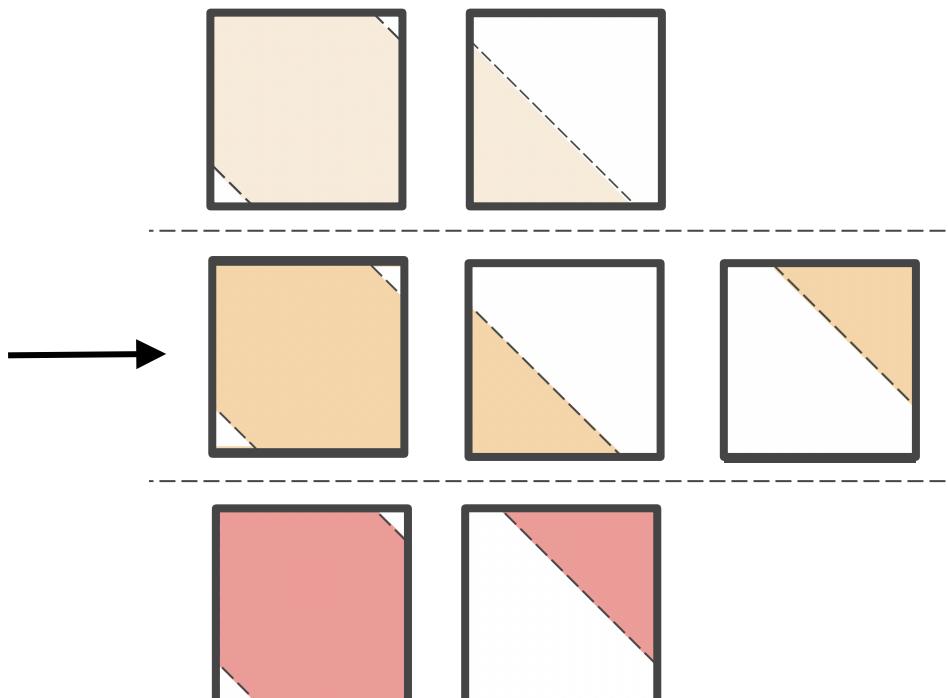
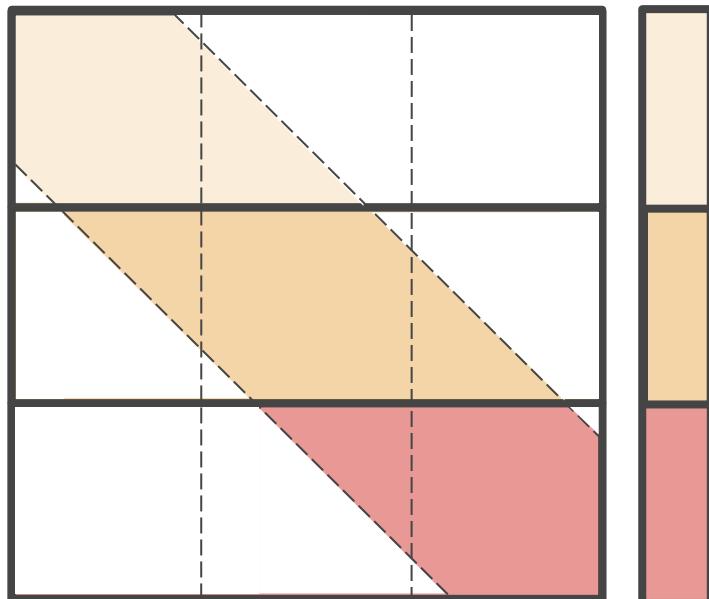
Block-wise distribution



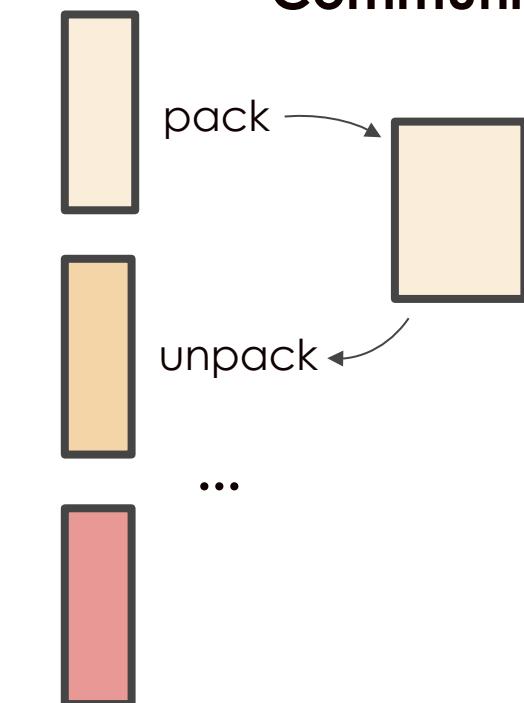
DISTRIBUTED ITERATIVE SOLVER



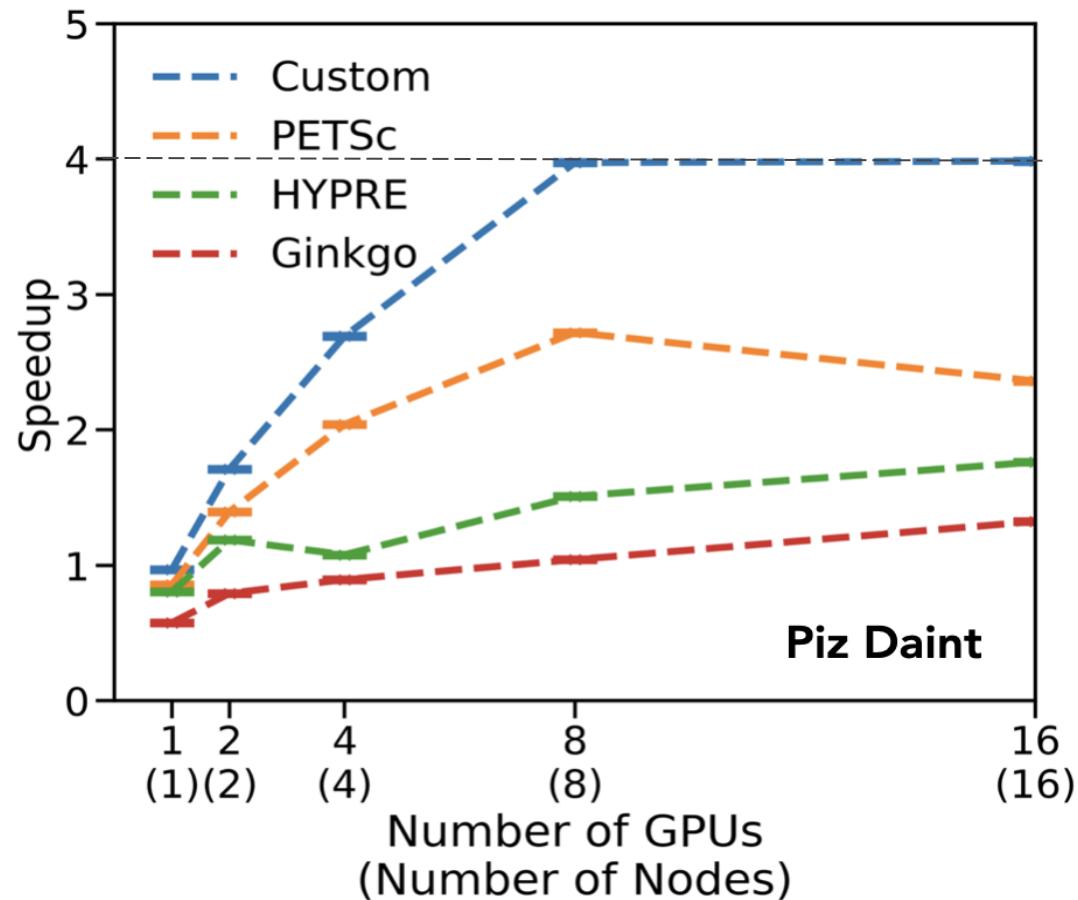
Block-wise distribution



Point-to-Point Communication



DISTRIBUTED ITERATIVE SOLVER

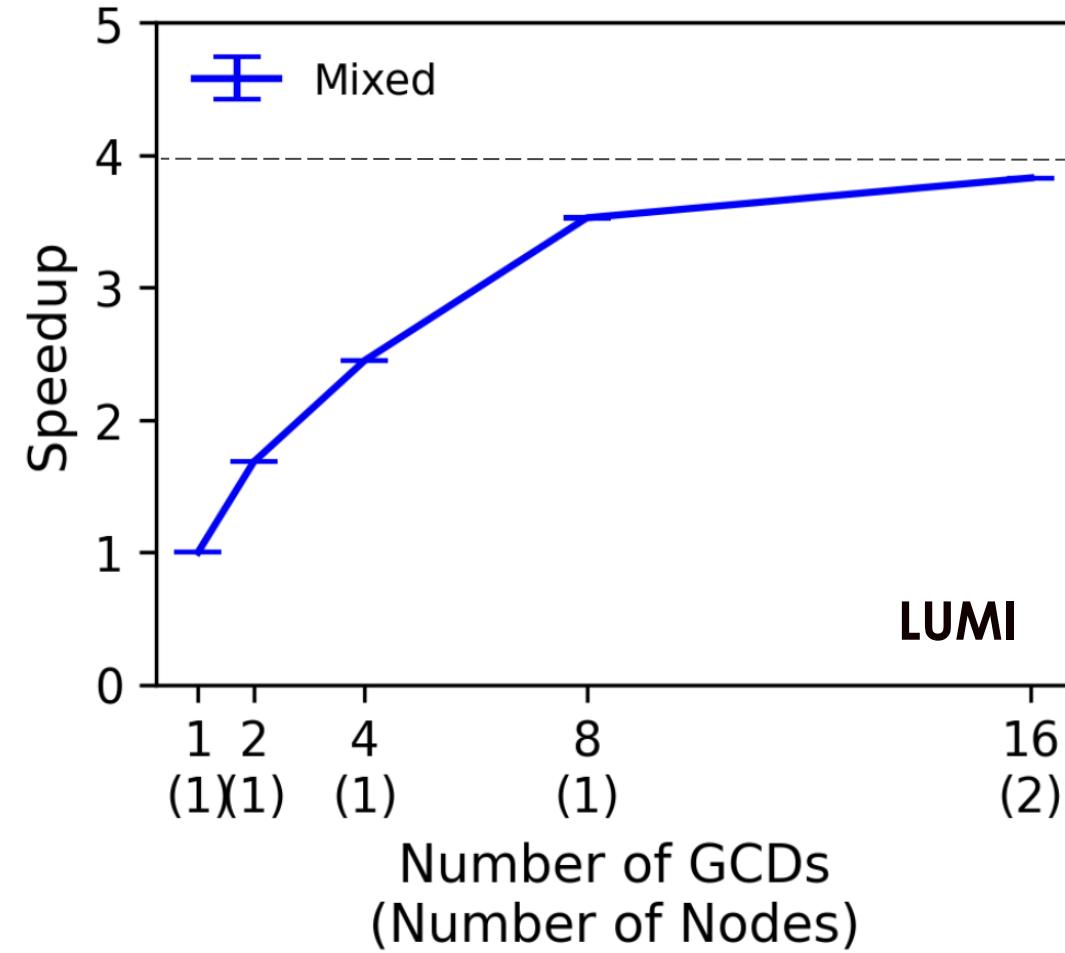
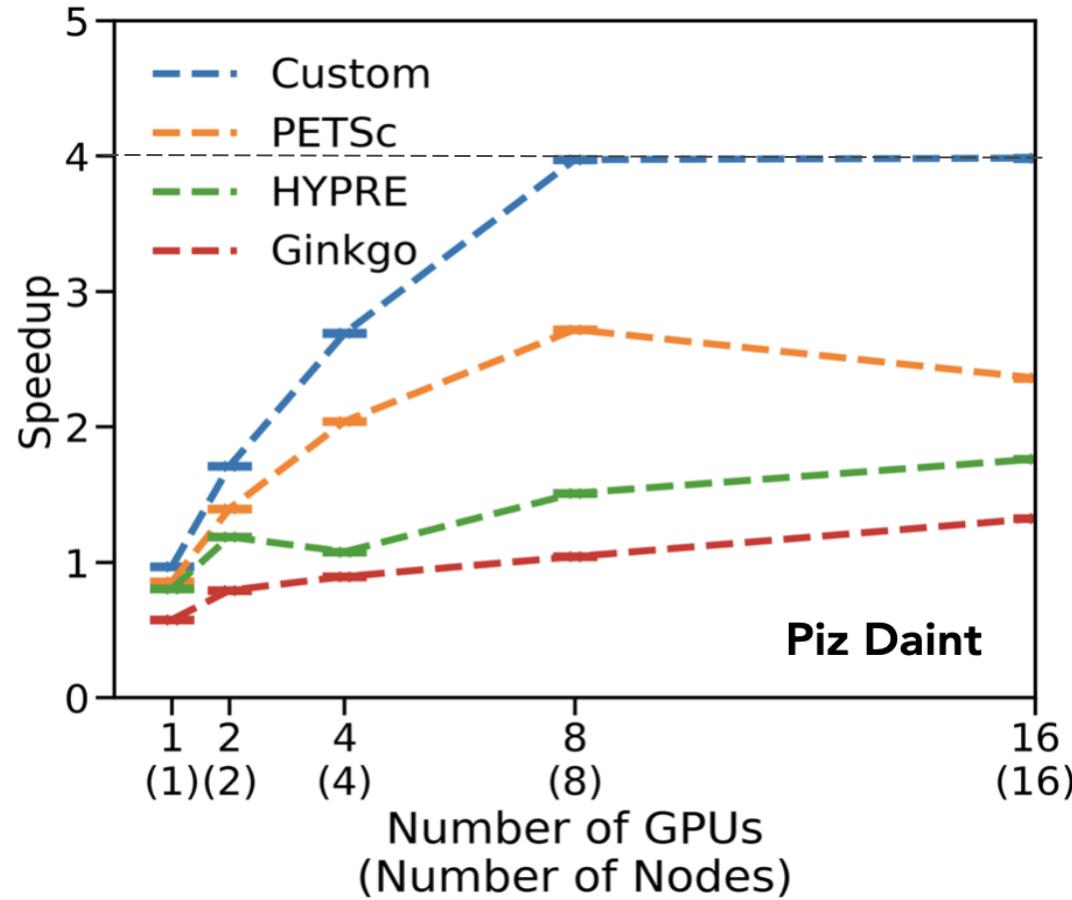


$$\|\vec{r}_n\|_{sym} = \vec{r}_n^T \mathbf{M} \vec{r}_n$$

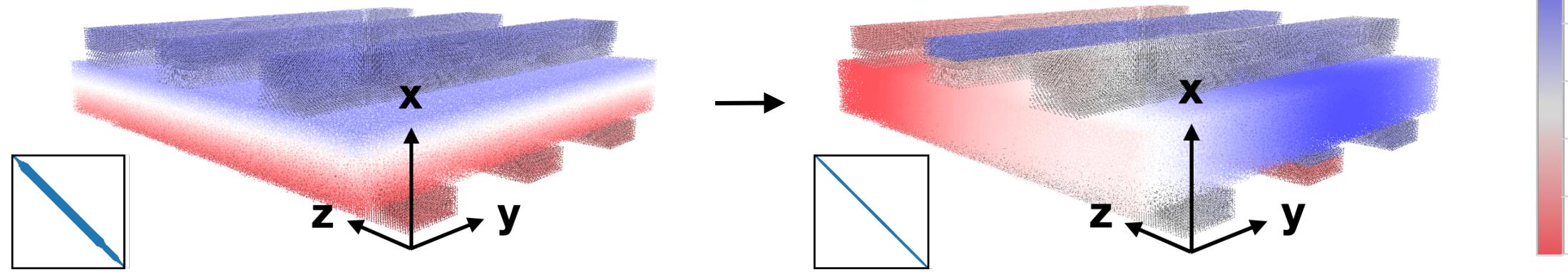
- $3 \rightarrow 2$ All reduce operations required



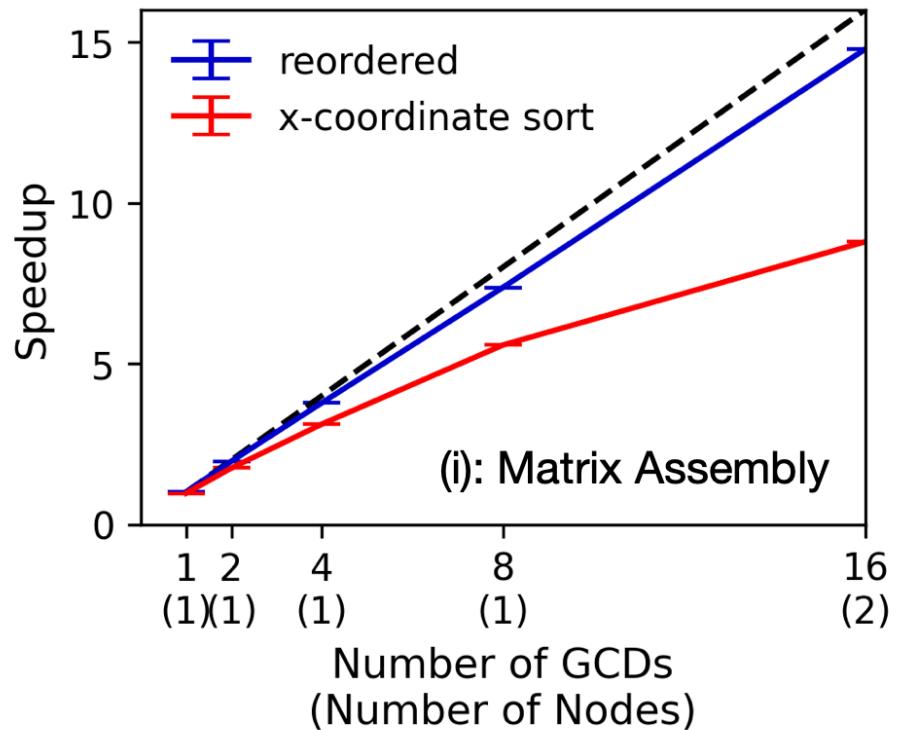
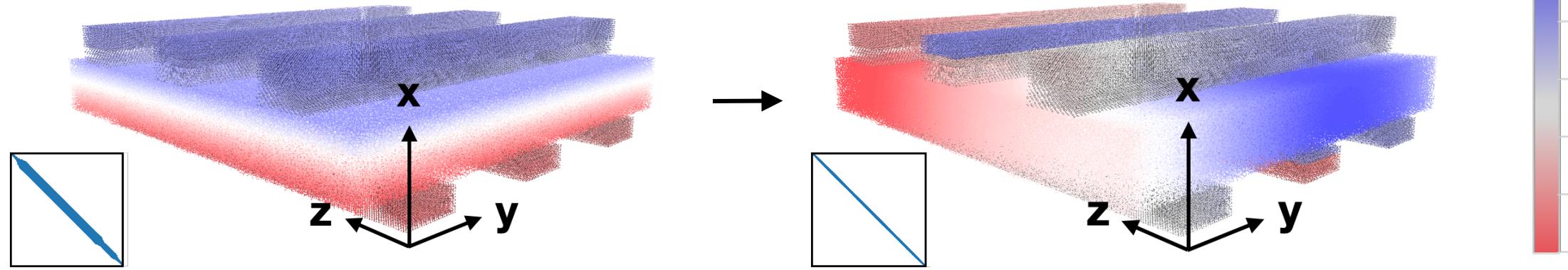
DISTRIBUTED ITERATIVE SOLVER



SPARSITY-SPECIFIC ITERATIVE SOLVERS



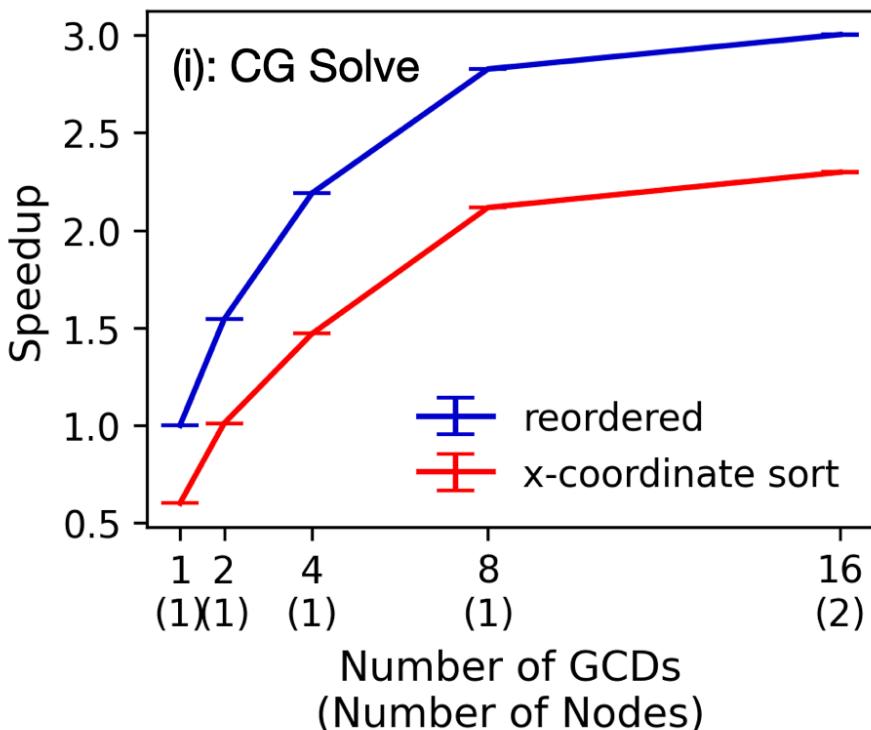
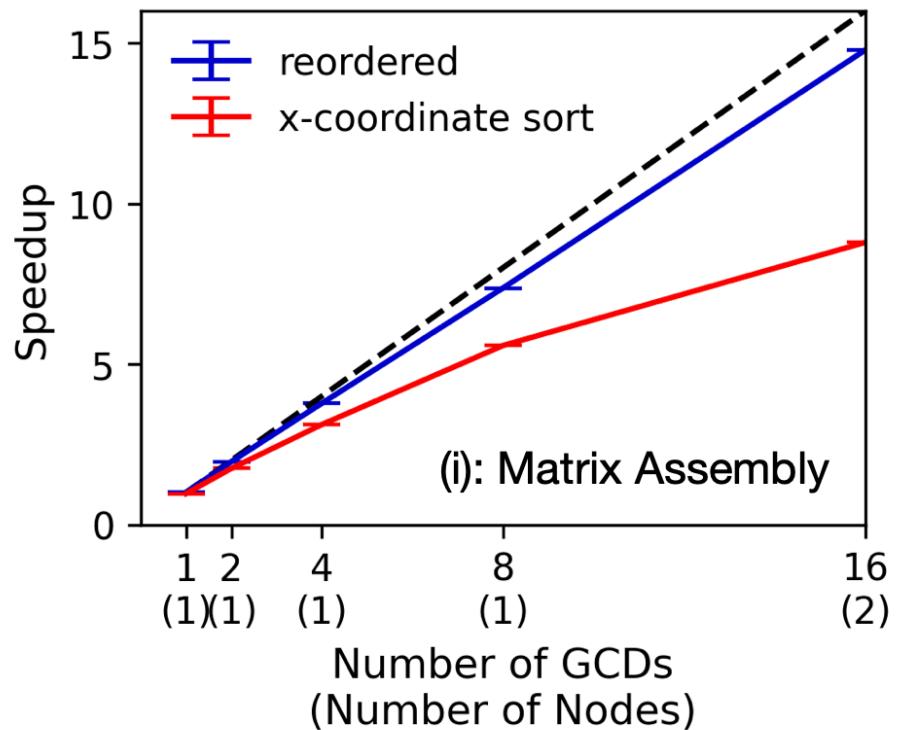
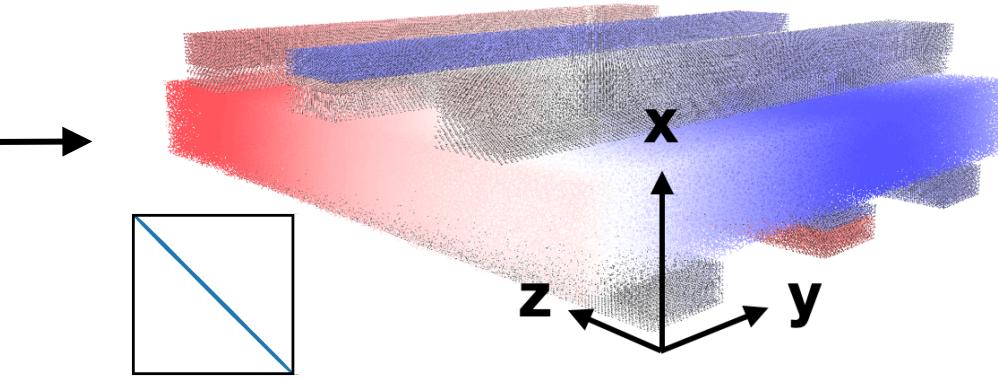
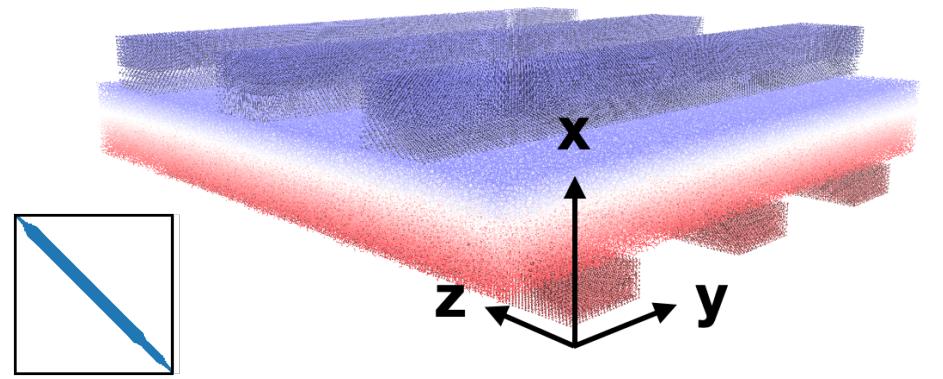
SPARSITY-SPECIFIC ITERATIVE SOLVERS



- Contiguous memory accesses



SPARSITY-SPECIFIC ITERATIVE SOLVERS



- Contiguous memory accesses
- Fewer block-neighbors for communication



KEY OPTIMIZATION AREAS

Field Updates



Development of a
sparsity-optimized
**distributed Conjugate
Gradient** solver

Event Selection



Distributed Monte Carlo
event **selection** process

Repeat supersteps



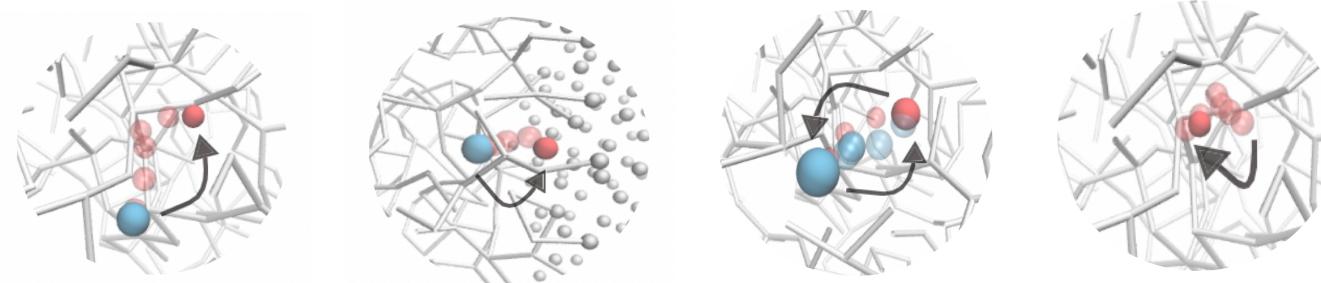
Task-based distribution
of application modules



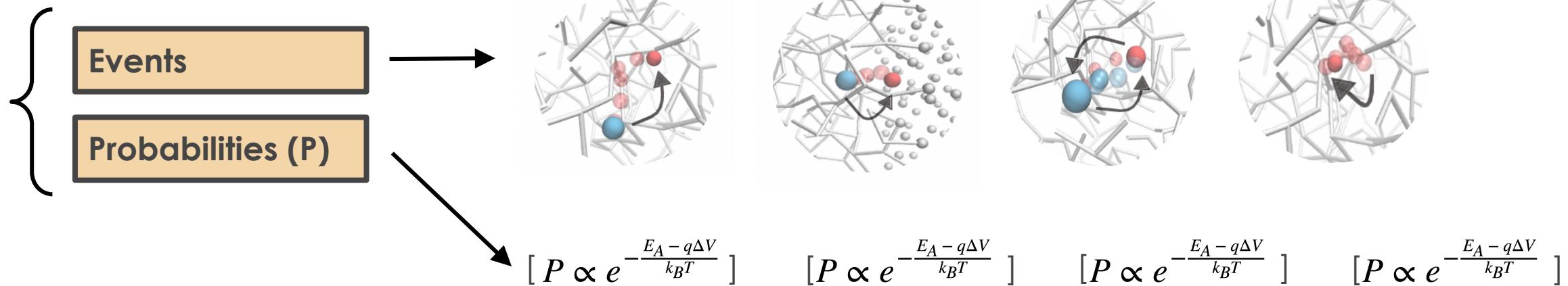
DISTRIBUTED MONTE CARLO SELECTION



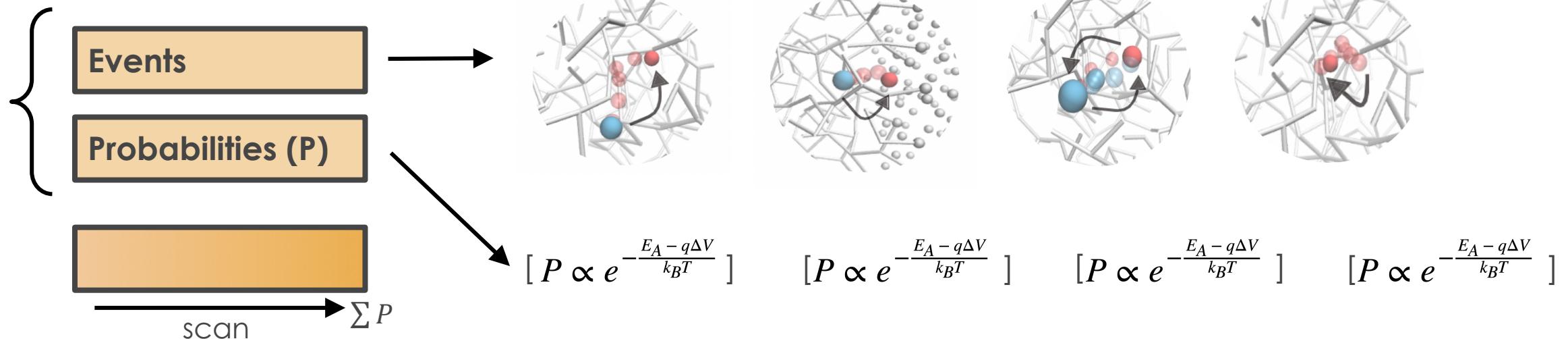
DISTRIBUTED MONTE CARLO SELECTION



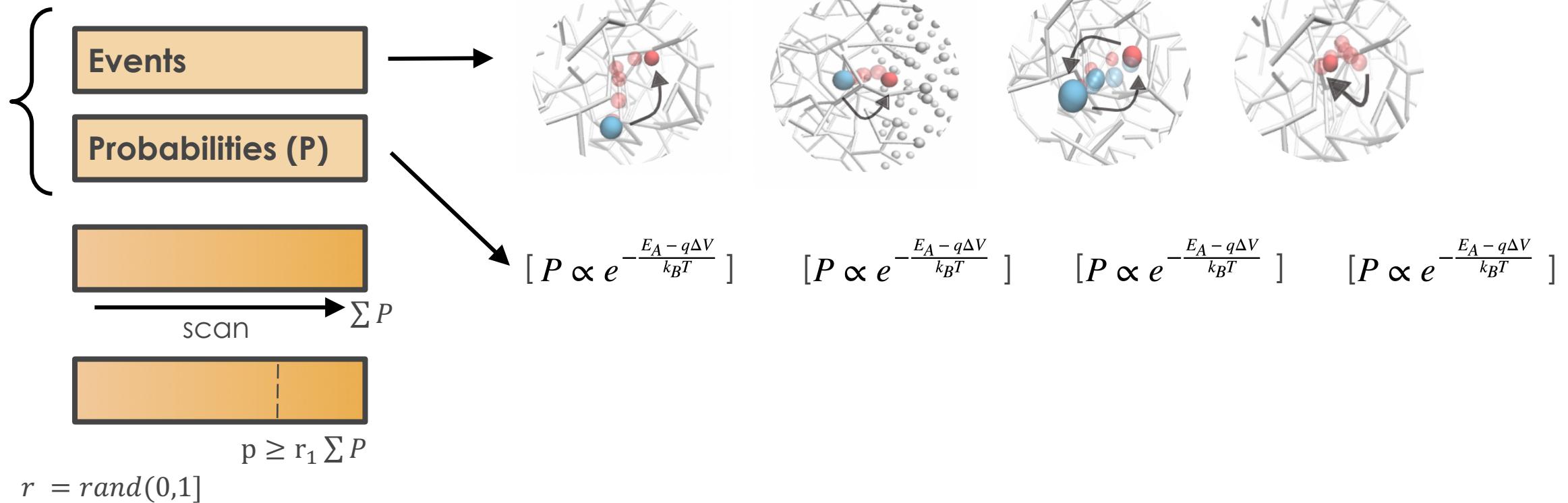
DISTRIBUTED MONTE CARLO SELECTION



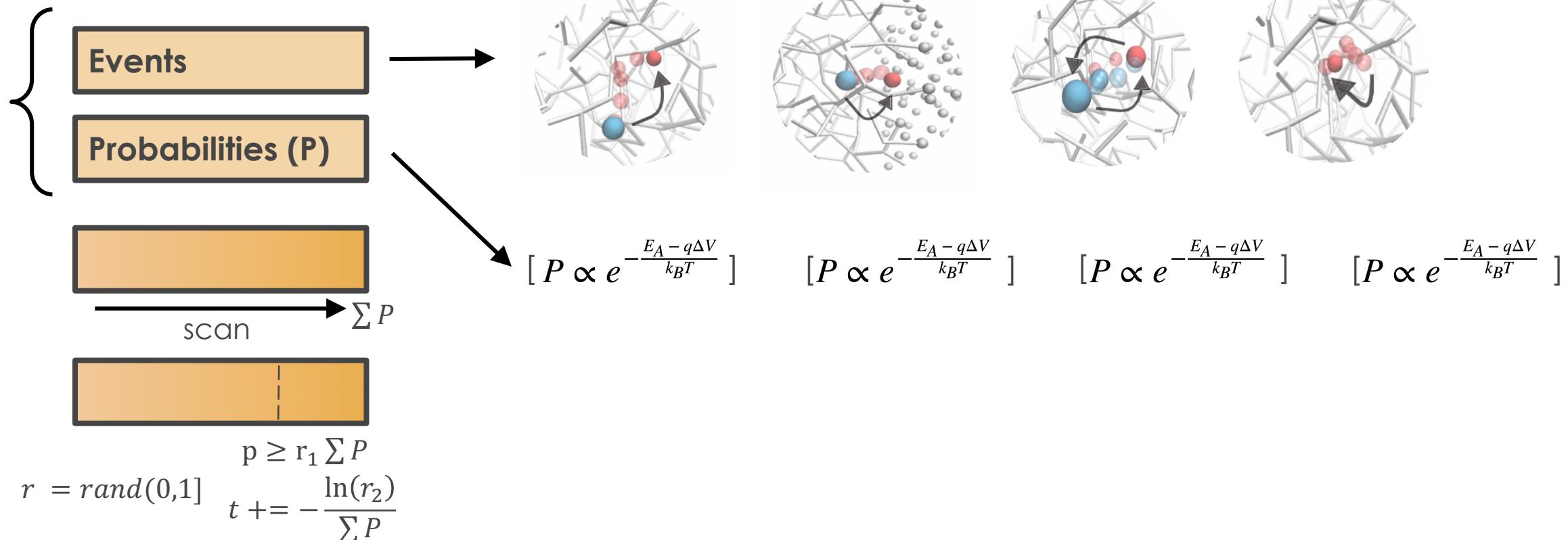
DISTRIBUTED MONTE CARLO SELECTION



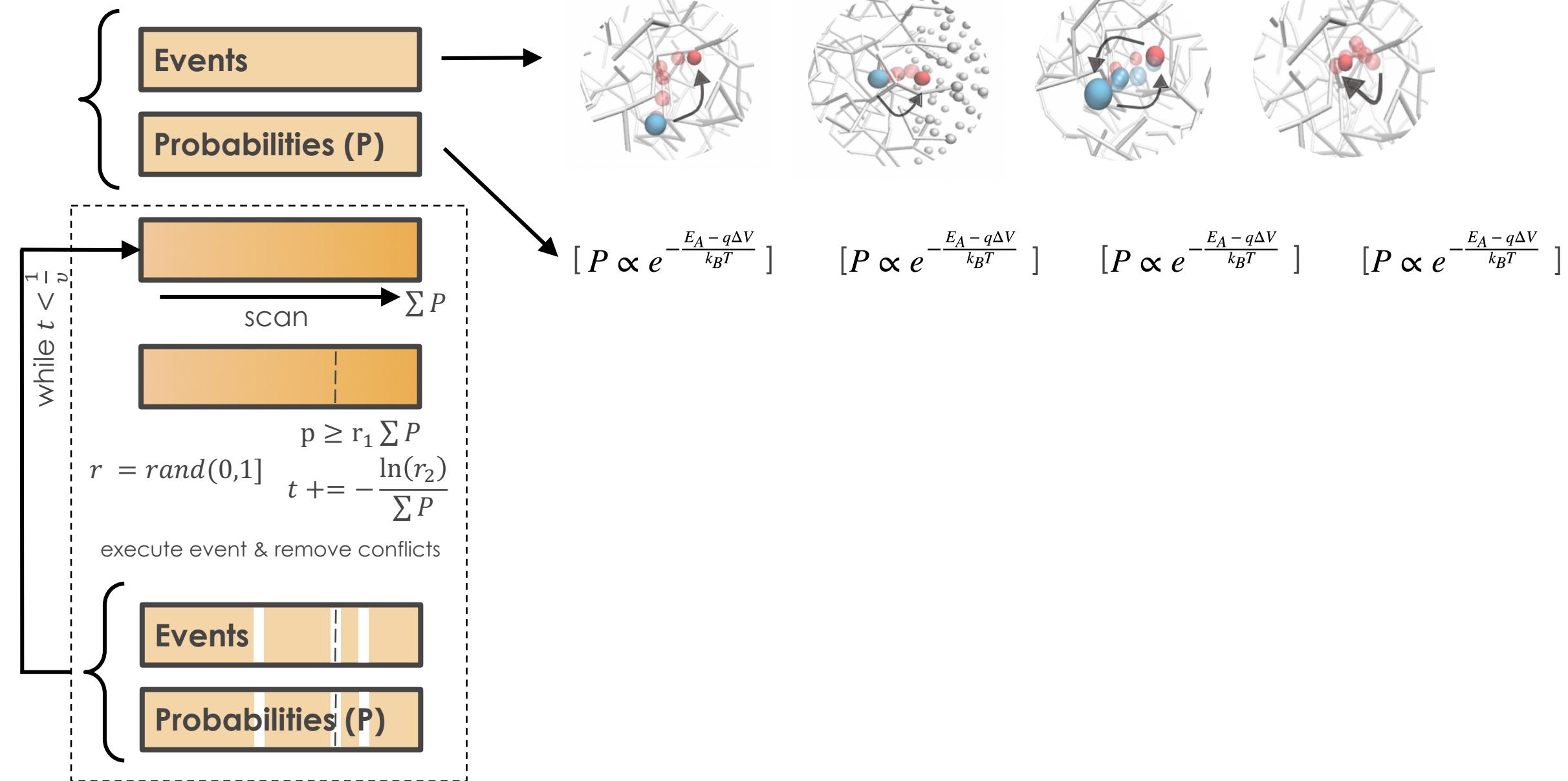
DISTRIBUTED MONTE CARLO SELECTION



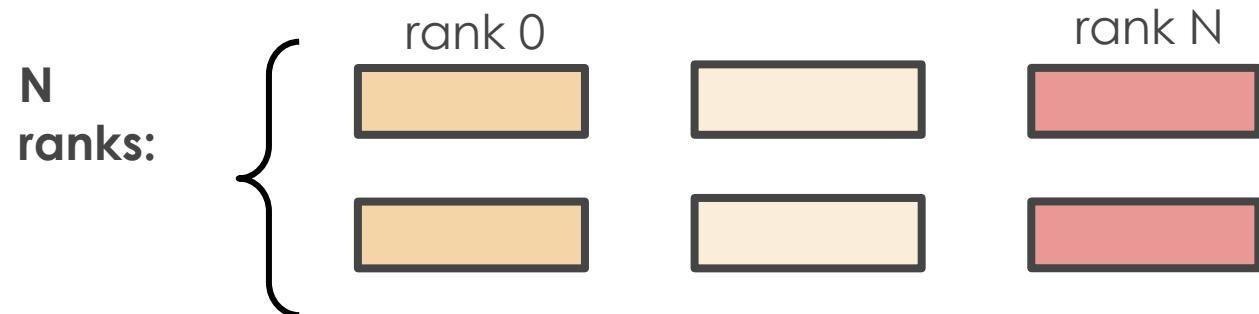
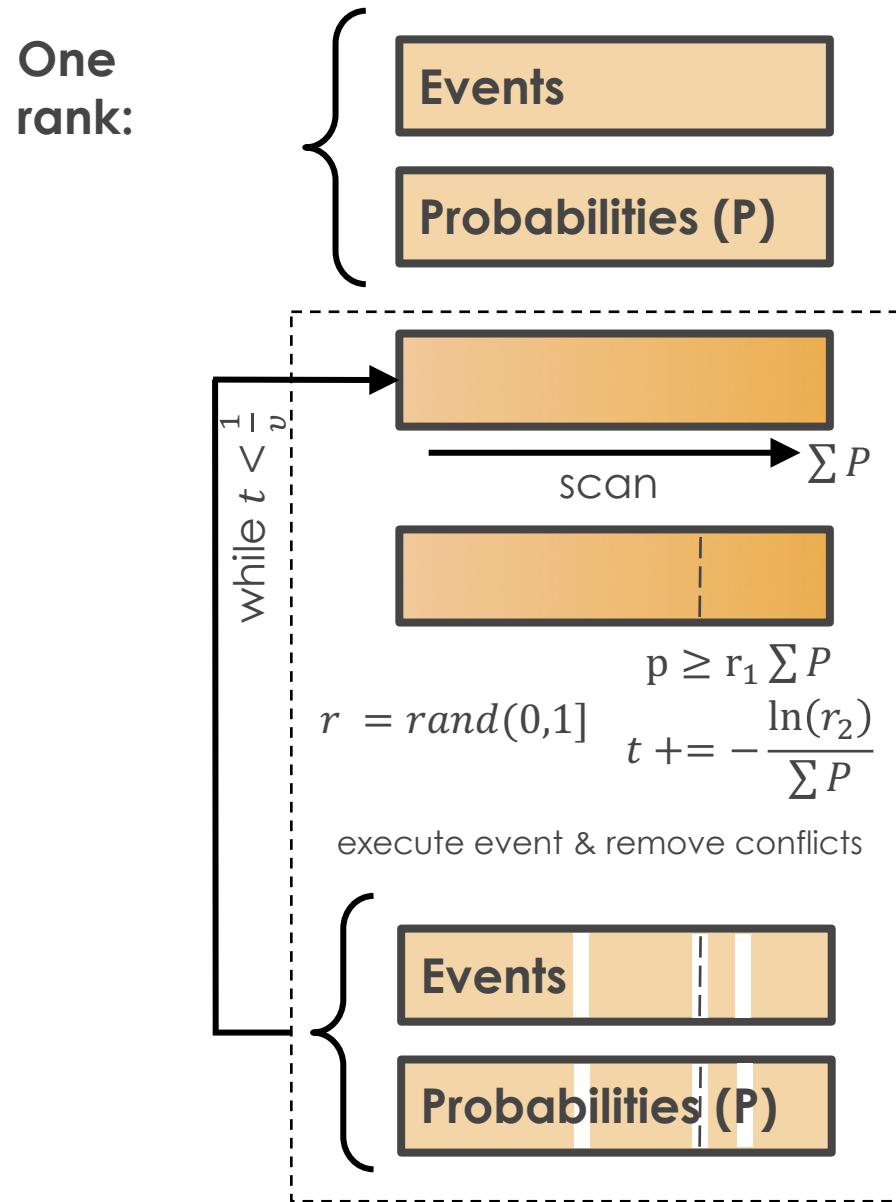
DISTRIBUTED MONTE CARLO SELECTION



DISTRIBUTED MONTE CARLO SELECTION

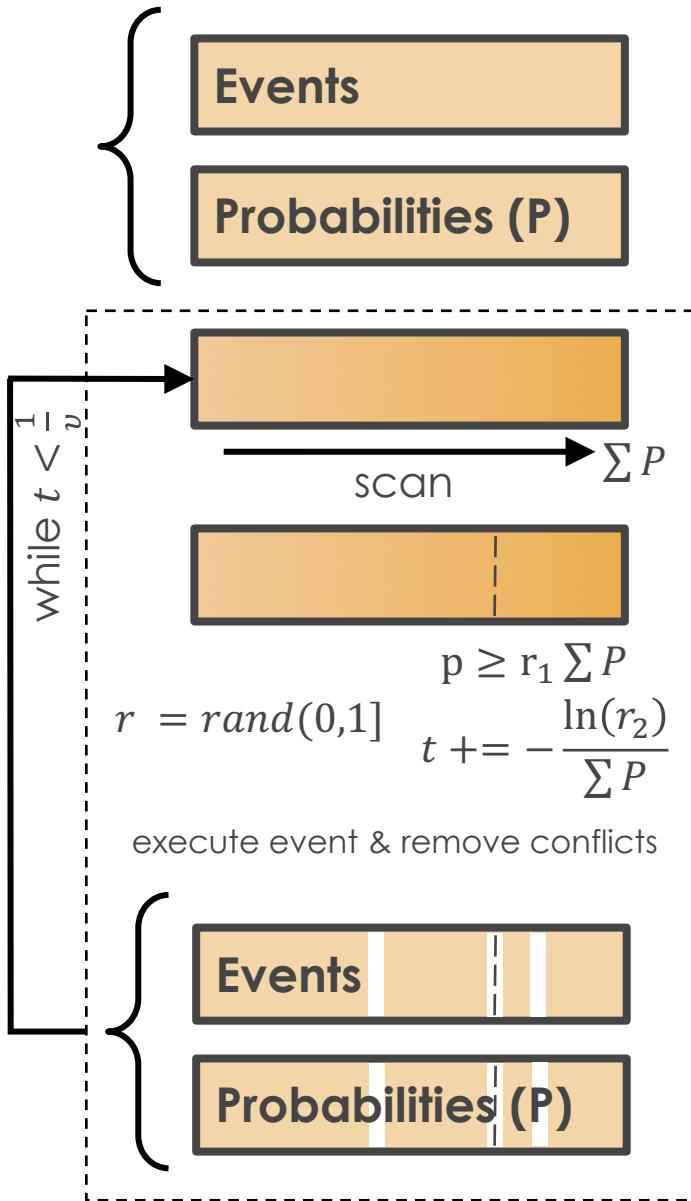


DISTRIBUTED MONTE CARLO SELECTION

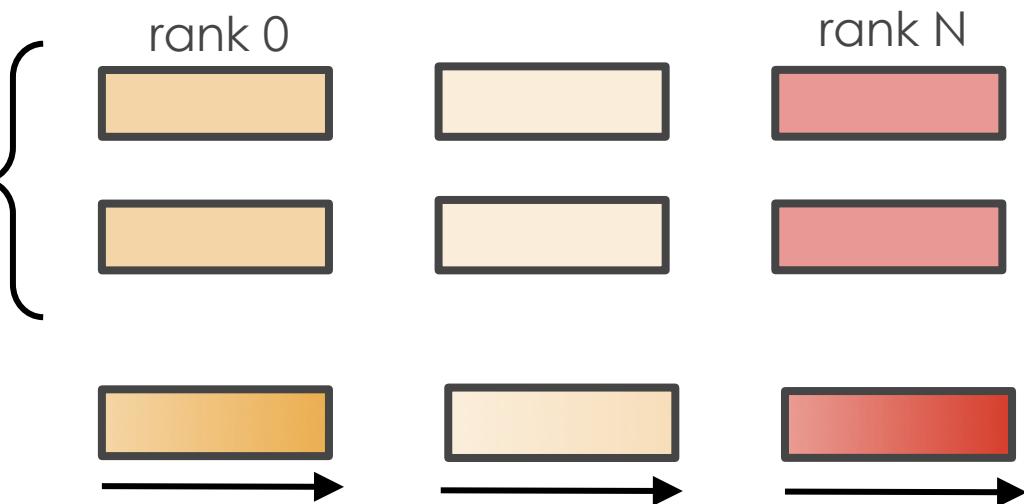


DISTRIBUTED MONTE CARLO SELECTION

One rank:

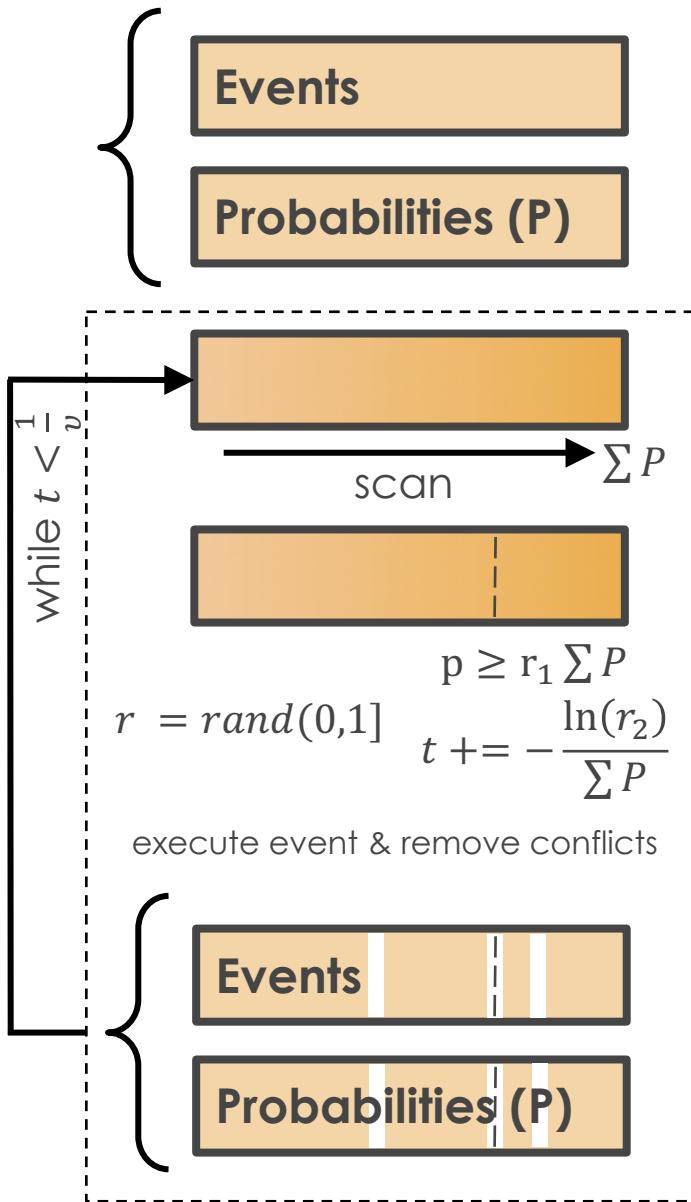


N ranks:

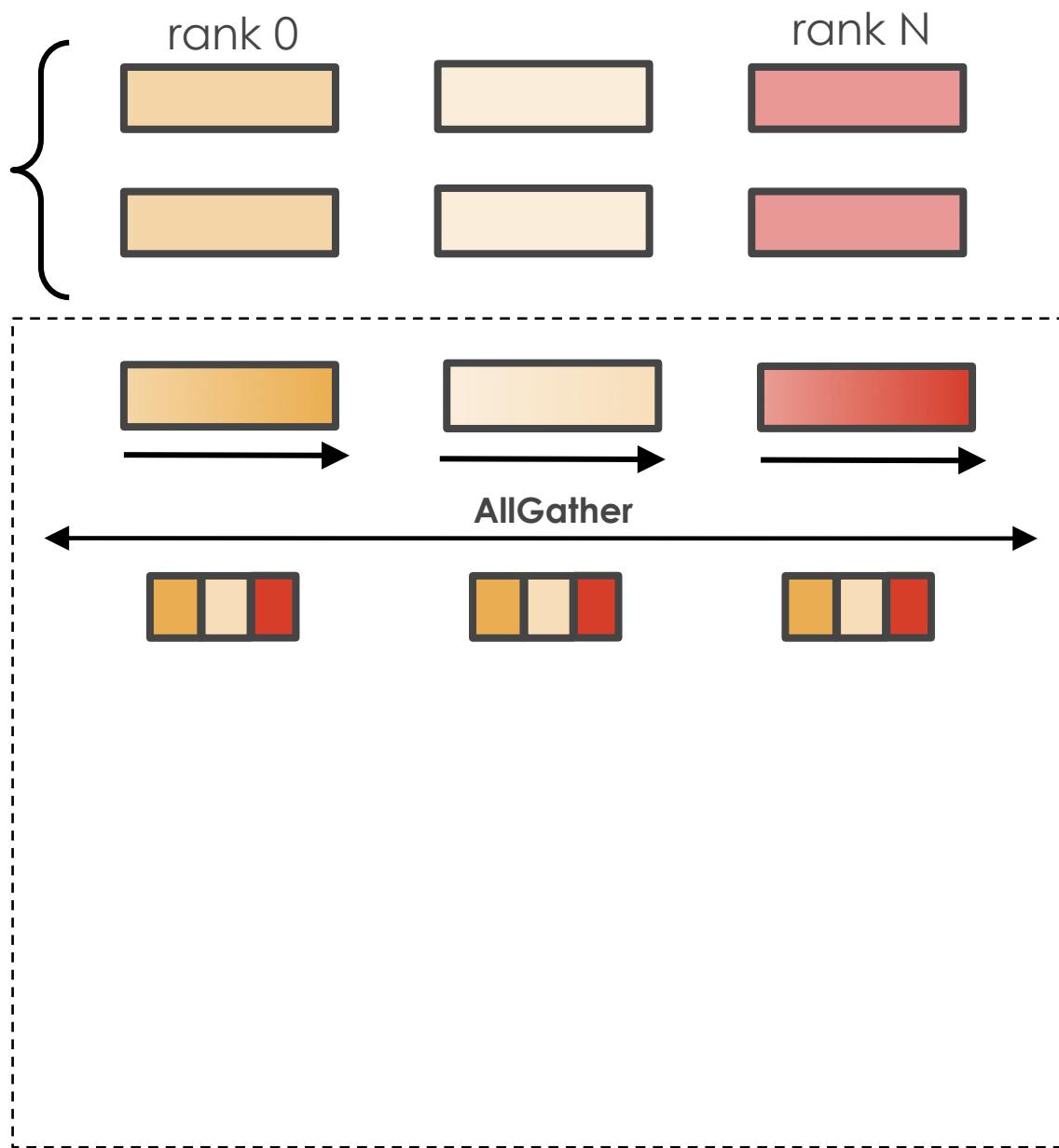


DISTRIBUTED MONTE CARLO SELECTION

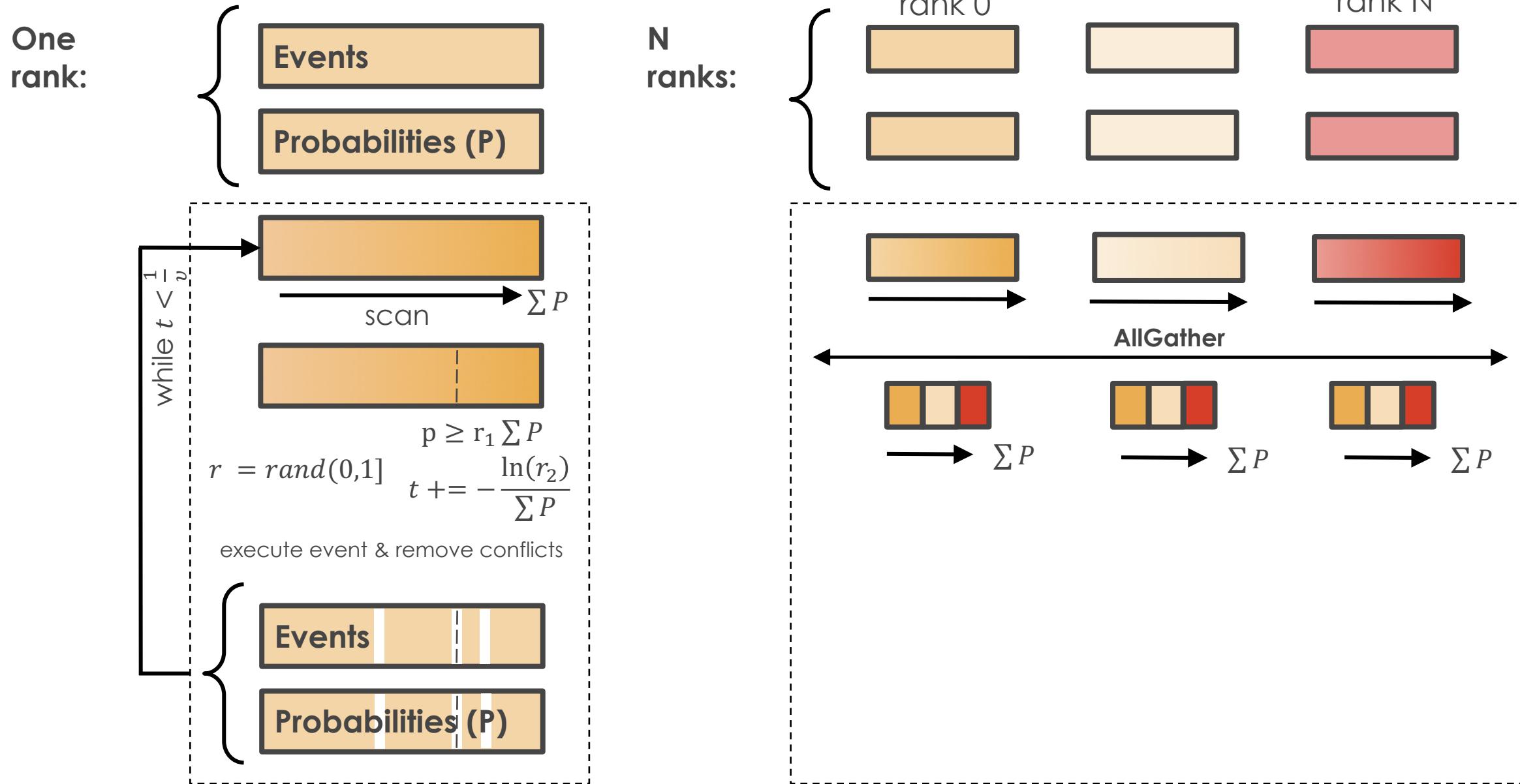
One rank:



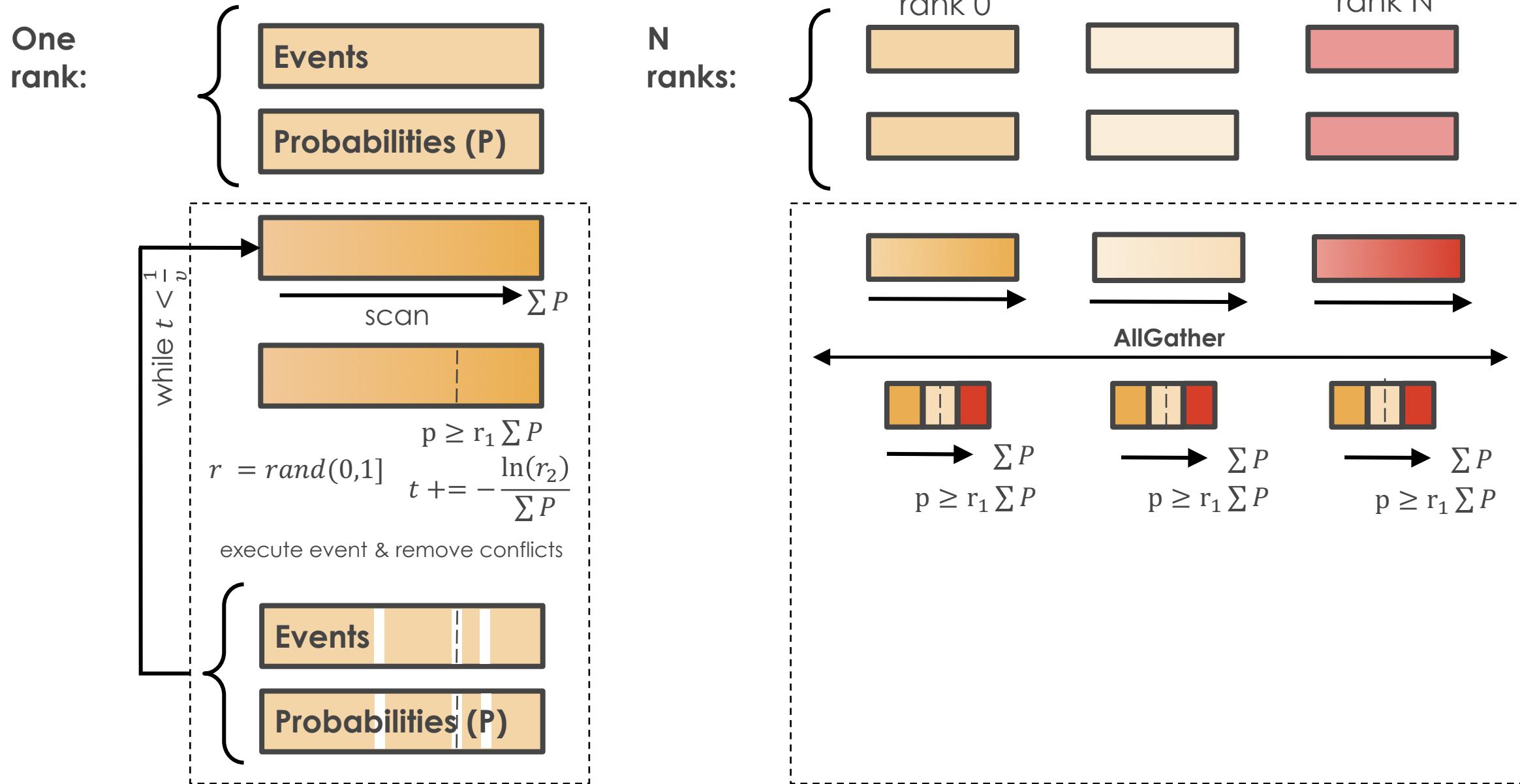
N ranks:



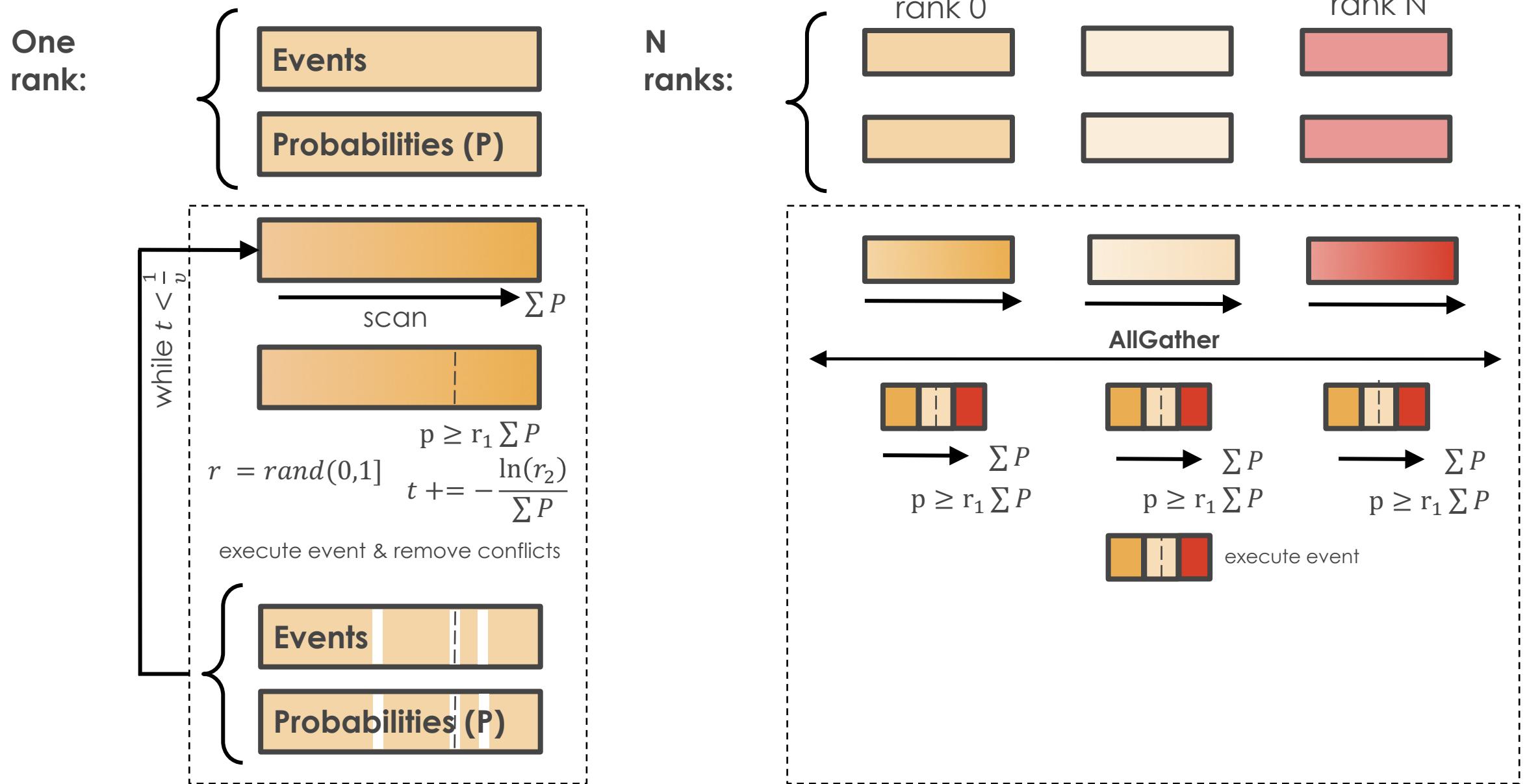
DISTRIBUTED MONTE CARLO SELECTION



DISTRIBUTED MONTE CARLO SELECTION

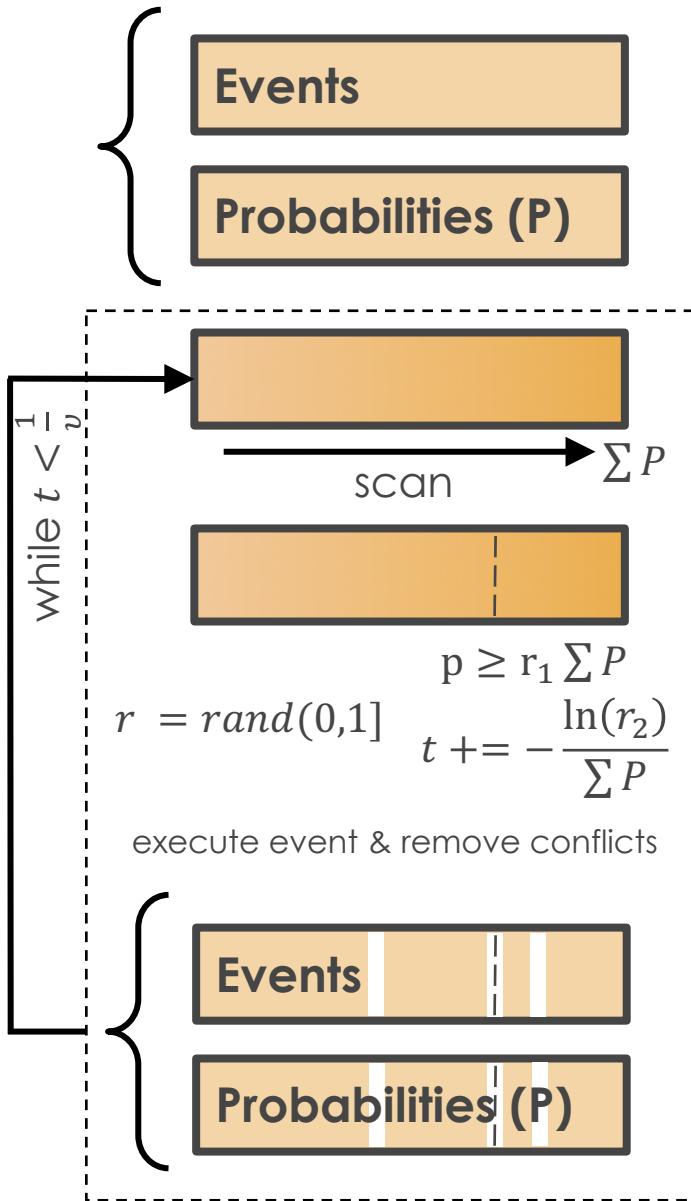


DISTRIBUTED MONTE CARLO SELECTION

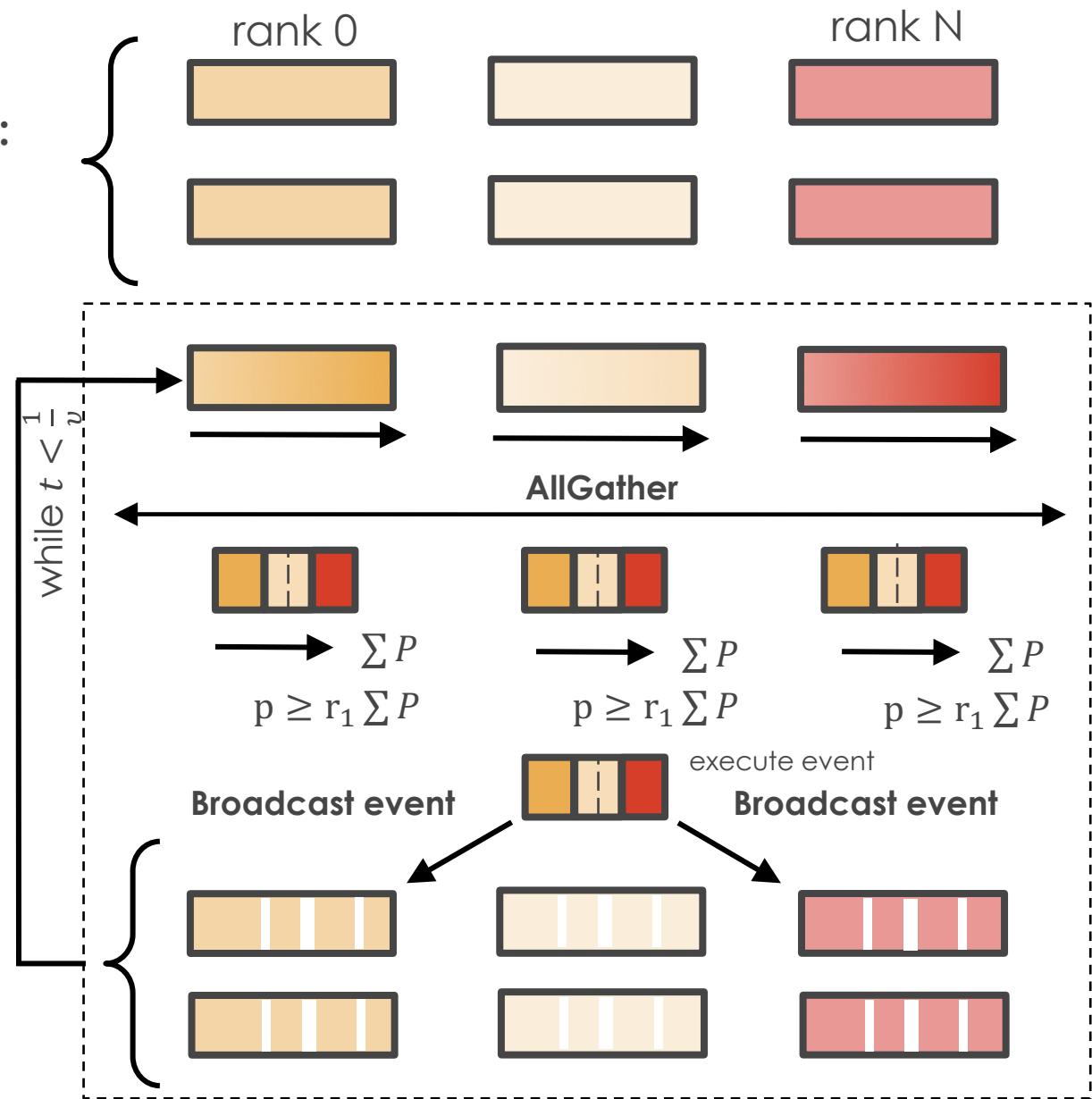


DISTRIBUTED MONTE CARLO SELECTION

One rank:



N ranks:



KEY OPTIMIZATION AREAS

Field Updates



Development of a
sparsity-optimized
**distributed Conjugate
Gradient** solver

Event Selection



Distributed Monte Carlo
event selection process

Repeat supersteps

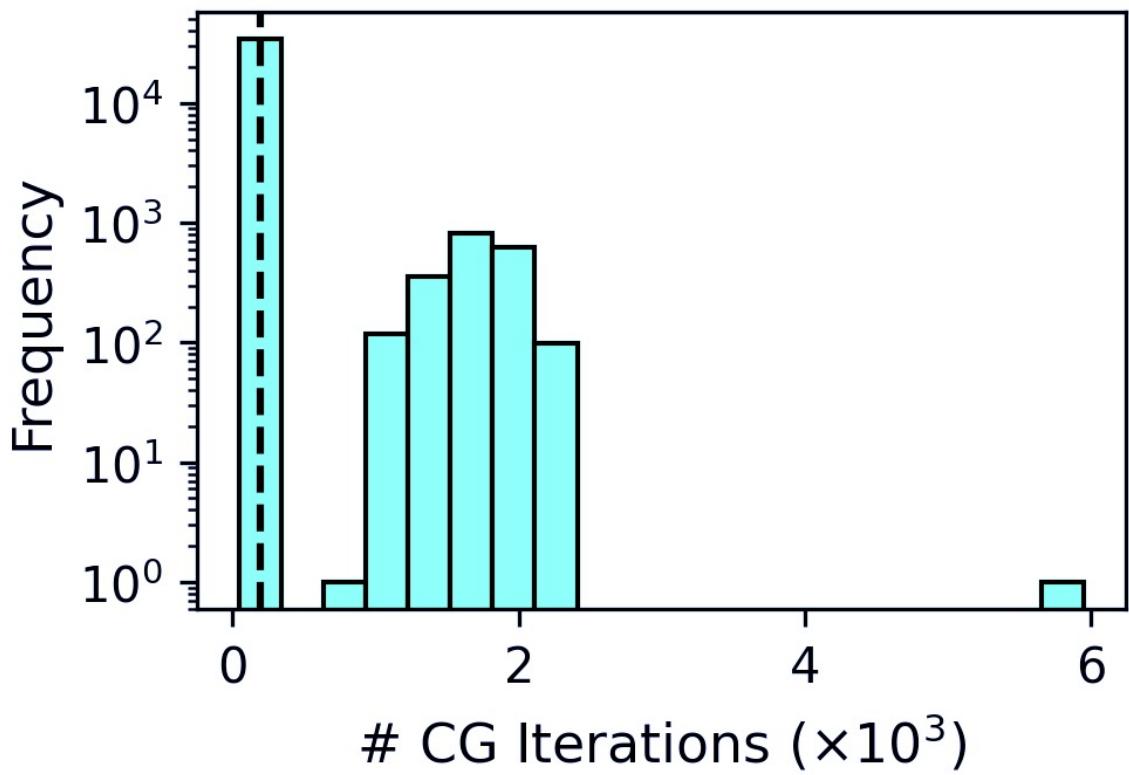


Task-based distribution
of application modules



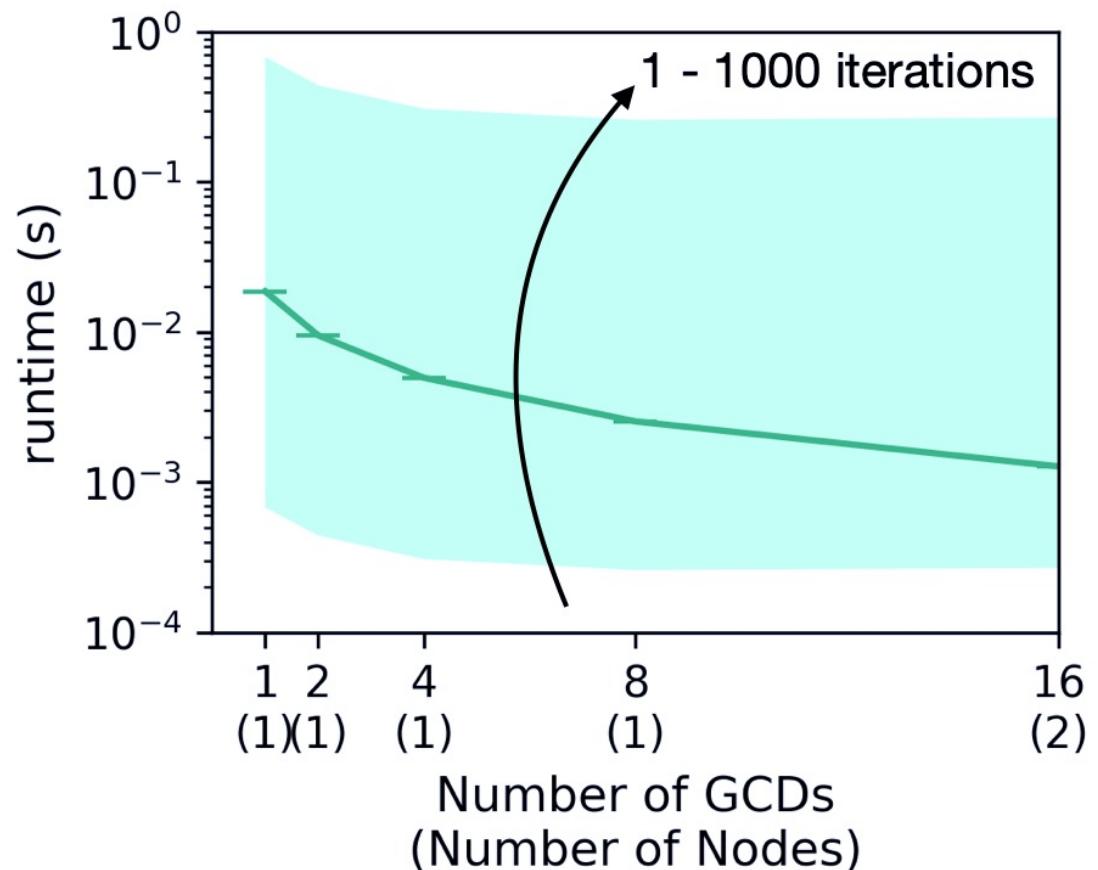
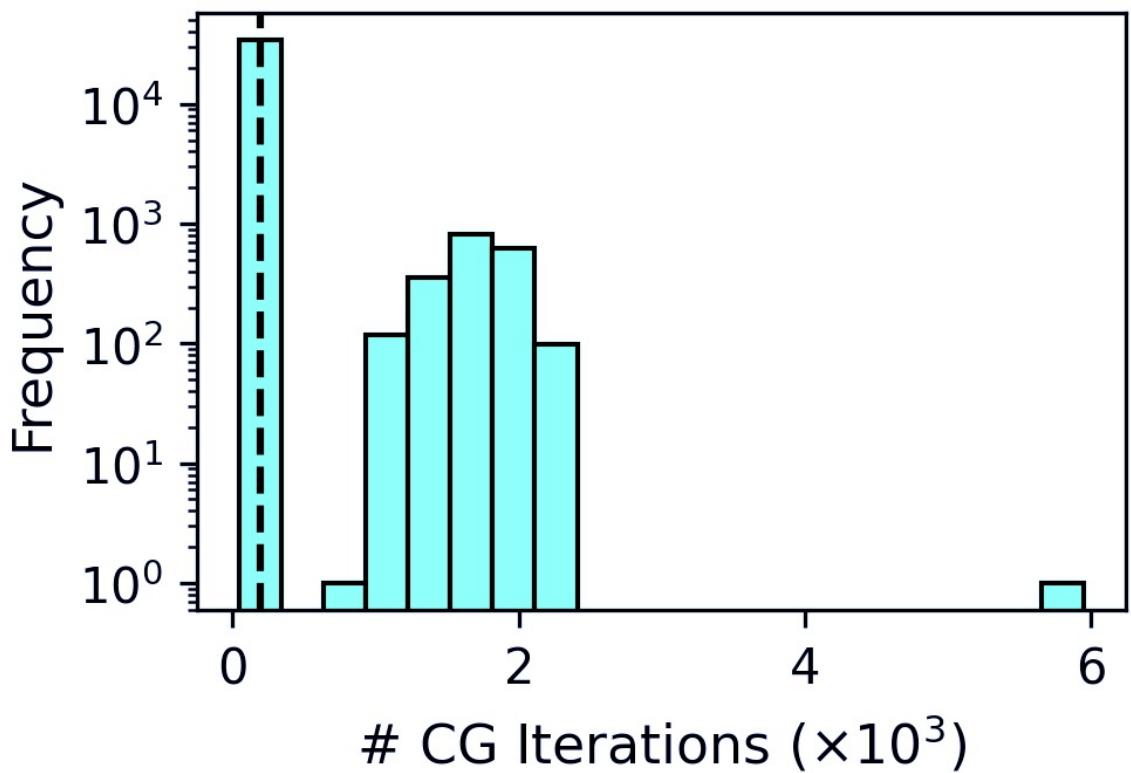
HOW TO DISTRIBUTE THE WORKLOAD WHEN...

... the **time** per module varies



HOW TO DISTRIBUTE THE WORKLOAD WHEN...

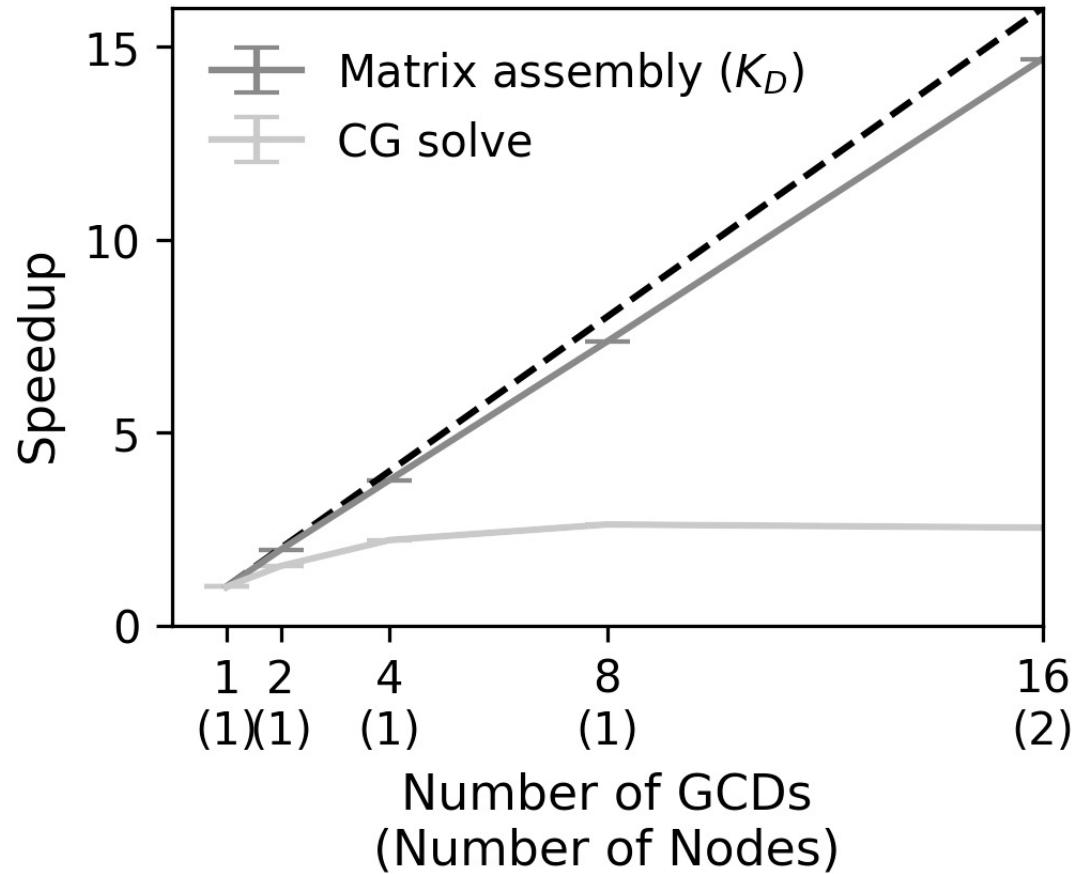
... the **time** per module varies



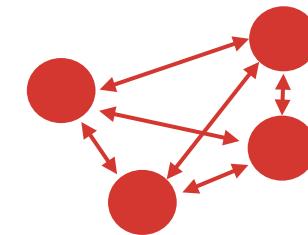
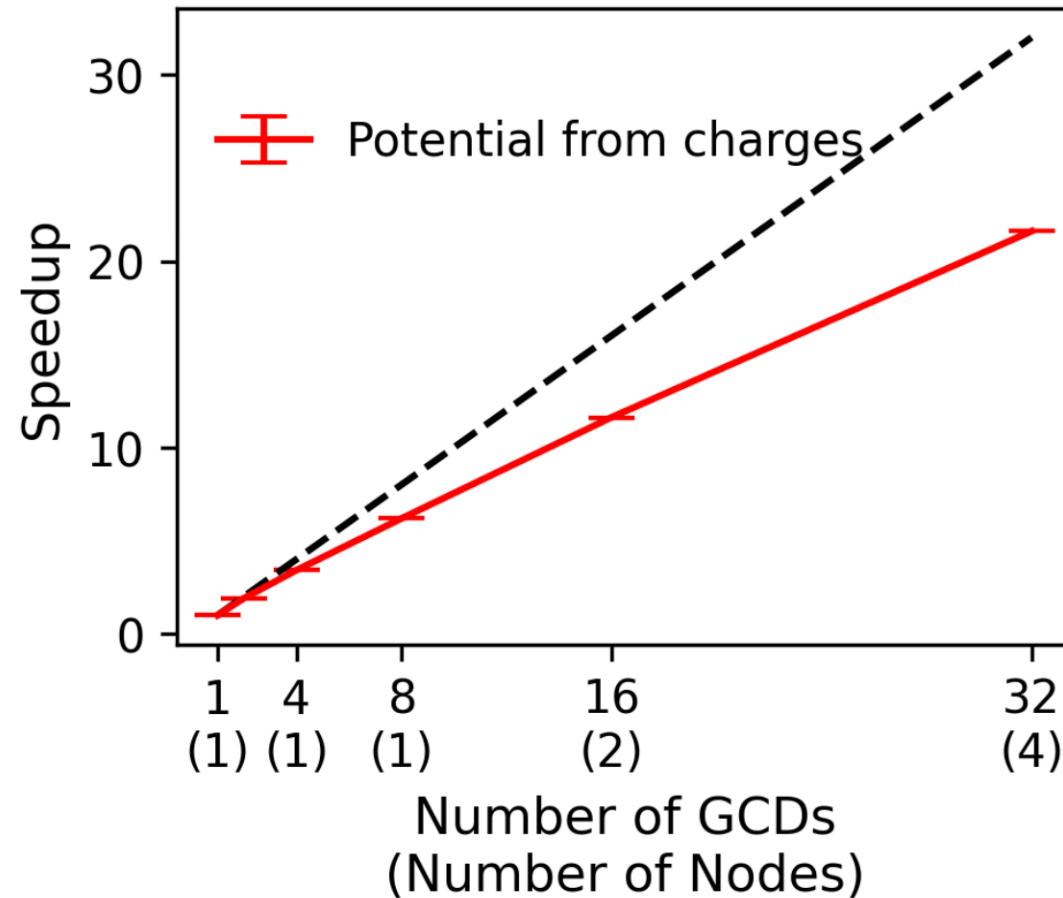
HOW TO DISTRIBUTE THE WORKLOAD WHEN...

... the **scalability** per module varies

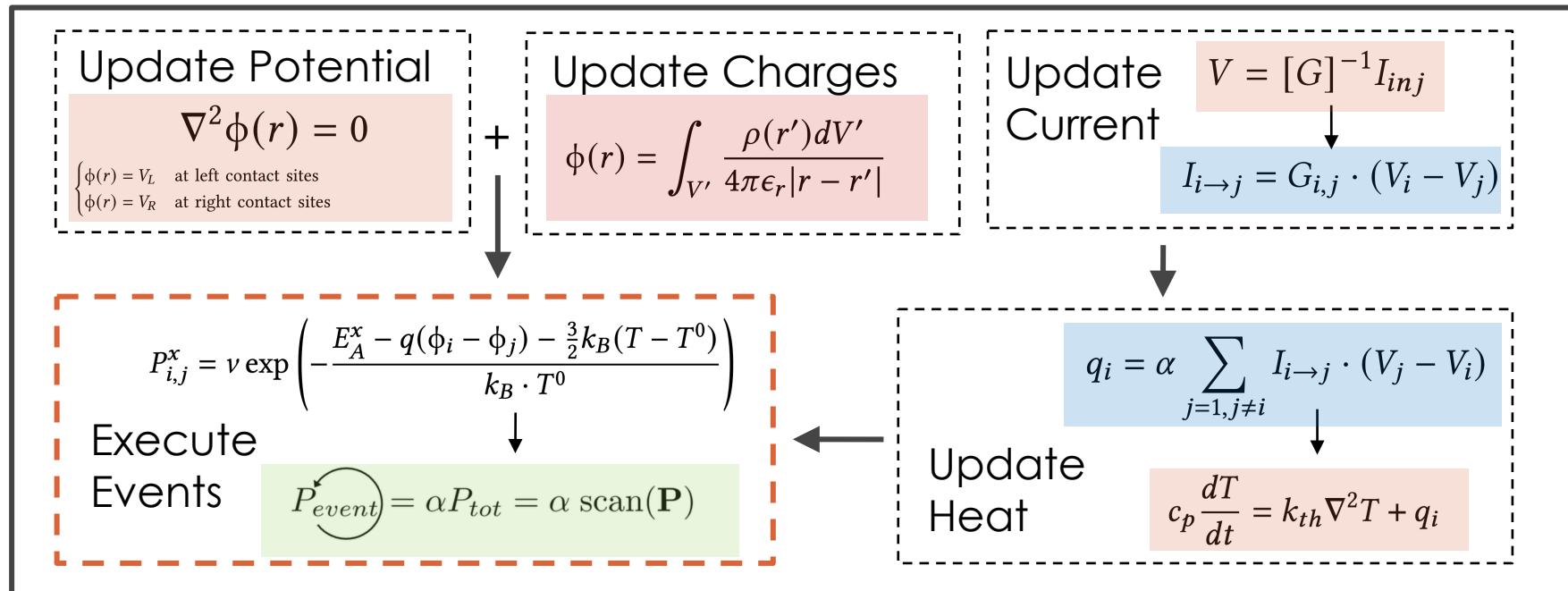
System of Linear Equations



Pair interactions



TASK BASED DISTRIBUTION



System of Linear Equations

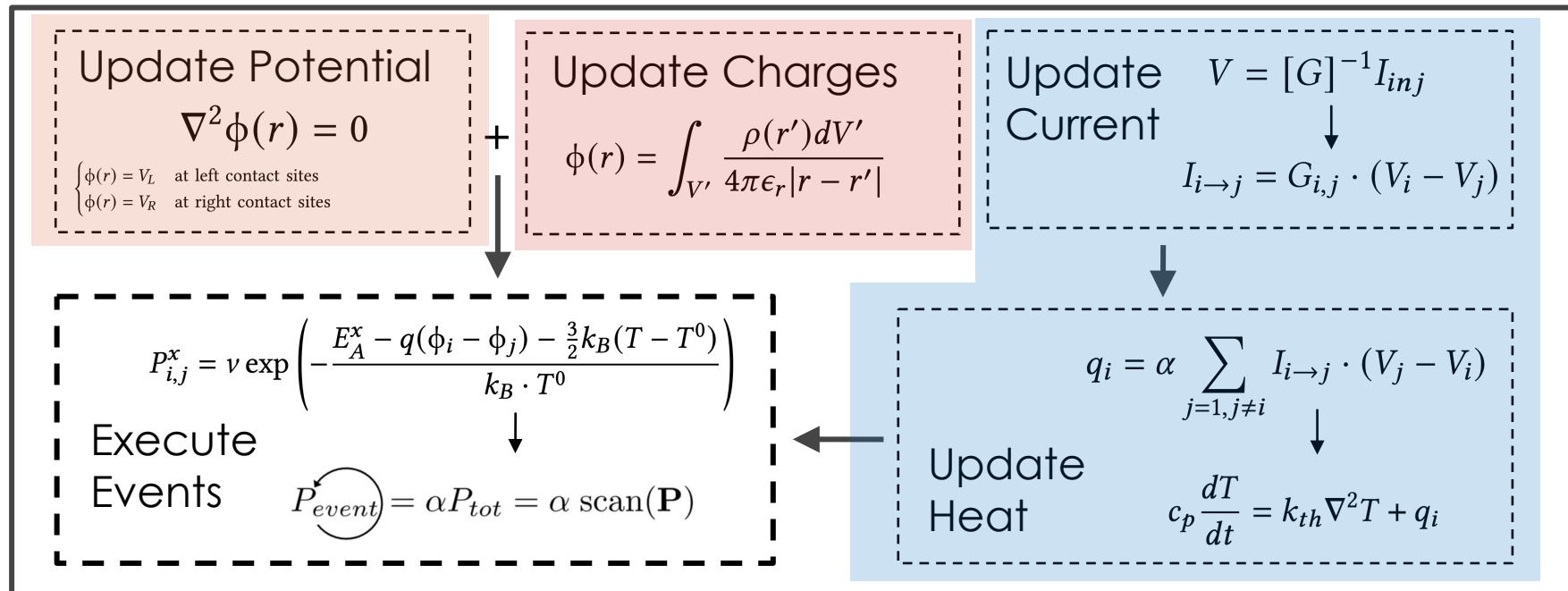
Pair interactions

SpMV

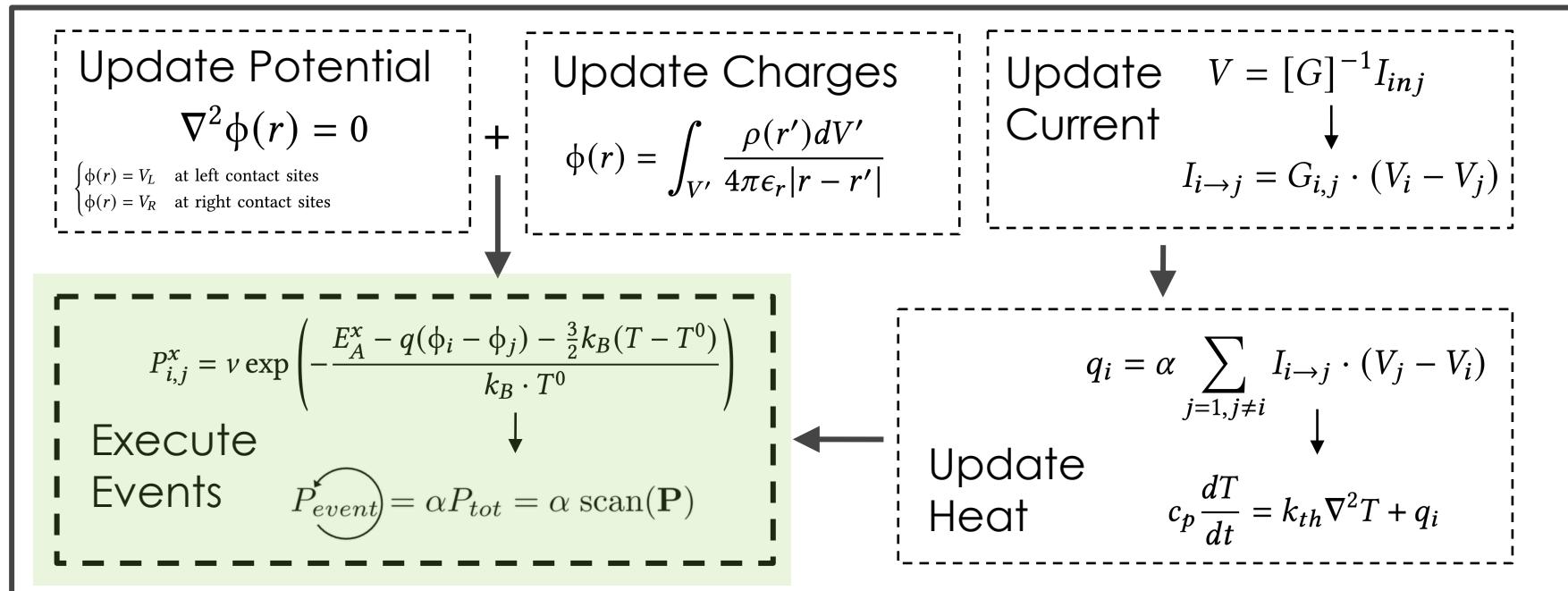
Prefix Sums



TASK BASED DISTRIBUTION



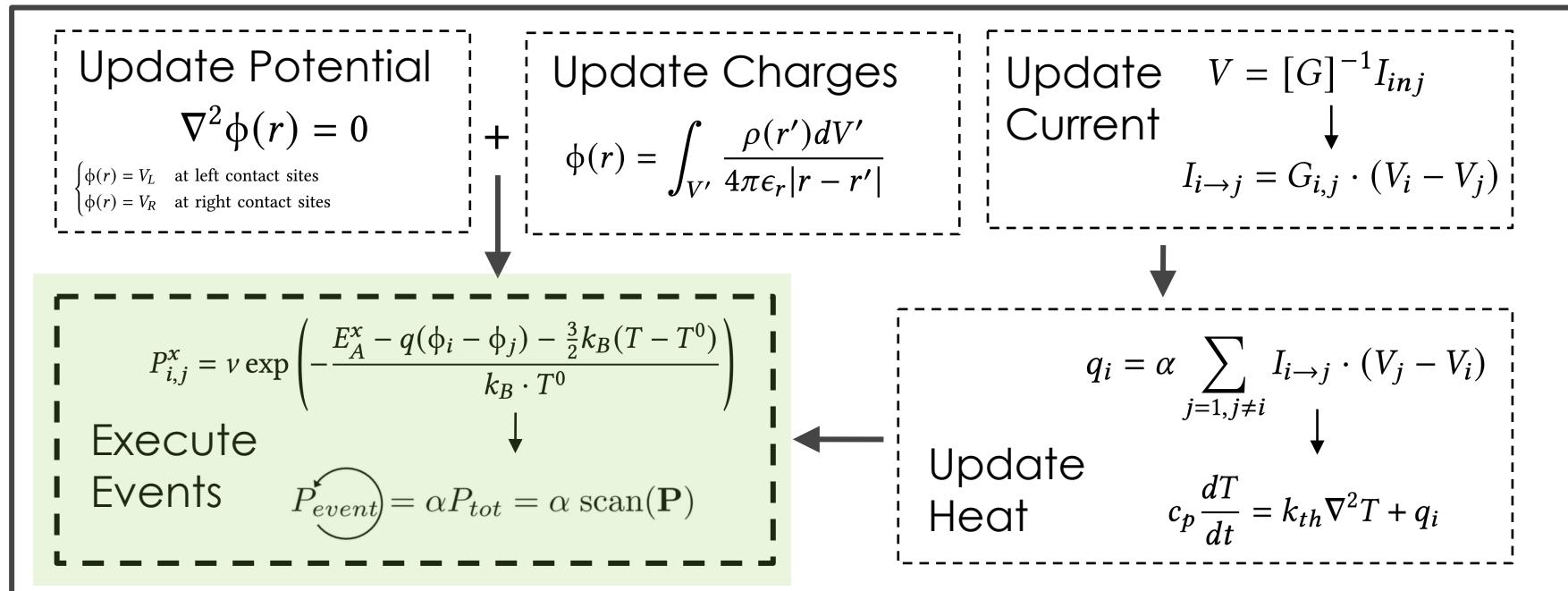
TASK BASED DISTRIBUTION



- Certain modules can be computed in parallel



TASK BASED DISTRIBUTION



- Certain modules can be computed in parallel
- Use of unevenly-divided MPI-subcommunicators



NAIVE DISTRIBUTION

Iterative CG

Update Potential

$$\nabla^2 \phi(r) = 0$$

$$\begin{cases} \phi(r) = V_L & \text{at left contact sites} \\ \phi(r) = V_R & \text{at right contact sites} \end{cases}$$



Pairwise interaction

Update Charges

$$\phi(r) = \int_{V'} \frac{\rho(r') dV'}{4\pi\epsilon_r |r - r'|}$$



$$P_{i,j}^x = v \exp \left(-\frac{E_A^x - q(\phi_i - \phi_j) - \frac{3}{2}k_B(T - T^0)}{k_B \cdot T^0} \right)$$

Execute

Events $P_{event} = \alpha P_{tot} = \alpha \text{ scan}(\mathbf{P})$



NAIVE DISTRIBUTION

Iterative CG

Update Potential

$$\nabla^2 \phi(r) = 0$$

$$\begin{cases} \phi(r) = V_L & \text{at left contact sites} \\ \phi(r) = V_R & \text{at right contact sites} \end{cases}$$



Update Charges

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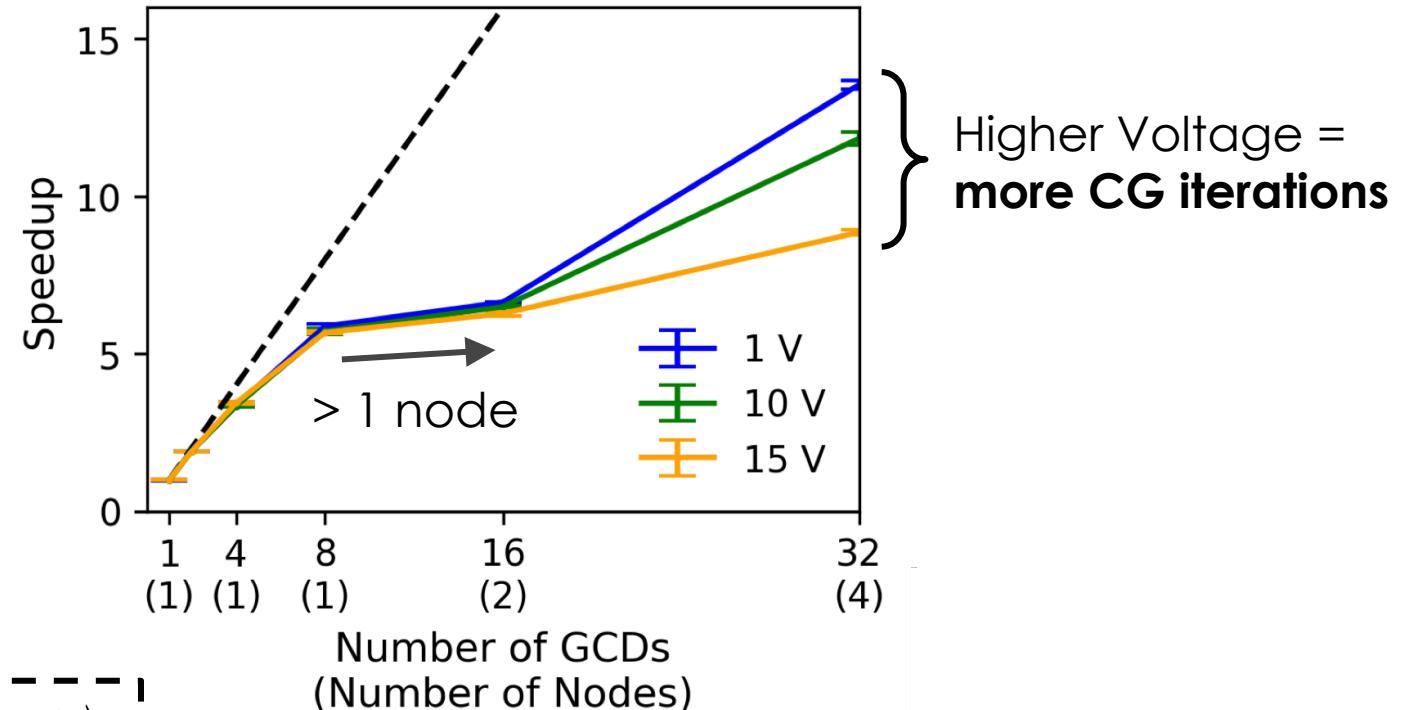


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NAIVE DISTRIBUTION

Iterative CG

Update Potential

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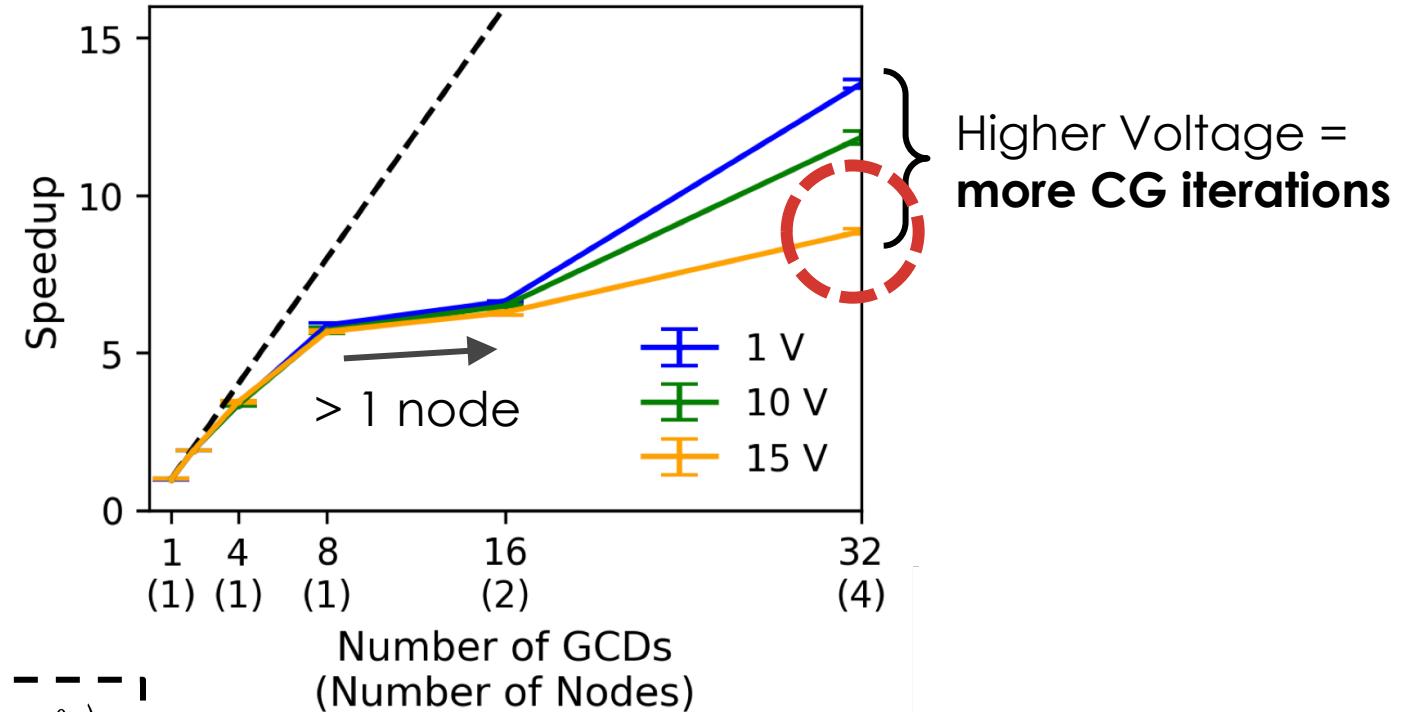
$$\begin{cases} \phi(r) = V_L & \text{at left contact sites} \\ \phi(r) = V_R & \text{at right contact sites} \end{cases}$$

+

Update Charges

$$\phi(r) = \int_{V'} \frac{\rho(r') dV'}{4\pi\epsilon_r |r - r'|}$$

Pairwise interaction



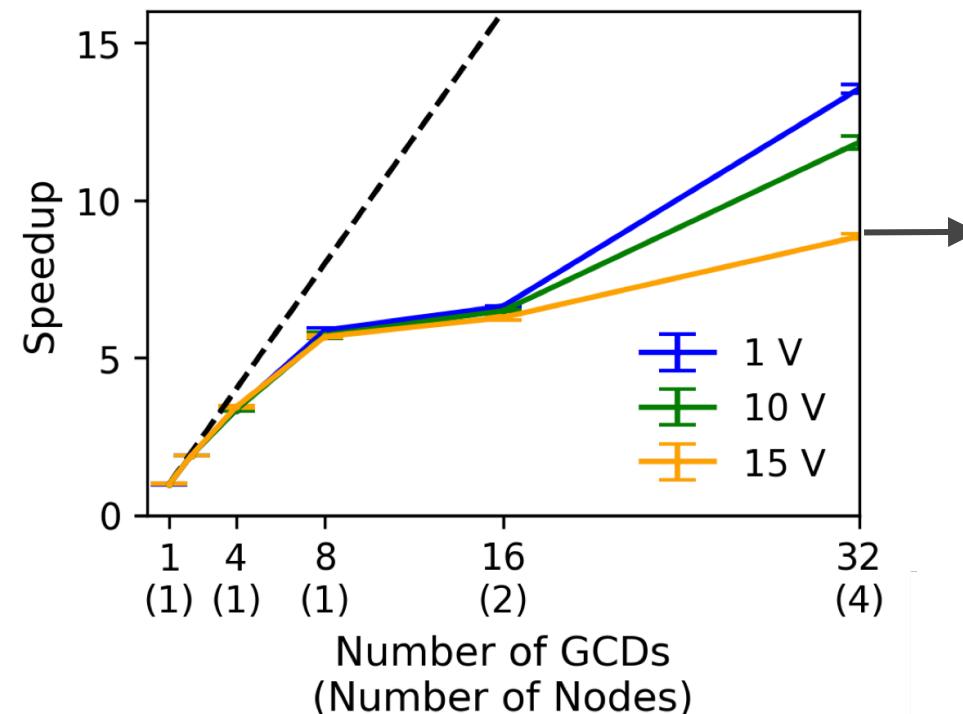
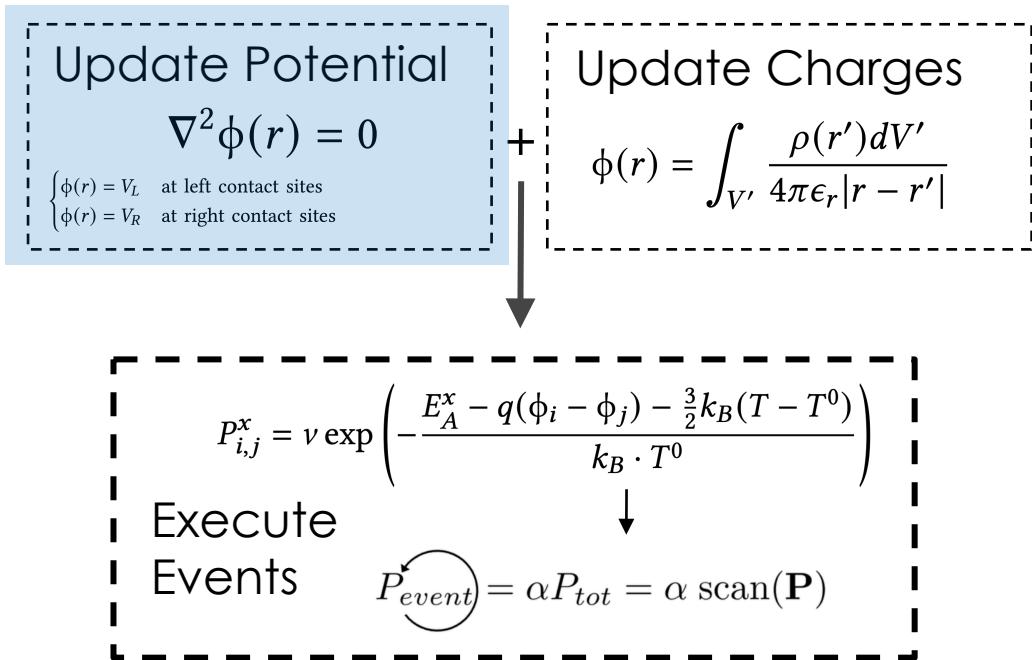
$P_{i,j}^x = v \exp \left(-\frac{E_A^x - q(\phi_i - \phi_j) - \frac{3}{2}k_B(T - T^0)}{k_B \cdot T^0} \right)$

Execute
Events $P_{event} = \alpha P_{tot} = \alpha \text{ scan}(\mathbf{P})$



TASK BASED DISTRIBUTION

Iterative CG: fast but scales poorly > 1 node



TASK BASED DISTRIBUTION

Iterative CG: fast but scales poorly > 1 node

Pairwise interaction: slow but parallel

Update Potential

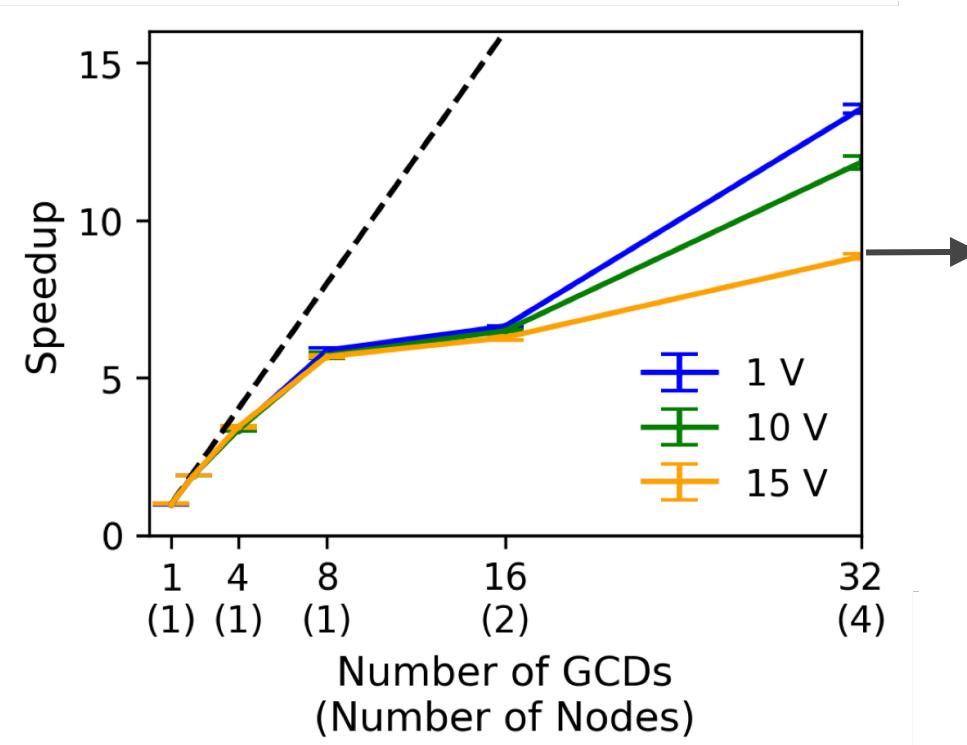
$$\nabla^2 \phi(r) = 0$$
$$\begin{cases} \phi(r) = V_L & \text{at left contact sites} \\ \phi(r) = V_R & \text{at right contact sites} \end{cases}$$

Update Charges

$$\phi(r) = \int_{V'} \frac{\rho(r') dV'}{4\pi\epsilon_r |r - r'|}$$

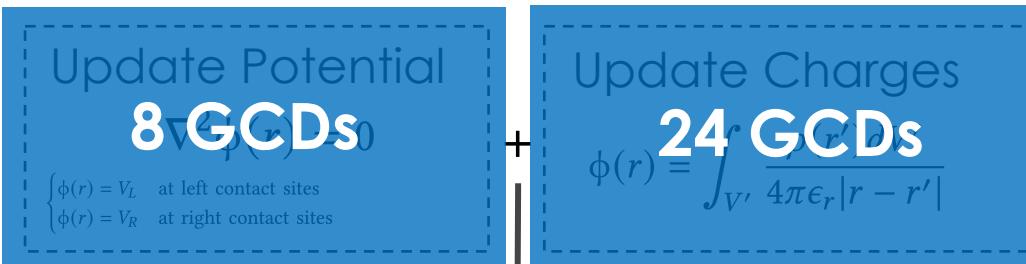
Execute Events

$$P_{i,j}^x = v \exp\left(-\frac{E_A^x - q(\phi_i - \phi_j) - \frac{3}{2}k_B(T - T^0)}{k_B \cdot T^0}\right)$$
$$P_{event} = \alpha P_{tot} = \alpha \text{ scan}(\mathbf{P})$$

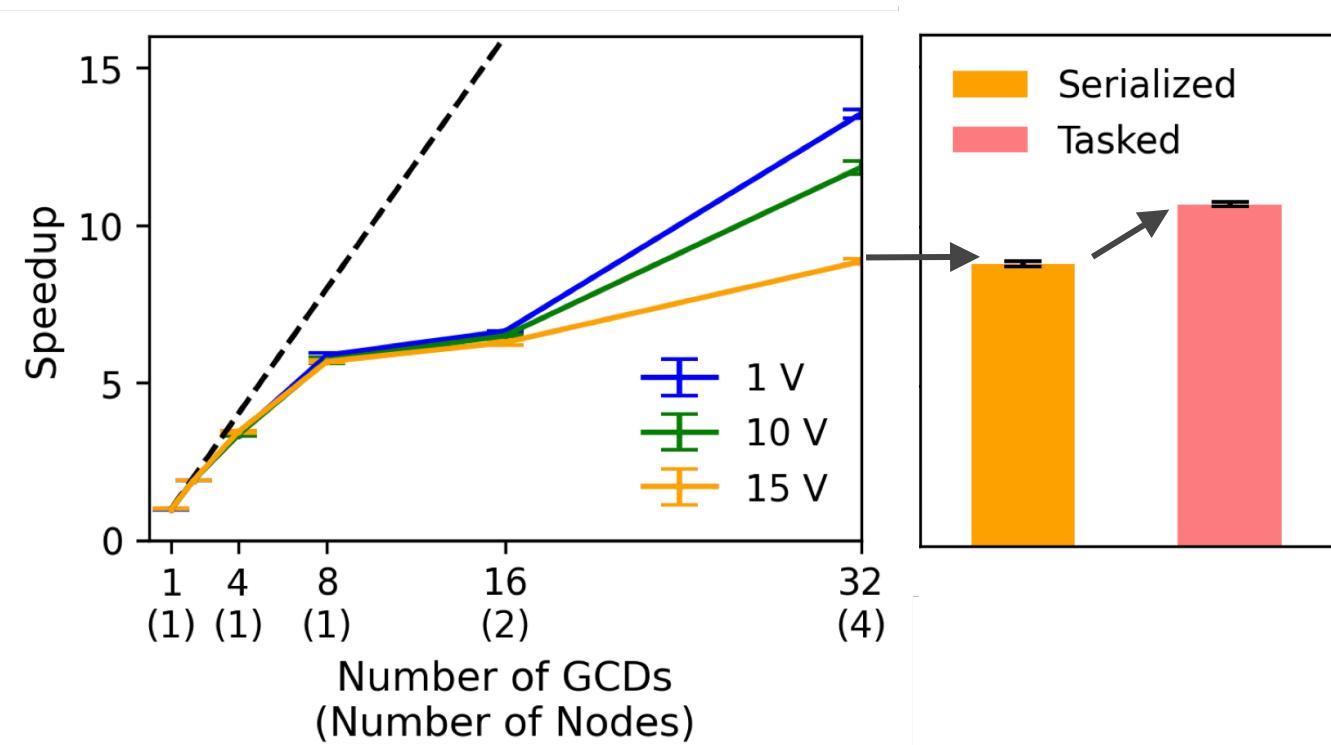
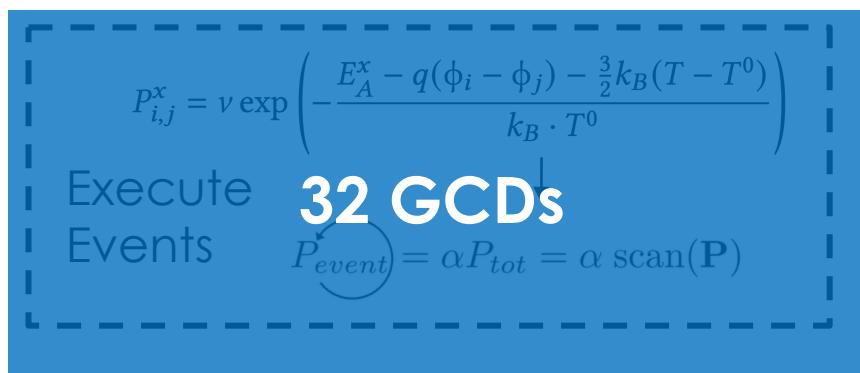


TASK BASED DISTRIBUTION

Iterative CG: fast but scales poorly > 1 node



Pairwise interaction:
slow but parallel



20% increase in achievable speedup with 4 nodes

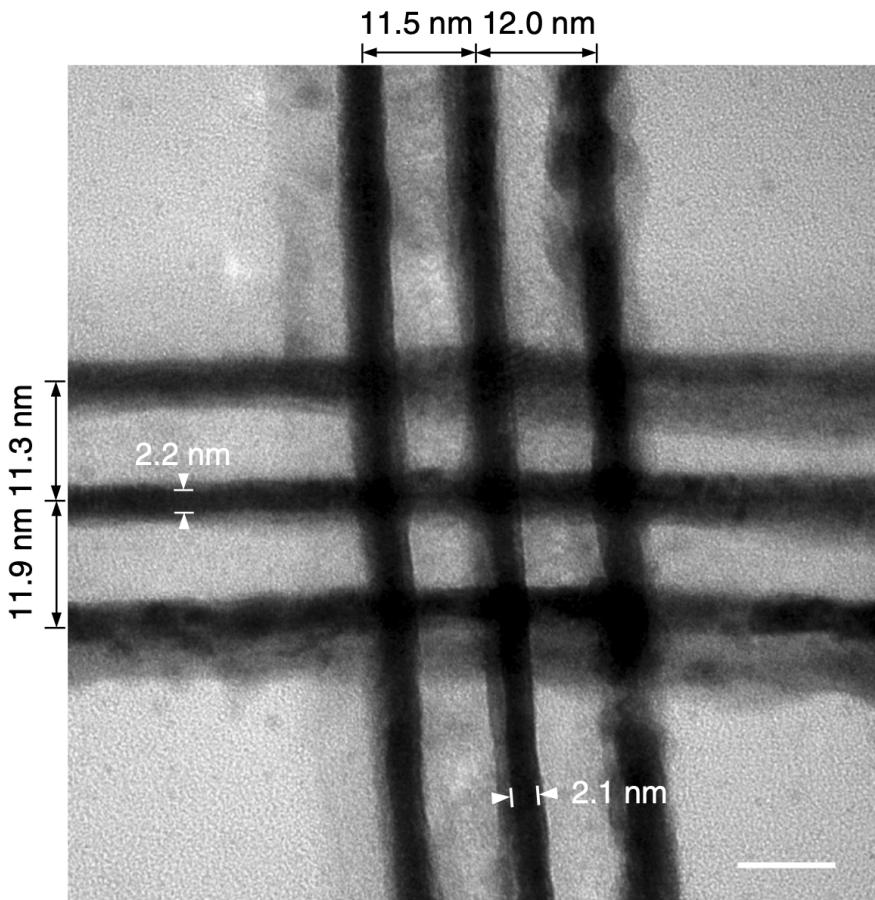


- Development of an application to simulate the kinetics of RRAM devices
- Enabling simulations of experimentally relevant geometries

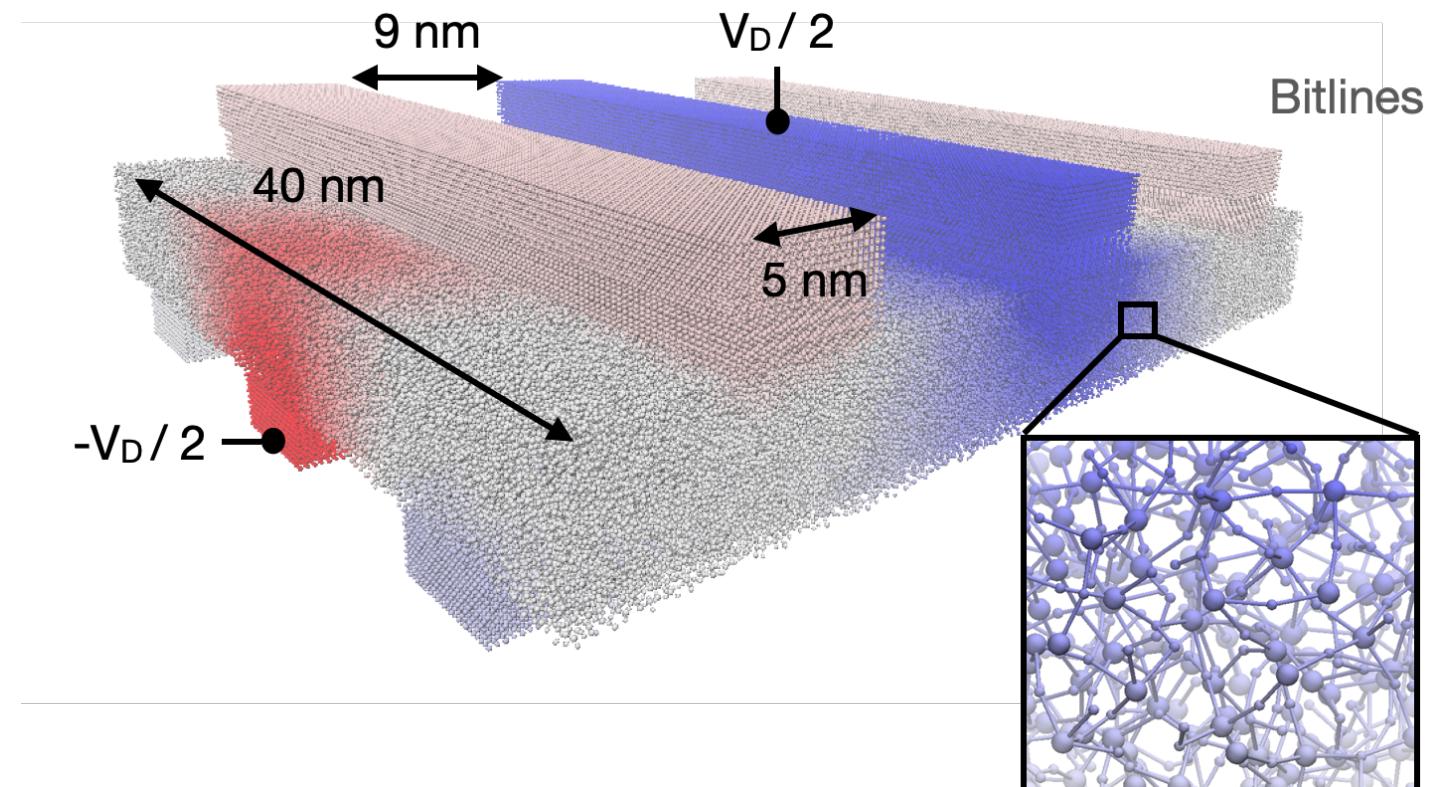
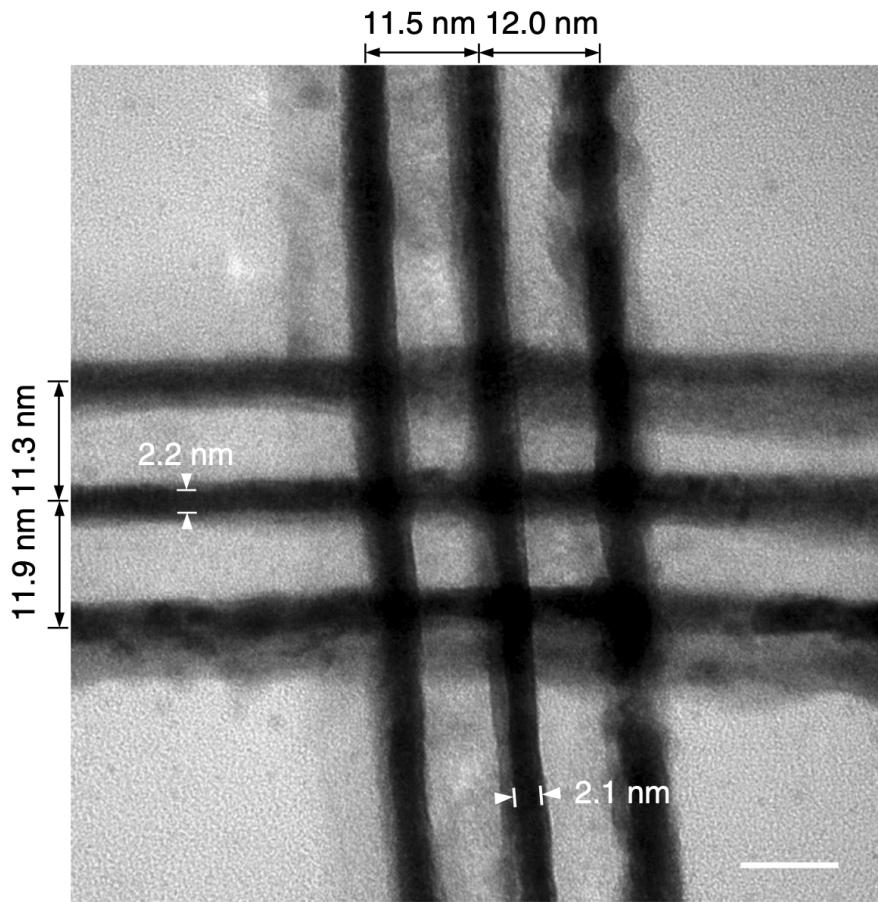
→ Computational explorations of device operation at the nanoscale



ARRAY ELECTROFORMING SIMULATIONS

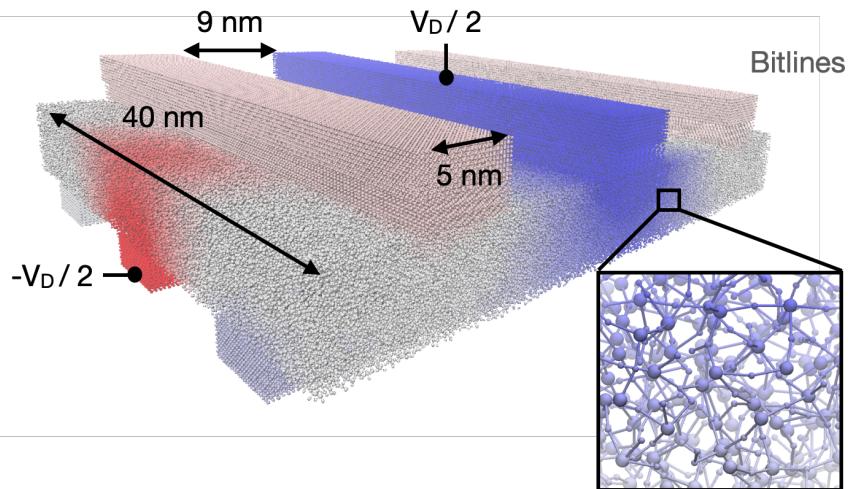


ARRAY ELECTROFORMING SIMULATIONS

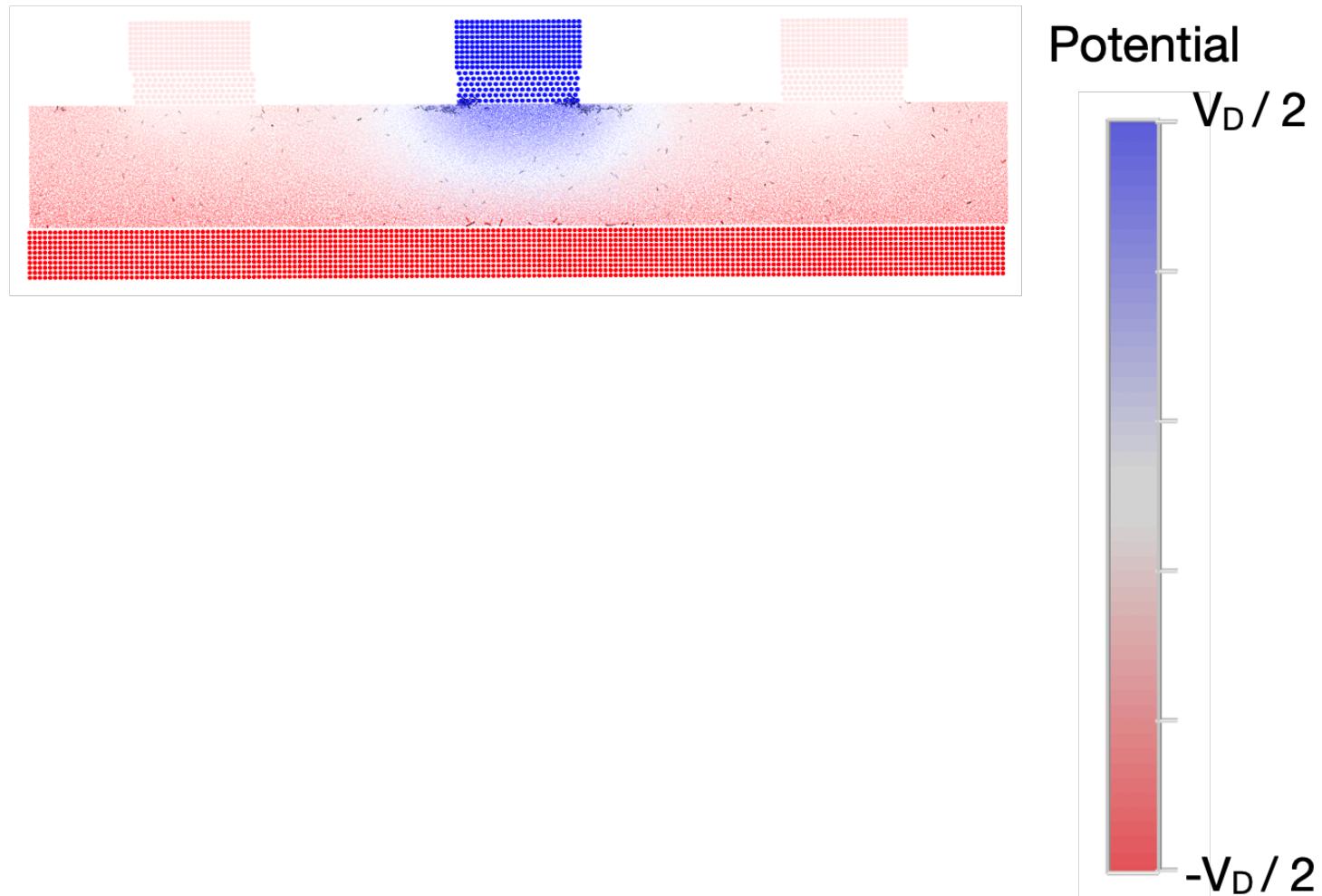


DEVICE SELECTION AND SET-PROCESS

- ~80k supersteps
- < 1s /superstep

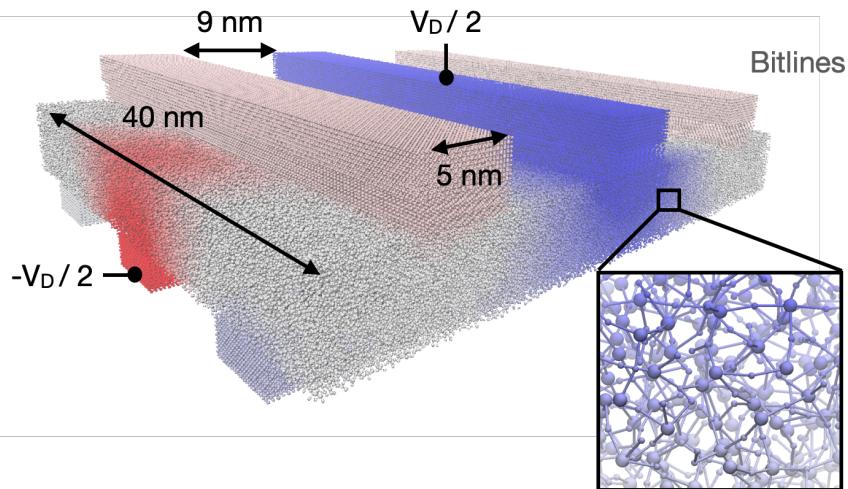


Simulation clock (ns)

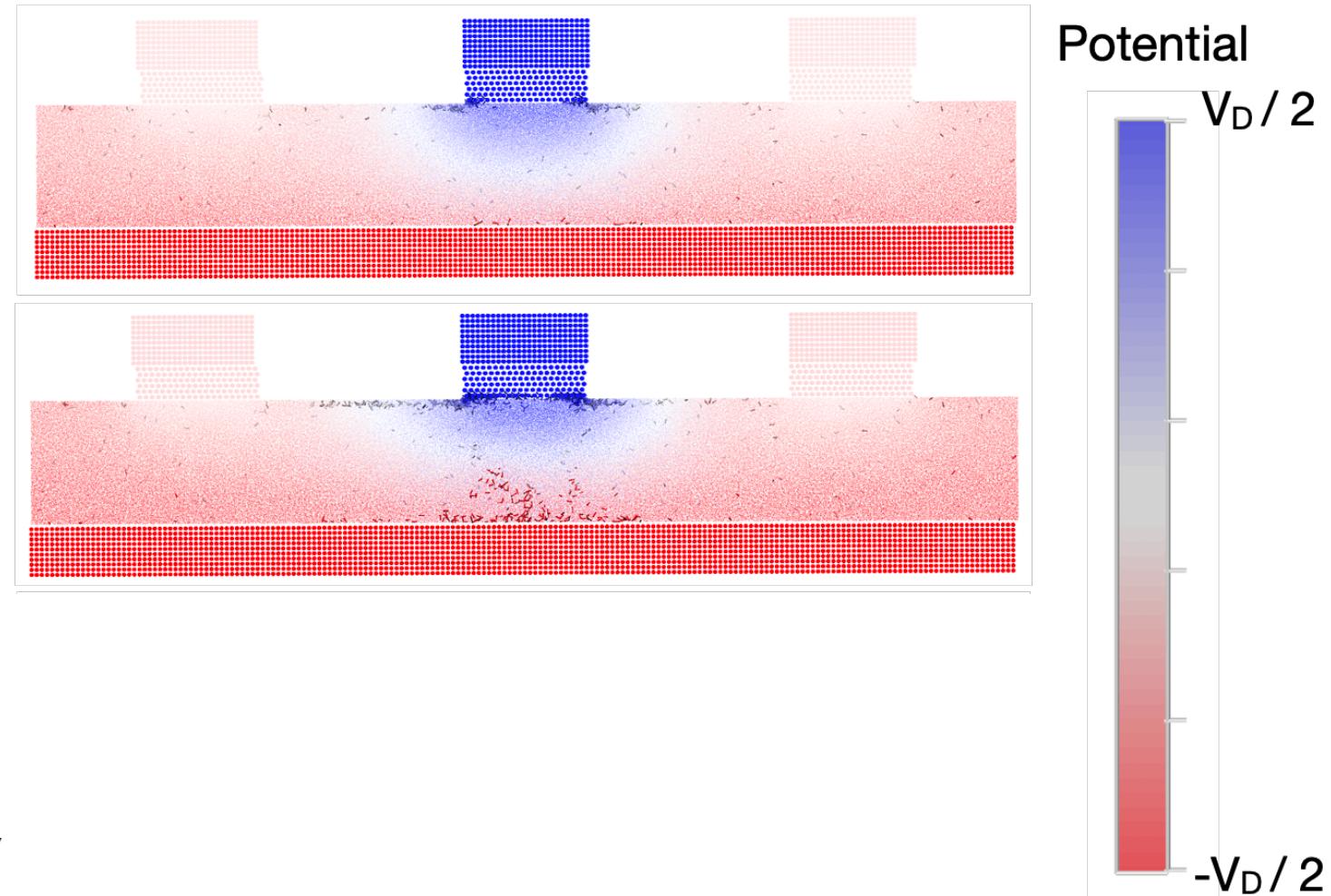


DEVICE SELECTION AND SET-PROCESS

- ~80k supersteps
- < 1s /superstep

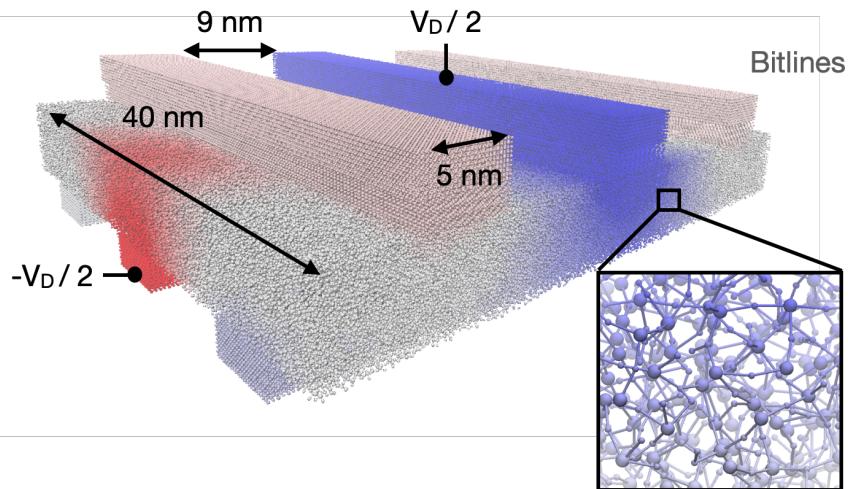


Simulation clock (ns)

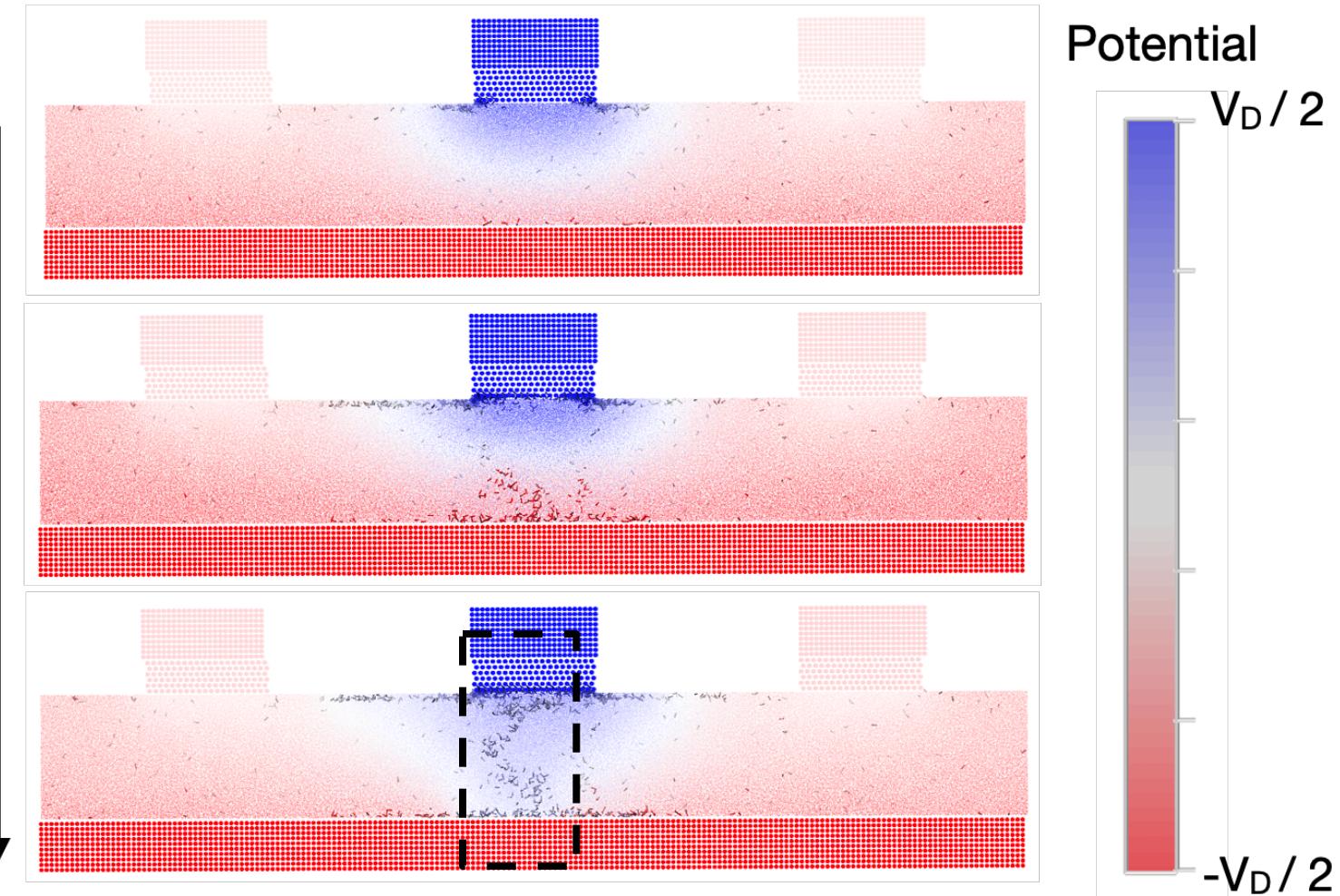


DEVICE SELECTION AND SET-PROCESS

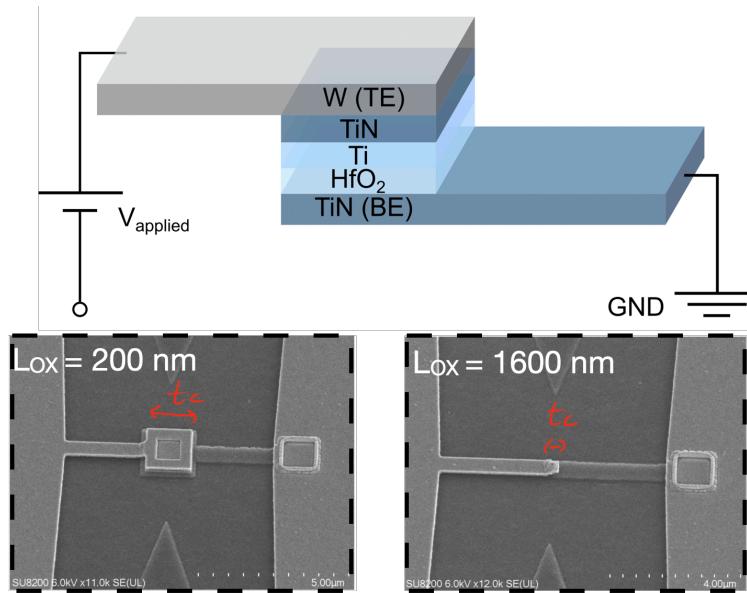
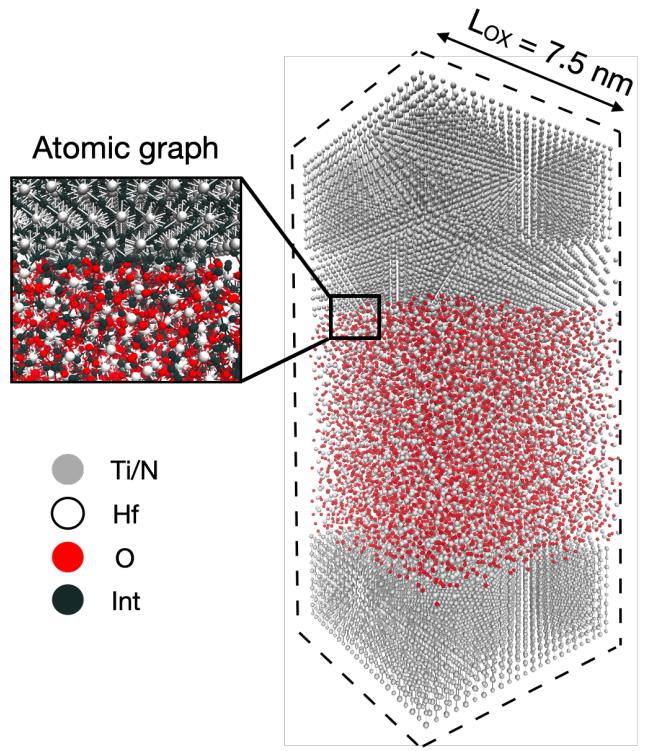
- ~80k supersteps
- < 1s /superstep



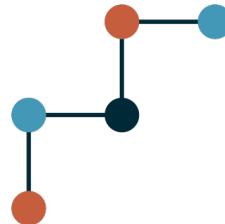
Simulation clock (ns)



CURRENT WORK



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