



# On Hybrid Lagrangian-Eulerian Simulation Methods

## Practical Notes and High-Performance Aspects

<http://mpm.graphics>

Yuanming Hu<sup>1</sup> Xinxin Zhang<sup>2</sup> Ming Gao<sup>2</sup> Chenfanfu Jiang<sup>3</sup>

<sup>1</sup>MIT CSAIL

<sup>2</sup>Tencent

<sup>3</sup>University of Pennsylvania

# Speakers

# Yuanming Hu



*PhD student*



# Dr. Xinxin Zhang

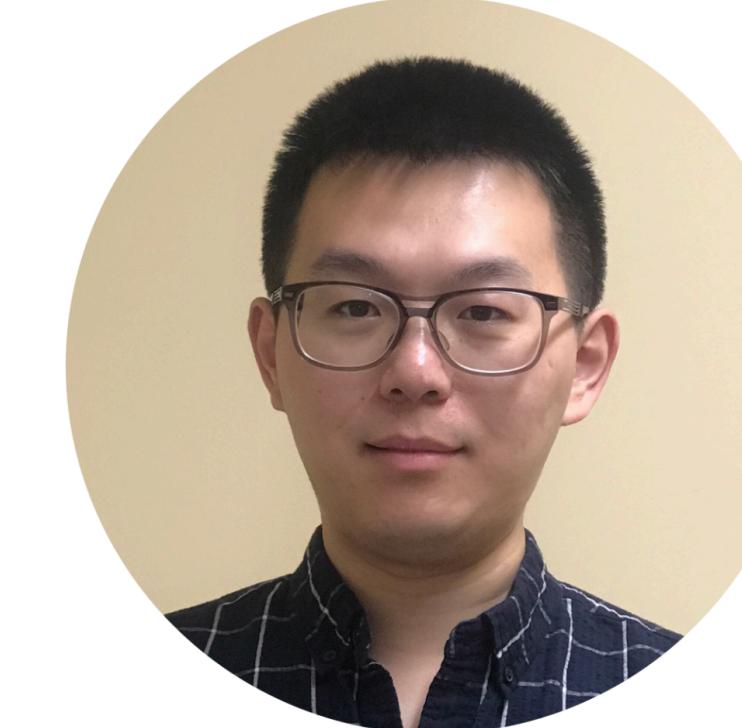


*Senior Graphics RnD*



**Tencent**

# Dr. Ming Gao



*Senior RnD researcher*



**Tencent**

# Dr. Chenfanfu Jiang

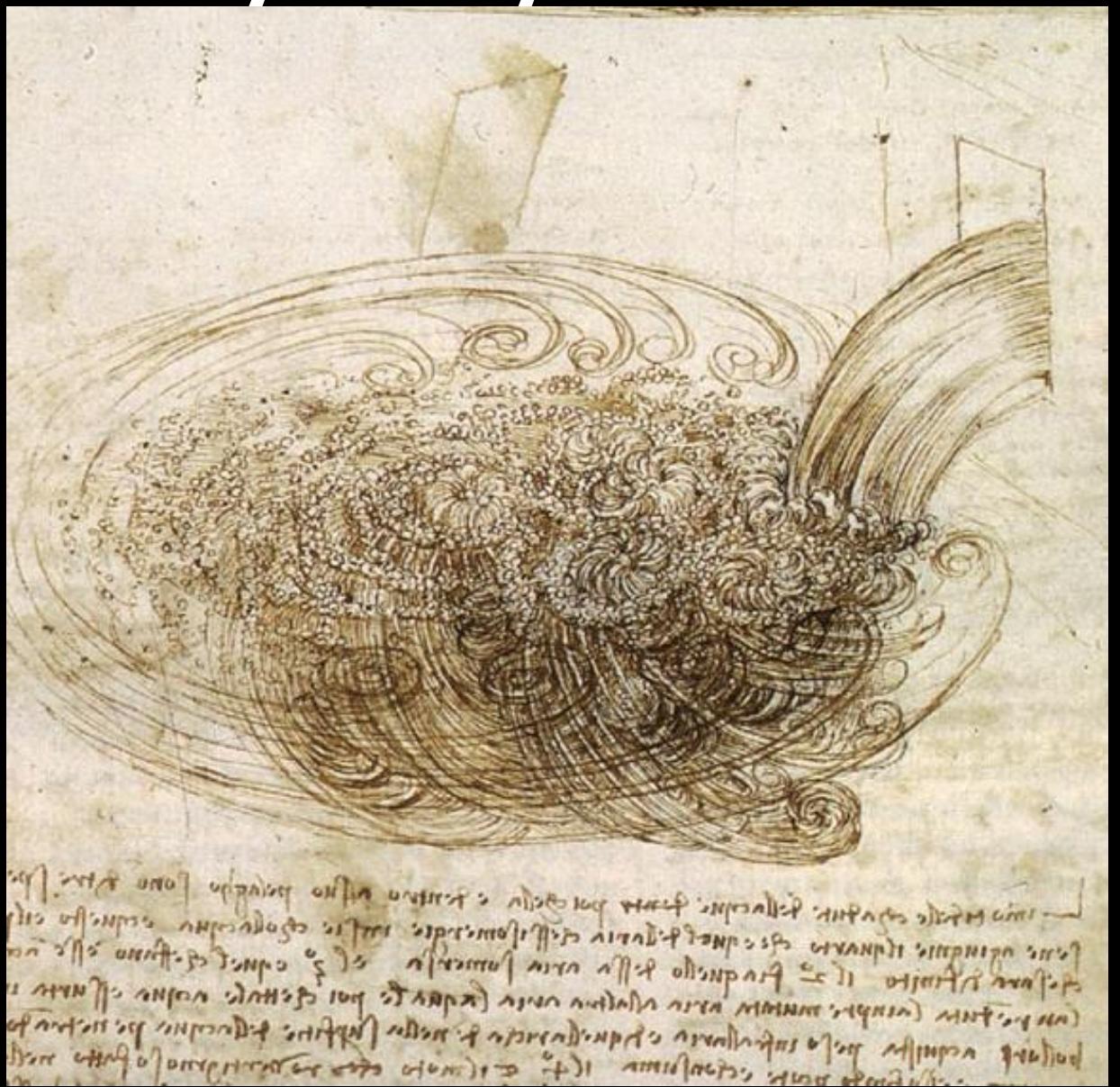


*Assistant professor*



# Particle-Particle Particle-Mesh Method for fast N-Body dynamics in Eulerian- Lagrangian Computations

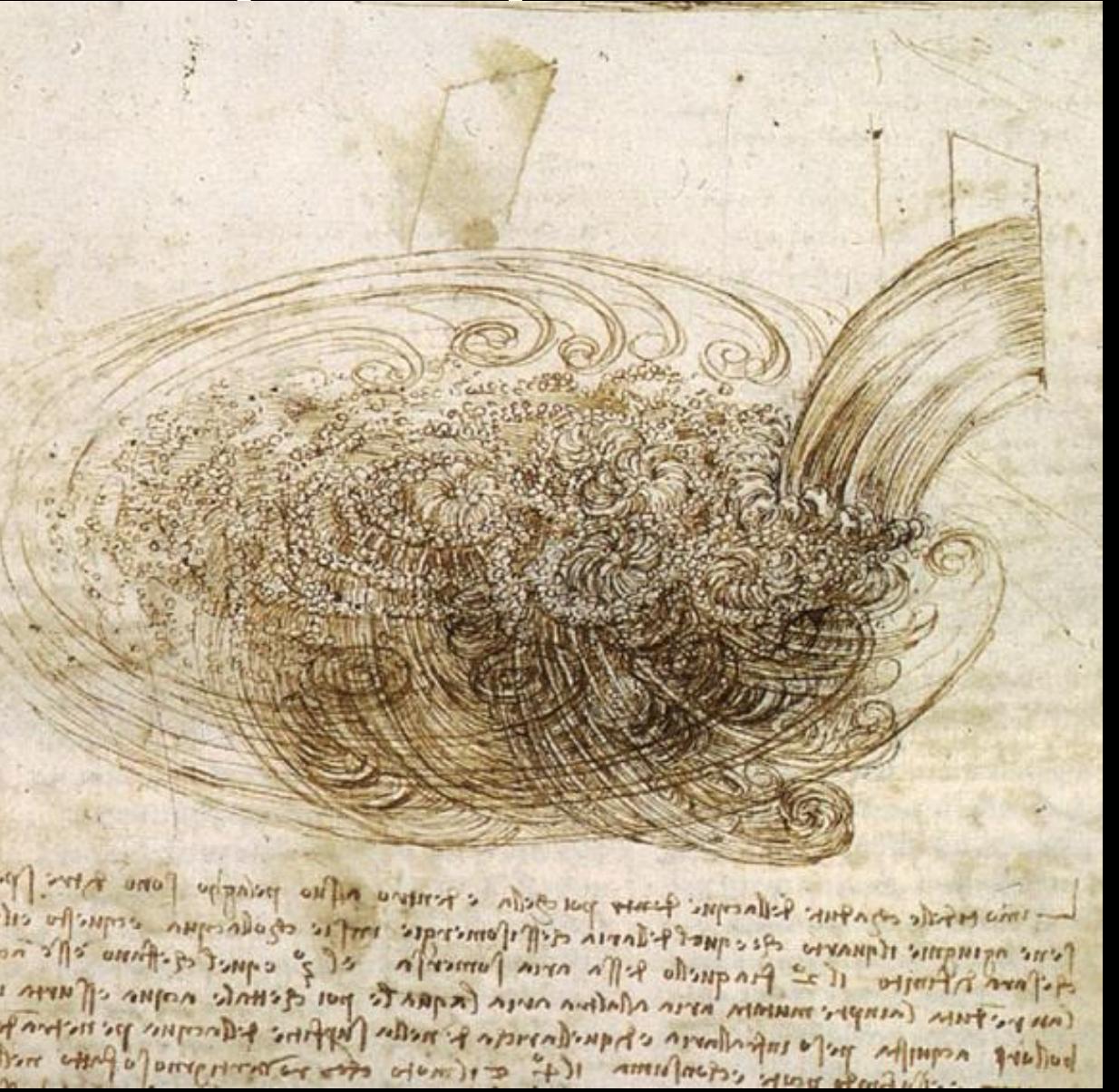
# N-Body Dynamics



$$u_i = \sum_{j=1, j \neq i}^N \frac{v_j \omega_j \times (x_i - x_j)}{4\pi \|x_i - x_j\|_2^3}$$

$$f_i = -\epsilon \sum_{j=1, j \neq i}^N \frac{\rho_j v_j (x_i - x_j)}{4\pi \|x_i - x_j\|_2^3}$$

# N-Body Dynamics

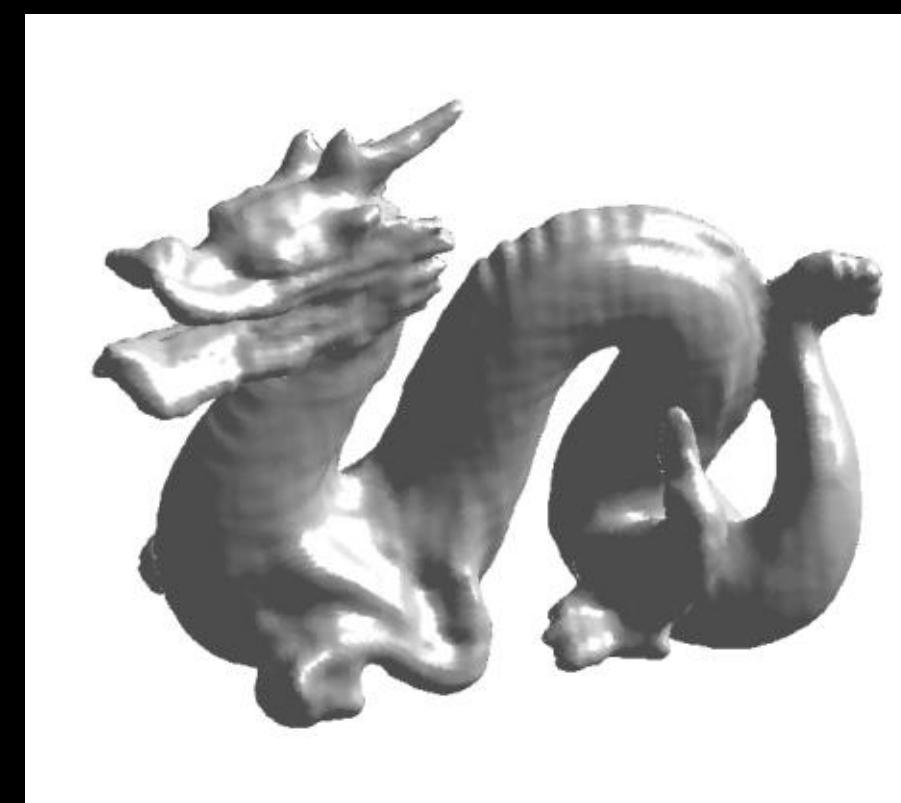


$$u_i = \sum_{j=1, j \neq i}^N \frac{v_j \omega_j \times (x_i - x_j)}{4\pi \|x_i - x_j\|_2^3}$$

*Given N particles and M evaluation position,  
direct computation requires O(NM) time!*



$$f_i = -\epsilon \sum_{j=1, j \neq i}^N \frac{\rho_j v_j (x_i - x_j)}{4\pi \|x_i - x_j\|_2^3}$$



*Surface reconstruction.*



*On the Accurate Large-scale Simulation of Ferrofluids.  
Huang et. al. SIGGRAPH 2019*

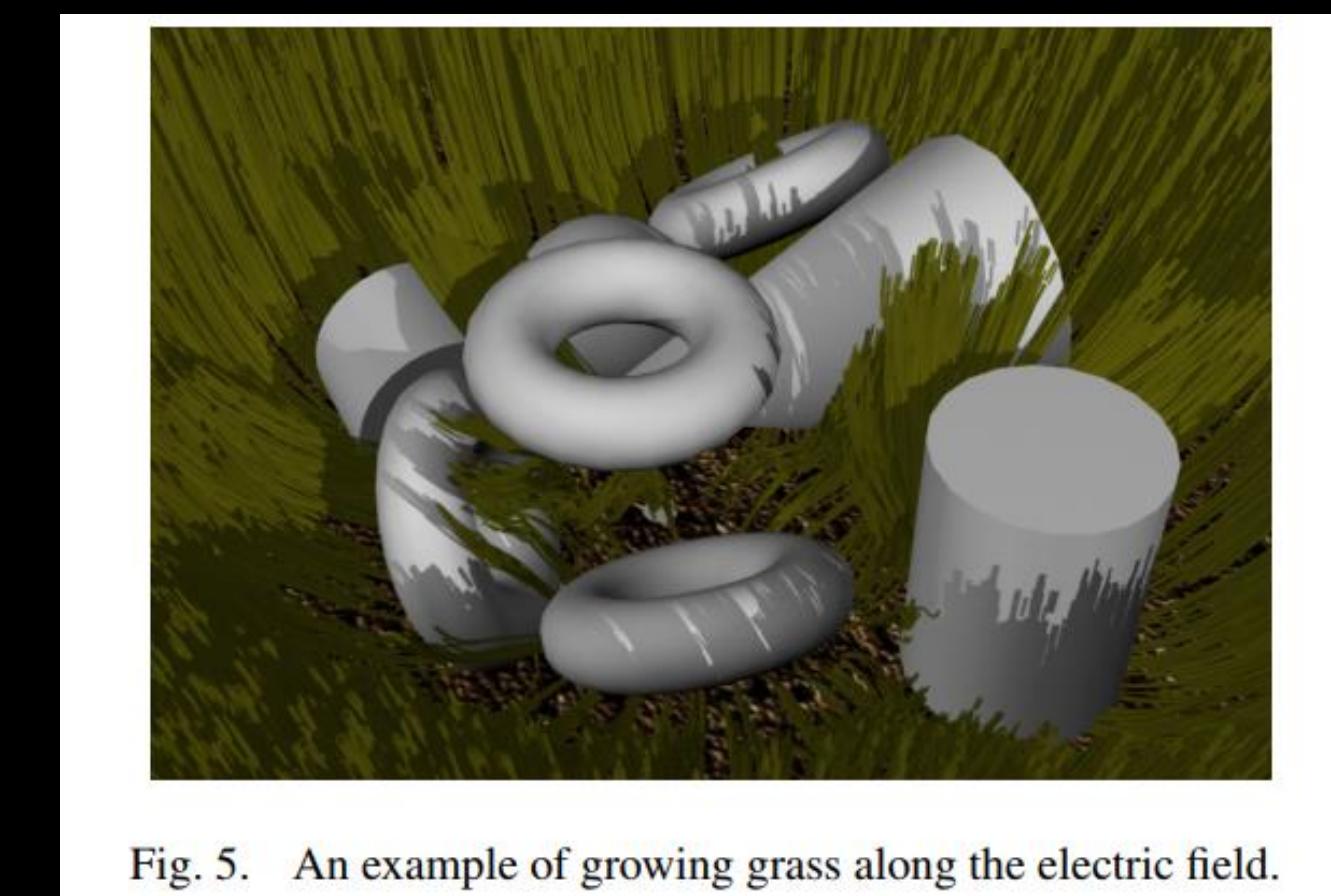
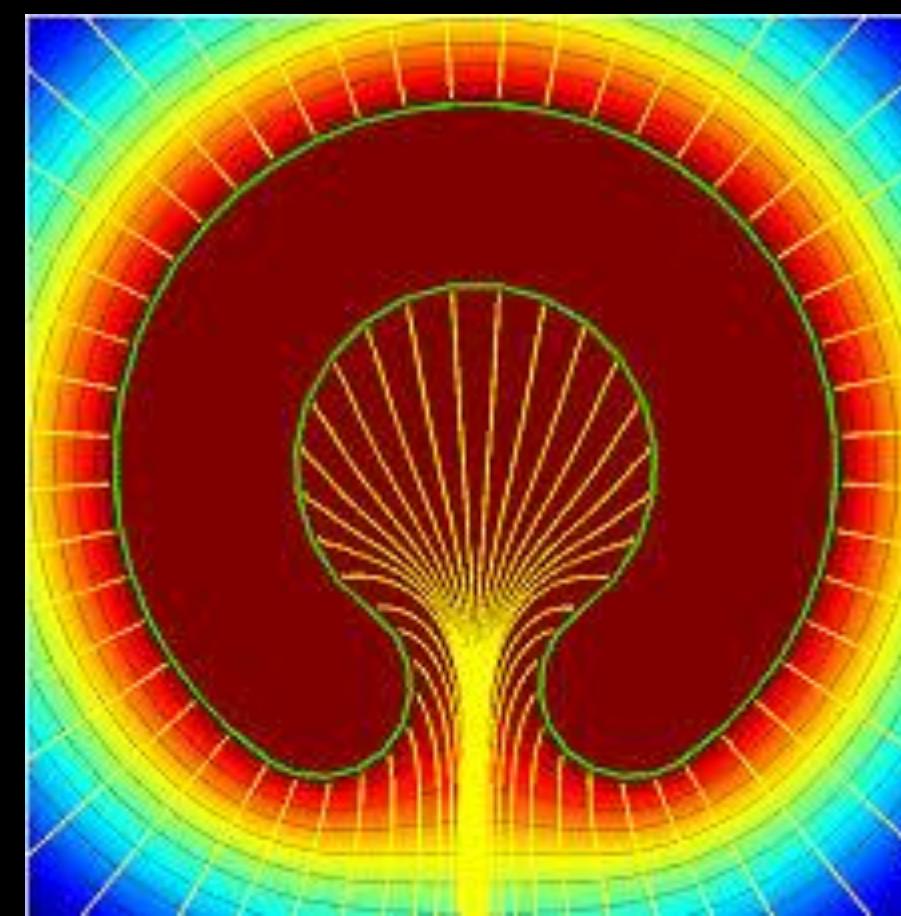


Fig. 5. An example of growing grass along the electric field.

*Harmonic Parameterization by Electrostatics. Wang et. al. ACM TOG*

# Fast N-body Summation is Non-Trivial

Solve dynamics with only near-by influence is wrong

cut-off influence

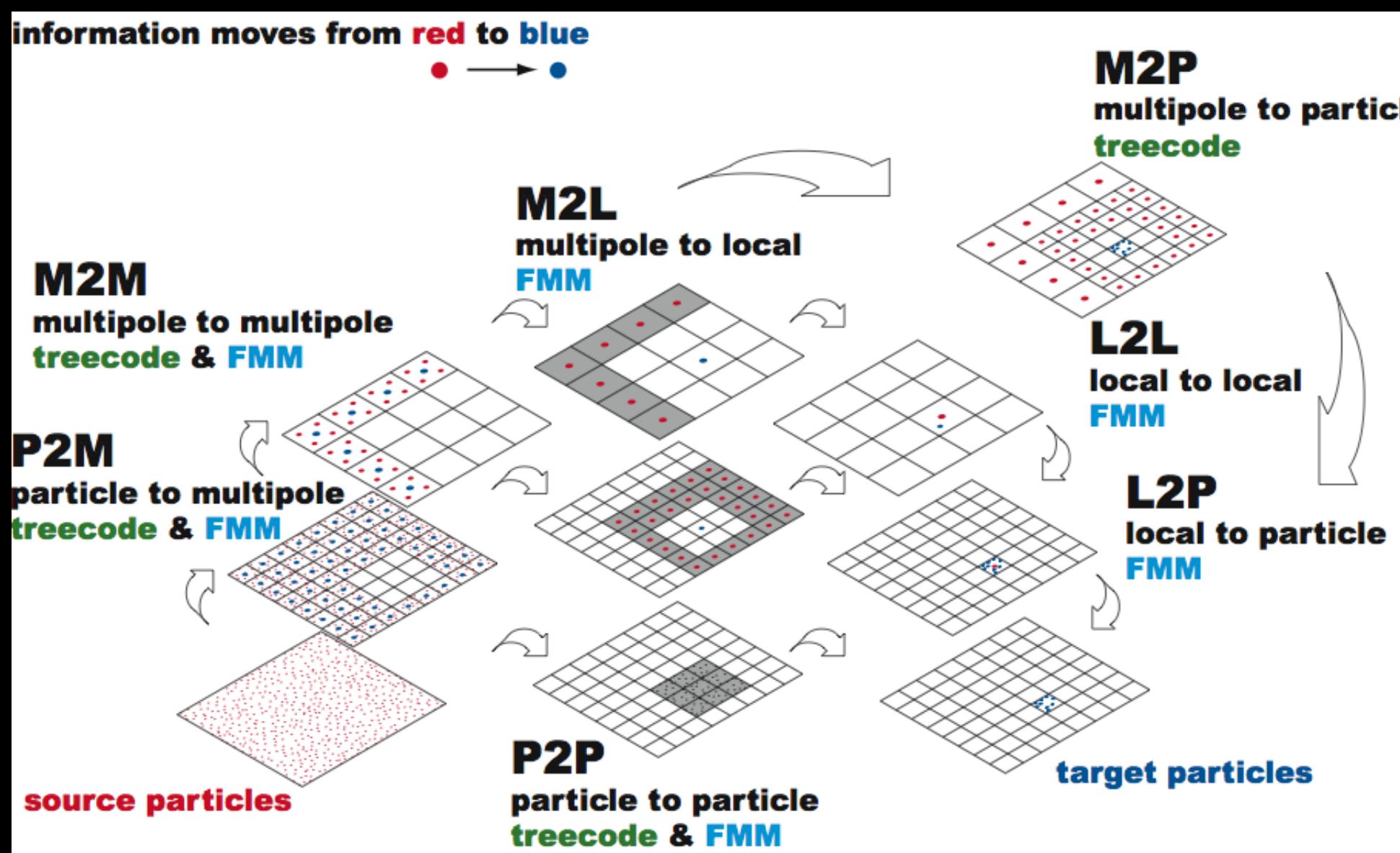


full influence



# Fast N-body Summations

- Solutions have been widely discovered to reduce this computation bottleneck.

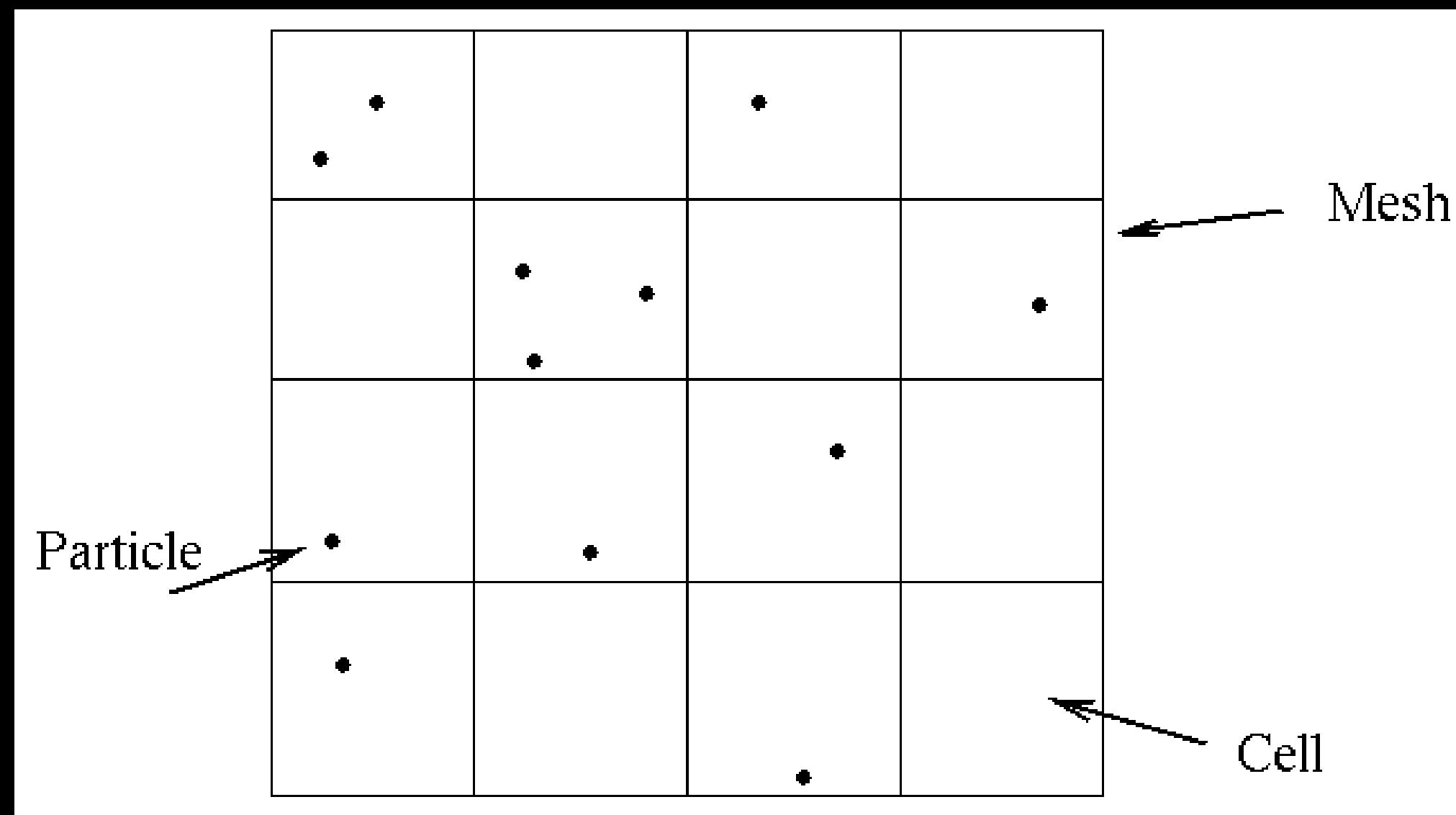


Accuracy	Efficiency	Code Complexity
Excellent	Good	Fair

$O(N)$  Fast Multipole Method(Rokhlin & Greengard)

# Fast N-body Summations

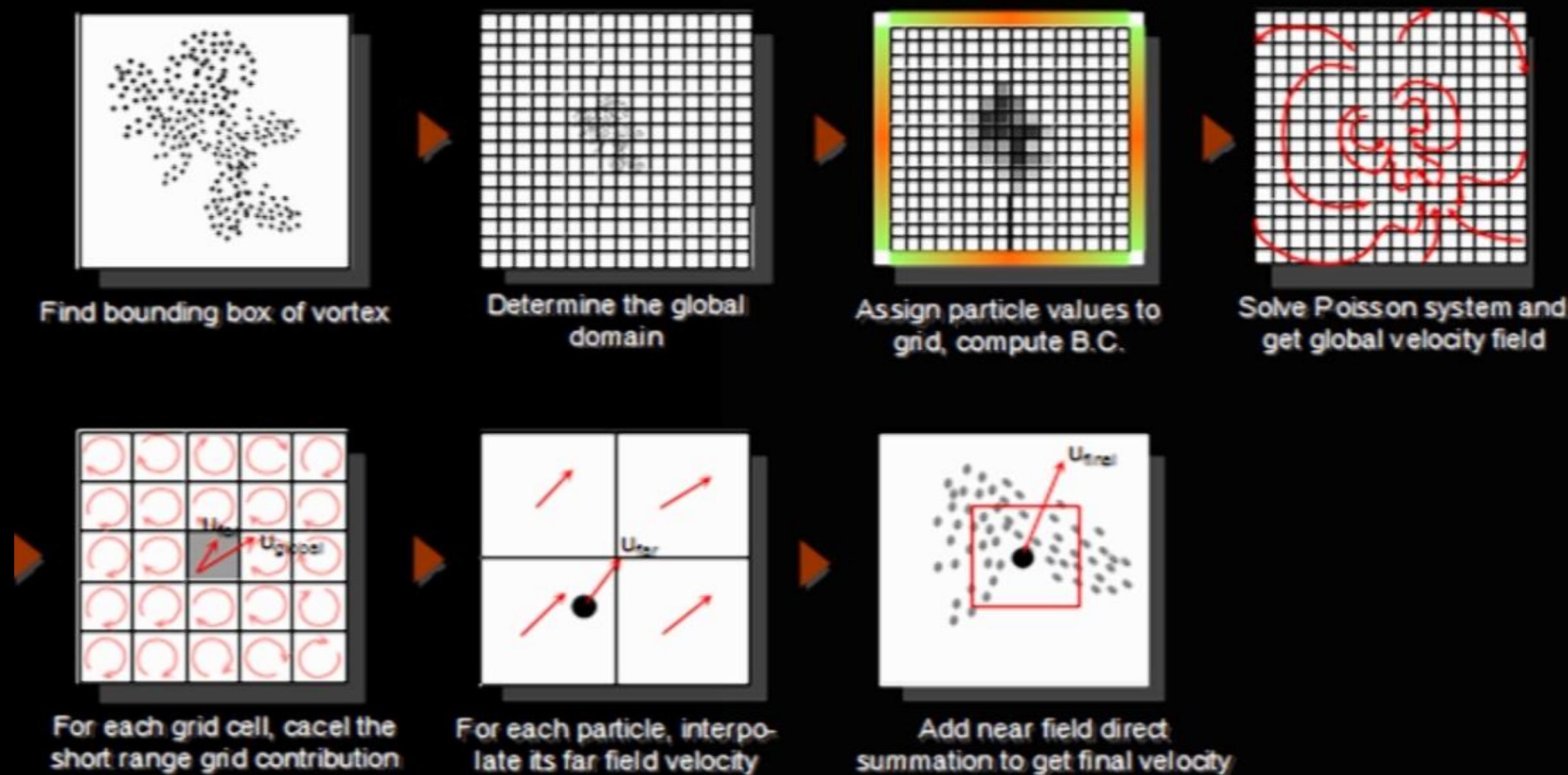
- Solutions have been widely discovered to reduce this computation bottleneck.



Accuracy	Efficiency	Code Complexity
Fair	Excellent	Excellent

$O(G)$  Particle Mesh Methods, Vortex-In-Cell.

# Fast N-body Summations: Particle-Particle, Particle-Mesh(PPPM)



Accuracy	Efficiency	Code Complexity
Good	Excellent	Excellent

# PPPM: Key idea

$$u_i = \sum_{j=1, j \neq i}^N \frac{v_j \omega_j \times (x_i - x_j)}{4\pi \|x_i - x_j\|_2^3}$$



$$\begin{aligned}\nabla^2 \psi &= -\omega \\ u &= \nabla \times \psi\end{aligned}$$

$$f_i = -\epsilon \sum_{j=1, j \neq i}^N \frac{\rho_j v_j (x_i - x_j)}{4\pi \|x_i - x_j\|_2^3}$$



$$\begin{aligned}\nabla^2 \phi &= \epsilon \rho \\ f &= \nabla \phi\end{aligned}$$

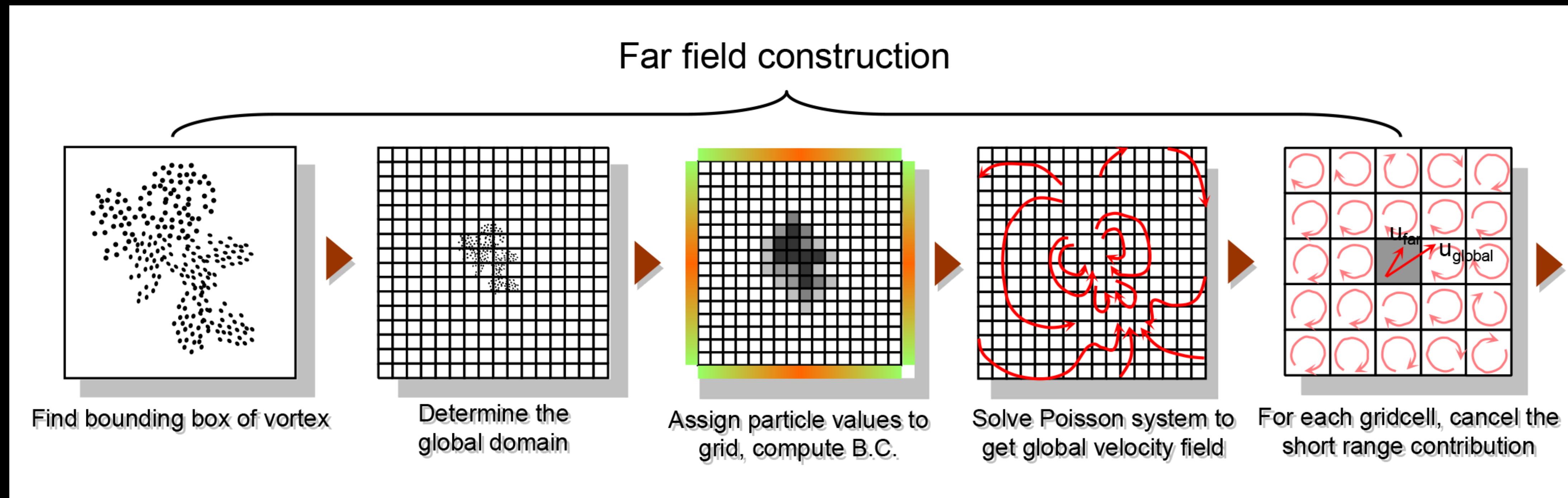
Direct summation for the turbulent part



Poisson's Equation for the smooth part

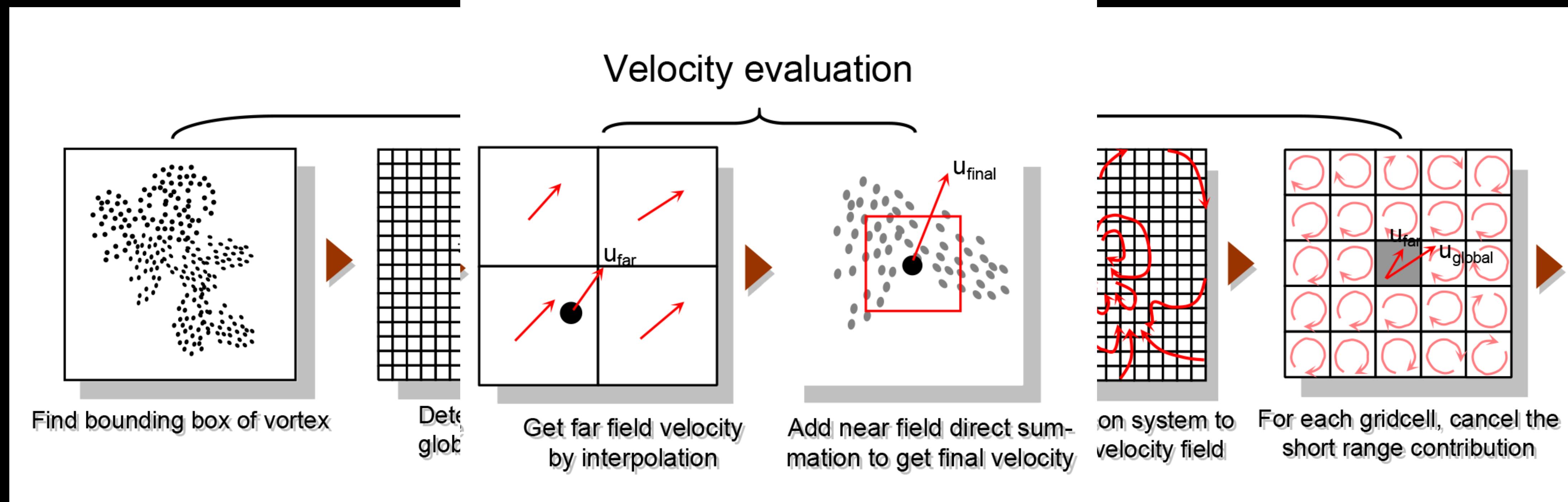
# PPPM

- Fast solution uses near-far decomposition to get acceleration. Can we do similar thing on a particle-mesh setup?

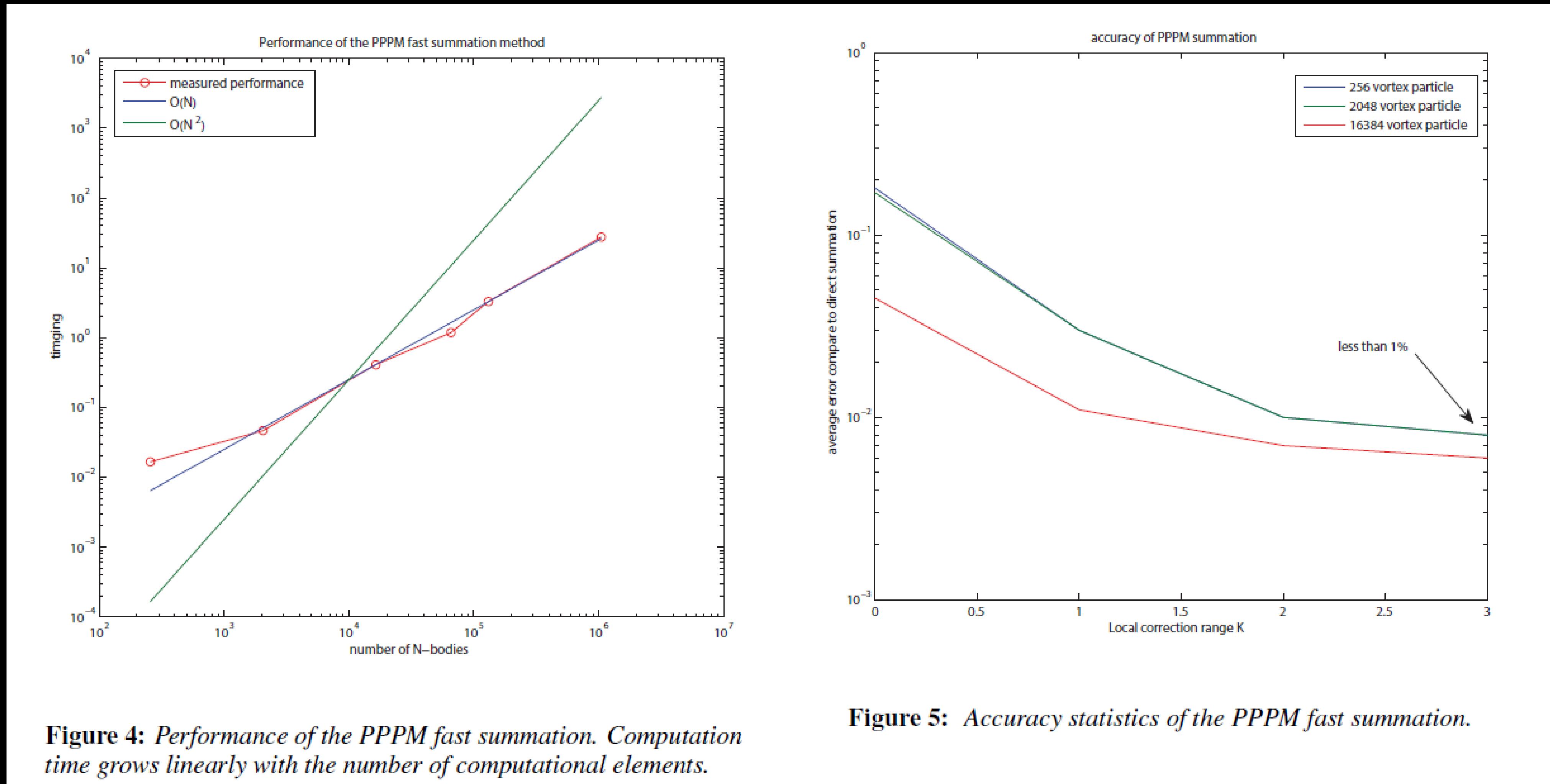


# PPPM

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# PPPM



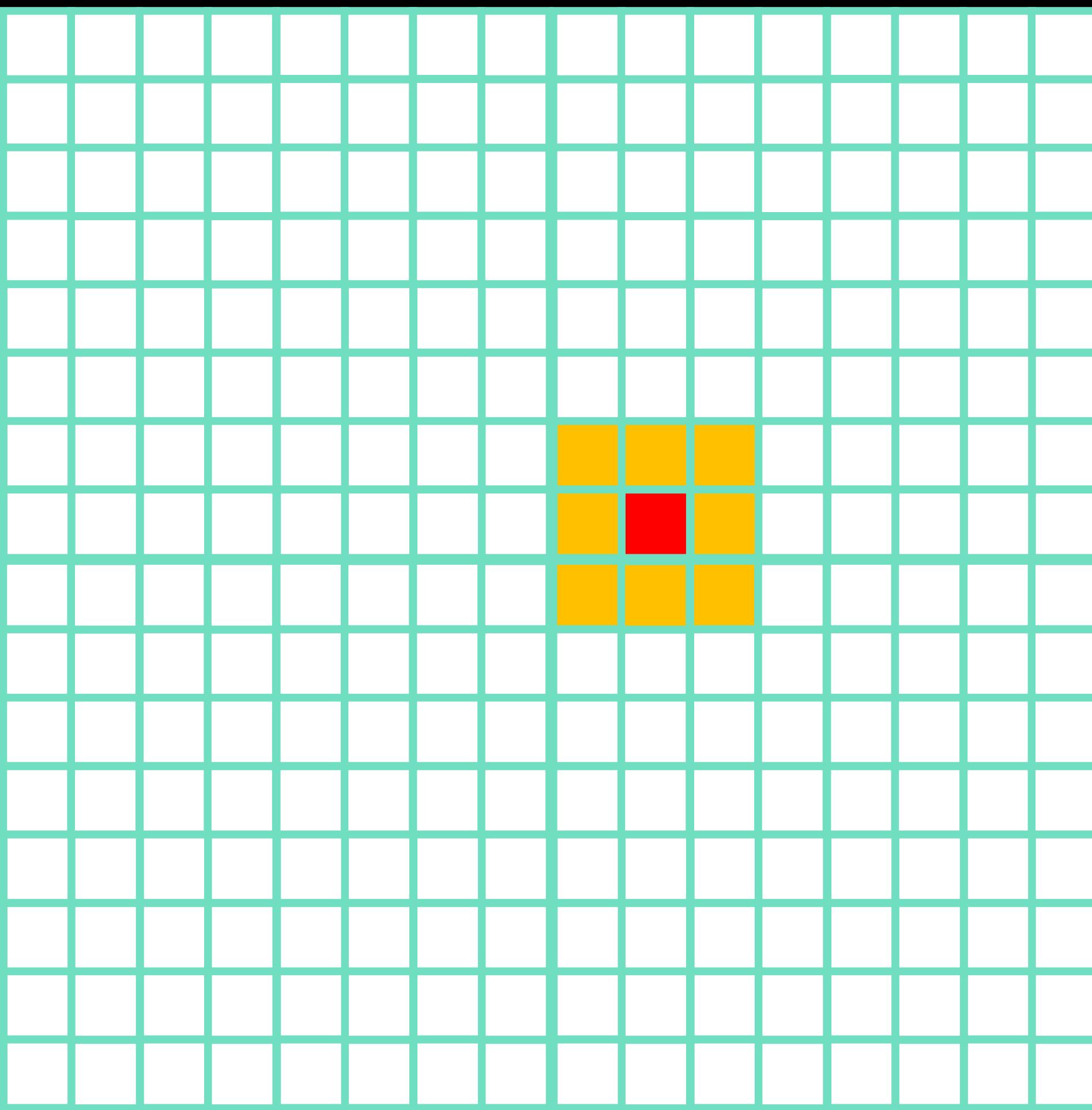
**Figure 4:** Performance of the PPPM fast summation. Computation time grows linearly with the number of computational elements.

**Figure 5:** Accuracy statistics of the PPPM fast summation.

# Local Correction

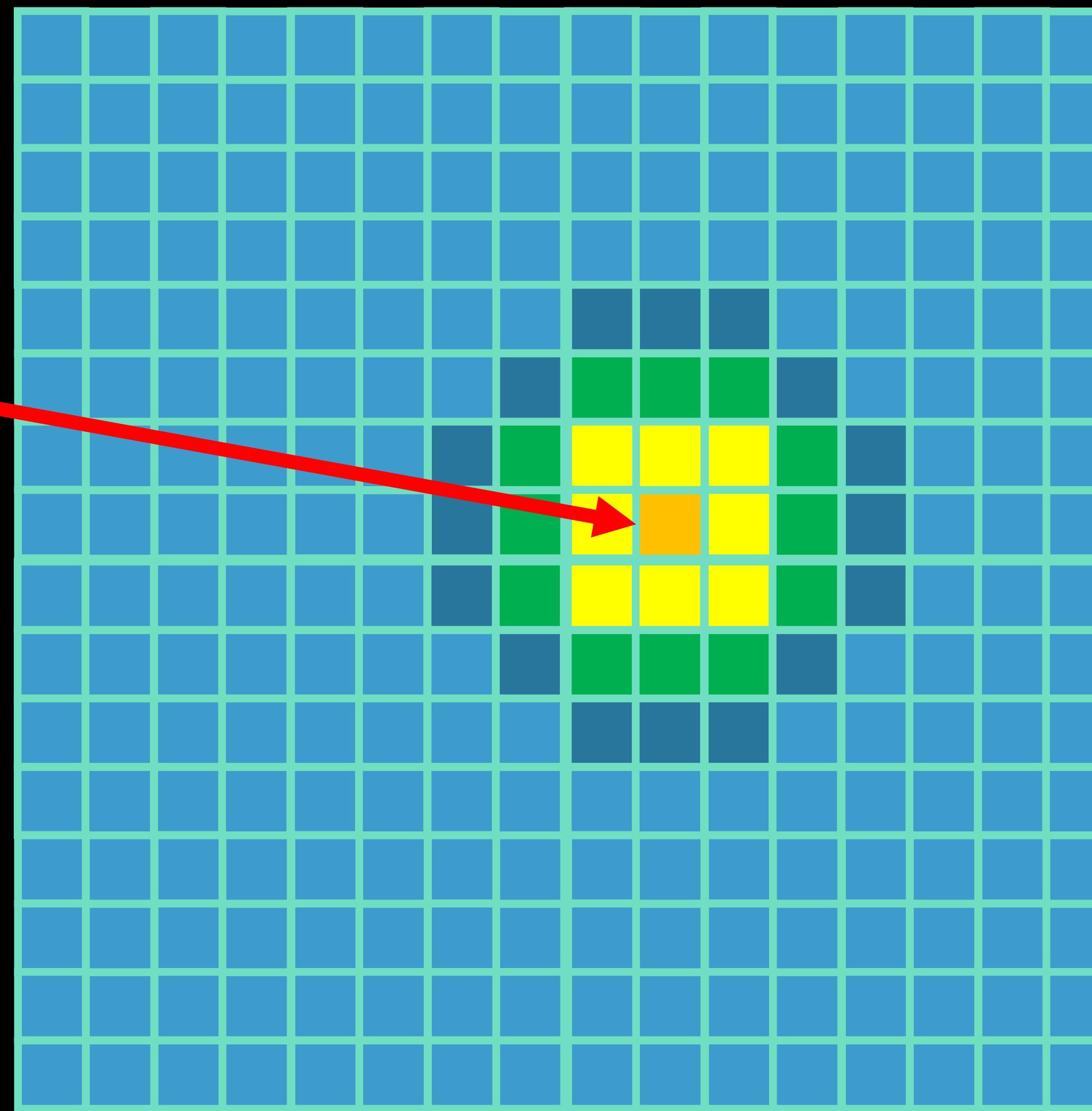
- In 3D, for a correction window of size  $K$  in each dimension, a local matrix of size  $K^3 \times K^3$  can be precomputed to cancel the local influence from grid.
- $T(N) = O(c K^6 N)$

# Local Correction



# Local Correction

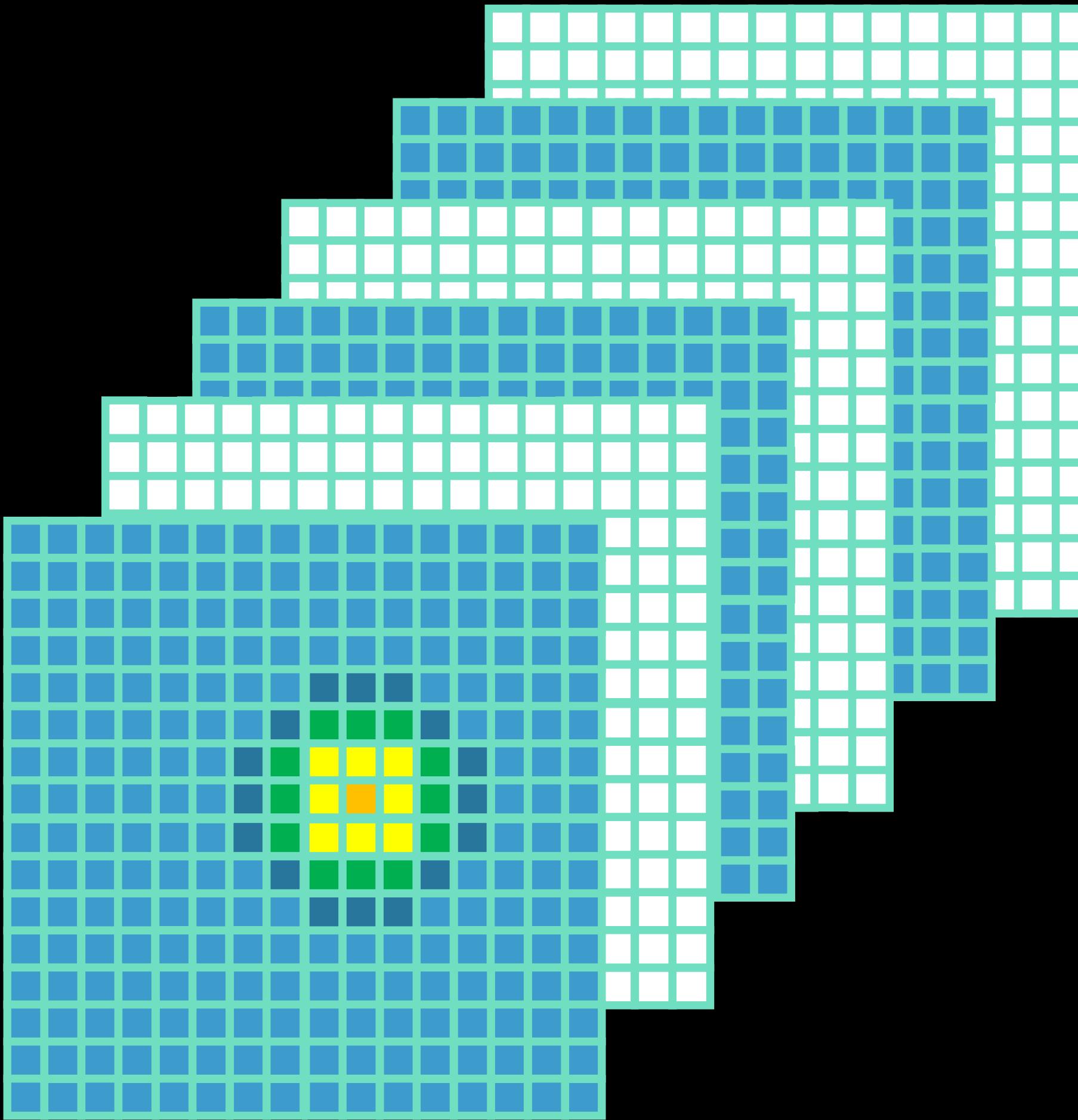
The influence made by  
neighbor cells.



# Local Correction

- *The matrix inverse reveals how the center cell's value depends linearly on its neighbors(including itself).*

$$s_c = \sum_{j \in \eta} a_j r_j$$



# One interesting finding

$$a_j \approx G_{cj} = \frac{1}{4\pi \|x_c - x_j\|_2}$$

# Even Simpler PPPM

- Decompose the velocity field as

$$u = u_{smooth} + u_{turbulent}$$

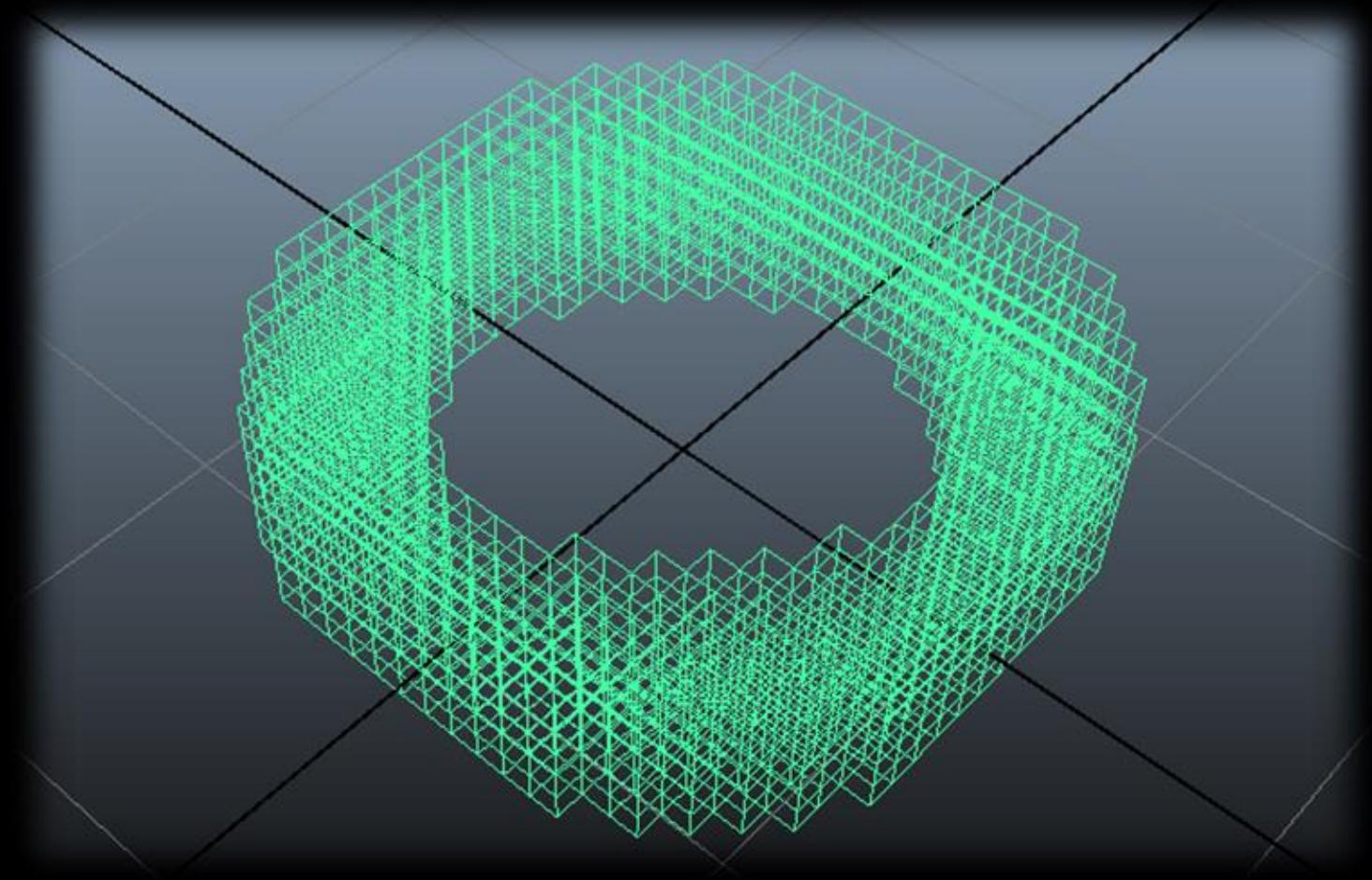
- Where

$u_{smooth} = \text{Interpolate}(PM\ Solution)$

$u_{turbulent} = \text{NearFieldSummation}(\omega_j - VIC)$

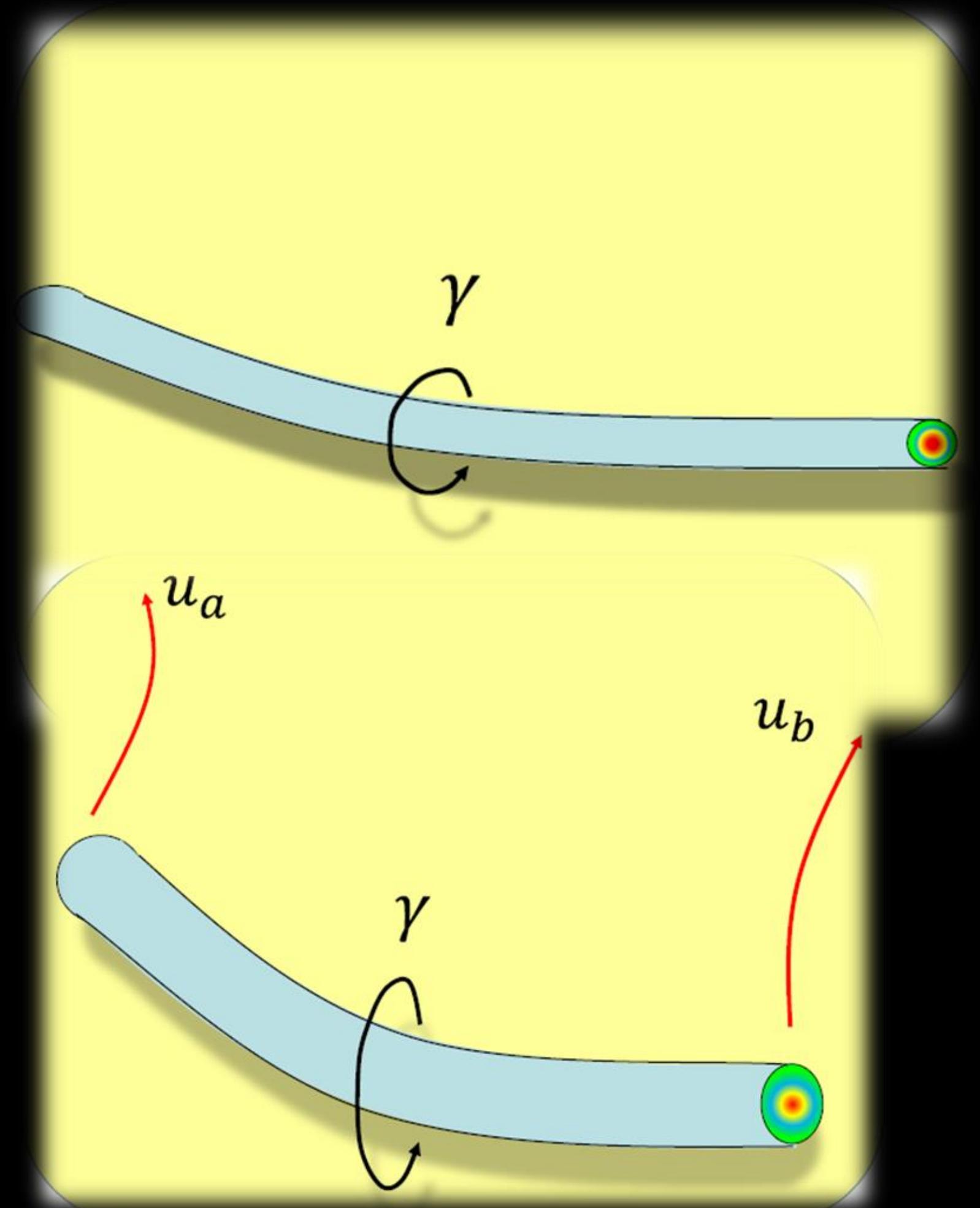
# Higher Order PPPM

- Compute Velocity Field not on Particles, but on SpGrid Nodes



- Allows tracking particle trajectories with higher order schemes, for example RK3.

# Stable Vortex Segments



$$|\omega_i^{n+1}|_2 = |\omega_i^n|_2 L_i^{n+1} / L_i^n$$

$$|\omega_i^n|_2 = \frac{|\omega_i^0|_2 L_i^n}{L_i^0} = \Gamma^0 L_i^n$$

# Better than remeshing

with remeshing only

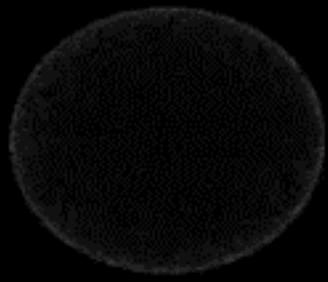


with particle splitting and remeshing



Raising vortex ring simulation,  
camera moving with the target

# Hybrid vortex-Eulerian simulation



# Continuum Mechanics and MPM

— Chenfanfu Jiang

# Constitutive modeling: basic example

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- ♦ **Keywords:** constitutive relationship/behavior, strain stress curve, ...

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- ♦ **Example:** Linear elasticity equilibrium (elastostatics)

**Kinematics describes strain and deformation**

infinitesimal strain (Cauchy strain):

$$\boldsymbol{\epsilon} = \frac{1}{2}(\mathbf{F} + \mathbf{F}^T) - \mathbf{I}$$

**Response comes from the constitutive model, relates to kinematics**

linear elasticity:

$$\Psi(\mathbf{F}) = \mu\boldsymbol{\epsilon} : \boldsymbol{\epsilon} + \frac{\lambda}{2}\text{tr}(\boldsymbol{\epsilon})^2 \quad \mathbf{P} = 2\mu\boldsymbol{\epsilon} + \lambda\text{tr}(\boldsymbol{\epsilon})\mathbf{I}$$

**Governing equations are the the PDEs to be solved**

force balance (equilibrium):

$$\nabla^{\mathbf{X}} \cdot \mathbf{P} + \mathbf{f}^{\text{ext}} = 0$$

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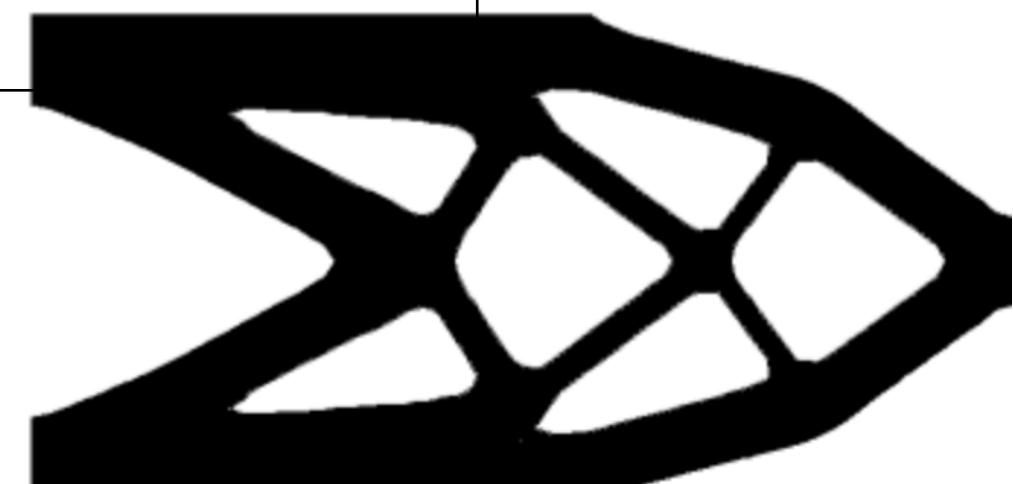
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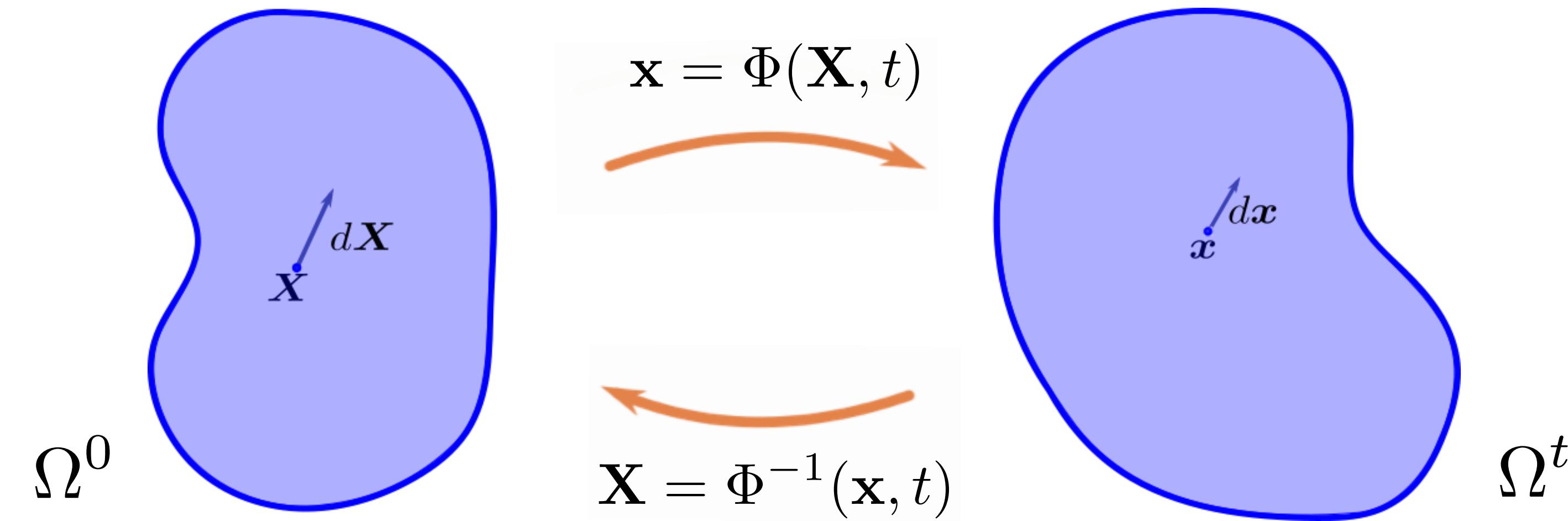
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A core model in topology optimization



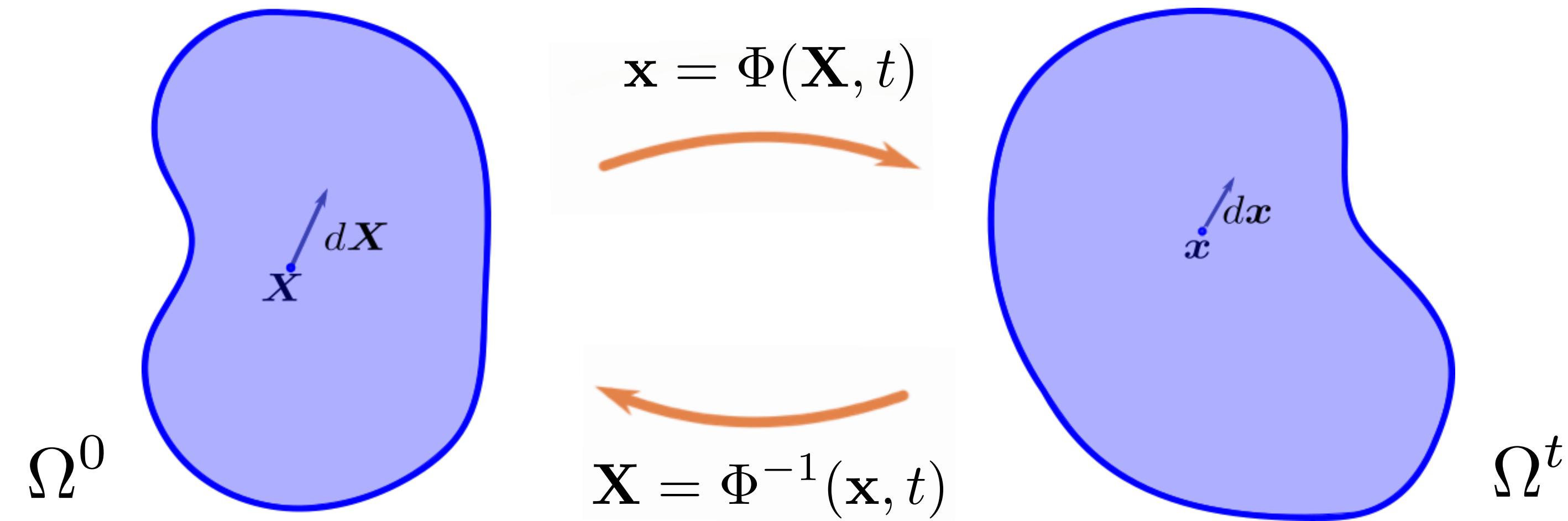
# Continuum assumption of material kinematics

## Continuum assumption



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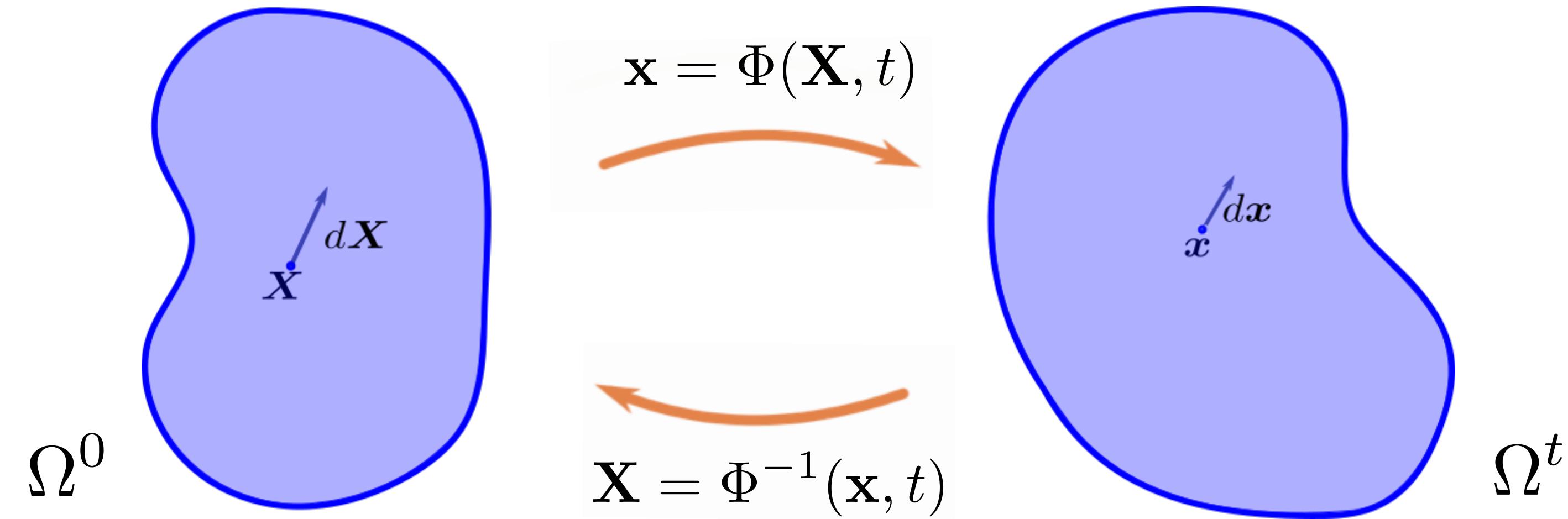
## Lagrangian kinematics

$$\mathbf{V}(\mathbf{X}, t) = \frac{\partial \Phi}{\partial t}$$

$$\mathbf{A}(\mathbf{X}, t) = \frac{\partial^2 \Phi}{\partial t^2}$$

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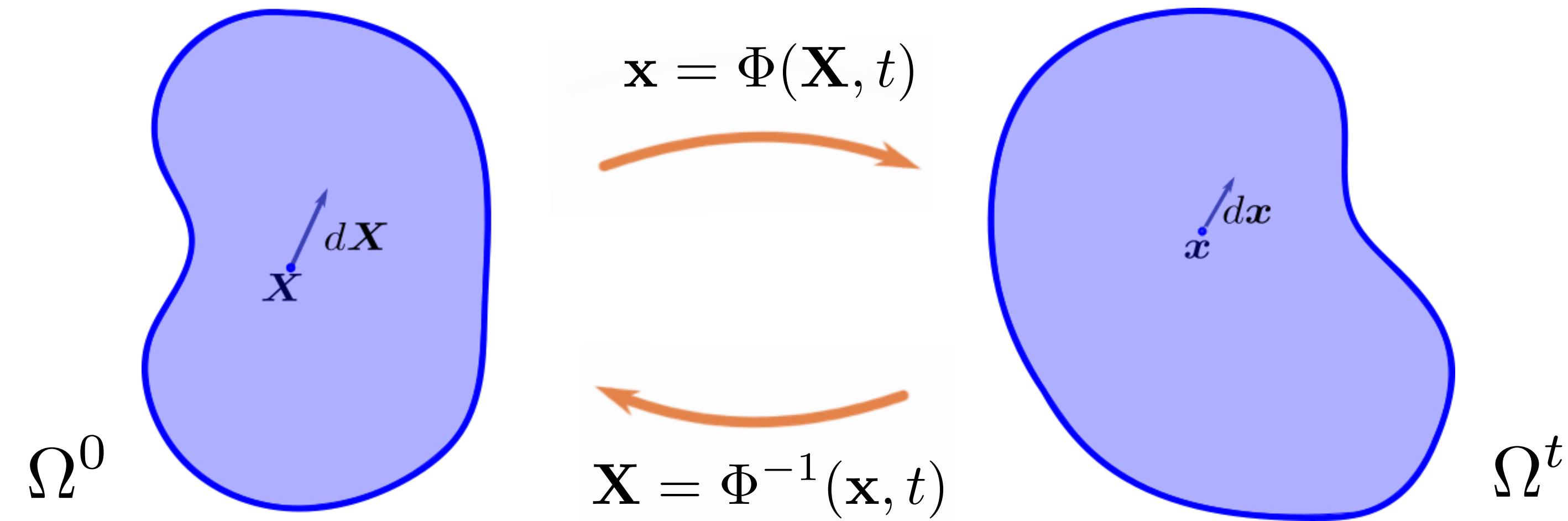
$$\mathbf{A}(\mathbf{X}, t) = \frac{\partial^2 \Phi}{\partial t^2}$$

## Eulerian velocity

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{V}(\Phi^{-1}(\mathbf{x}, t), t)$$

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## Lagrangian kinematics

$$\mathbf{v}(\mathbf{X}, t) = \frac{\partial \Phi}{\partial t}$$

$$\mathbf{A}(\mathbf{X}, t) = \frac{\partial^2 \Phi}{\partial t^2}$$

## Deformation gradient

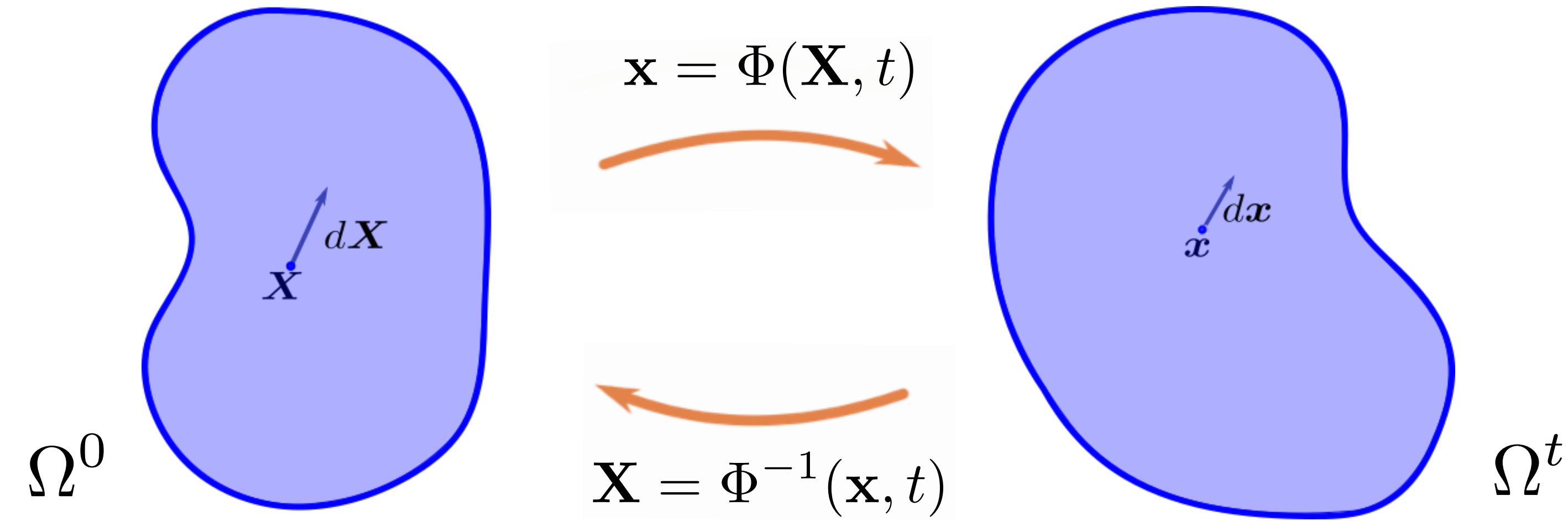
$$\mathbf{F}(\mathbf{X}, t) = \frac{\partial \Phi}{\partial \mathbf{X}}$$

## Eulerian velocity

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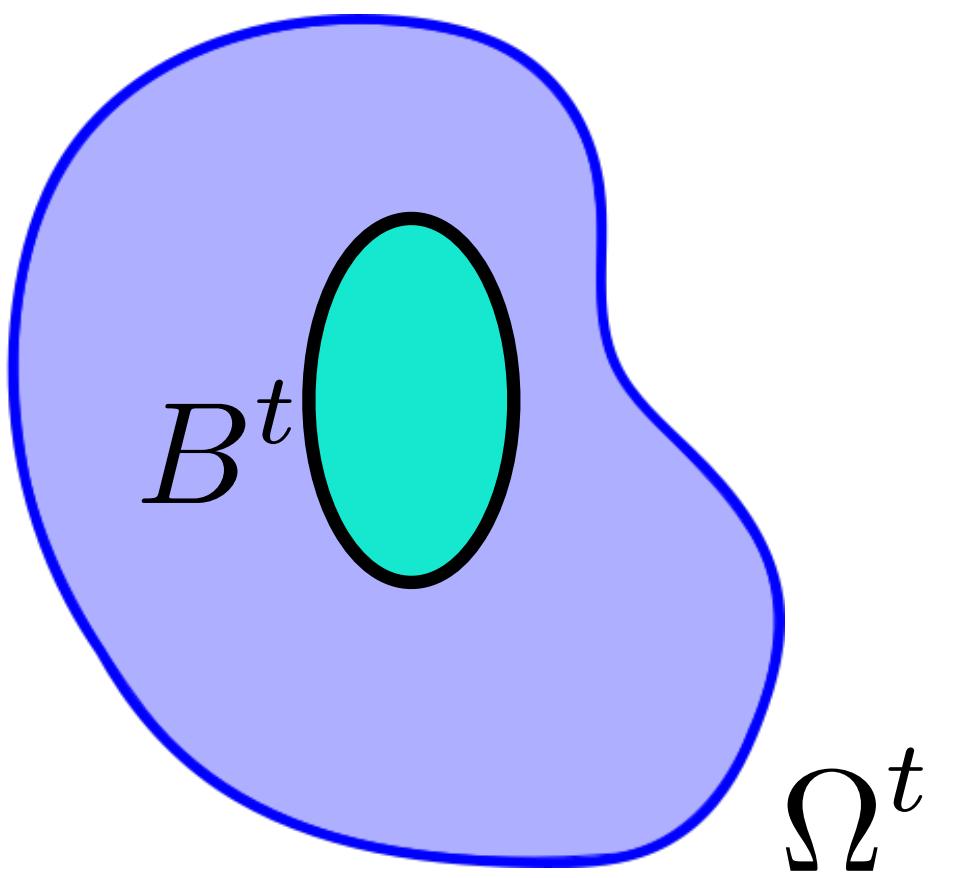
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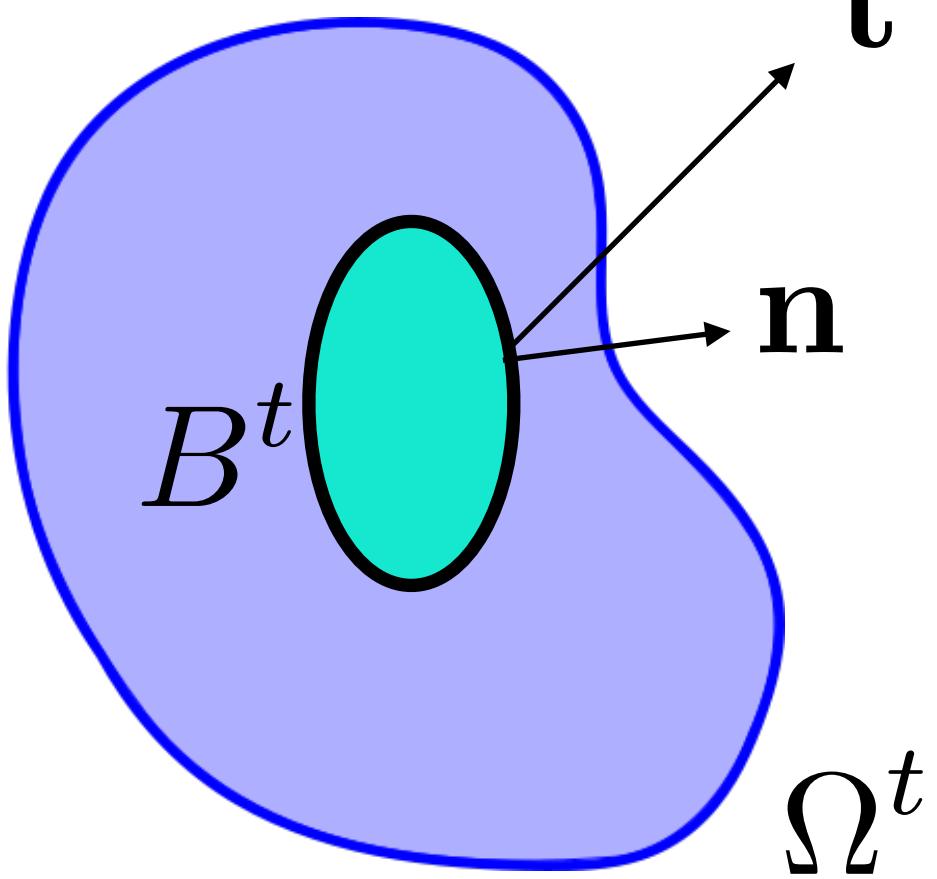
## Volume change

$$J(\mathbf{X}, t) = \det(\mathbf{F}(\mathbf{X}, t))$$

# Stress and dynamics



# Stress and dynamics

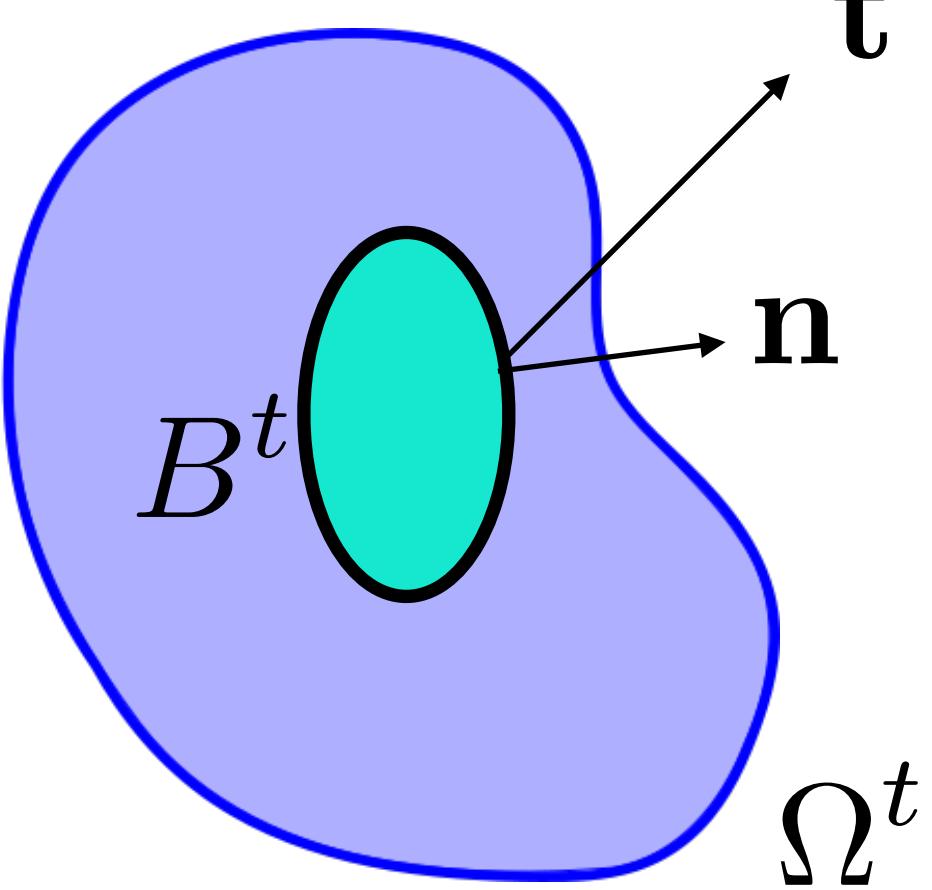


$t = \sigma n$  **traction: force per unit area**

**outward pointing normal**

$\sigma$  **Cauchy stress tensor**

# Stress and dynamics



$t = \sigma n$  **traction: force per unit area**

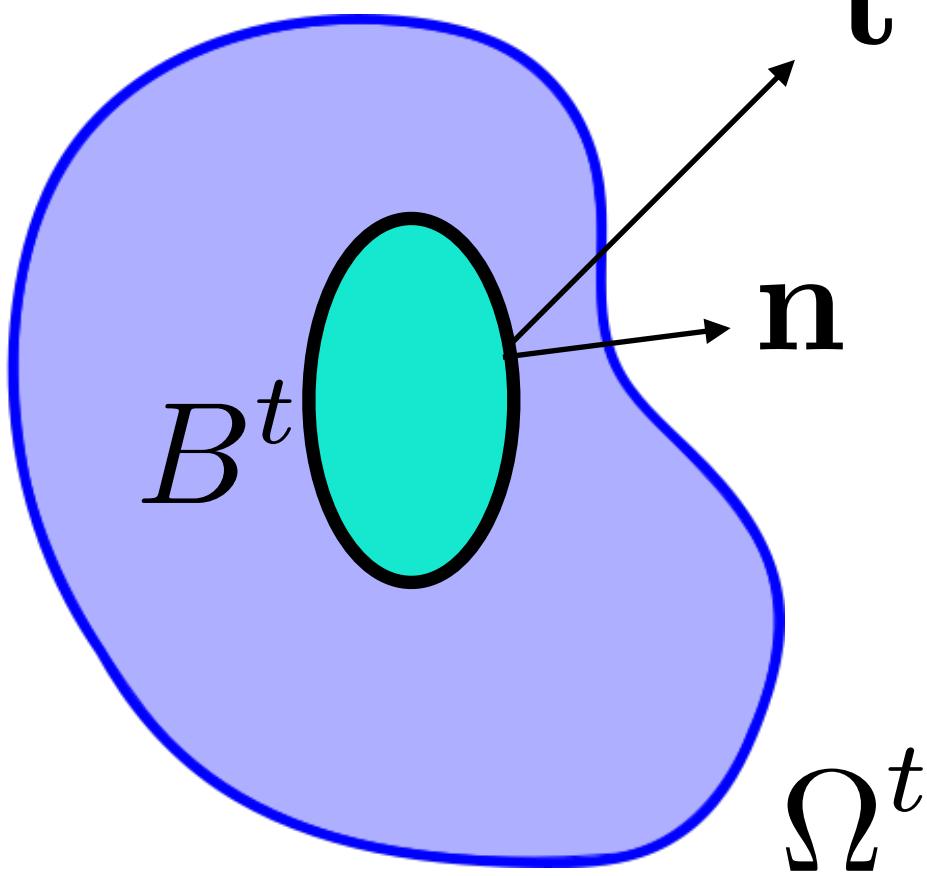
**outward pointing normal**

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**Net force due to contact with exterior**

$$\mathbf{f}_{B^t} = \int_{\partial B^t} \mathbf{t} ds(\mathbf{x}) = \int_{\partial B^t} \sigma \mathbf{n} ds(\mathbf{x}) = \int_{B^t} \nabla^{\mathbf{x}} \cdot \sigma d\mathbf{x}$$

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**Conservation of momentum**

$$\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g}.$$

# MPM and MLS-MPM from the weak form

**Strong form**

$$\rho \frac{D\mathbf{v}}{Dt} = \nabla \cdot \boldsymbol{\sigma} + \rho g \quad (\text{conservation of momentum})$$

**Weak form**

$$\begin{aligned} & \frac{1}{\Delta t} \int_{\Omega^{t^n}} \rho(\mathbf{x}, t^n) \left( \hat{v}_\alpha^{n+1}(\mathbf{x}) - v_\alpha^n(\mathbf{x}) \right) q_\alpha(\mathbf{x}, t^n) d\mathbf{x} \\ &= \int_{\partial\Omega^{t^n}} q_\alpha(\mathbf{x}, t^n) \mathcal{T}_\alpha(\mathbf{x}, t^n) ds - \int_{\Omega^{t^n}} q_{\alpha,\beta}(\mathbf{x}, t^n) \sigma_{\alpha\beta}(\mathbf{x}, t^n) d\mathbf{x} \end{aligned}$$

**B-Spline MPM kernels**

$$q_\alpha(\mathbf{x}, t^n) = N_i(\mathbf{x}) q_{i\alpha}^n$$

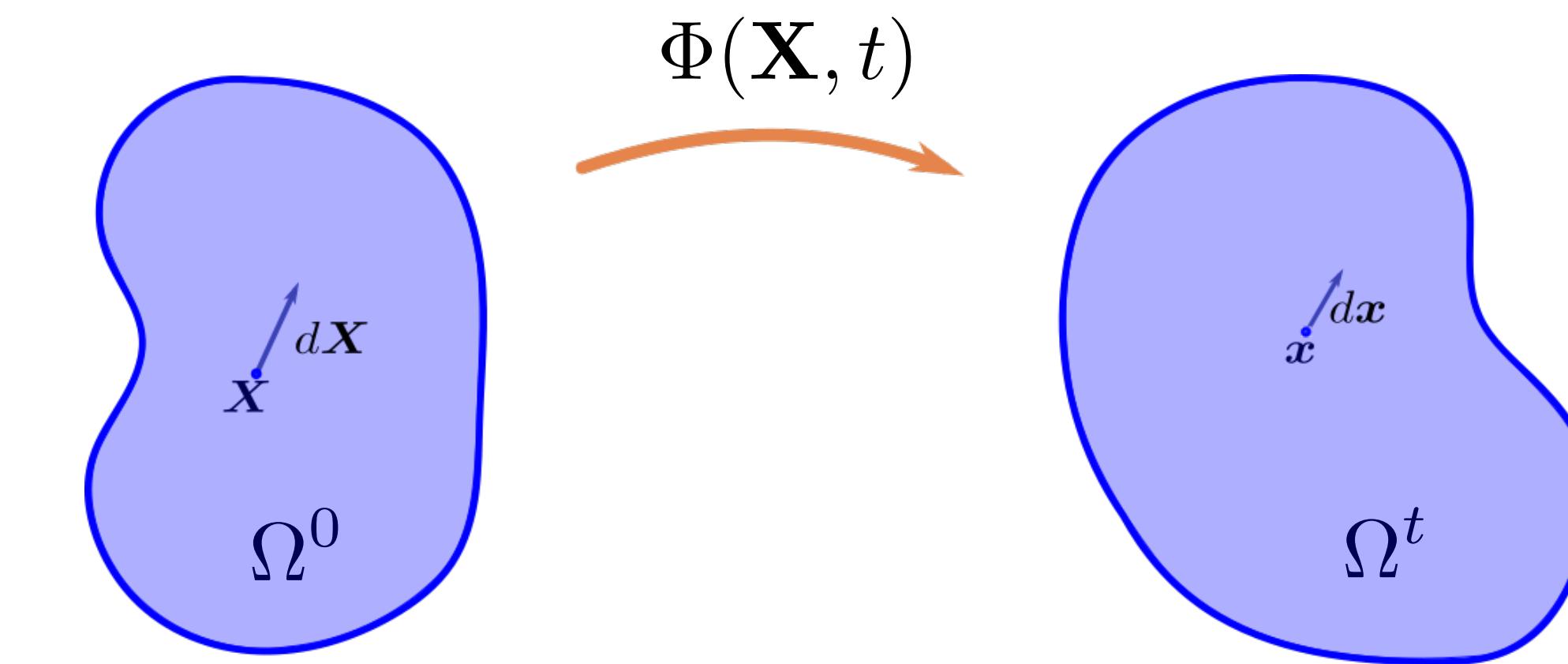
**MLS-MPM kernels**

$$q_\alpha(\mathbf{x}, t^n) = \mathbf{P}^T (\mathbf{x} - \mathbf{x}_p^n) \mathbf{M}^{-1}(\mathbf{x}_p^n) \xi_{\hat{i}}(\mathbf{x}_p^n) \mathbf{P} (\mathbf{x}_{\hat{i}} - \mathbf{x}_p^n) \delta_{\alpha\hat{\alpha}}$$

# Lagrangian Kinematics of Continuum

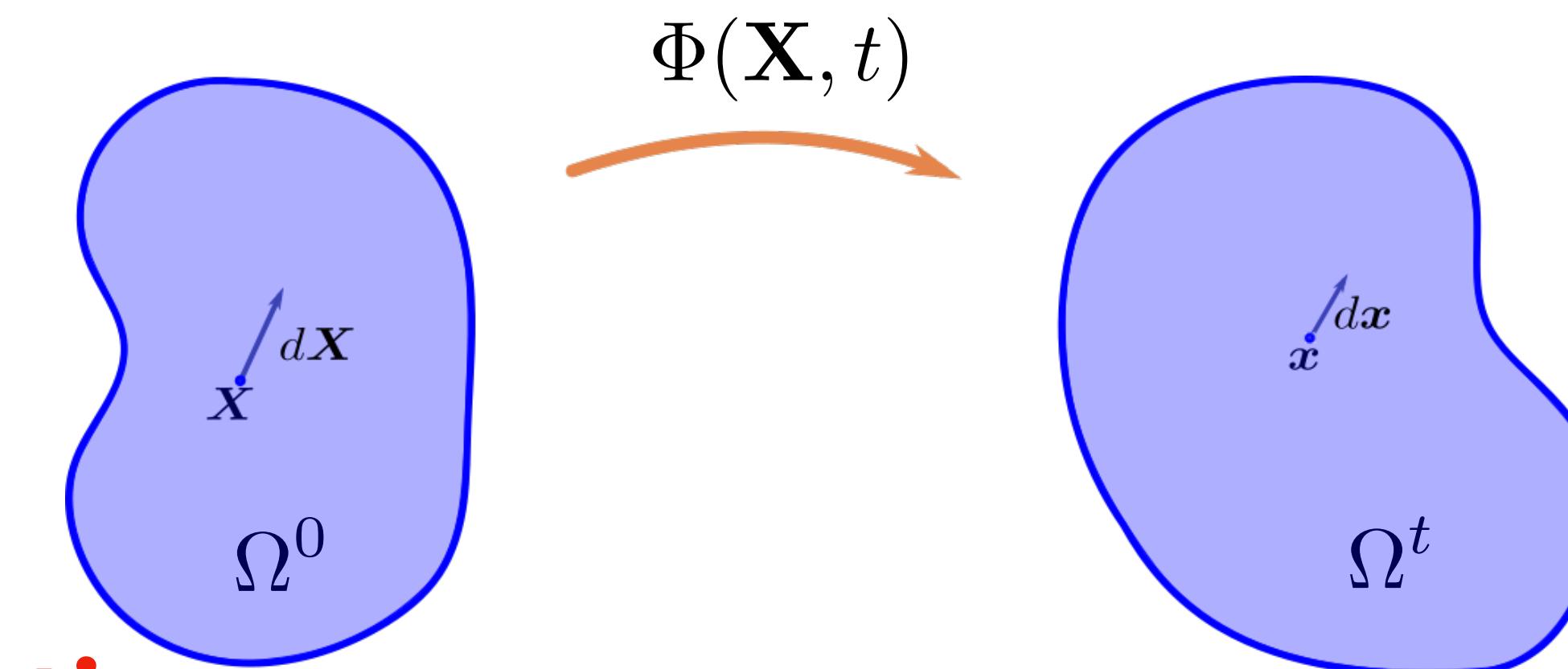
# Lagrangian Kinematics of Continuum

**Full Lagrangian kinematics**

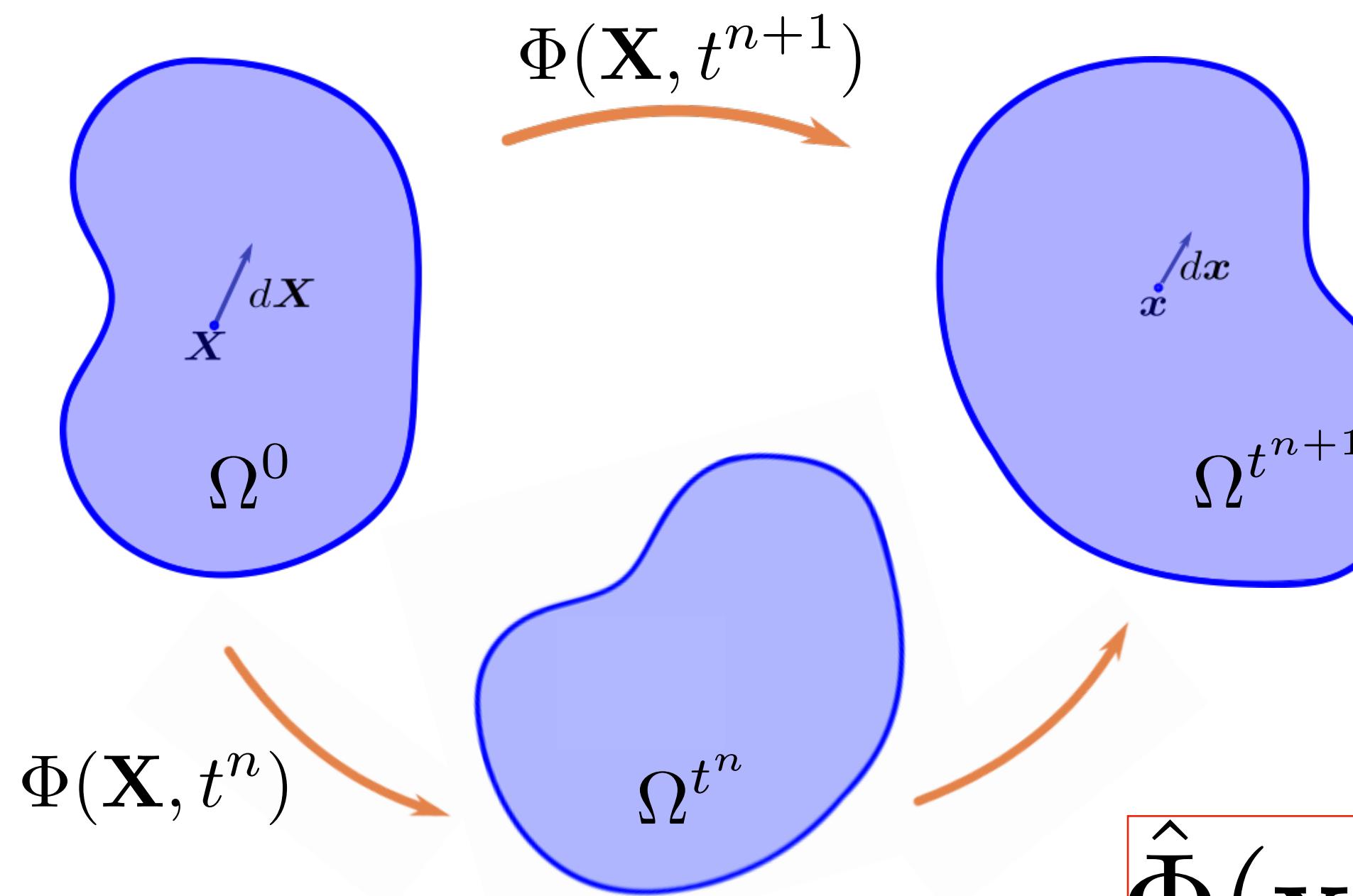


# Lagrangian Kinematics of Continuum

Full Lagrangian kinematics



Updated Lagrangian kinematics



The deformation flows through updating the current configuration.

$$\hat{\Phi}(\mathbf{x}^n) = \Phi(\Phi^{-1}(\mathbf{x}^n, t^n), t^{n+1})$$

# Evolve the deformation

$$\mathbf{F}_p^{n+1} = (\mathbf{I} + \Delta t \nabla \mathbf{v}_p^{n+1}) \mathbf{F}_p^n$$

# Evolve the deformation

$$\hat{\Phi}(\mathbf{x}_p^n) = \Phi(\Phi^{-1}(\mathbf{x}_p^n, t^n), t^{n+1})$$

$$\frac{\partial \hat{\Phi}}{\partial \mathbf{x}_p^n} = \frac{\partial \Phi}{\partial \mathbf{X}}(\mathbf{X}, t^{n+1}) \left( \frac{\partial \Phi}{\partial \mathbf{X}}(\mathbf{X}, t^n) \right)^{-1}$$

$$\hat{\mathbf{f}} = \mathbf{F}^{n+1} (\mathbf{F}^n)^{-1}$$

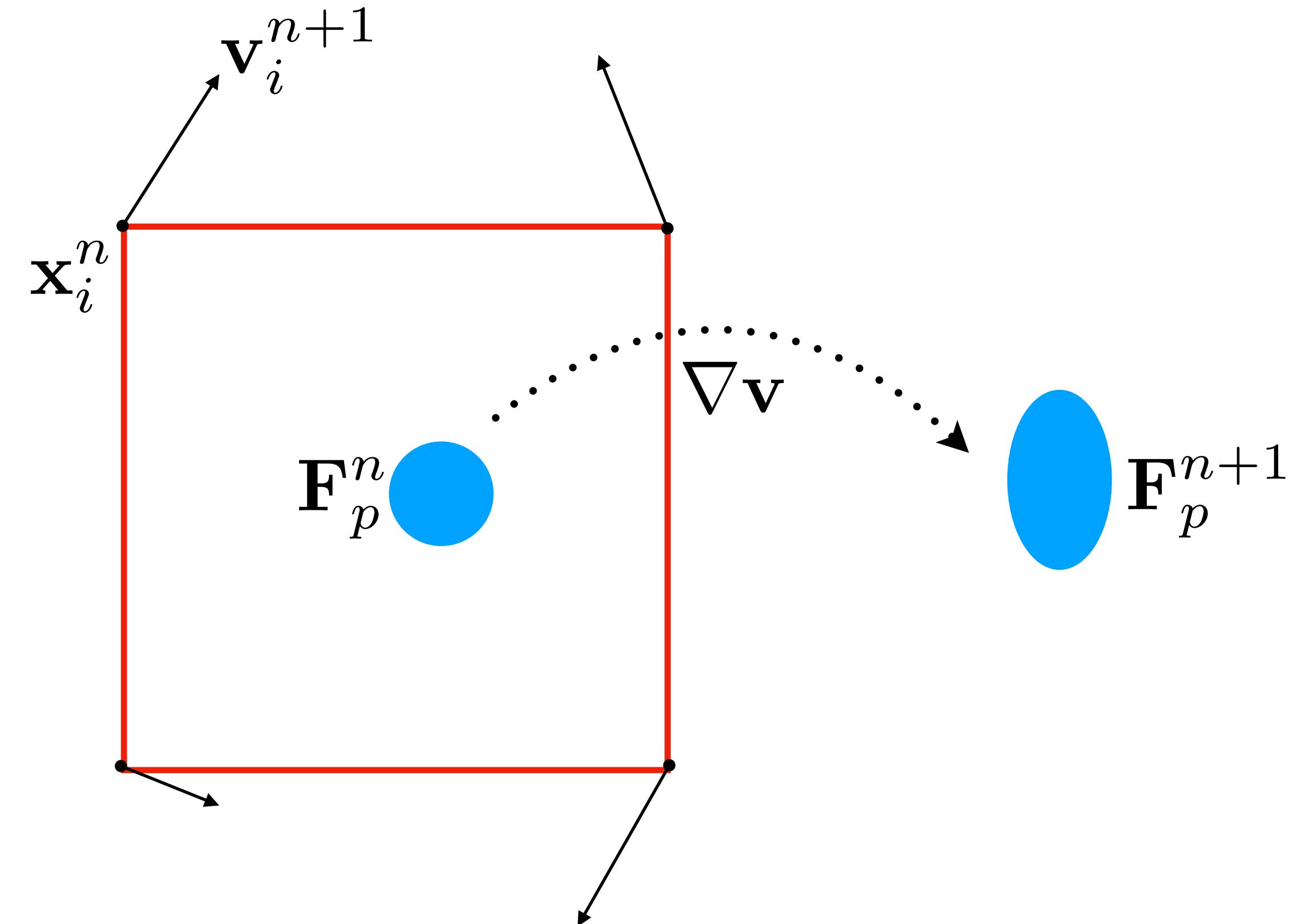
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$$\hat{\Phi} = \mathbf{x}_p^n + \Delta t \sum_i \mathbf{v}_i^{n+1} w_{ip}^n$$

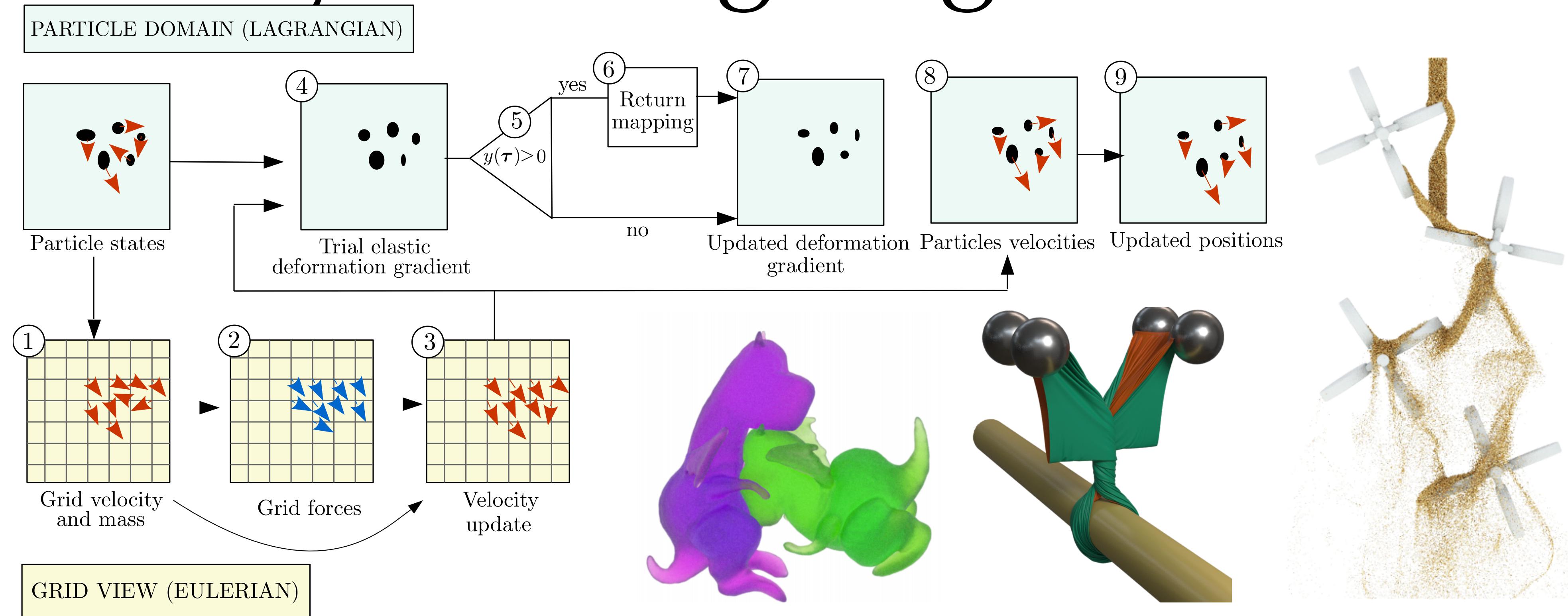
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$$\hat{\mathbf{f}} = \mathbf{I} + \Delta t \sum_i \mathbf{v}_i^{n+1} \nabla w_{ip}^n$$

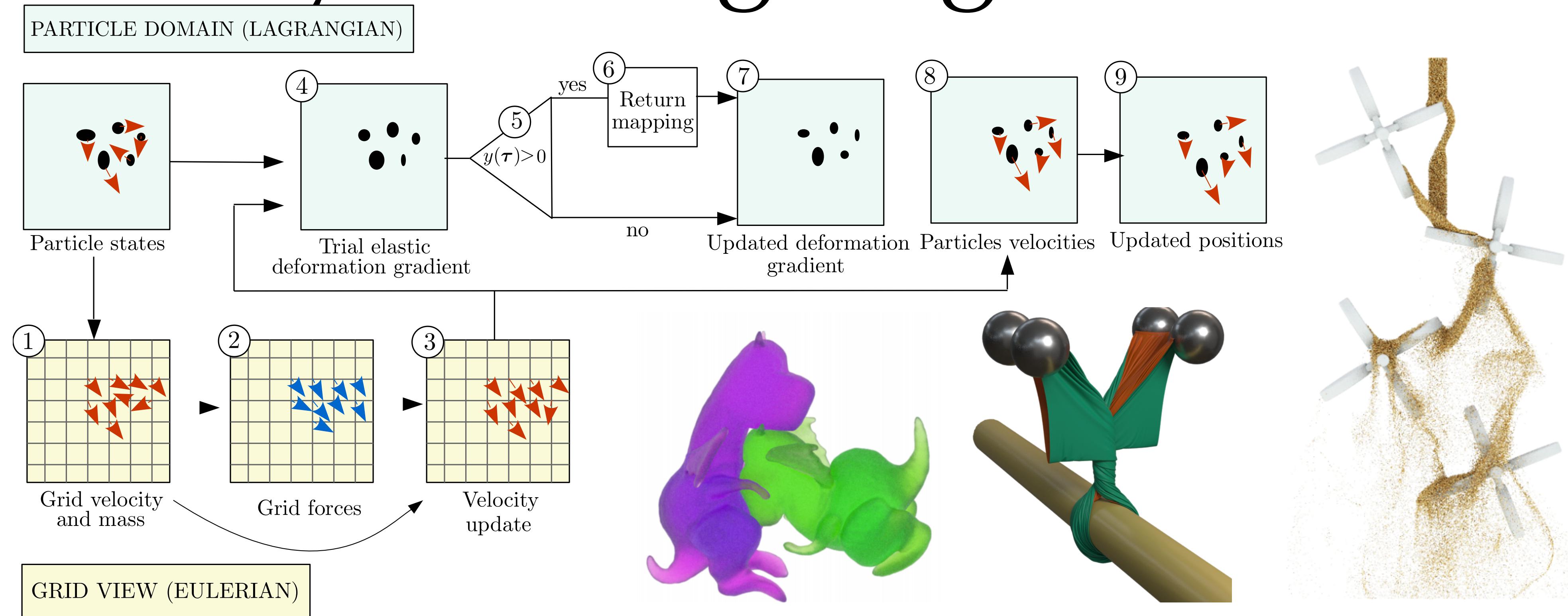
**F is updated using velocity gradient**



# MPM is hybrid Lagrangian/Eulerian

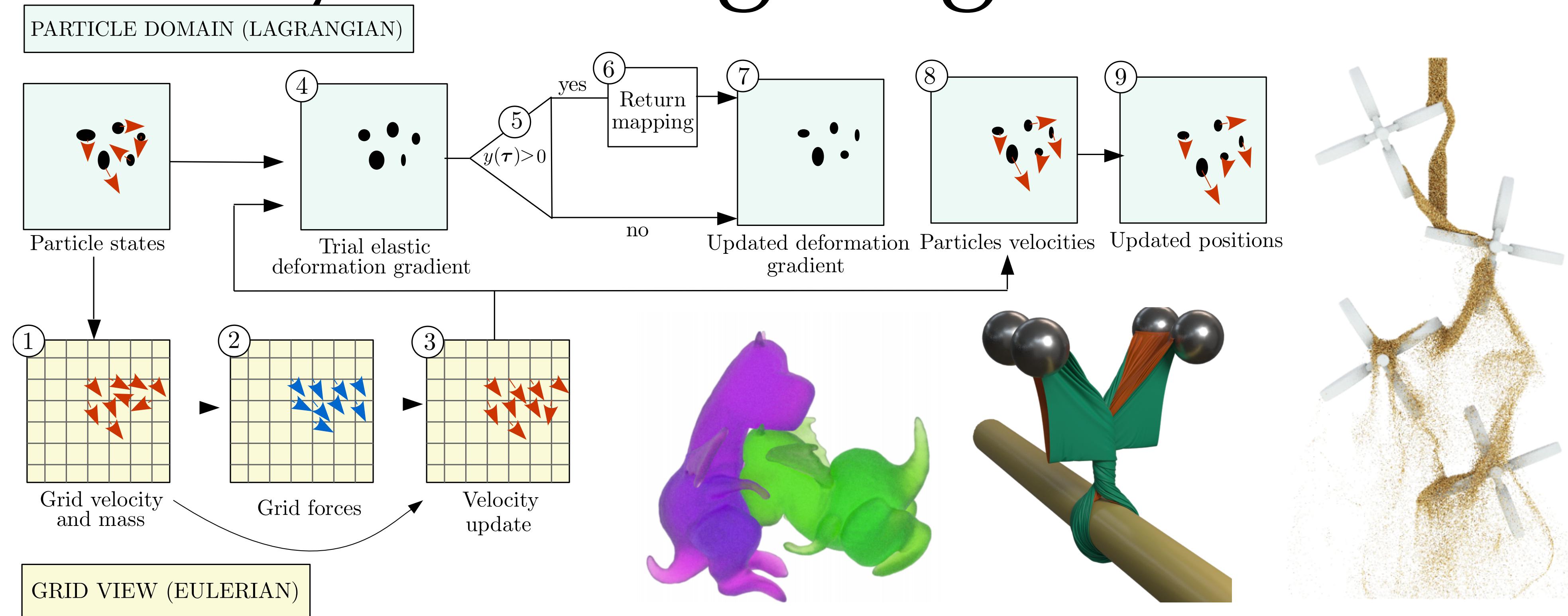


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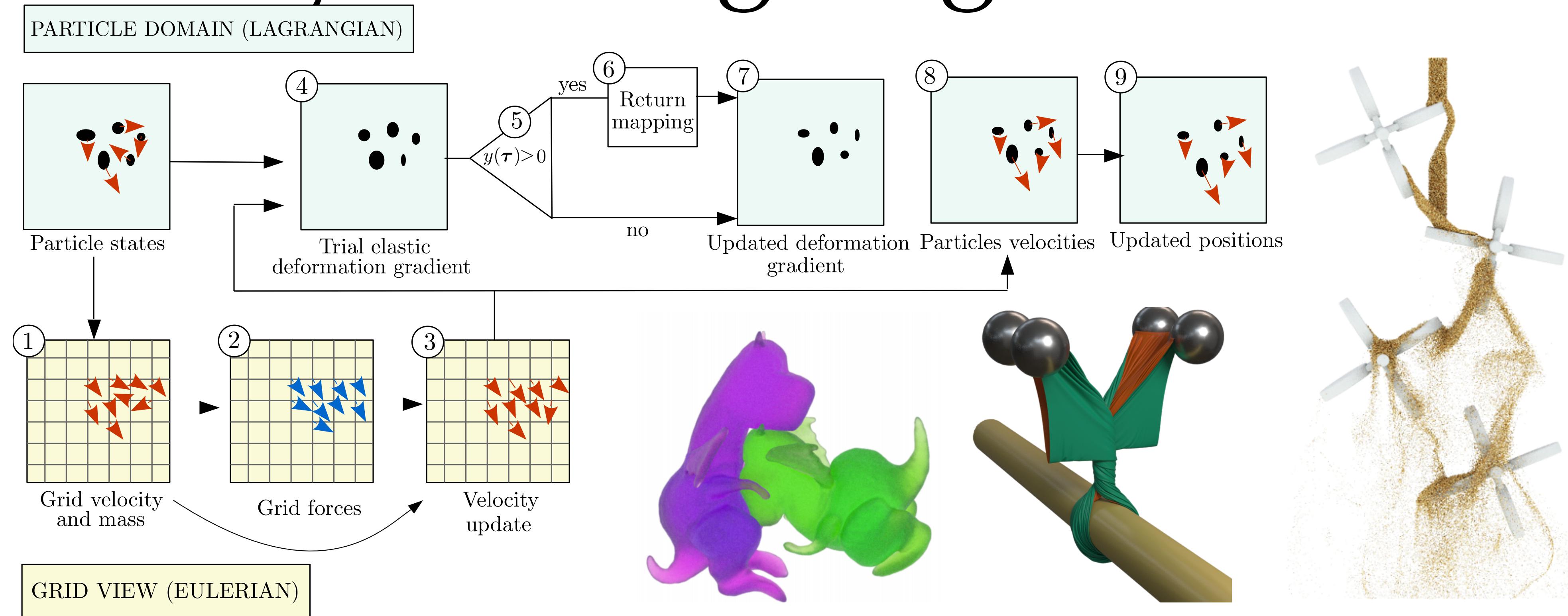
♦ Grid handles: the Galerkin DOFs, discretization, function space, ....

# MPM is hybrid Lagrangian/Eulerian



- ♦ Grid handles: the Galerkin DOFs, discretization, function space, ....
- ♦ The transfer/embedding handles: coupling, quadrature rule, non-penetration, topology change, ...

# MPM is hybrid Lagrangian/Eulerian



- ♦ Grid handles: the Galerkin DOFs, discretization, function space, ....
- ♦ The transfer/embedding handles: coupling, quadrature rule, non-penetration, topology change, ...
- ♦ Each individual particle handles: constitutive modeling - the physics

# Elasticity, hyperelasticity

## ♦ Hyperelasticity is convenient

- Capturing real materials
- Artistic design
- Anisotropy, damping ...

$$\Psi(\mathbf{F}) = \frac{\mu}{2} (\text{tr}(\mathbf{FF}^T) - 3) - \mu \log(J) + \frac{\lambda}{2} \log^2(J)$$

$$\Psi(\mathbf{F}) = \mu \|\mathbf{F} - \mathbf{R}\|_F^2 + \frac{\lambda}{2} (\det(\mathbf{F}) - 1)^2$$

$$\Psi(\mathbf{F}) = \mu \text{tr}((\log \Sigma)^2) + \frac{\lambda}{2} (\text{tr}(\log \Sigma))^2$$

$$\Psi(\mathbf{F}) = f(\sigma_1) + f(\sigma_2) + f(\sigma_3) + g(\sigma_1\sigma_2) + g(\sigma_2\sigma_3) + g(\sigma_3\sigma_1) + h(\sigma_1\sigma_2\sigma_3)$$



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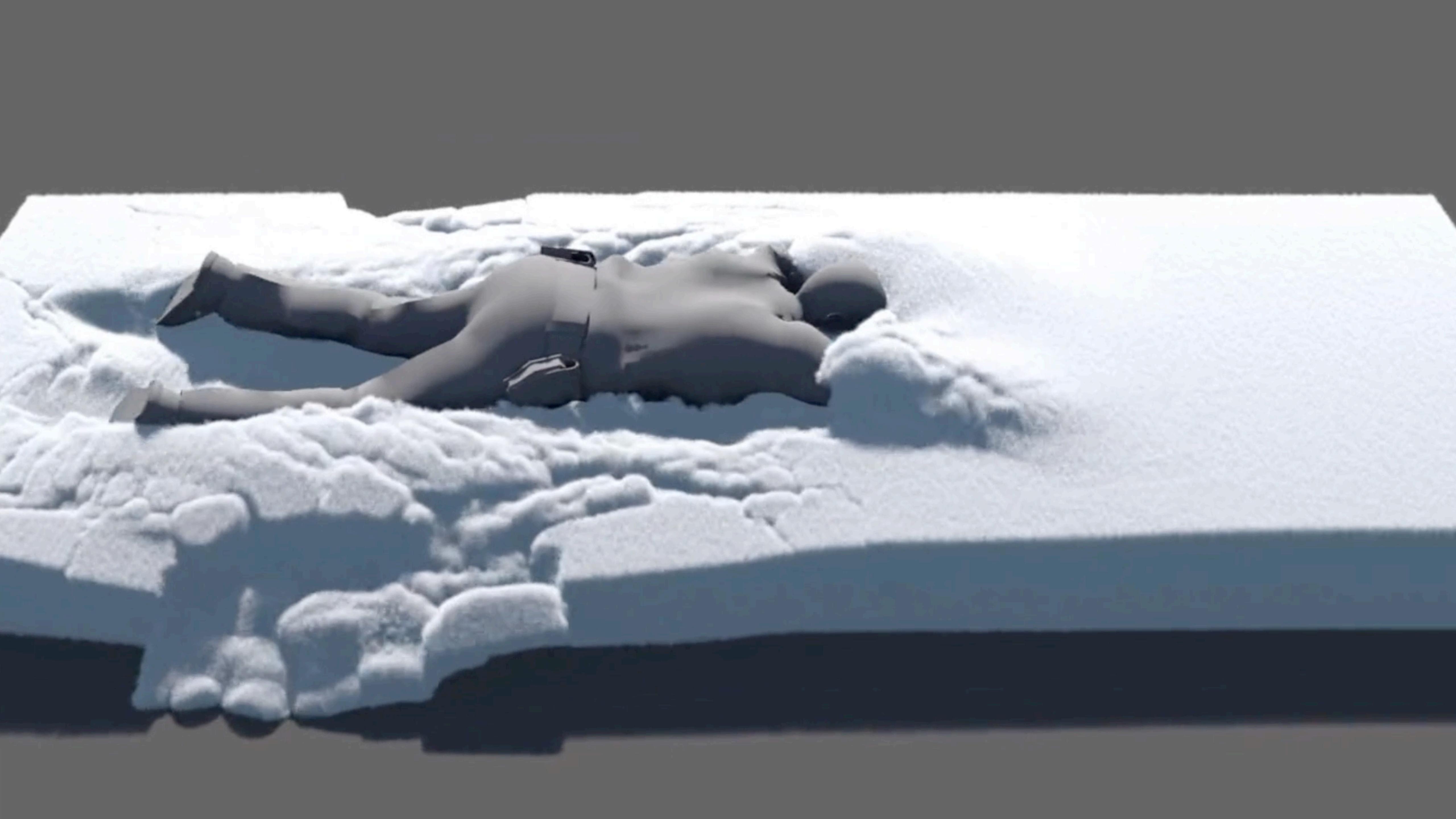
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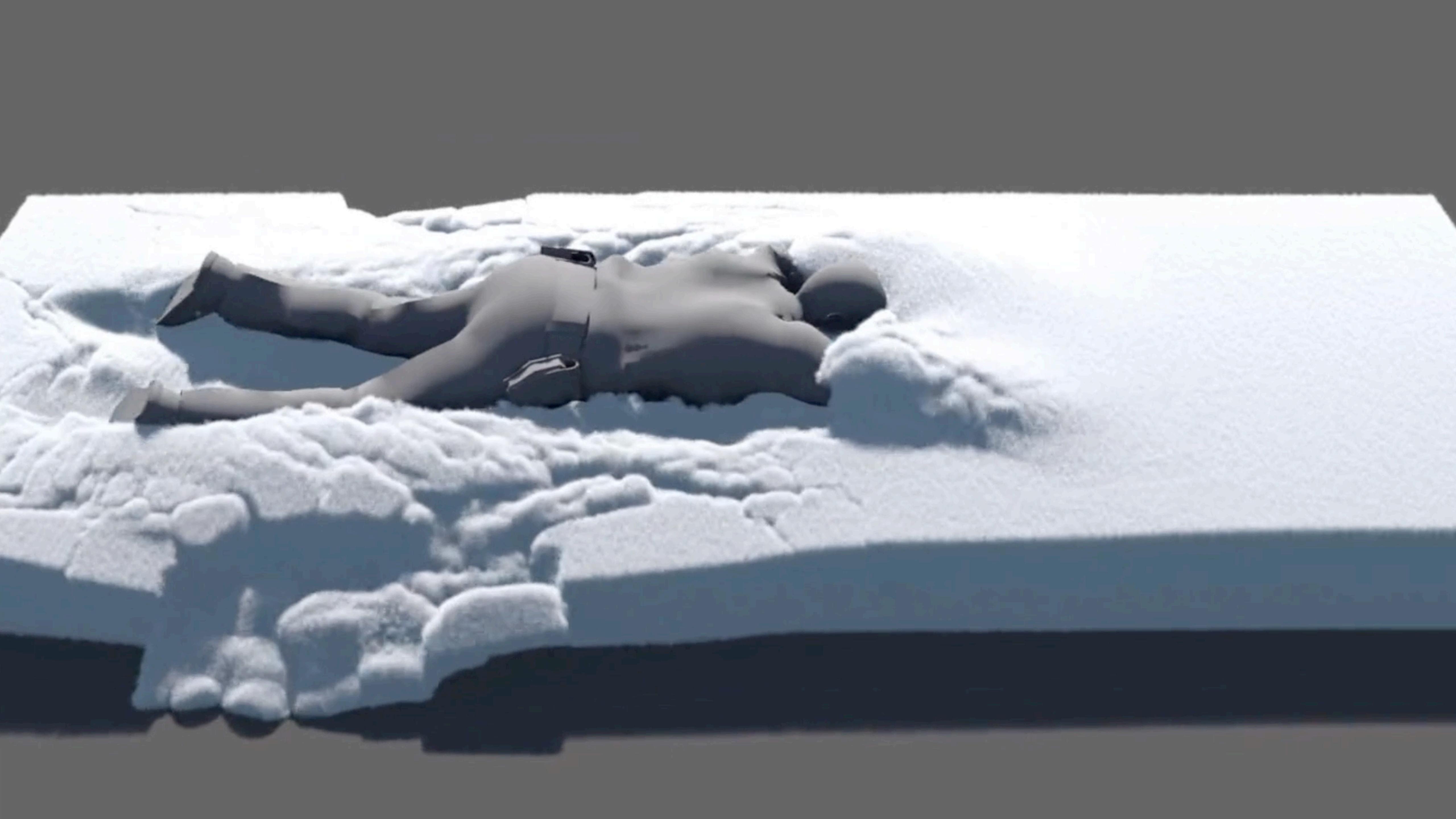
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# Inelasticity



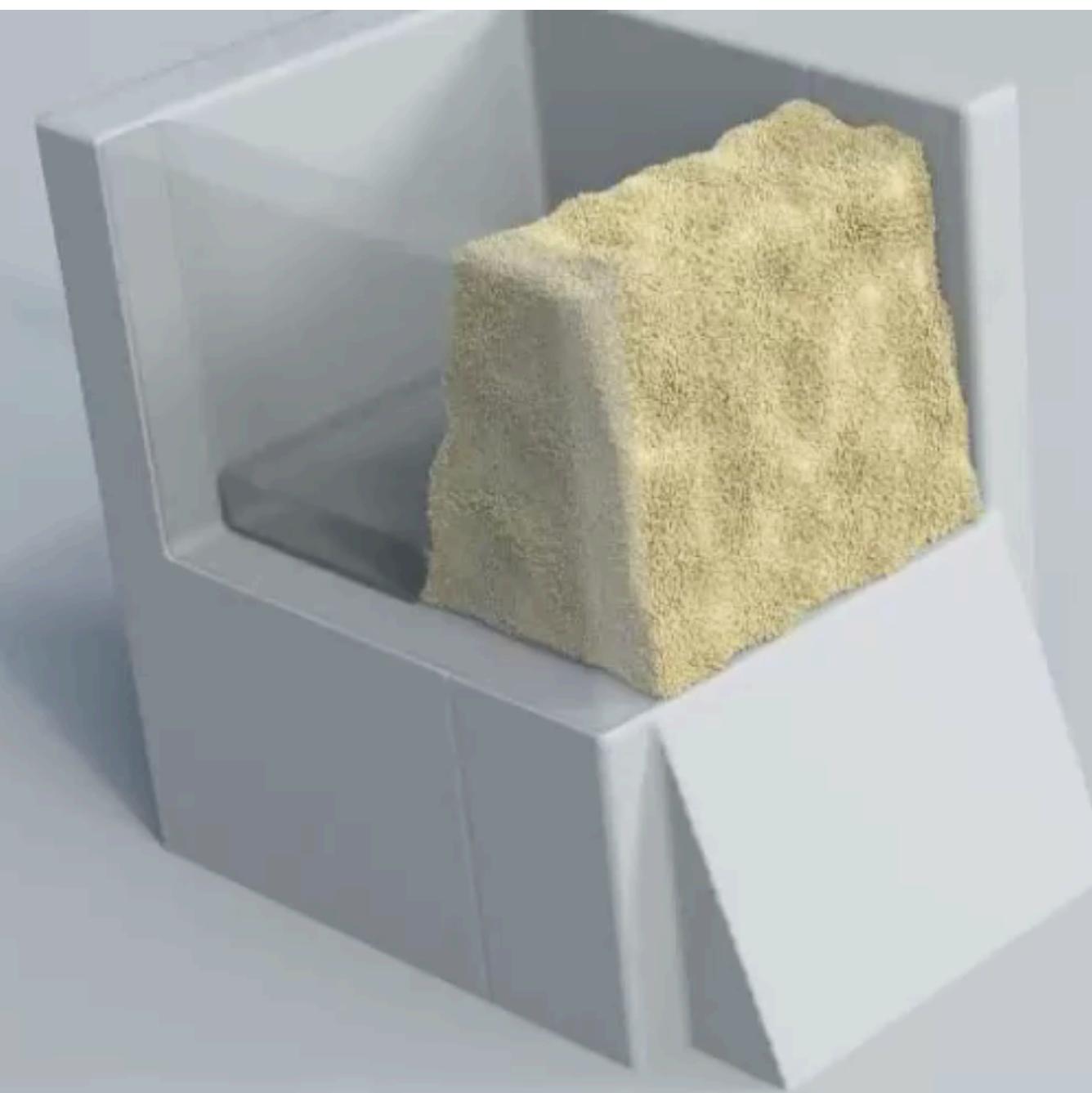


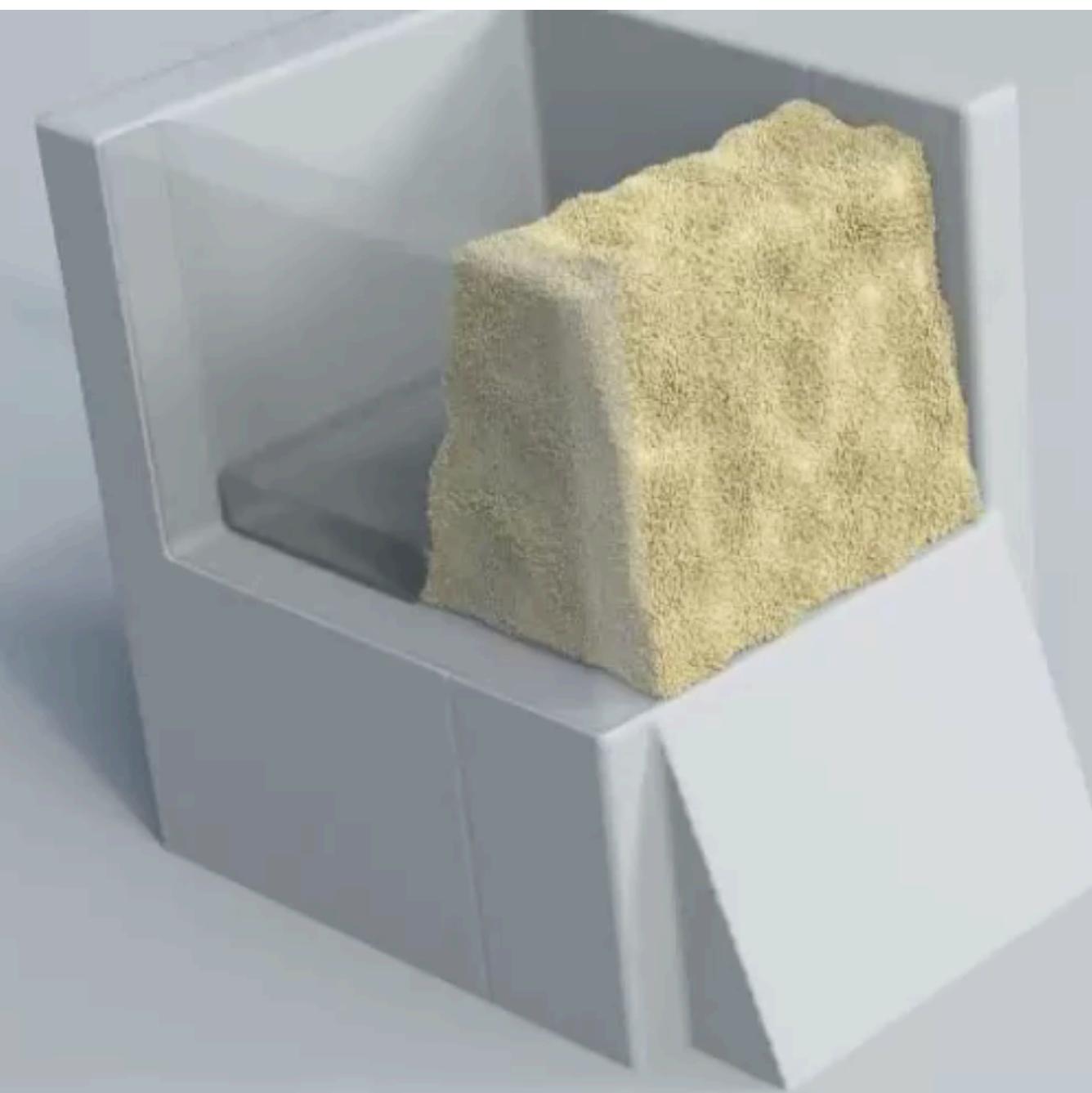


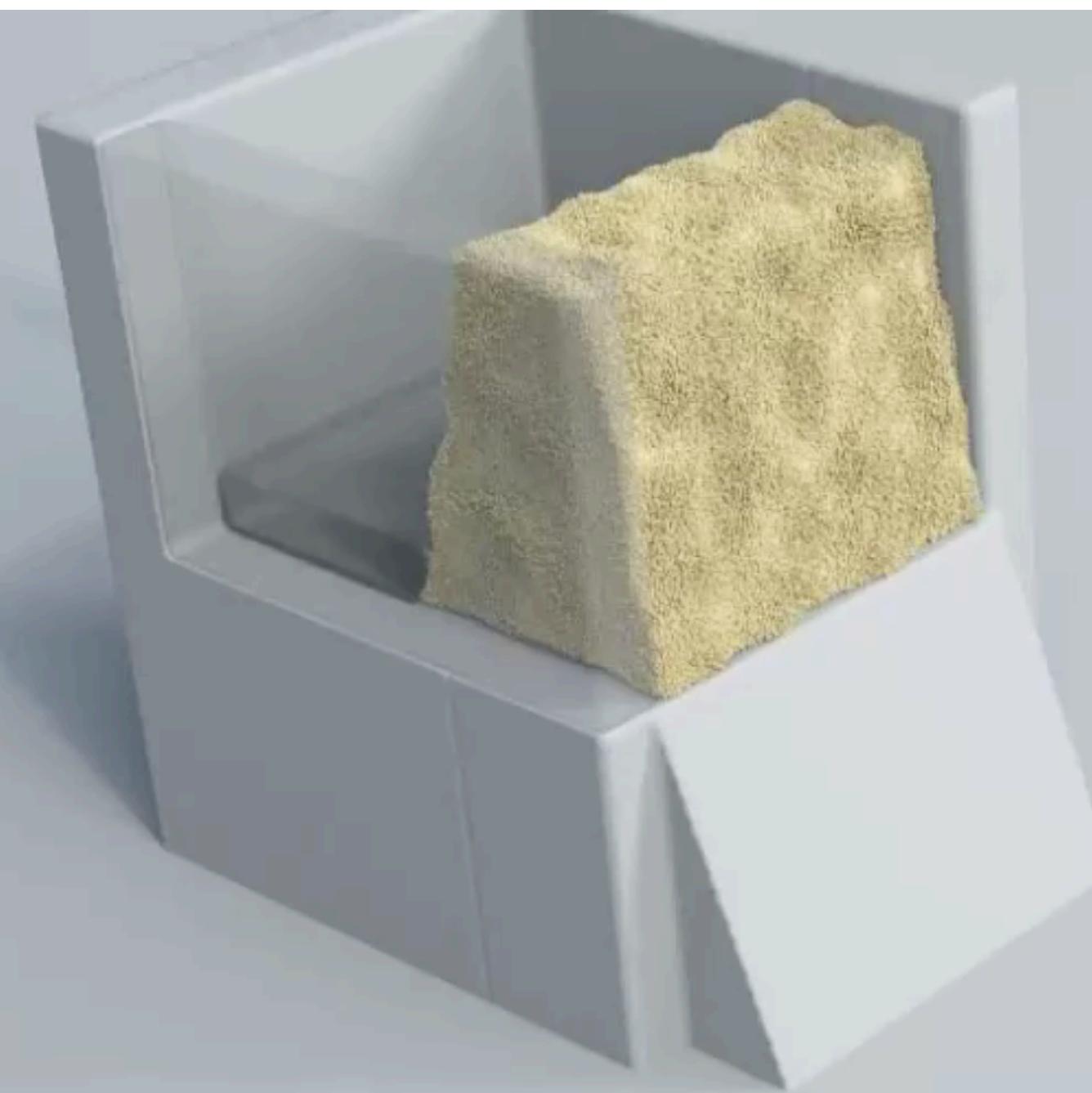


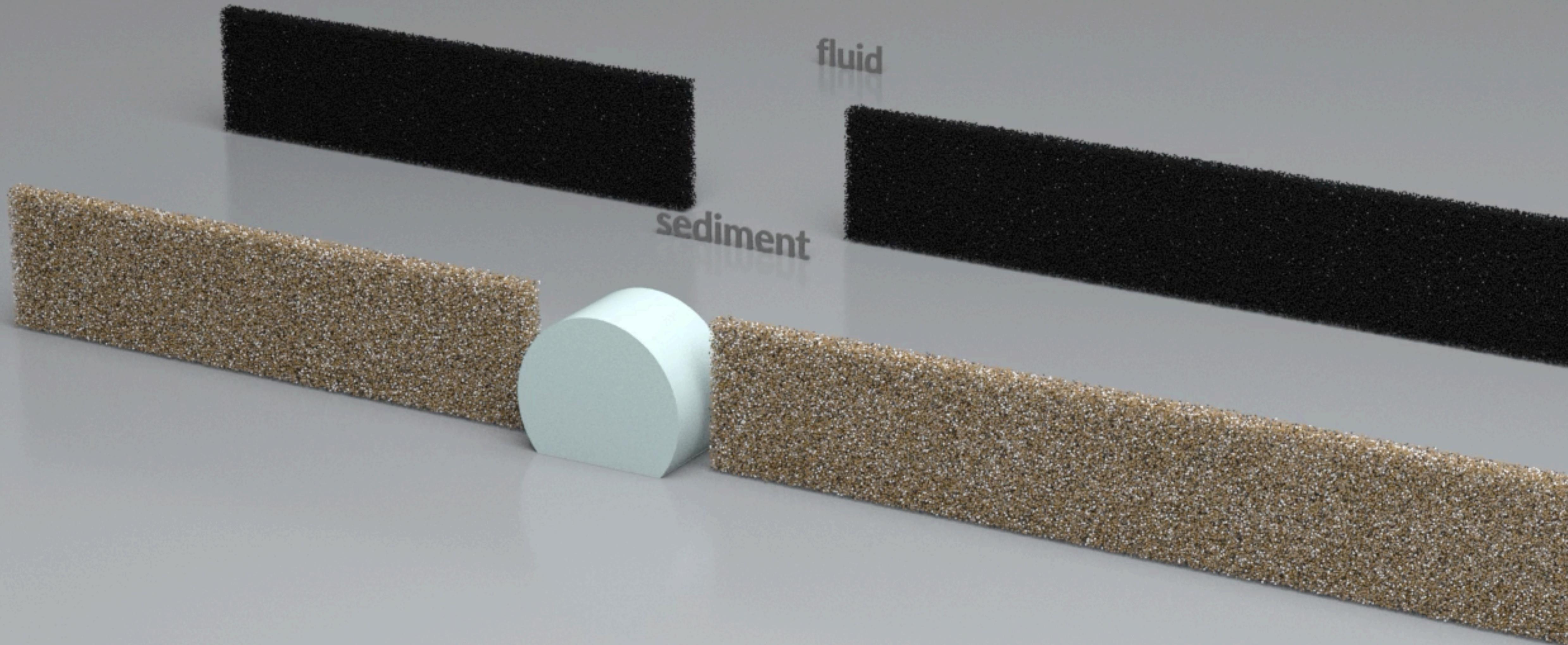


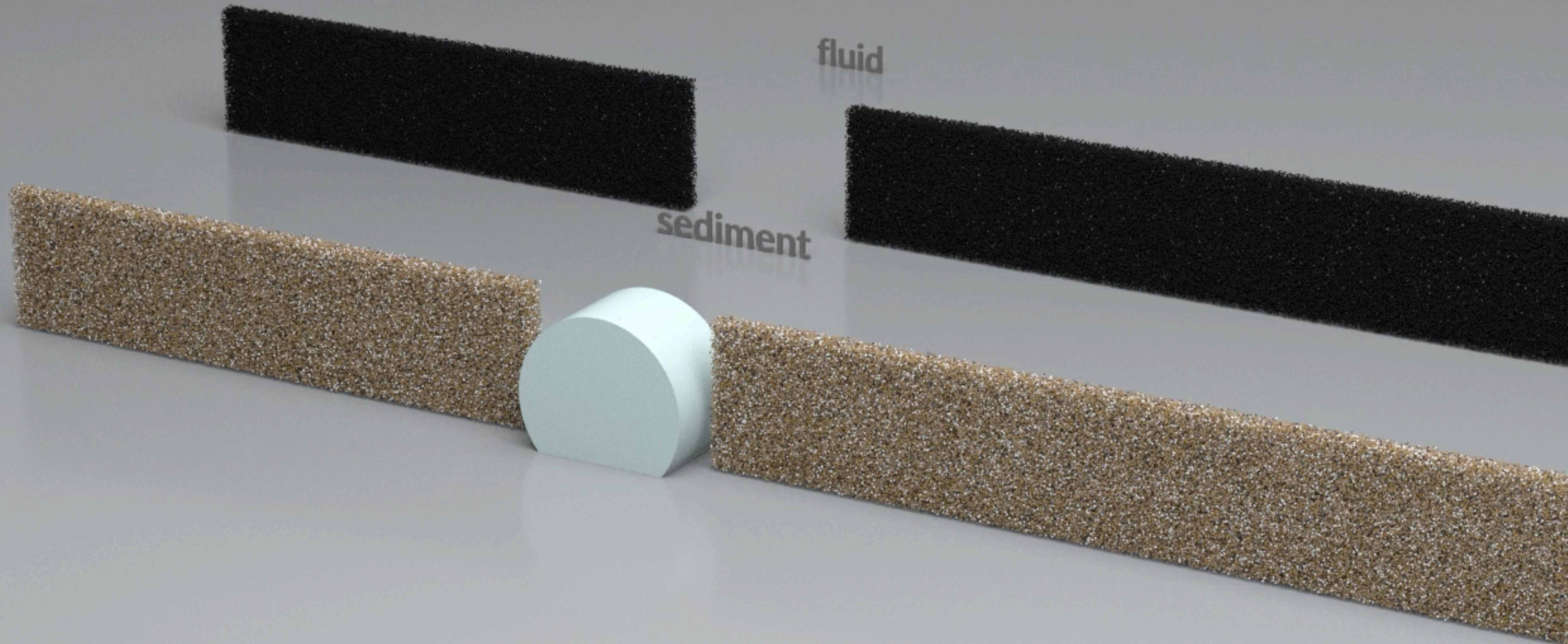


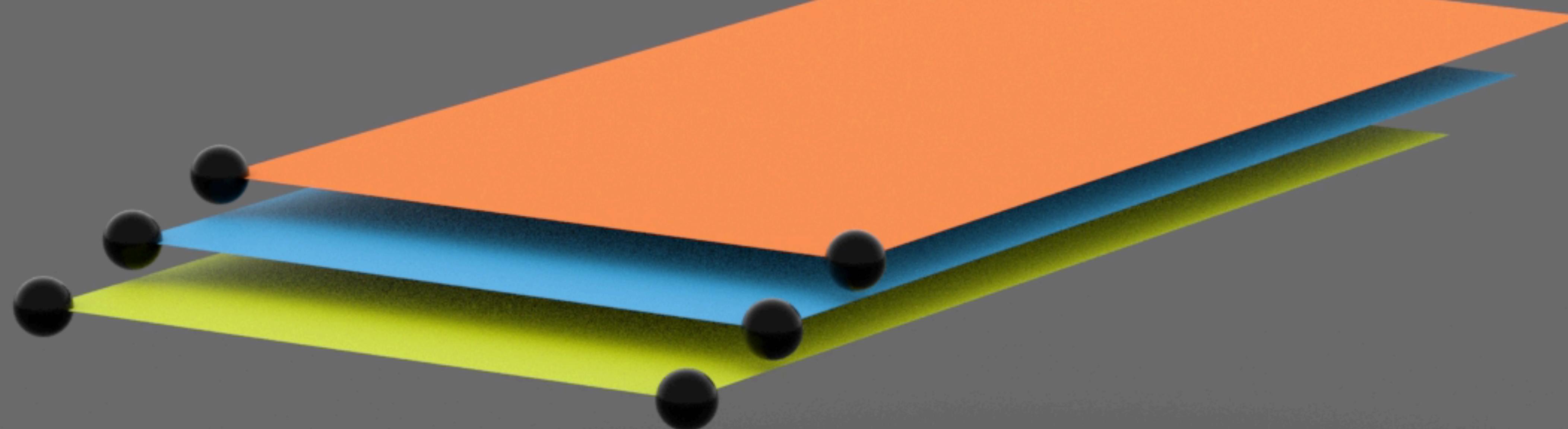




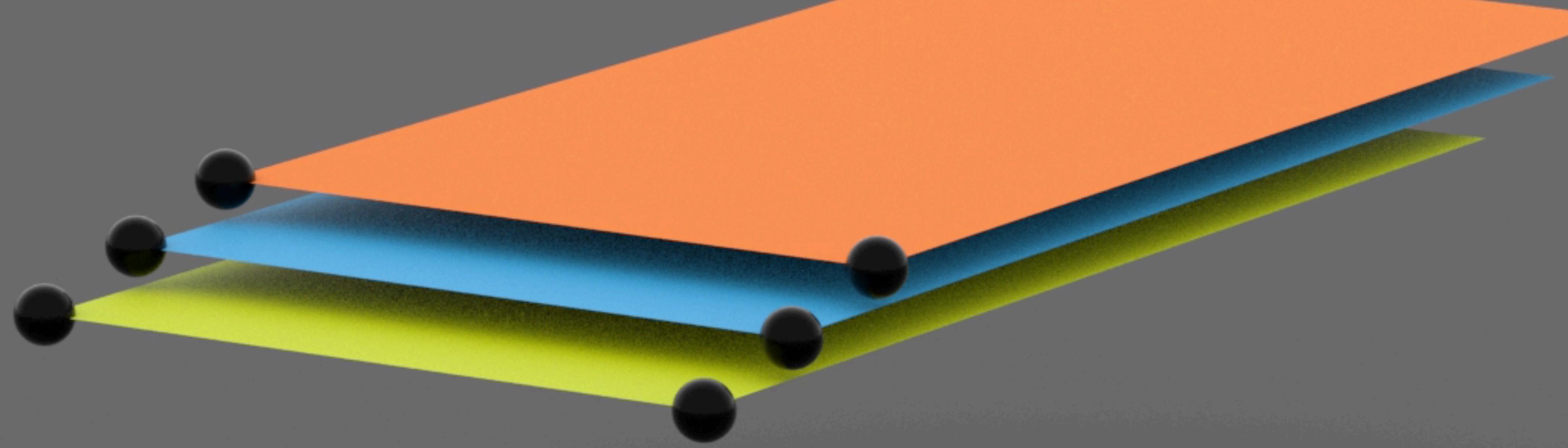




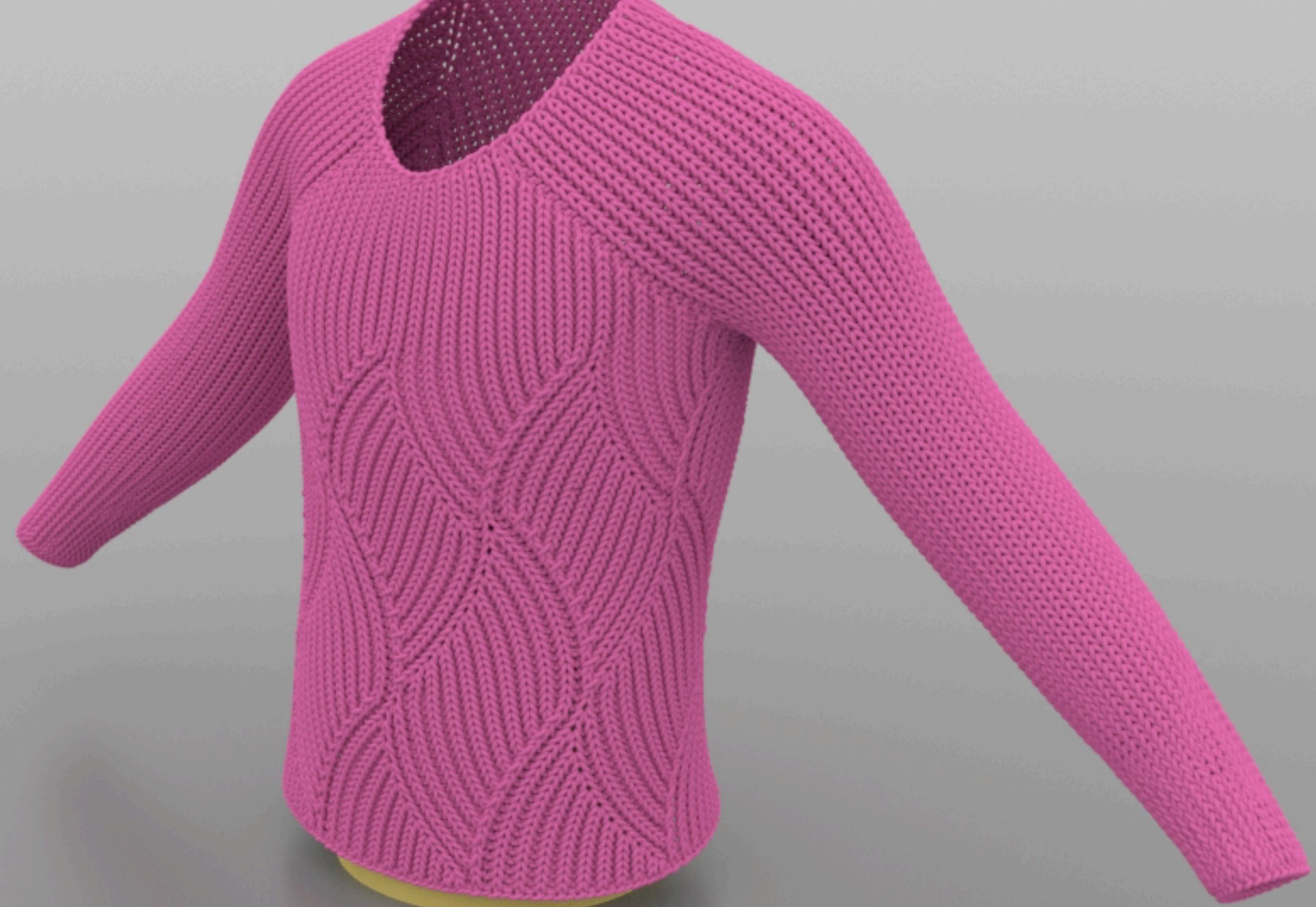


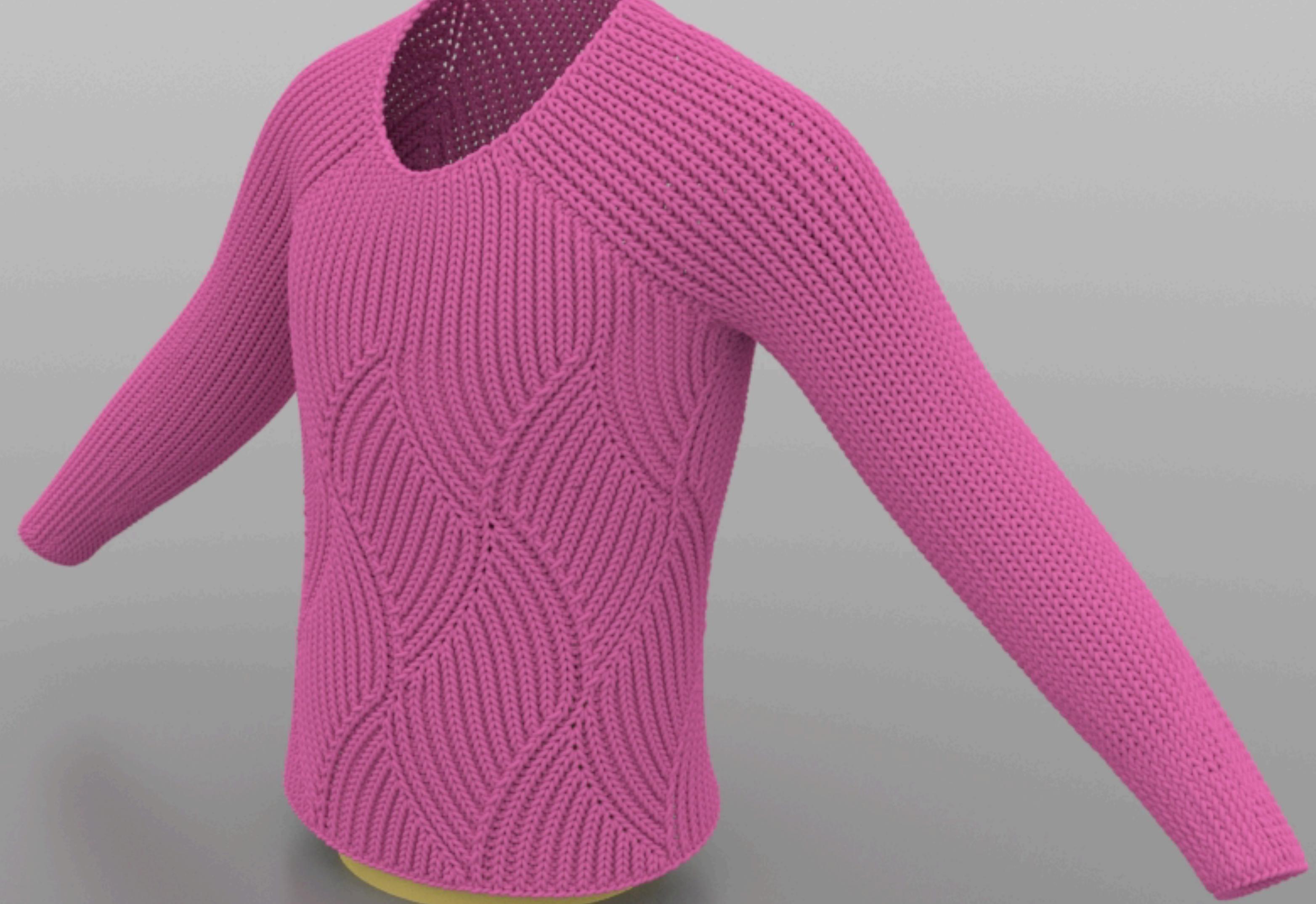


[Jiang17] Anisotropic Elastoplasticity for Cloth, Knit and Hair under Contact, Chenfanfu Jiang, Theodore Gast, Joseph Teran,  
SIGGRAPH 2017



[Jiang17] Anisotropic Elastoplasticity for Cloth, Knit and Hair under Contact, Chenfanfu Jiang, Theodore Gast, Joseph Teran,  
SIGGRAPH 2017





















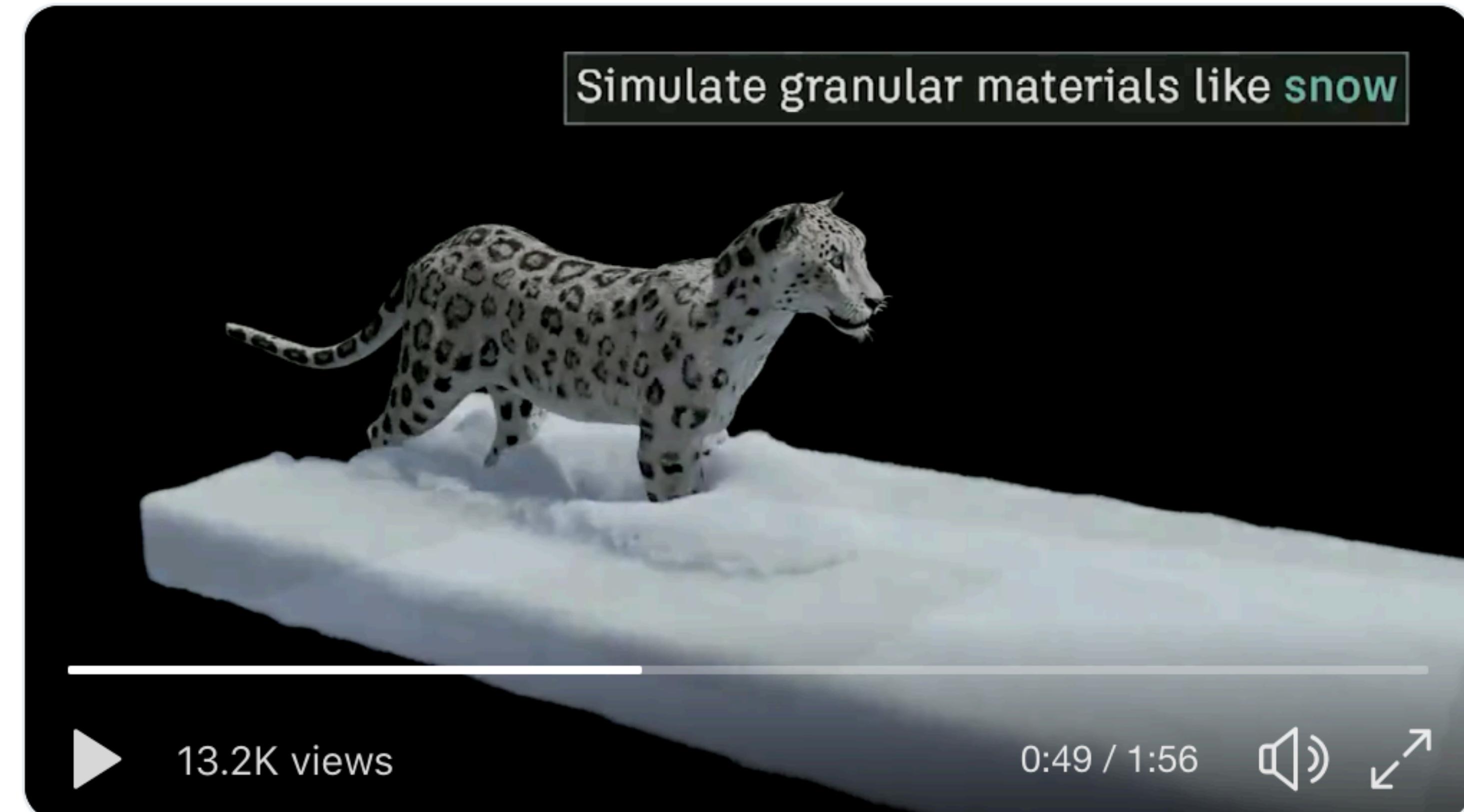
MPM is in  
Bifrost[Maya]  
starting  
yesterday

**TRY IT  
NOW!**



**Autodesk Maya** @AdskMaya · 23h

Coming July 31 – #Bifrost for Maya empowers #3D artists and TDs to create blockbuster-worthy effects using a new visual programming environment. Learn about the powerful dynamic solvers, ready-to-use graphs, and more here: [bit.ly/bifrost-maya](http://bit.ly/bifrost-maya)



# MPM is in Bifrost[Maya] starting yesterday

**TRY IT  
NOW!**



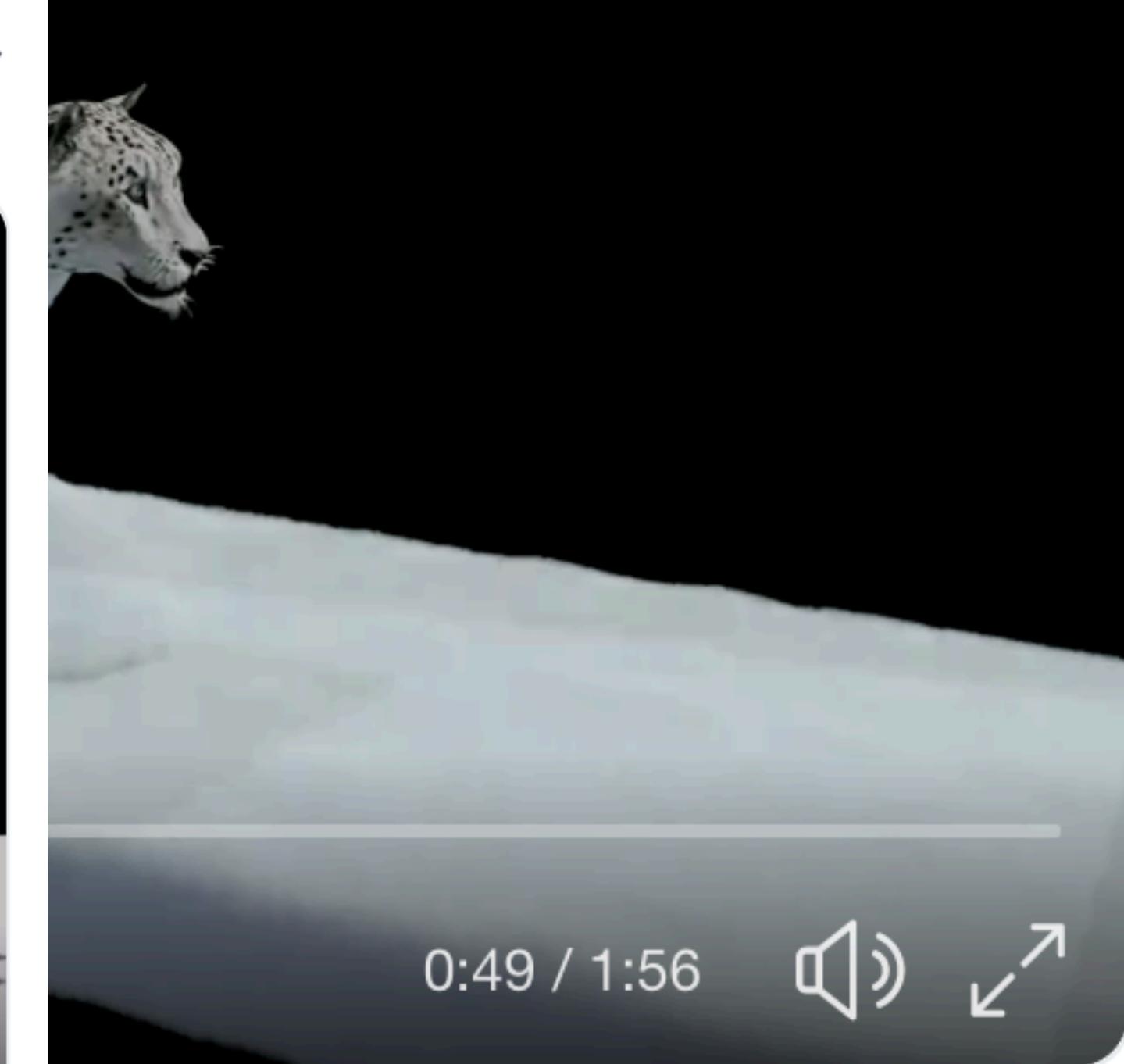
**Autodesk Maya** @AdskMaya · 23h

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Simulate granular materials like **snow**



**Autodesk Maya** @AdskMaya · Jul 23  
7.31.19



# MPM is in Bifrost[Maya] starting yesterday

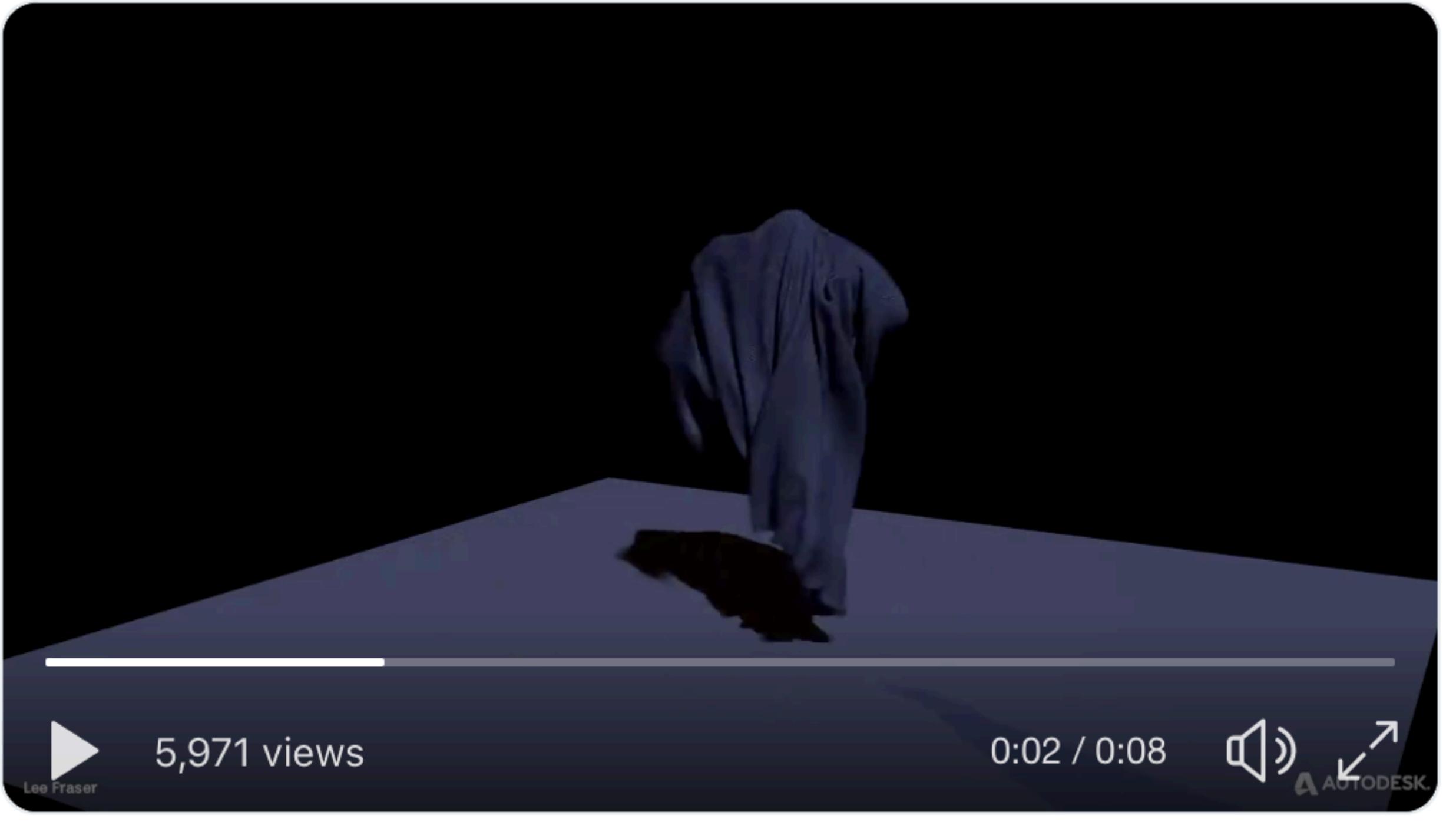


Autodec  
7.31.19

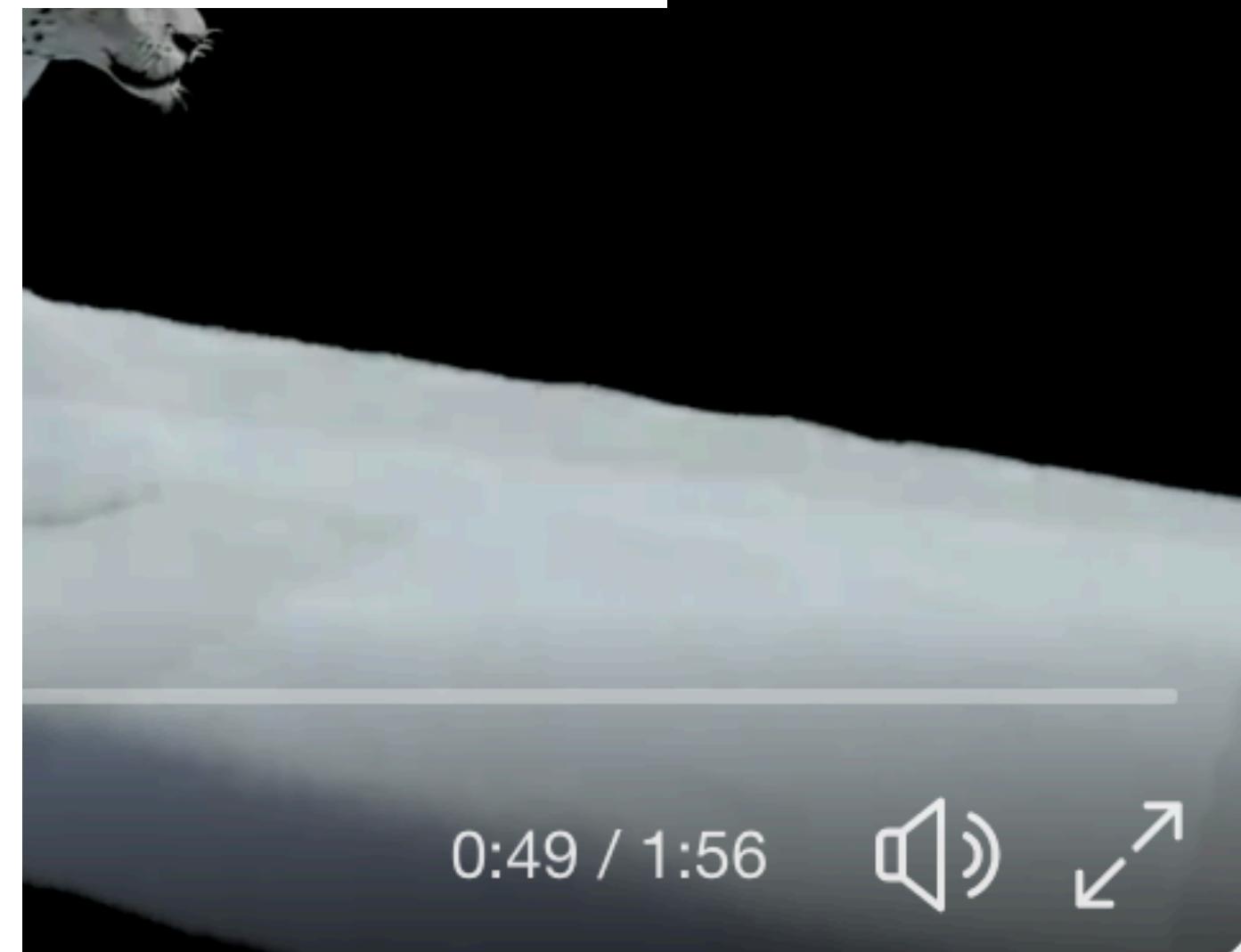
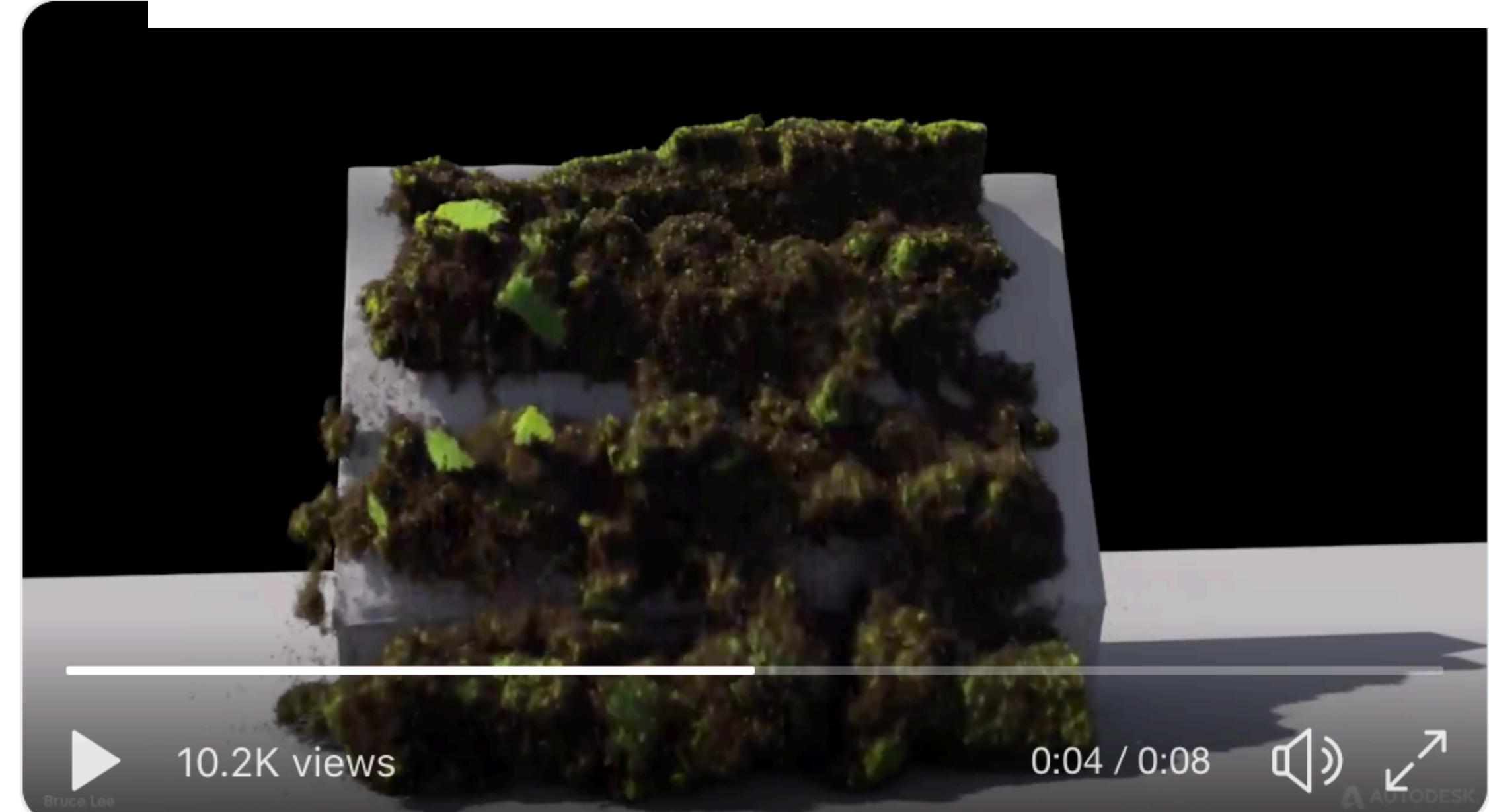
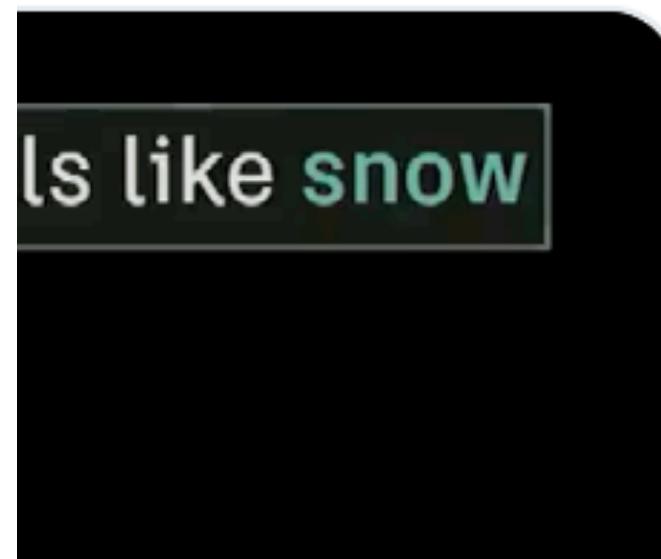
**TRY IT  
NOW!**



Autodesk Maya @AdskMaya · Jul 28  
7.31.19



TDs to create  
environment. Learn  
more here:

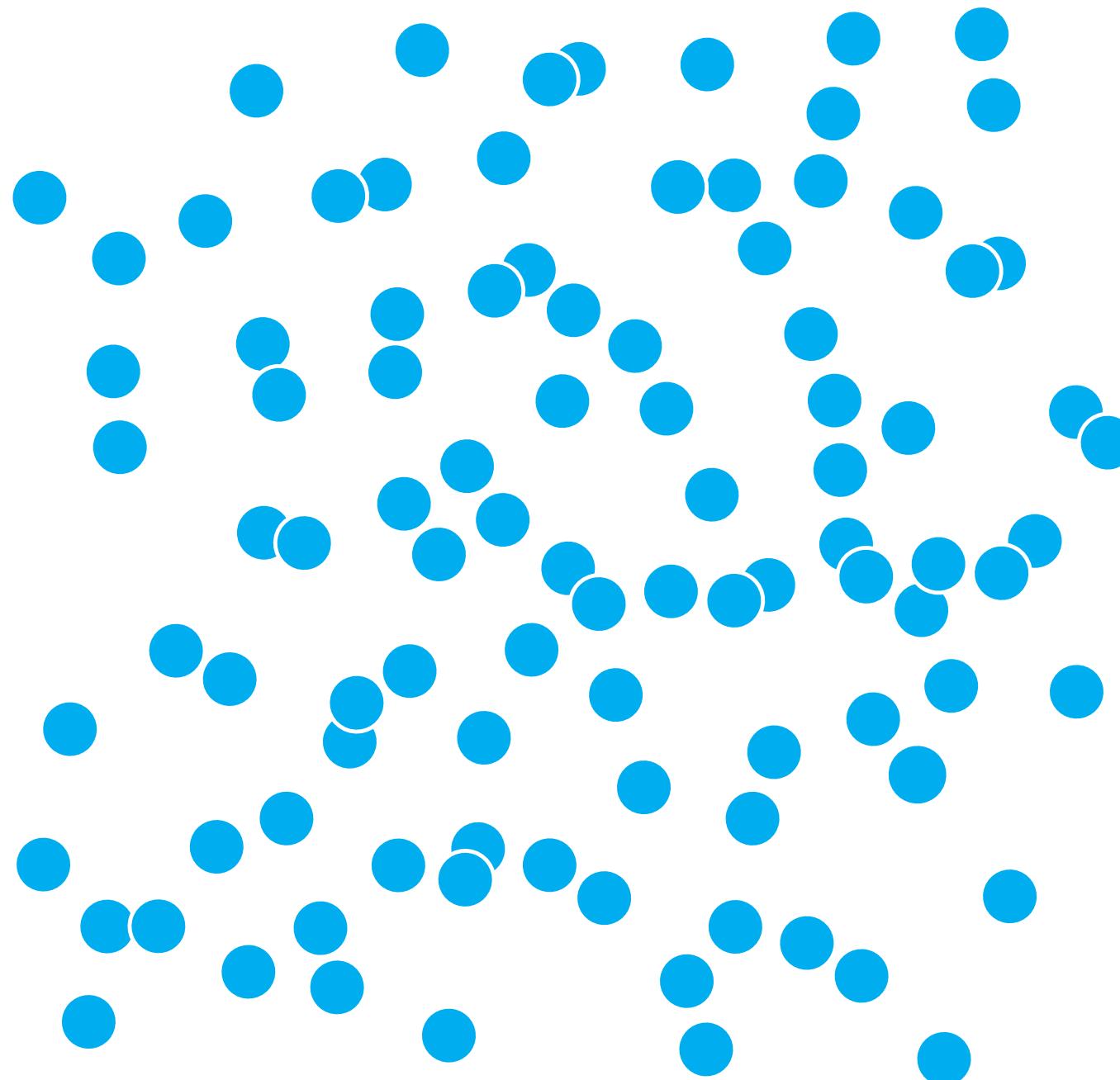


# MPM Implementation & Performance Considerations

Yuanming Hu  
MIT CSAIL

# The Material Point Method (MPM)

# The Material Point Method (MPM)



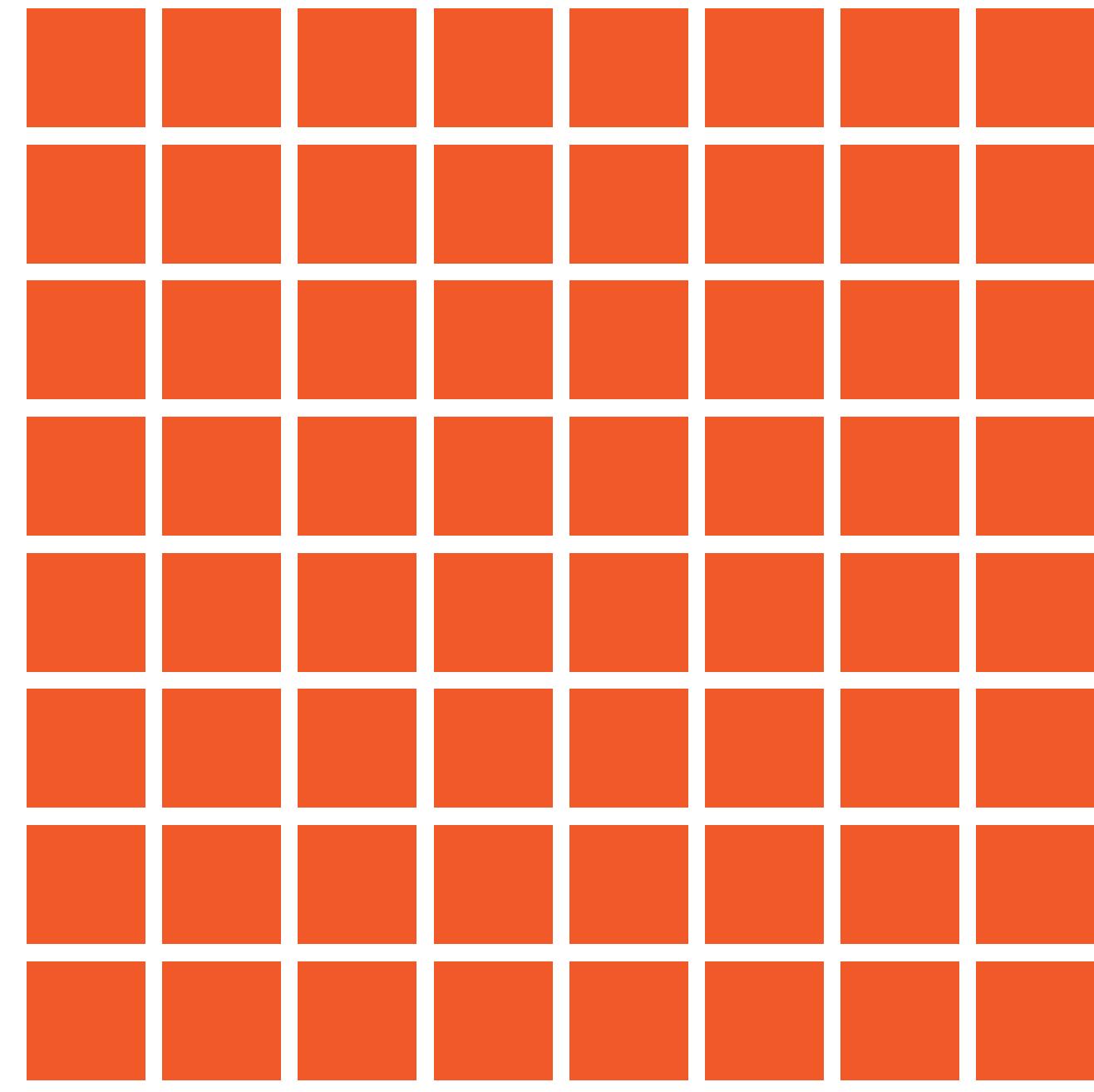
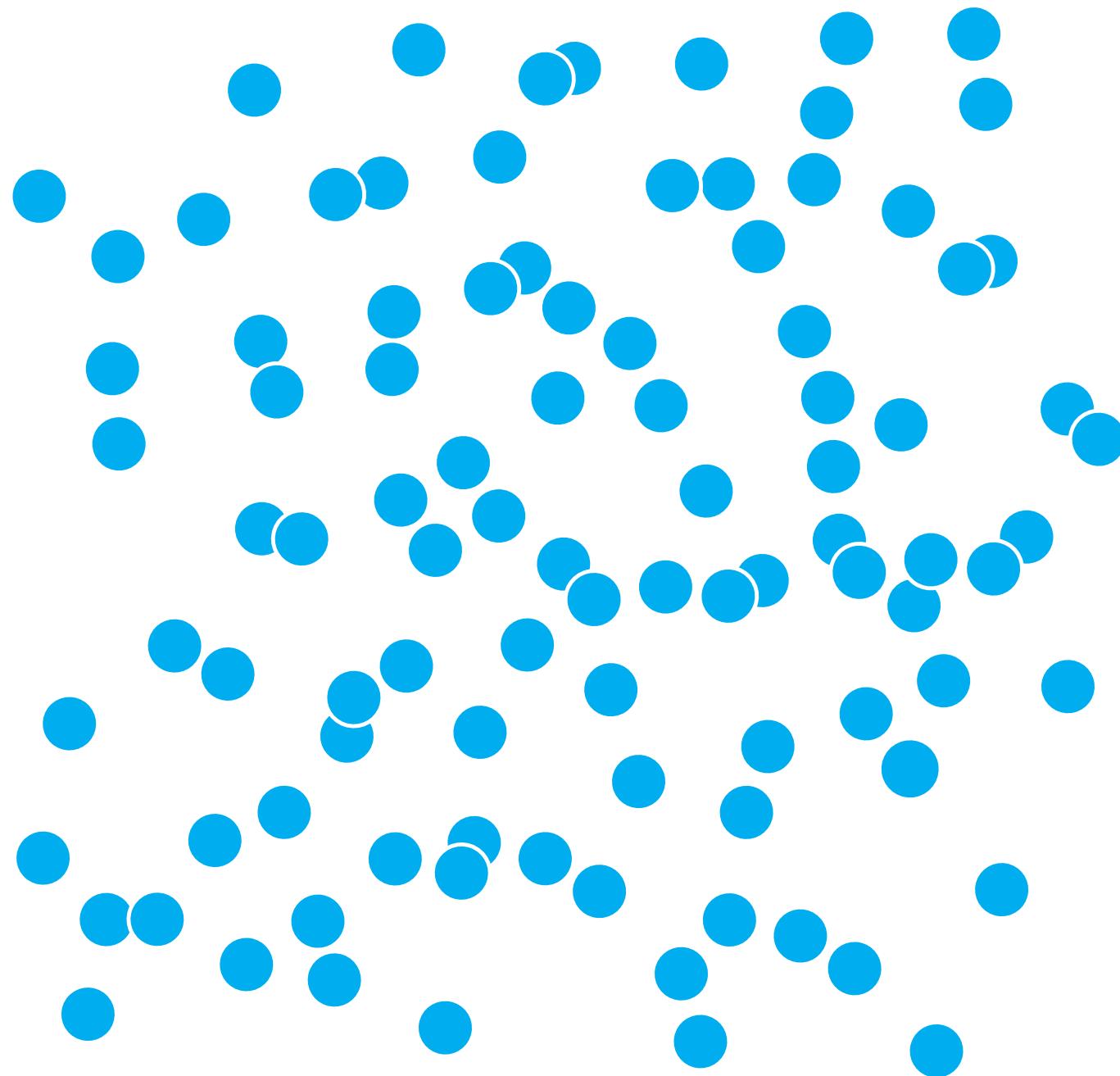
## Particles (Constitutive models)

Snow [Stomakhin et al. 2013],

Foam [Ram et al. 2015, Yue et al. 2015]

Sand [Klar et al. 2015, Pradhana et al 2017]

# The Material Point Method (MPM)



**Grid**

SPGrid [Setaluri et al. 2014],  
OpenVDB [Museth 2013]  
Multiple Grids  
[Pradhana et al. 2015]

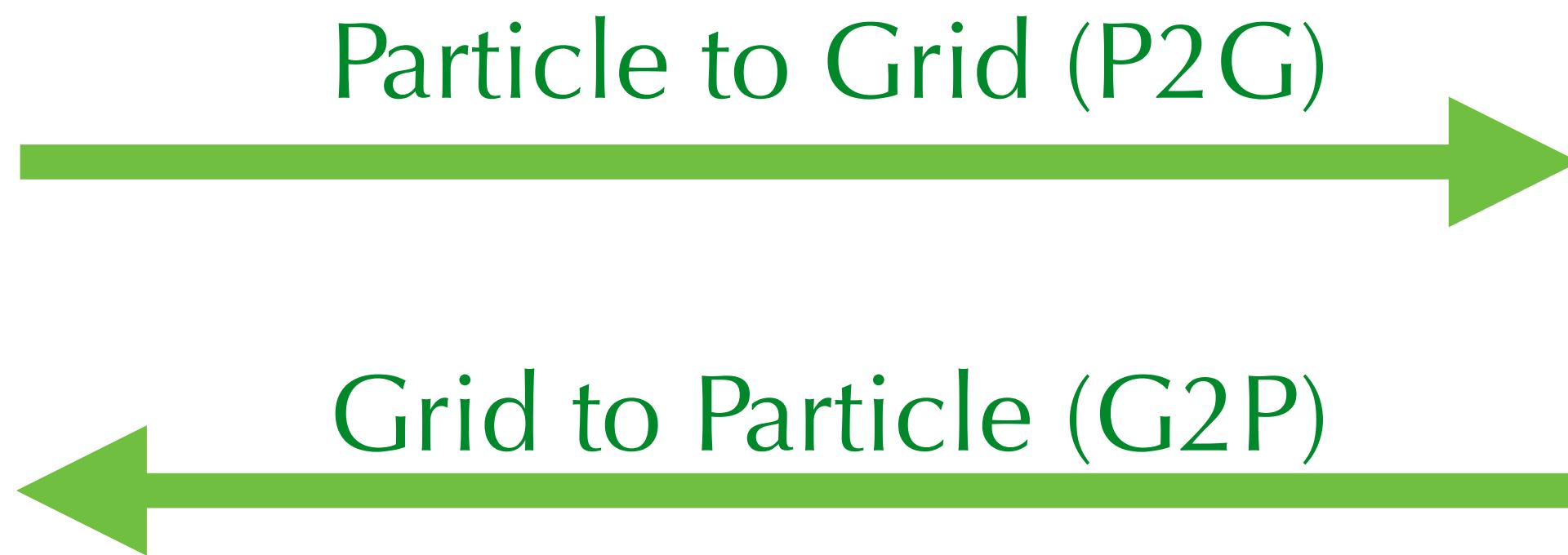
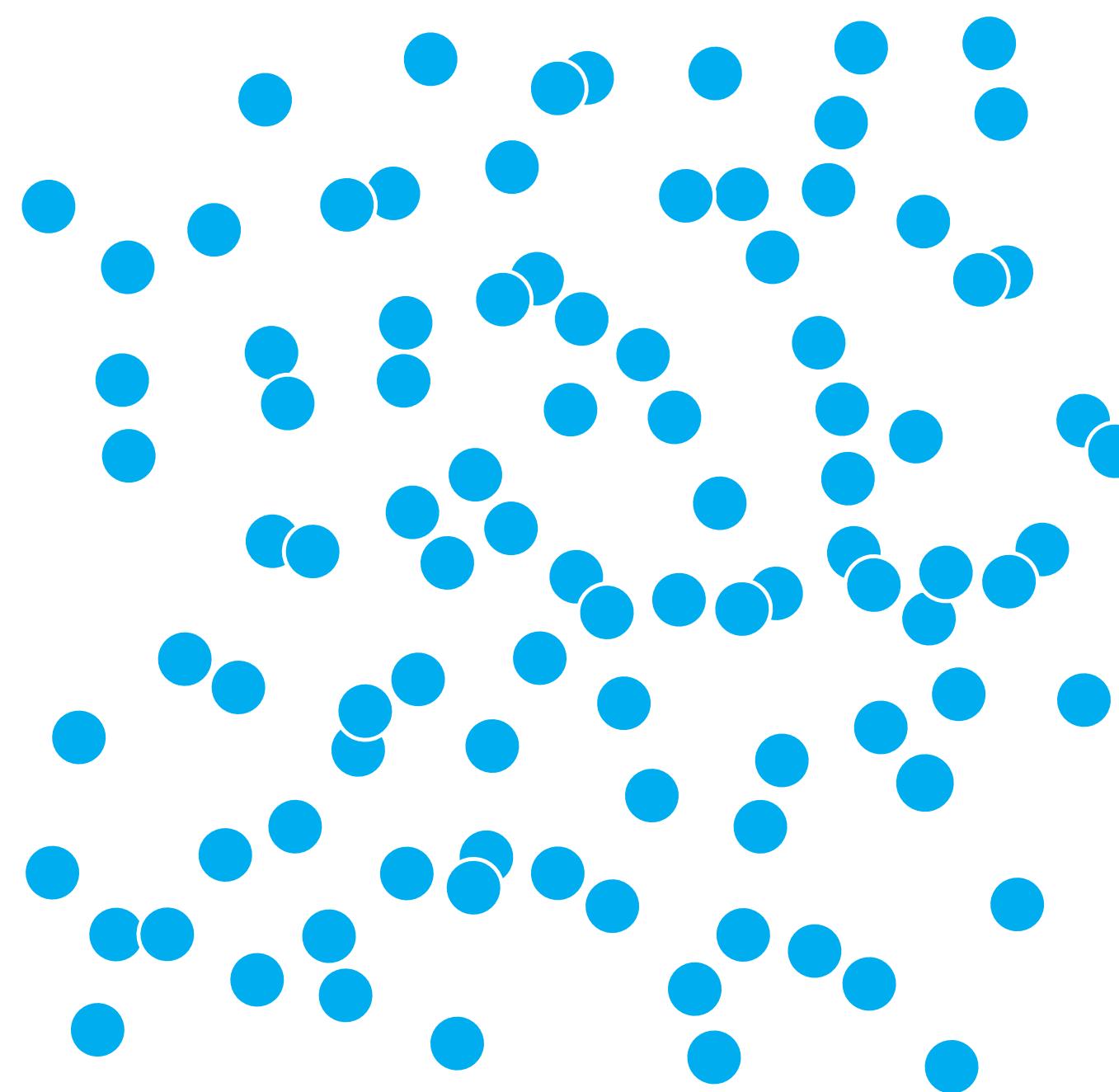
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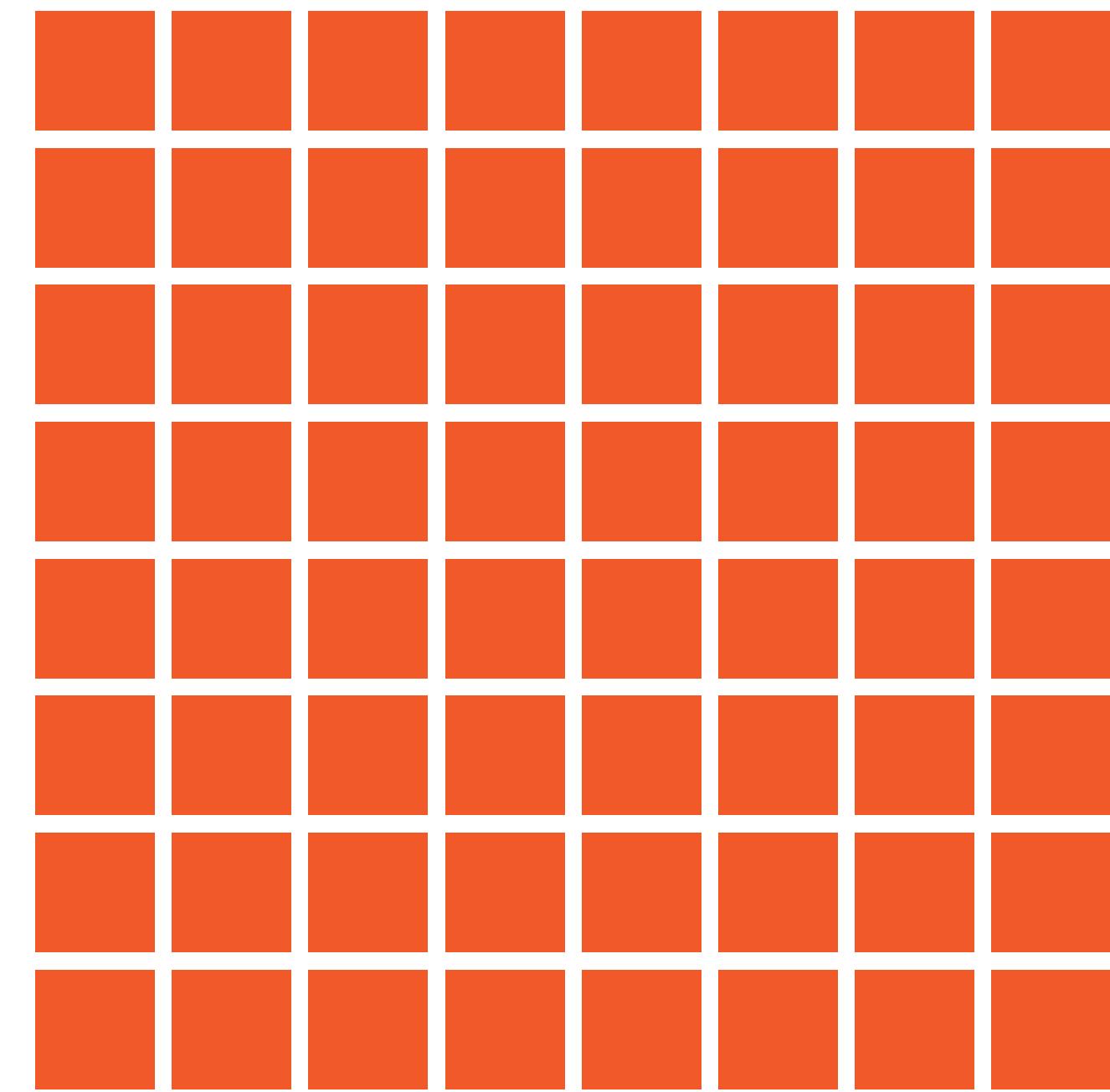
# The Material Point Method (MPM)



## Transfer (Particle in Cell, PIC)

- Affine PIC, APIC [Jiang et al. 2016]
- Polynomial PIC, PolyPIC [Fu et al. 2017]
- High-performance GIMP [Gao et al. 2017]
- Moving Least Squares [Hu et al. 2018]
- Compatible PIC [Hu et al. 2018]

...



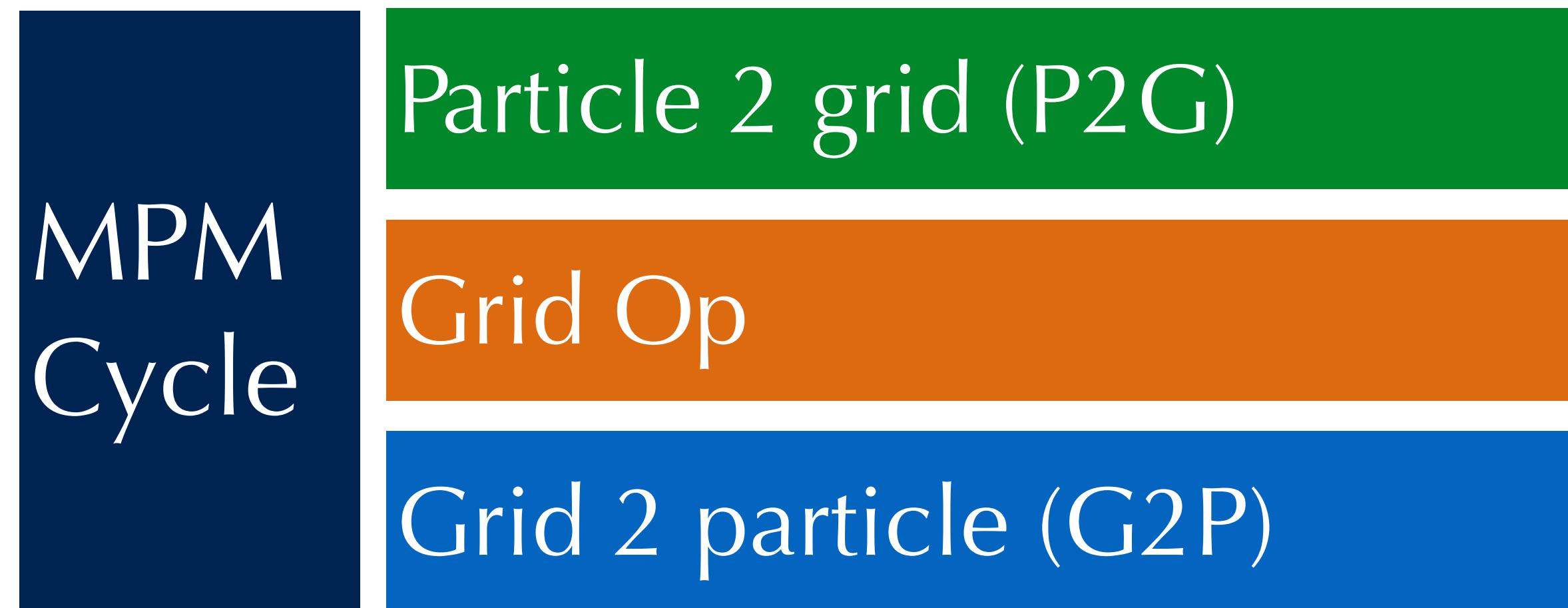
**Grid**

- SPGrid [Setaluri et al. 2014],
- OpenVDB [Museth 2013]
- Multiple Grids [Pradhana et al. 2015]

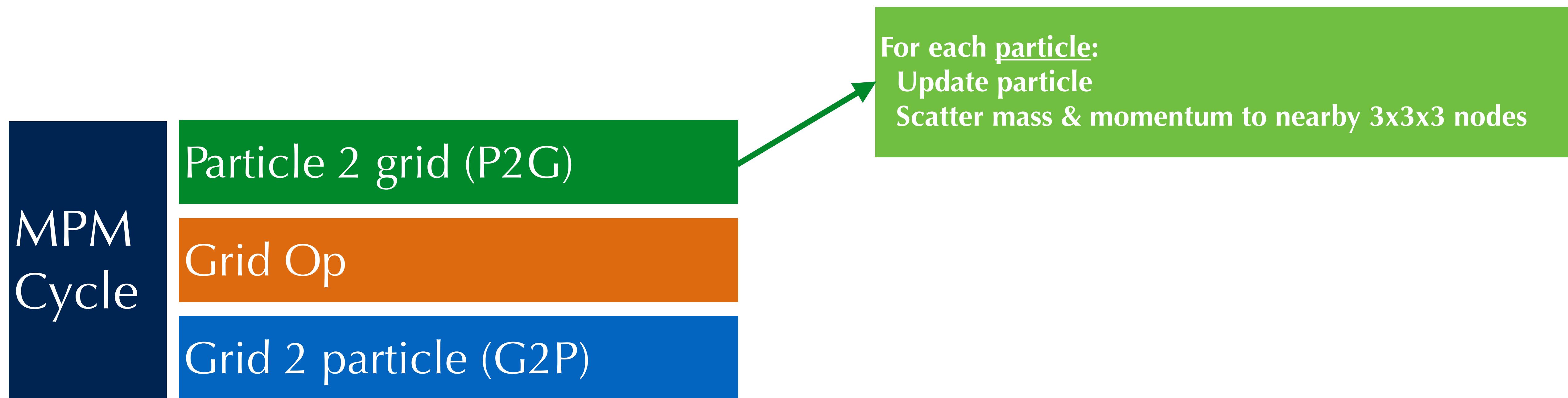
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- Snow [Stomakhin et al. 2013],
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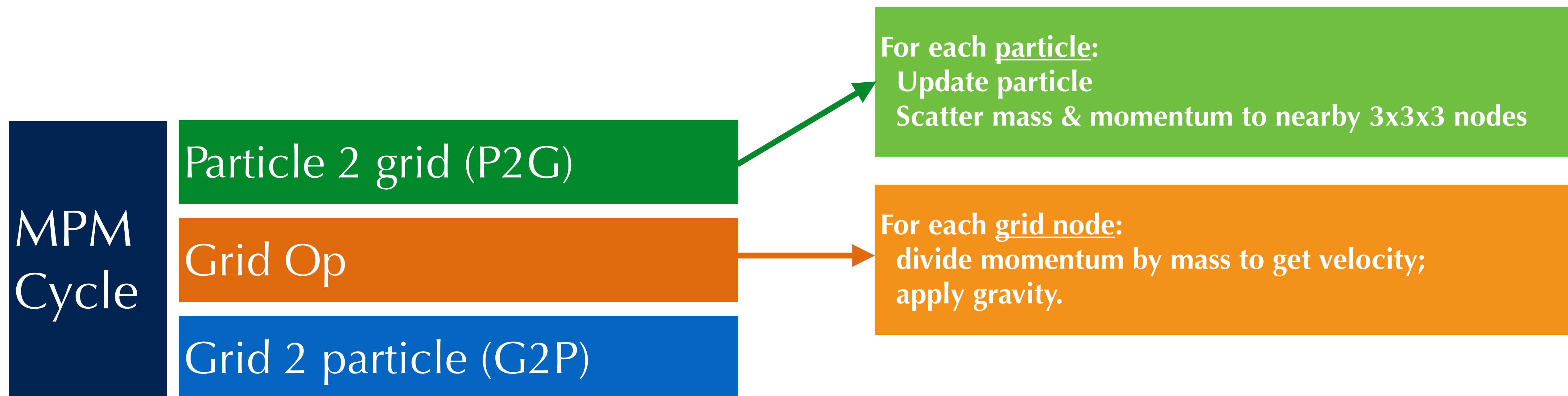
# The MPM Simulation Cycle



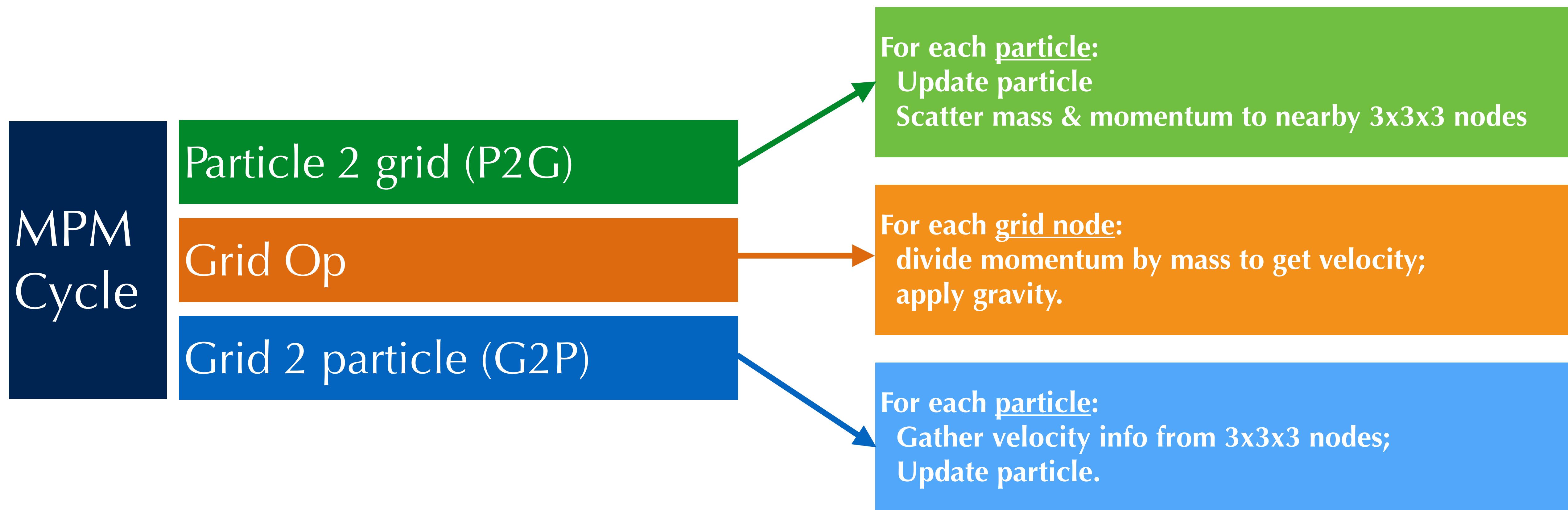
# The MPM Simulation Cycle



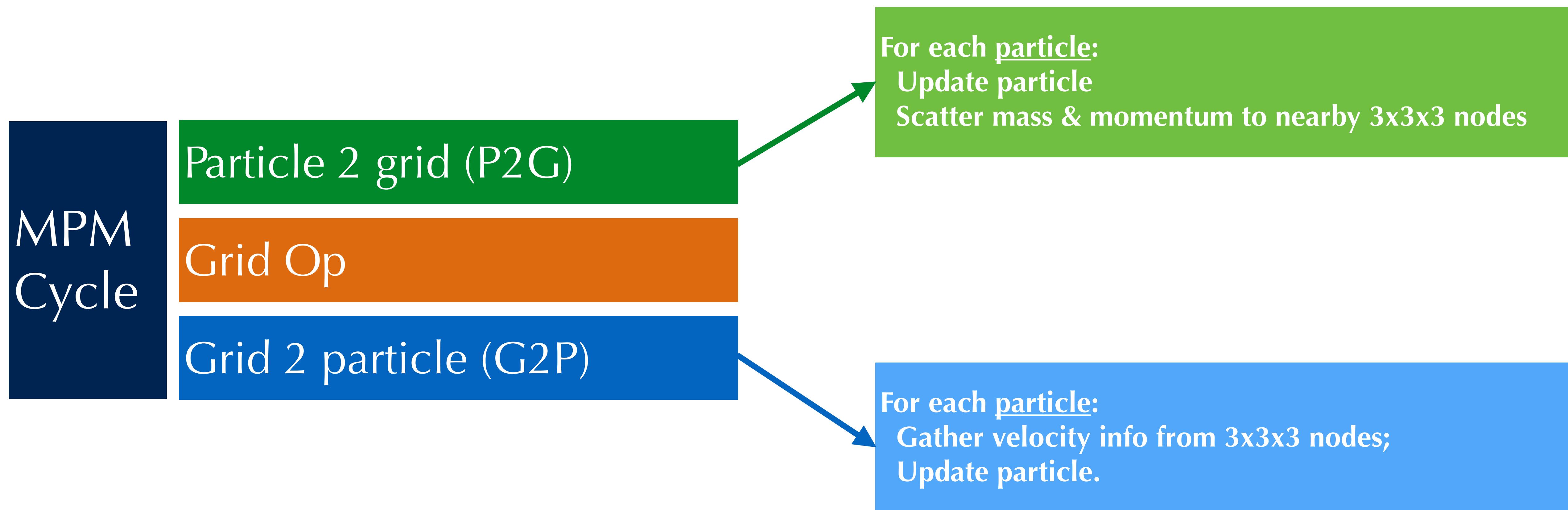
# The MPM Simulation Cycle



# The MPM Simulation Cycle



# The MPM Simulation Cycle



```

void advance(real dt) {
    std::memset(grid, 0, sizeof(grid)); // Reset grid
    for (auto &p : particles) { // P2G
        Vector2i base_coord=(p.x*inv_dx-Vec(0.5_f)).cast<int>(); //element-wise floor
        Vec fx = p.x * inv_dx - base_coord.cast<real>();
        // Quadratic kernels [http://mpm.graphics Eqn. 123, with x=fx, fx-1,fx-2]
        Vec w[3]{Vec(0.5) * sqr(Vec(1.5) - fx), Vec(0.75) - sqr(fx - Vec(1.0)),
                  Vec(0.5) * sqr(fx - Vec(0.5))};
        auto e = std::exp(hardening * (1.0_f - p.Jp)), mu=mu_0*e, lambda=lambda_0*e;
        real J = determinant(p.F); // Current volume
        Mat r, s; polar_decomp(p.F, r, s); //Polar decomp. for fixed corotated model
        auto stress = // Cauchy stress times dt and inv_dx
            -4*inv_dx*inv_dx*dt*vol*(2*mu*(p.F-r) * transposed(p.F)+lambda*(J-1)*J);
        auto affine = stress+particle_mass*p.C;
        for (int i = 0; i < 3; i++) for (int j = 0; j < 3; j++) { // Scatter to grid
            auto dpos = (Vec(i, j) - fx) * dx;
            Vector3 mv(p.v * particle_mass, particle_mass); //translational momentum
            grid[base_coord.x + i][base_coord.y + j] +=
                w[i].x*w[j].y * (mv + Vector3(affine*dpos, 0));
        }
    }

    for(int i = 0; i <= n; i++) for(int j = 0; j <= n; j++) { //For all grid nodes
        auto &g = grid[i][j];
        if (g[2] > 0) { // No need for epsilon here
            g /= g[2]; // Normalize by mass
            g += dt * Vector3(0, -200, 0); // Gravity
            real boundary=0.05,x=(real)i/n,y=real(j)/n; //boundary thick.,node coord
            if (x < boundary||x > 1-boundary||y > 1-boundary) g=Vector3(0); //Sticky
            if (y < boundary) g[1] = std::max(0.0_f, g[1]); //Separate
        }
    }

    for (auto &p : particles) { // Grid to particle
        Vector2i base_coord=(p.x*inv_dx-Vec(0.5_f)).cast<int>(); //element-wise floor
        Vec fx = p.x * inv_dx - base_coord.cast<real>();
        Vec w[3]{Vec(0.5) * sqr(Vec(1.5) - fx), Vec(0.75) - sqr(fx - Vec(1.0)),
                  Vec(0.5) * sqr(fx - Vec(0.5))};
        p.C = Mat(0); p.v = Vec(0);
        for (int i = 0; i < 3; i++) for (int j = 0; j < 3; j++) {
            auto dpos = (Vec(i, j) - fx),
                grid_v = Vec(grid[base_coord.x + i][base_coord.y + j]);
            auto weight = w[i].x * w[j].y;
            p.v += weight * grid_v; // Velocity
            p.C += 4 * inv_dx * Mat::outer_product(weight * grid_v, dpos); // APIC C
        }
        p.x += dt * p.v; // Advection
        auto F = (Mat(1) + dt * p.C) * p.F; // MLS-MPM F-update
        Mat svd_u, sig, svd_v; svd(F, svd_u, sig, svd_v);
        for (int i = 0; i < 2 * int(plastic); i++) // Snow Plasticity
            sig[i][i] = clamp(sig[i][i], 1.0_f - 2.5e-2_f, 1.0_f + 7.5e-3_f);
        real oldJ = determinant(F); F = svd_u * sig * transposed(svd_v);
        real Jp_new = clamp(p.Jp * oldJ / determinant(F), 0.6_f, 20.0_f);
        p.Jp = Jp_new; p.F = F;
    }
}

```

P2G

Grid Op

G2P

# 88 Lines of C++

[https://github.com/yuanming-hu/taichi\\_mpm](https://github.com/yuanming-hu/taichi_mpm)

- 88-Line MLS-MPM (cross-platform)
- High-Performance 3D MLS-MPM+CPIC Solver on CPUs
- MLS-MPM Tetris Game
- **niall**'s MLS-MPM implementation and tutorial in *Unity*
- **Roberto Toro** made *mls-mpm.js* that runs in your browser
- **David Medina** contributed *mls-mpm88-explained.cpp*

main simulation loop:

→ **void advance(float dt) [54 lines]**

# Demos!

# Particle 2 Grid

```
for (auto &p : particles) {                                     // P2G
    Vector2i base_coord=(p.x*inv_dx-Vec(0.5_f)).cast<int>(); //element-wise floor
    Vec fx = p.x * inv_dx - base_coord.cast<real>();
    // Quadratic kernels [http://mpm.graphics Eqn. 123, with x=fx, fx-1,fx-2]
    Vec w[3]{Vec(0.5) * sqr(Vec(1.5) - fx), Vec(0.75) - sqr(fx - Vec(1.0)),
              Vec(0.5) * sqr(fx - Vec(0.5))};
    auto e = std::exp(hardening * (1.0_f - p.Jp)), mu=mu_0*e, lambda=lambda_0*e;
    real J = determinant(p.F);           // Current volume
    Mat r, s; polar_decomp(p.F, r, s); //Polar decomp. for fixed corotated model
    auto stress =                      // Cauchy stress times dt and inv_dx
        -4*inv_dx*inv_dx*dt*vol*(2*mu*(p.F-r) * transposed(p.F)+lambda*(J-1)*J);
    auto affine = stress+particle_mass*p.C;
    for (int i = 0; i < 3; i++) for (int j = 0; j < 3; j++) { // Scatter to grid
        auto dpos = (Vec(i, j) - fx) * dx;
        Vector3 mv(p.v * particle_mass, particle_mass); //translational momentum
        grid[base_coord.x + i][base_coord.y + j] +=
            w[i].x*w[j].y * (mv + Vector3(affine*dpos, 0));
    }
}
```

# Particle 2 Grid

```
for (auto &p : particles) { // P2G
    Vector2i base_coord=(p.x*inv_dx-Vec(0.5_f)).cast<int>(); //element-wise floor
    Vec fx = p.x * inv_dx - base_coord.cast<real>();
    // Quadratic kernels [http://mpm.graphics Eqn. 123, with x=fx, fx-1,fx-2]
    Vec w[3]{Vec(0.5) * sqr(Vec(1.5) - fx), Vec(0.75) - sqr(fx - Vec(1.0)),
              Vec(0.5) * sqr(fx - Vec(0.5))};
    auto e = std::exp(hardening * (1.0_f - p.Jp)), mu=mu_0*e, lambda=lambda_0*e;
    real J = determinant(p.F); // Current volume
    Mat r, s; polar_decomp(p.F, r, s); //Polar decomp. for fixed corotated model
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    for (int i = 0; i < 3; i++) for (int j = 0; j < 3; j++) { // Scatter to grid
        auto dpos = (Vec(i, j) - fx) * dx;
        Vector3 mv(p.v * particle_mass, particle_mass); //translational momentum
        grid[base_coord.x + i][base_coord.y + j] +=
            w[i].x*w[j].y * (mv + Vector3(affine*dpos, 0));
    }
}
```

Particle Processing

# Particle 2 Grid

```
for (auto &p : particles) { // P2G
    Vector2i base_coord=(p.x*inv_dx-Vec(0.5_f)).cast<int>(); //element-wise floor
    Vec fx = p.x * inv_dx - base_coord.cast<real>();
    // Quadratic kernels [http://mpm.graphics Eqn. 123, with x=fx, fx-1,fx-2]
    Vec w[3]{Vec(0.5) * sqr(Vec(1.5) - fx), Vec(0.75) - sqr(fx - Vec(1.0)),
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    auto e = std::exp(hardening * (1.0_f - p.Jp)), mu=mu_0*e, lambda=lambda_0*e;
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        auto dpos = (Vec(i, j) - fx) * dx;
        Vector3 mv(p.v * particle_mass, particle_mass); //translational momentum
        grid[base_coord.x + i][base_coord.y + j] +=
            w[i].x*w[j].y * (mv + Vector3(affine*dpos, 0));
    }
}
```

Particle Processing

Grid Rasterization  
( $3^3=27$  nodes in 3D!)

# Grid 2 Particle

```
for (auto &p : particles) {                                     // Grid to particle
    Vector2i base_coord=(p.x*inv_dx-Vec(0.5_f)).cast<int>(); //element-wise floor
    Vec fx = p.x * inv_dx - base_coord.cast<real>();
    Vec w[3]{Vec(0.5) * sqr(Vec(1.5) - fx), Vec(0.75) - sqr(fx - Vec(1.0)),
              Vec(0.5) * sqr(fx - Vec(0.5))};
    p.C = Mat(0); p.v = Vec(0);
    for (int i = 0; i < 3; i++) for (int j = 0; j < 3; j++) {
        auto dpos = (Vec(i, j) - fx),
             grid_v = Vec(grid[base_coord.x + i][base_coord.y + j]);
        auto weight = w[i].x * w[j].y;
        p.v += weight * grid_v;                                // Velocity
        p.C += 4 * inv_dx * Mat::outer_product(weight * grid_v, dpos); // APIC C
    }
    p.x += dt * p.v;                                         // Advection
    auto F = (Mat(1) + dt * p.C) * p.F;                      // MLS-MPM F-update
    Mat svd_u, sig, svd_v; svd(F, svd_u, sig, svd_v);
    for (int i = 0; i < 2 * int(plastic); i++)           // Snow Plasticity
        sig[i][i] = clamp(sig[i][i], 1.0_f - 2.5e-2_f, 1.0_f + 7.5e-3_f);
    real oldJ = determinant(F); F = svd_u * sig * transposed(svd_v);
    real Jp_new = clamp(p.Jp * oldJ / determinant(F), 0.6_f, 20.0_f);
    p.Jp = Jp_new; p.F = F;
}
```

# Grid 2 Particle

```
for (auto &p : particles) {                                     // Grid to particle
    Vector2i base_coord=(p.x*inv_dx-Vec(0.5_f)).cast<int>(); //element-wise floor
    Vec fx = p.x * inv_dx - base_coord.cast<real>();
    Vec w[3]{Vec(0.5) * sqr(Vec(1.5) - fx), Vec(0.75) - sqr(fx - Vec(1.0)),
              Vec(0.5) * sqr(fx - Vec(0.5))};
    p.C = Mat(0); p.v = Vec(0);
    for (int i = 0; i < 3; i++) for (int j = 0; j < 3; j++) {
        auto dpos = (Vec(i, j) - fx),
             grid_v = Vec(grid[base_coord.x + i][base_coord.y + j]);
        auto weight = w[i].x * w[j].y;
        p.v += weight * grid_v;                                // Velocity
        p.C += 4 * inv_dx * Mat::outer_product(weight * grid_v, dpos); // APIC C
    }
    p.x += dt * p.v;                                         // Advection
    auto F = (Mat(1) + dt * p.C) * p.F;                      // MLS-MPM F-update
    Mat svd_u, sig, svd_v; svd(F, svd_u, sig, svd_v);
    for (int i = 0; i < 2 * int(plastic); i++)           // Snow Plasticity
        sig[i][i] = clamp(sig[i][i], 1.0_f - 2.5e-2_f, 1.0_f + 7.5e-3_f);
    real oldJ = determinant(F); F = svd_u * sig * transposed(svd_v);
    real Jp_new = clamp(p.Jp * oldJ / determinant(F), 0.6_f, 20.0_f);
    p.Jp = Jp_new; p.F = F;
}
```

Particle Processing

# Grid 2 Particle

```
for (auto &p : particles) {                                     // Grid to particle
    Vector2i base_coord=(p.x*inv_dx-Vec(0.5_f)).cast<int>(); //element-wise floor
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    p.C = Mat(0); p.v = Vec(0);
    for (int i = 0; i < 3; i++) for (int j = 0; j < 3; j++) {
        auto dpos = (Vec(i, j) - fx),
             grid_v = Vec(grid[base_coord.x + i][base_coord.y + j]);
        auto weight = w[i].x * w[j].y;
        p.v += weight * grid_v;                                // Velocity
        p.C += 4 * inv_dx * Mat::outer_product(weight * grid_v, dpos); // APIC C
    }
    p.x += dt * p.v;                                         // Advection
    auto F = (Mat(1) + dt * p.C) * p.F;                      // MLS-MPM F-update
    Mat svd_u, sig, svd_v; svd(F, svd_u, sig, svd_v);
    for (int i = 0; i < 2 * int(plastic); i++)           // Snow Plasticity
        sig[i][i] = clamp(sig[i][i], 1.0_f - 2.5e-2_f, 1.0_f + 7.5e-3_f);
    real oldJ = determinant(F); F = svd_u * sig * transposed(svd_v);
    real Jp_new = clamp(p.Jp * oldJ / determinant(F), 0.6_f, 20.0_f);
    p.Jp = Jp_new; p.F = F;
}
```

Particle Processing

Grid Gathering  
( $3^3=27$  nodes in 3D!)

# Grid 2 Particle

```
for (auto &p : particles) {                                     // Grid to particle
    Vector2i base_coord=(p.x*inv_dx-Vec(0.5_f)).cast<int>(); //element-wise floor
    Vec fx = p.x * inv_dx - base_coord.cast<real>();
    Vec w[3]{Vec(0.5) * sqr(Vec(1.5) - fx), Vec(0.75) - sqr(fx - Vec(1.0)),
              Vec(0.5) * sqr(fx - Vec(0.5))};
    p.C = Mat(0); p.v = Vec(0);
    for (int i = 0; i < 3; i++) for (int j = 0; j < 3; j++) {
        auto dpos = (Vec(i, j) - fx),
             grid_v = Vec(grid[base_coord.x + i][base_coord.y + j]);
        auto weight = w[i].x * w[j].y;
        p.v += weight * grid_v;                                // Velocity
        p.C += 4 * inv_dx * Mat::outer_product(weight * grid_v, dpos); // APIC C
    }
    p.x += dt * p.v;                                         // Advection
    auto F = (Mat(1) + dt * p.C) * p.F;                      // MLS-MPM F-update
    Mat svd_u, sig, svd_v; svd(F, svd_u, sig, svd_v);
    for (int i = 0; i < 2 * int(plastic); i++)           // Snow Plasticity
        sig[i][i] = clamp(sig[i][i], 1.0_f - 2.5e-2_f, 1.0_f + 7.5e-3_f);
    real oldJ = determinant(F); F = svd_u * sig * transposed(svd_v);
    real Jp_new = clamp(p.Jp * oldJ / determinant(F), 0.6_f, 20.0_f);
    p.Jp = Jp_new; p.F = F;
}
```

Particle Processing

Grid Gathering  
( $3^3=27$  nodes in 3D!)

Particle Processing

# Key Computational Patterns:

- a) Streaming Particle Data
- b) Particle-Grid Interaction

How much do implementation practices  
affect performance?

40% ?

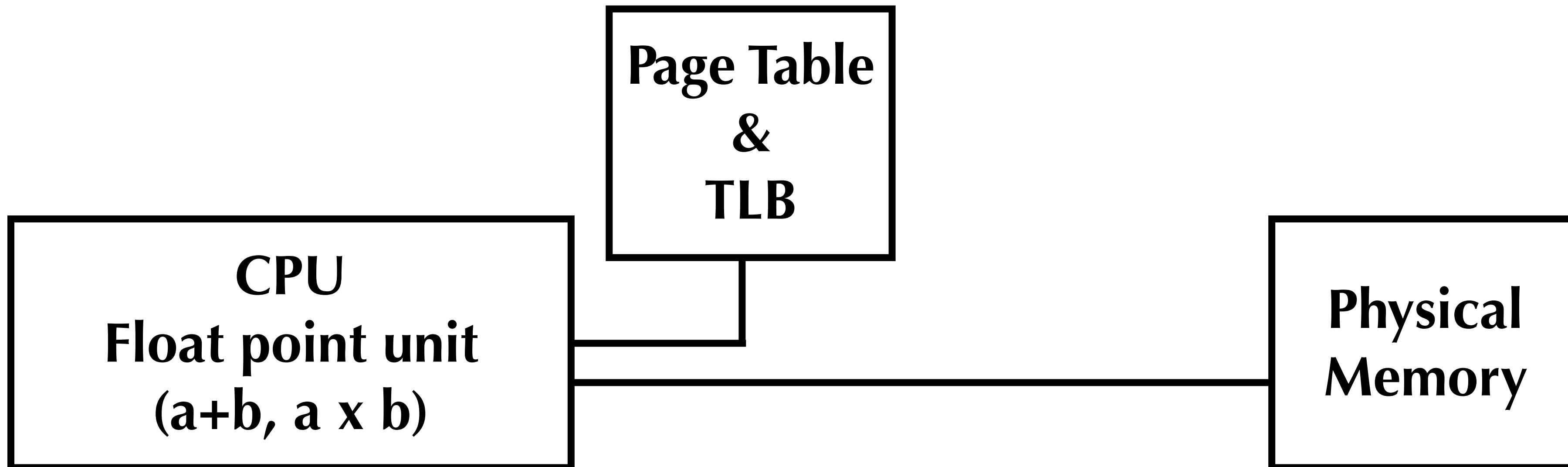
# How much do implementation practices affect performance?

## 10x higher performance!

without multithreading

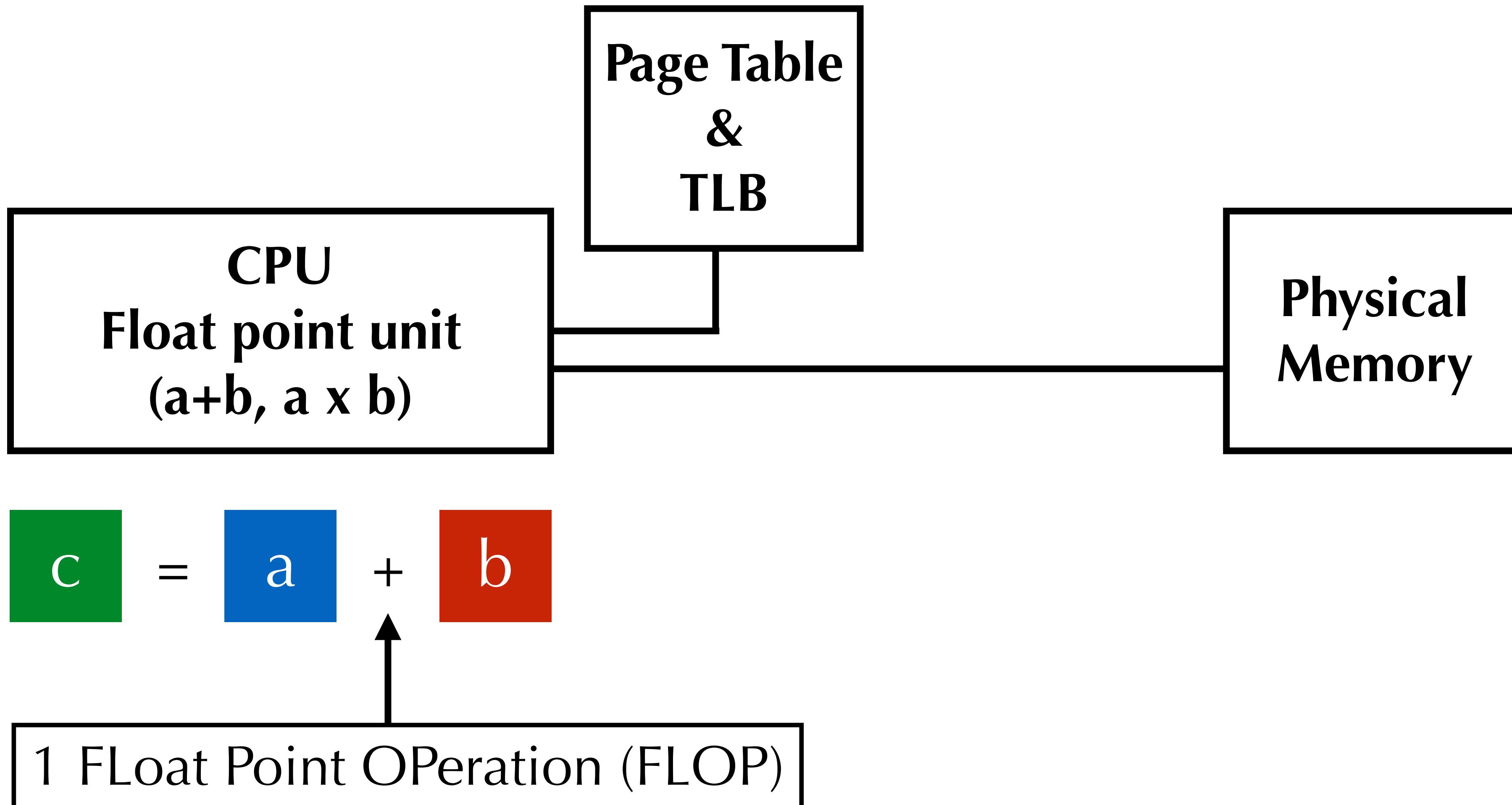
- Instruction-level parallelism
- Vectorization
- High-quality instruction generation
- Lock-free parallelization
- Bandwidth-saving data structures
- ...

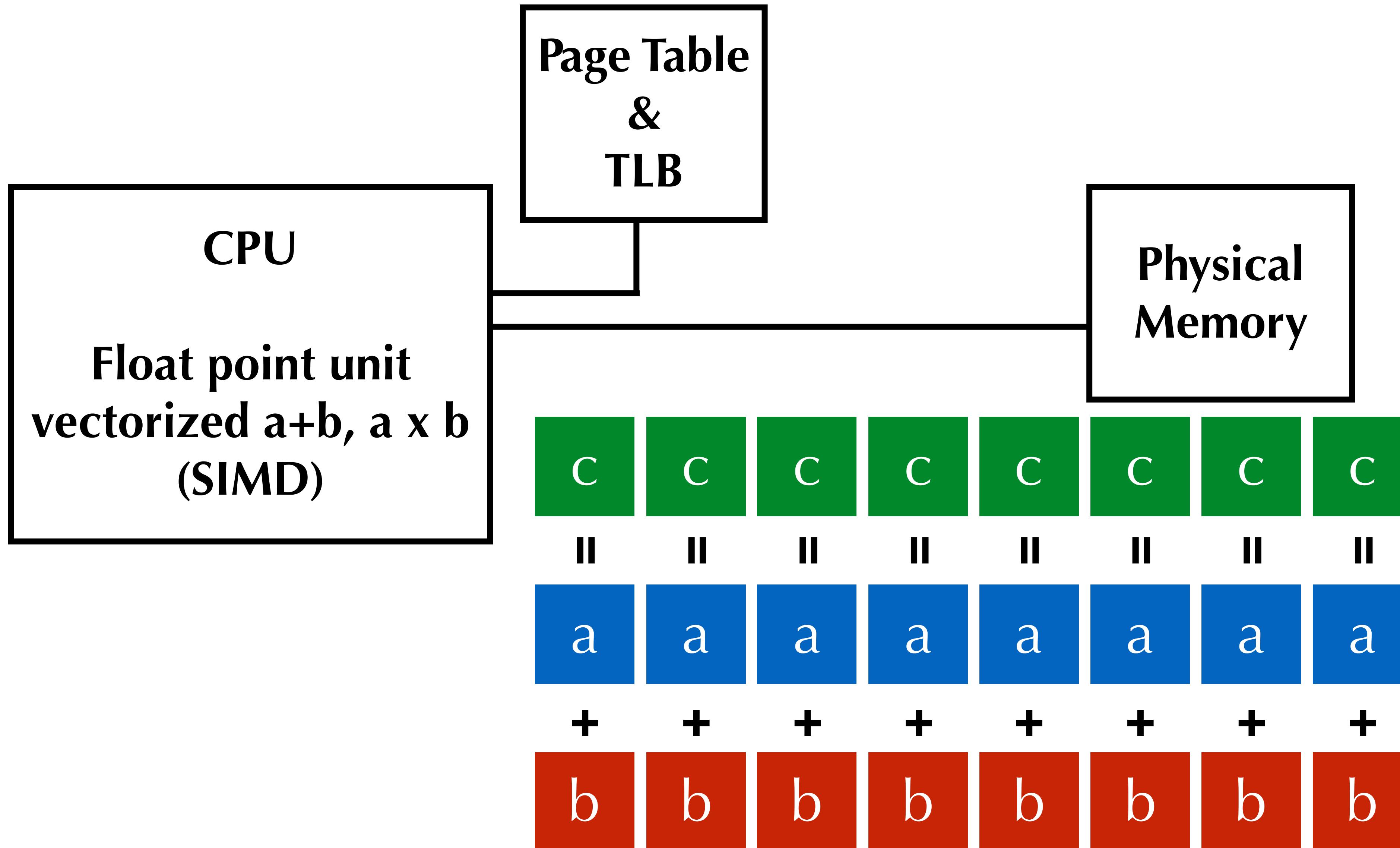
# Recap: Modern Computer Architecture



$$c = a + b$$

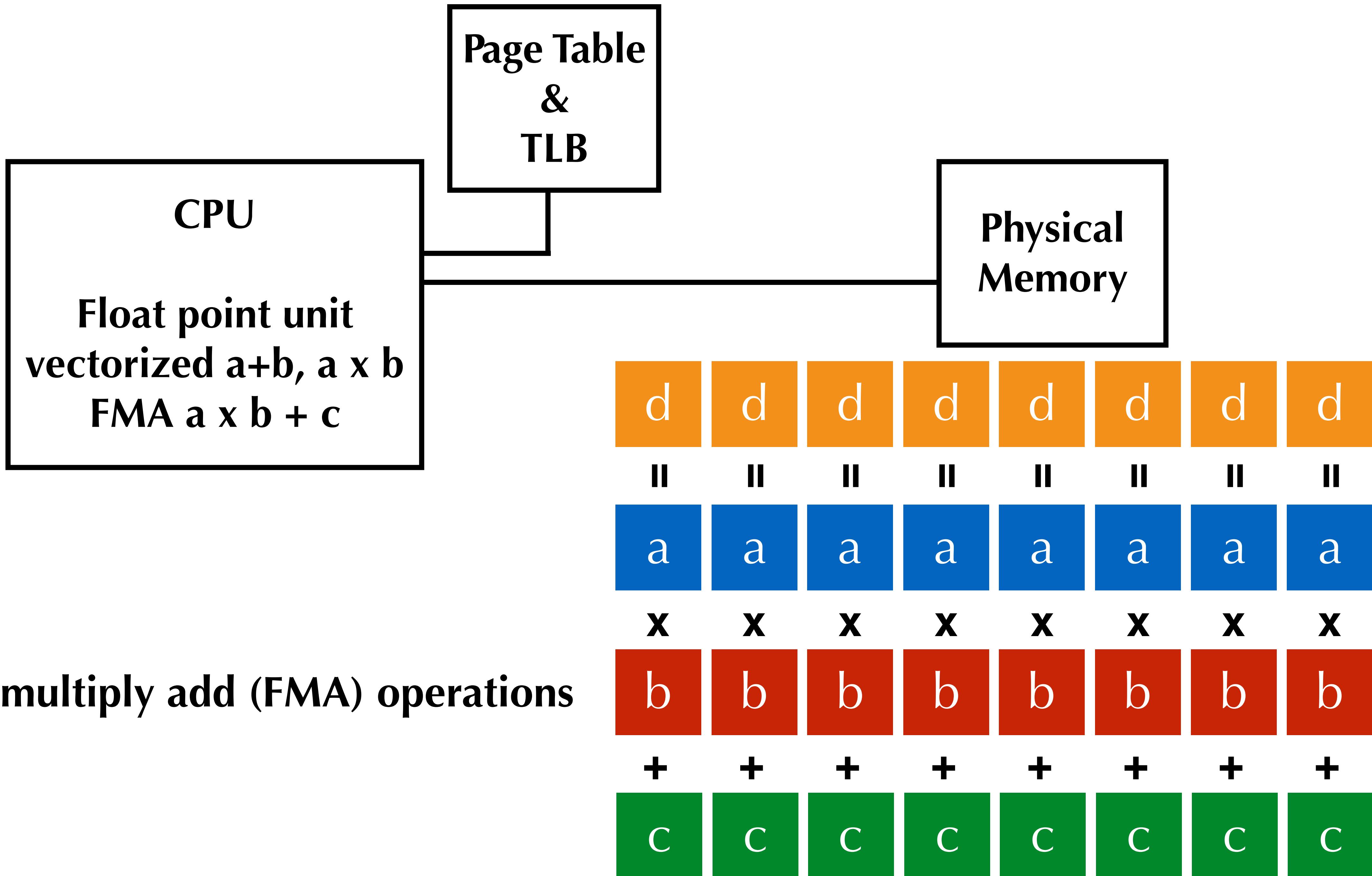
# Recap: Modern Computer Architecture

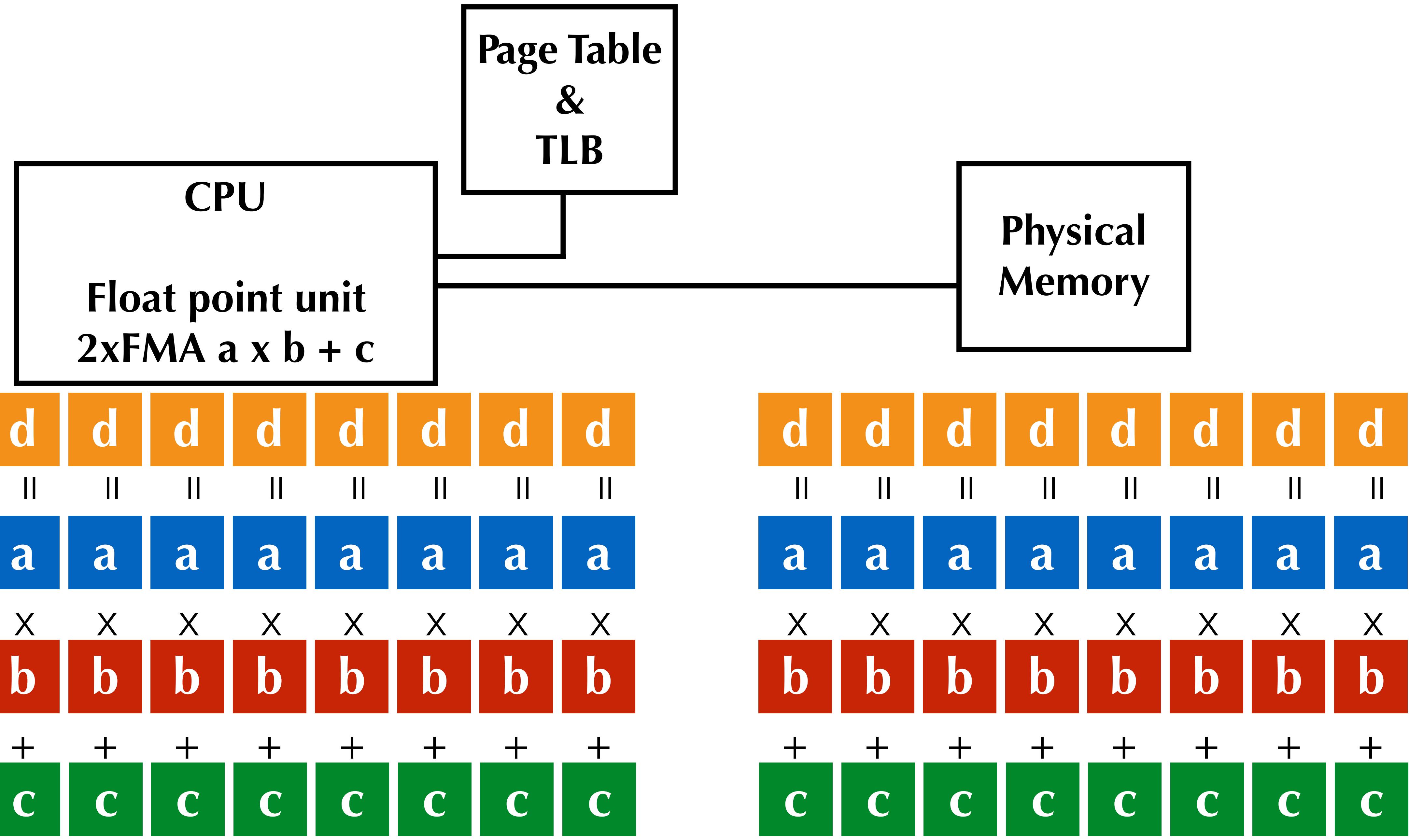




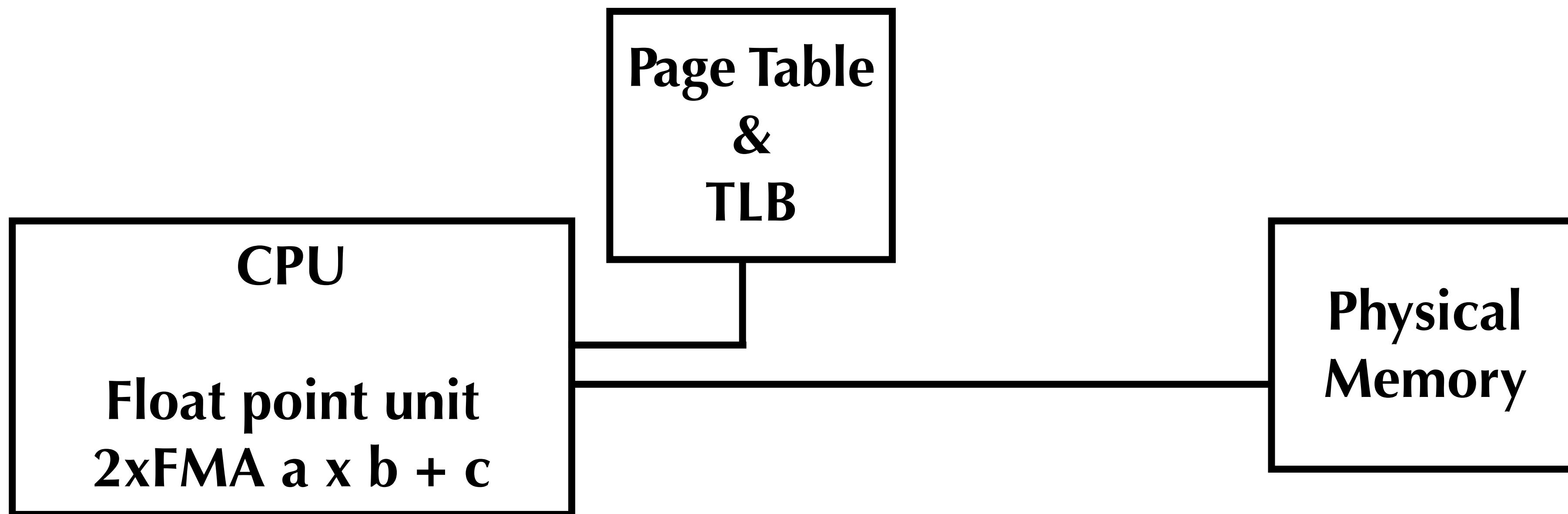
**AVX2:** 8 single precision/4 double precision float point number operations in a row

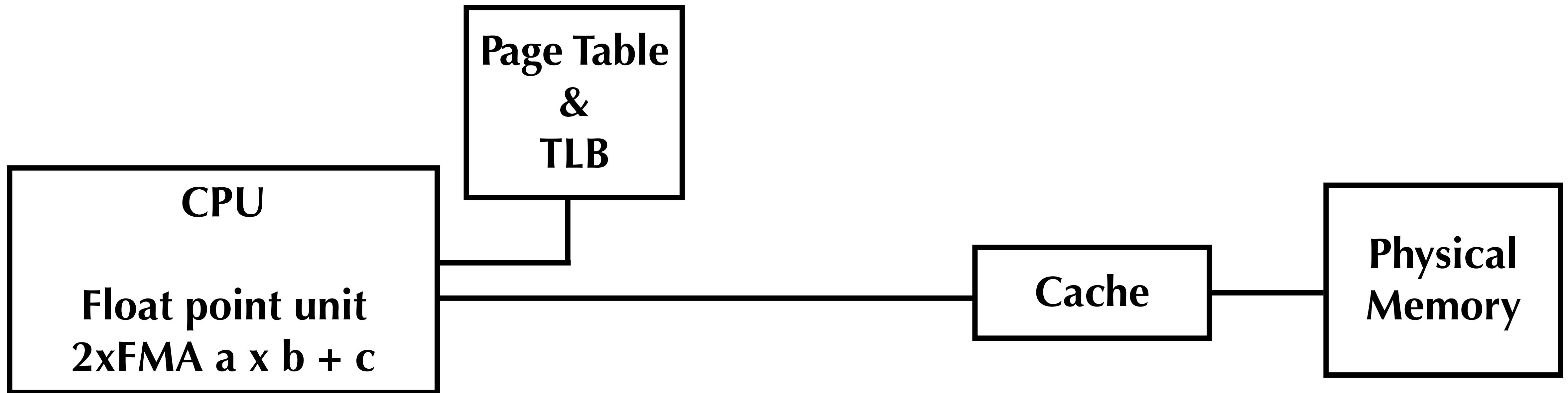
**AVX512:** 16 single precision/8 double precision float point number operations in a row

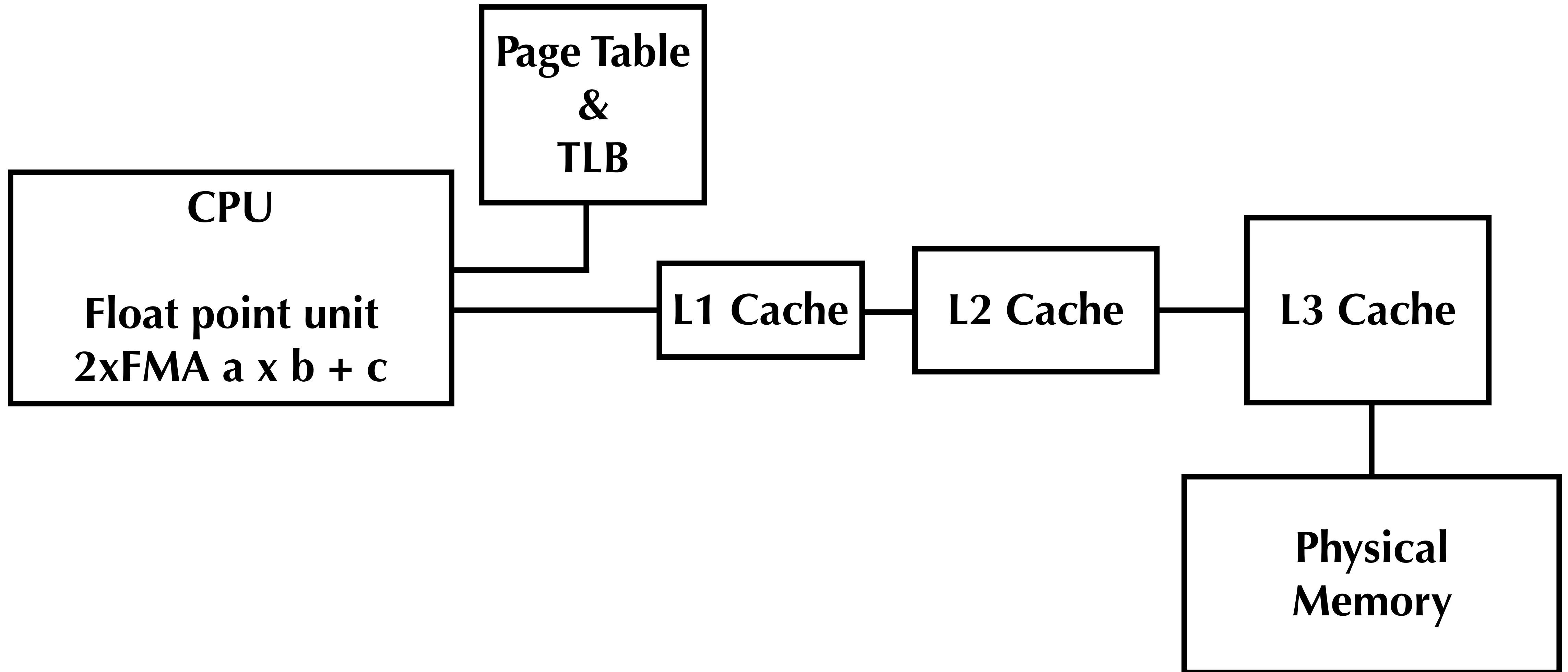




$$4.2\text{G Hz} \times 2 \text{ FMA/cycle} \times 16 \text{ FLOPs/FMA} \times 4 \text{ cores} = 538\text{G FLOPs}$$







**Main Memory**  
**35.8 GB/s**  
**256 cyc latency**

**L3 cache 2M/core**  
**134.4 GB/s**  
**42 cyc latency**

**L2 cache 256KB**  
**268.8 GB/s**  
**12 cyc latency**

**L2 Unified TLB (STLB)**  
4 KB/2MB pages - 1536 entries  
1G pages - 16 entries

**L1 data cache 32KB**  
**403.2 GB/s**  
**4 cyc latency**

**L1 Data TLB**  
4 KB pages - 64 entries  
2/4 MB pages - 32 entries  
1G pages - 4 entries

**CPU core**

**Integer Physical Registers**  
8 bytes per entry, 180 entries  
**1 cyc latency**

**Vector Physical Registers**  
32 byte entries, 168 entries  
**1 cyc latency**

**Execution Engine**  
**4.20 GHz**  
**134.4 G FLOP/s, i.e. 806.4 GB/s bandwidth requirement**

# (Part of) the Memory Hierarchy

- \* Figures are not drawn to scale.
- \* Instruction caches are omitted.
- \* Main memory BW is shared by all cores.

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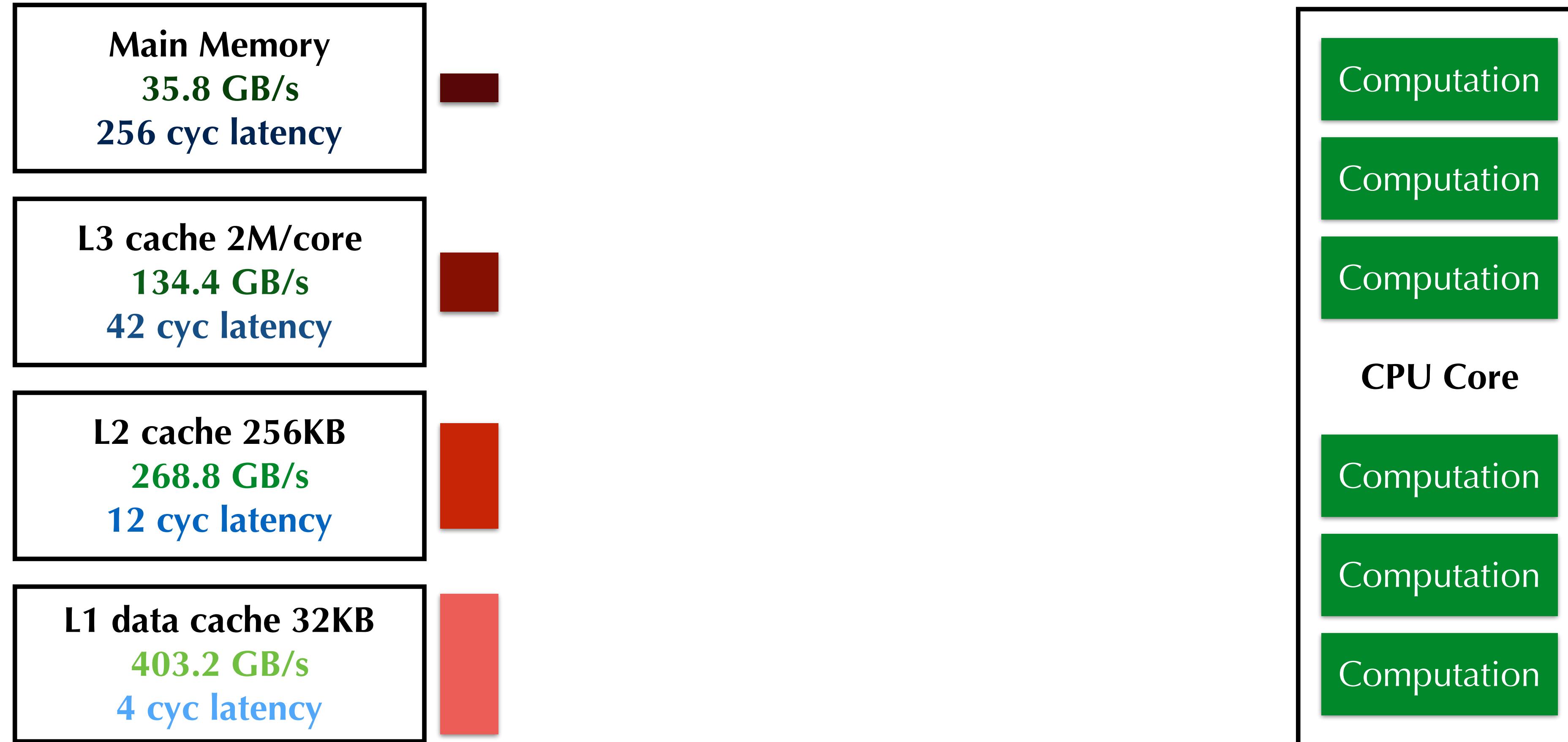
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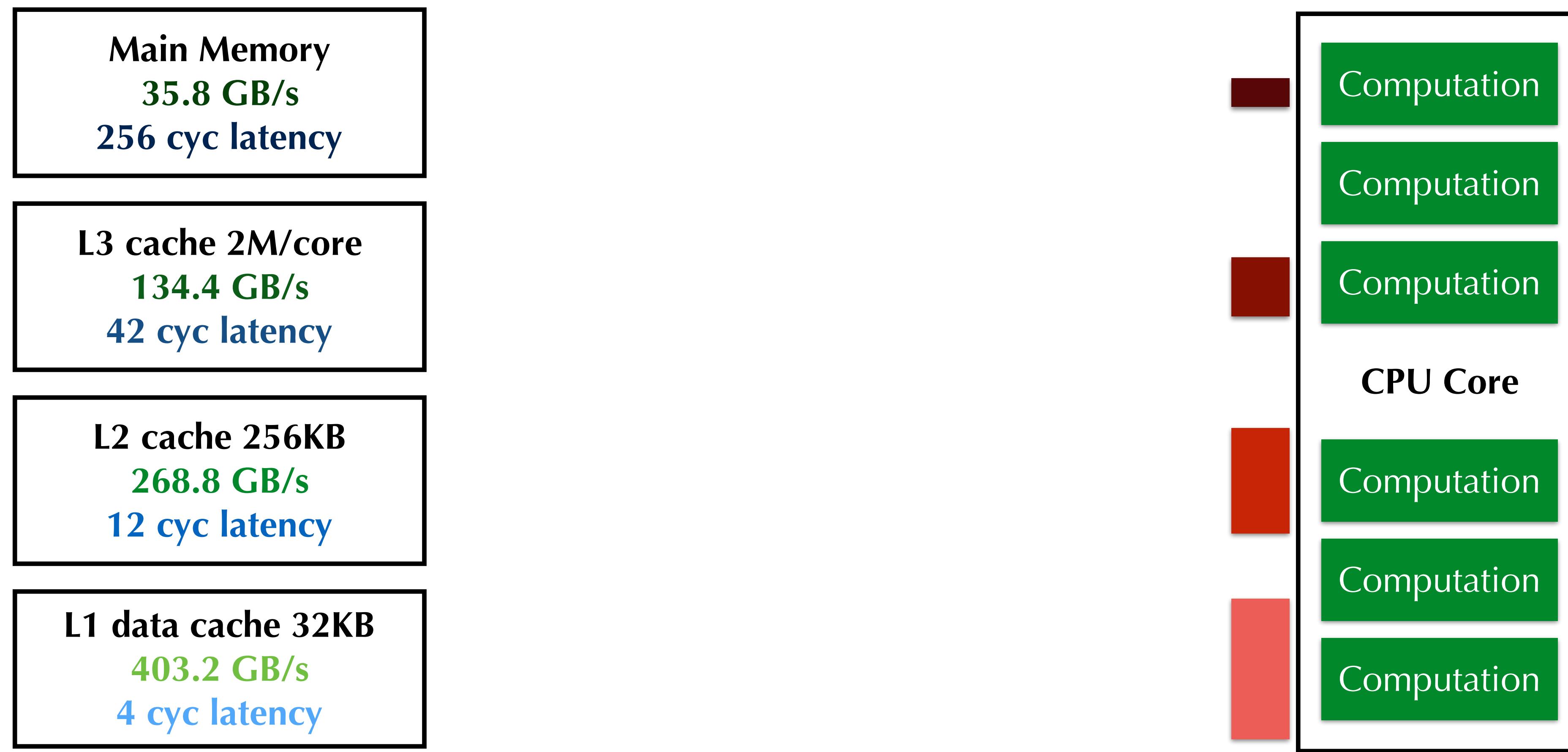
Vector Physical Registers  
32 byte entries, 168 entries  
1 cyc latency

Execution Engine  
4.20 GHz  
134.4 G FLOP/s, i.e. 806.4 GB/s bandwidth requirement

closer to CPU,  
smaller capacity,  
lower latency,  
higher bandwidth.



- \* Caches are not drawn to scale.
- \* Data collected from the Intel Skylake architecture, single core.
- \* There can be multiple data transfers happening simultaneously.
- \* Access to slower memory is invoked by faster memory cache miss.



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- \* Data collected from the Intel Skylake architecture, single core.
- \* There can be multiple data transfers happening simultaneously.
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# Locality

- ♦ **Spatial locality:** try to access spatially neighboring data in main memory
  - Higher cacheline utilization
  - Fewer Cache/TLB misses
  - Better hardware prefetching on CPUs
- ♦ **Temporal locality:** reuse the data as much as you can
  - Higher cache-hit rates
  - Lower main memory bandwidth pressure
- ♦ Shrink the working set, so that data resides in lower-level (higher throughput, lower latency) memory

Main Memory  
35.8 GB/s in total, **9 GB/s per core**  
256 cyc latency

Execution Engine  
4.20 GHz  
134.4 G FLOP/s, i.e. **806.4 GB/s bandwidth requirement**

Main Memory  
35.8 GB/s in total, **9 GB/s per core**  
256 cyc latency

Without data reuse (temporal locality),  
Processors need 100x higher bandwidth than  
what they actually have!

Execution Engine  
4.20 GHz  
134.4 G FLOP/s, i.e. **806.4 GB/s bandwidth requirement**

# The era of slow memory...

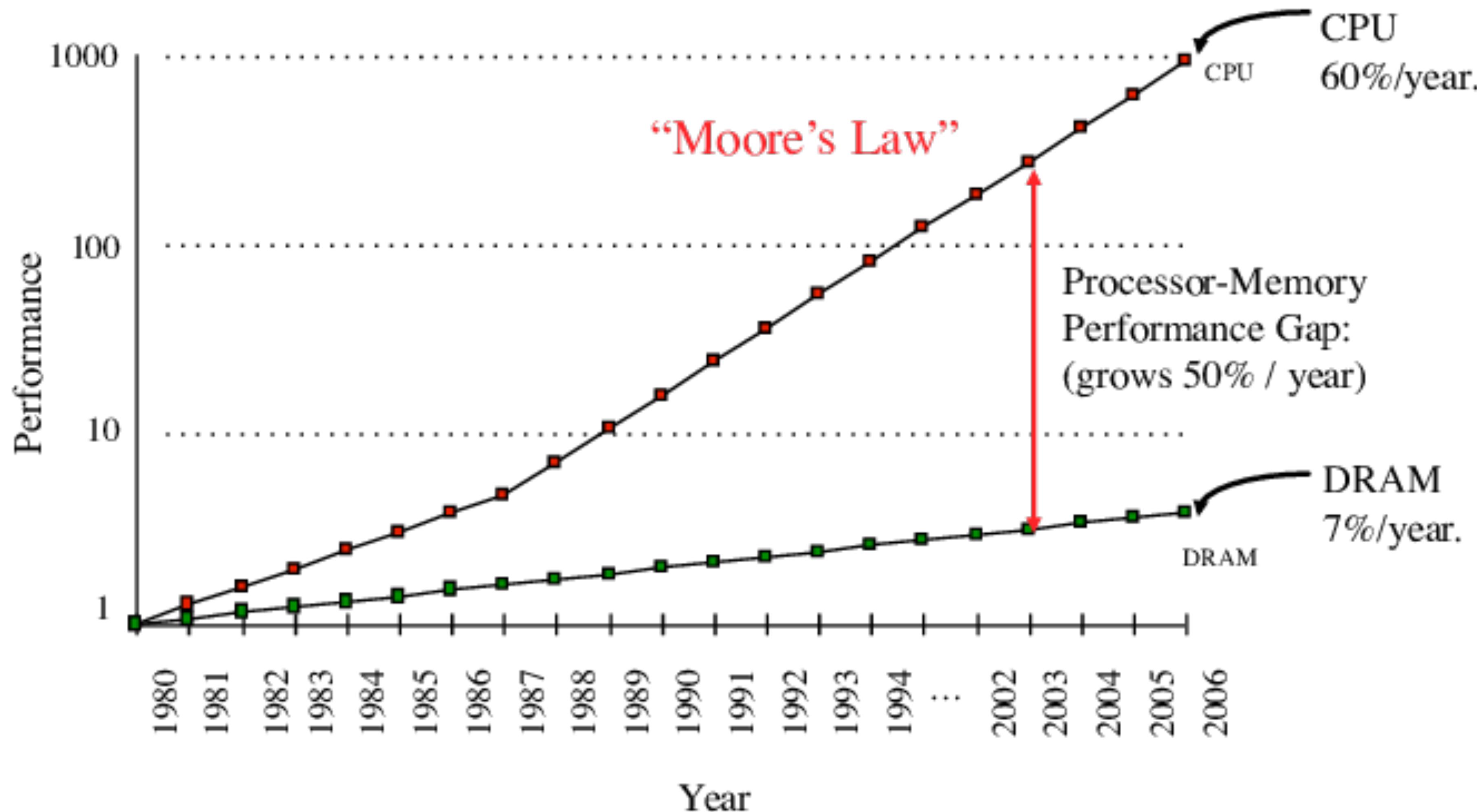
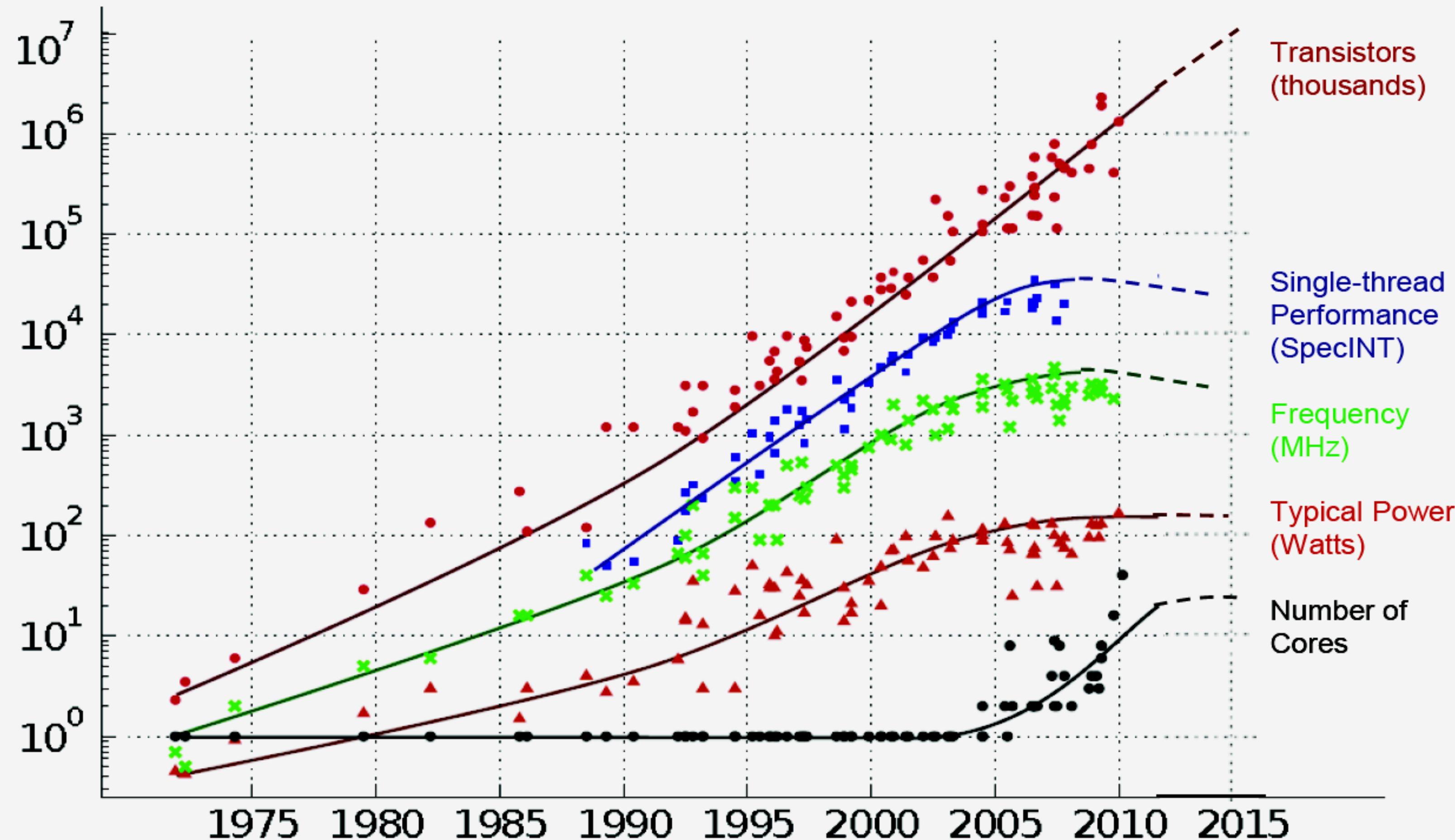


Figure from *High Performance by Exploiting Information Locality through Reverse Computing*, Bahi & Eisenbeis

# ...and parallelism.

## 35 YEARS OF MICROPROCESSOR TREND DATA

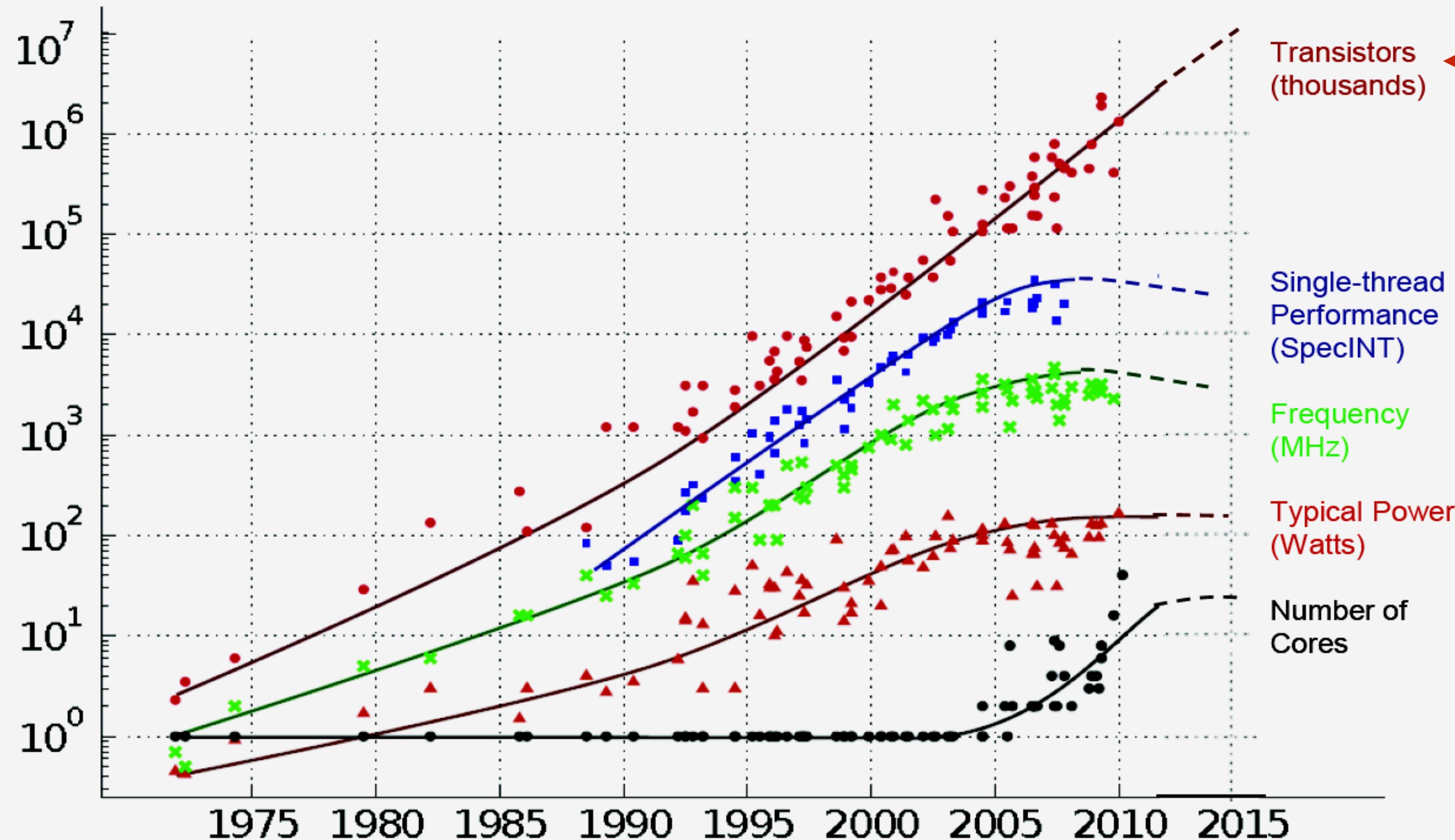


<https://www.karlrupp.net/2015/06/40-years-of-microprocessor-trend-data/>

Original data collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond and C. Batten  
Dotted line extrapolations by C. Moore

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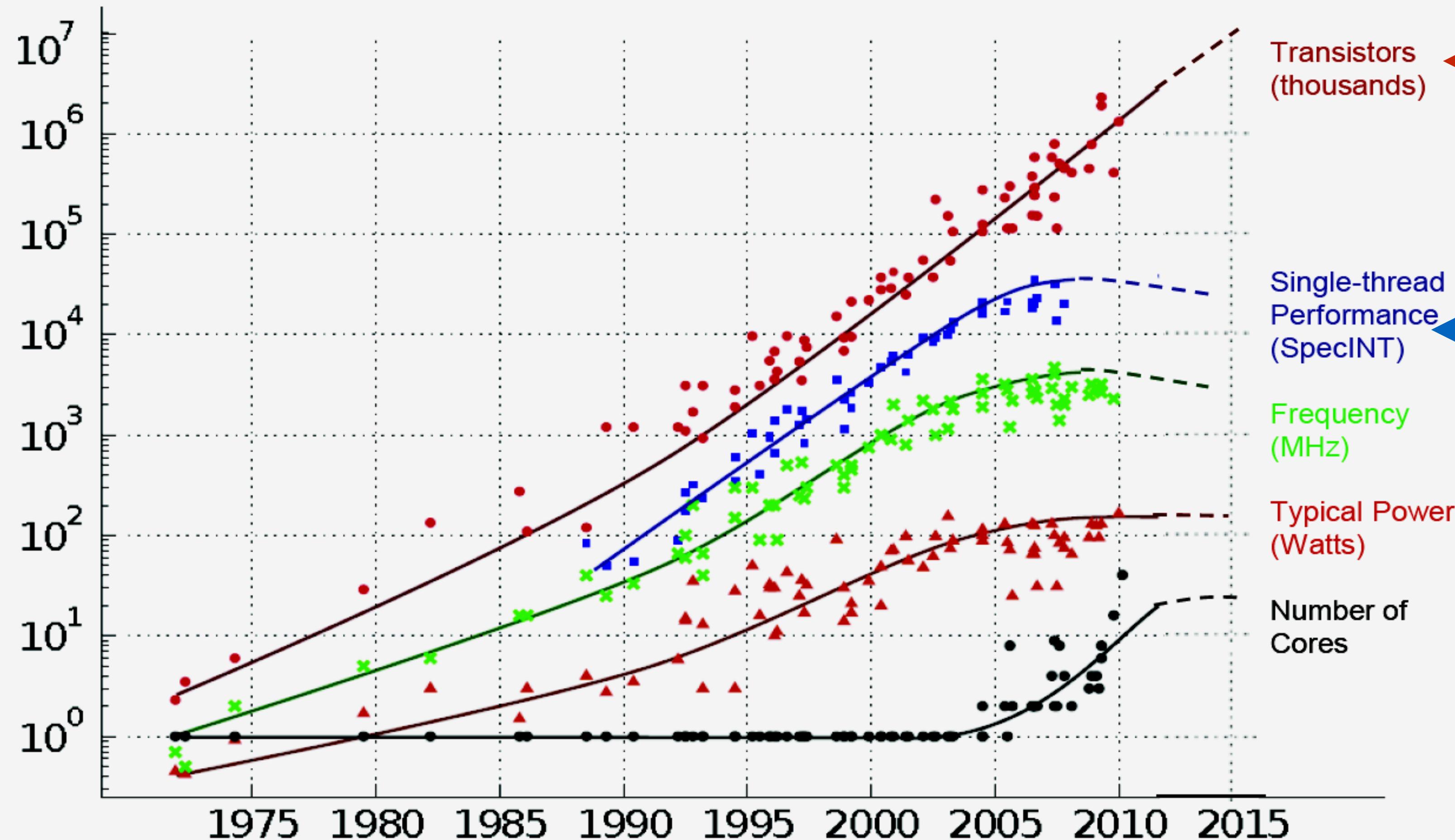


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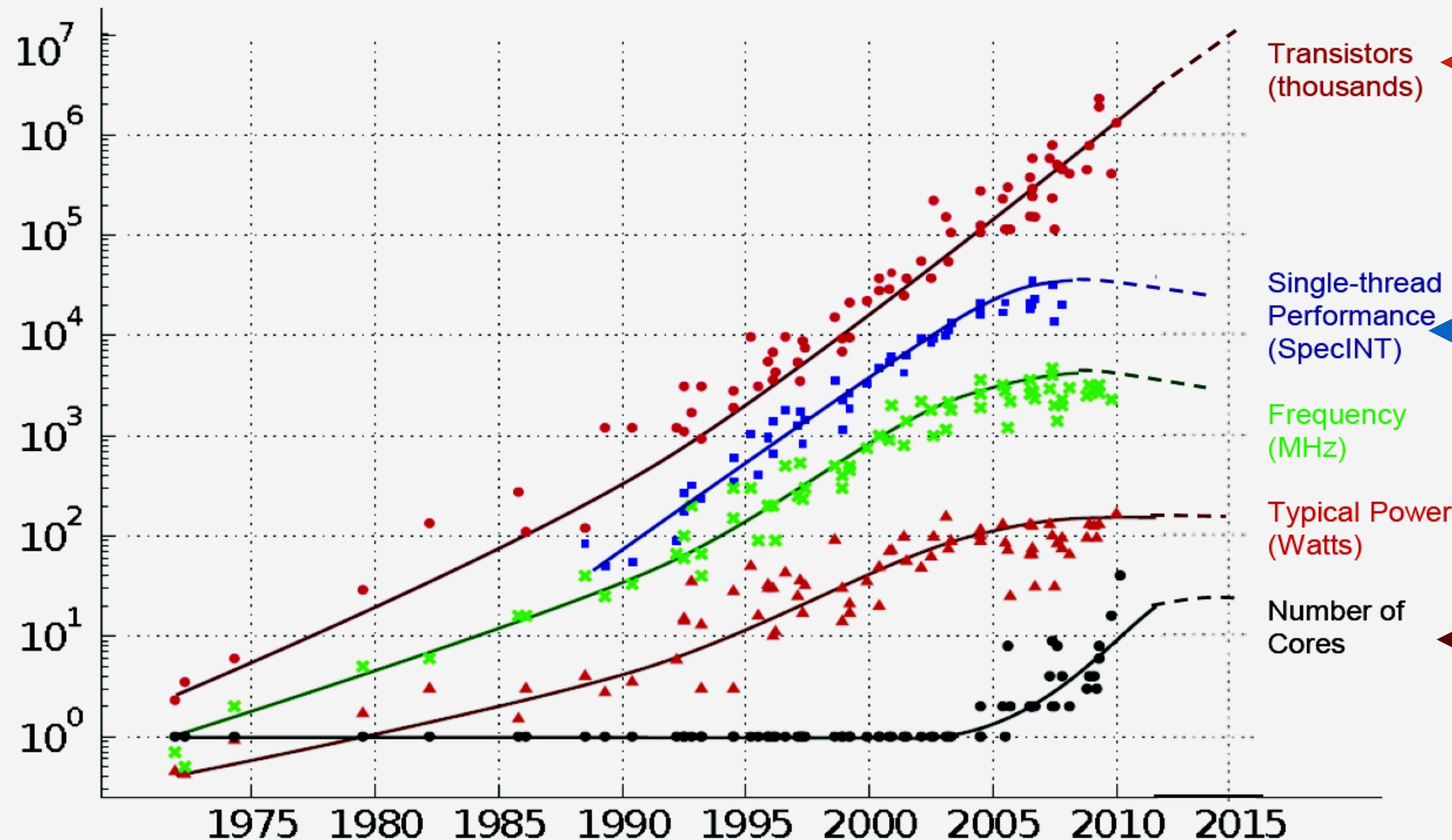


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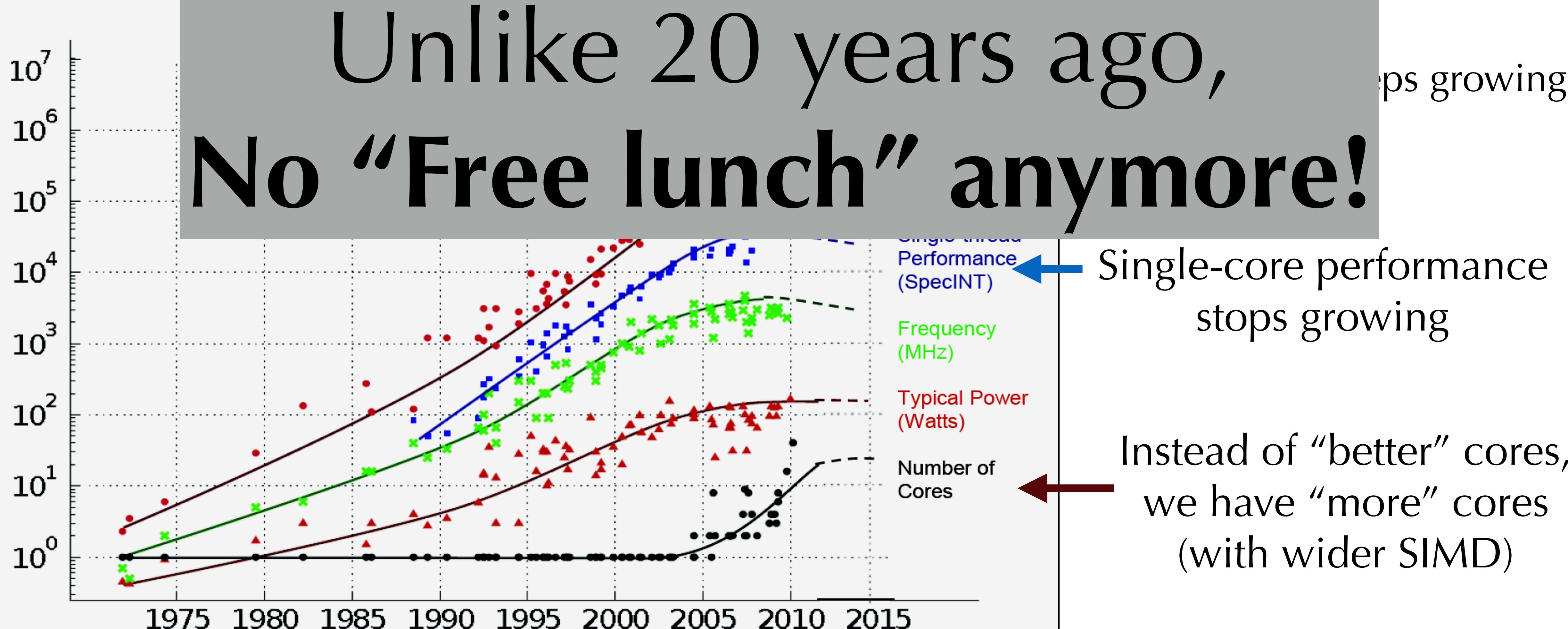


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# Takeaways:

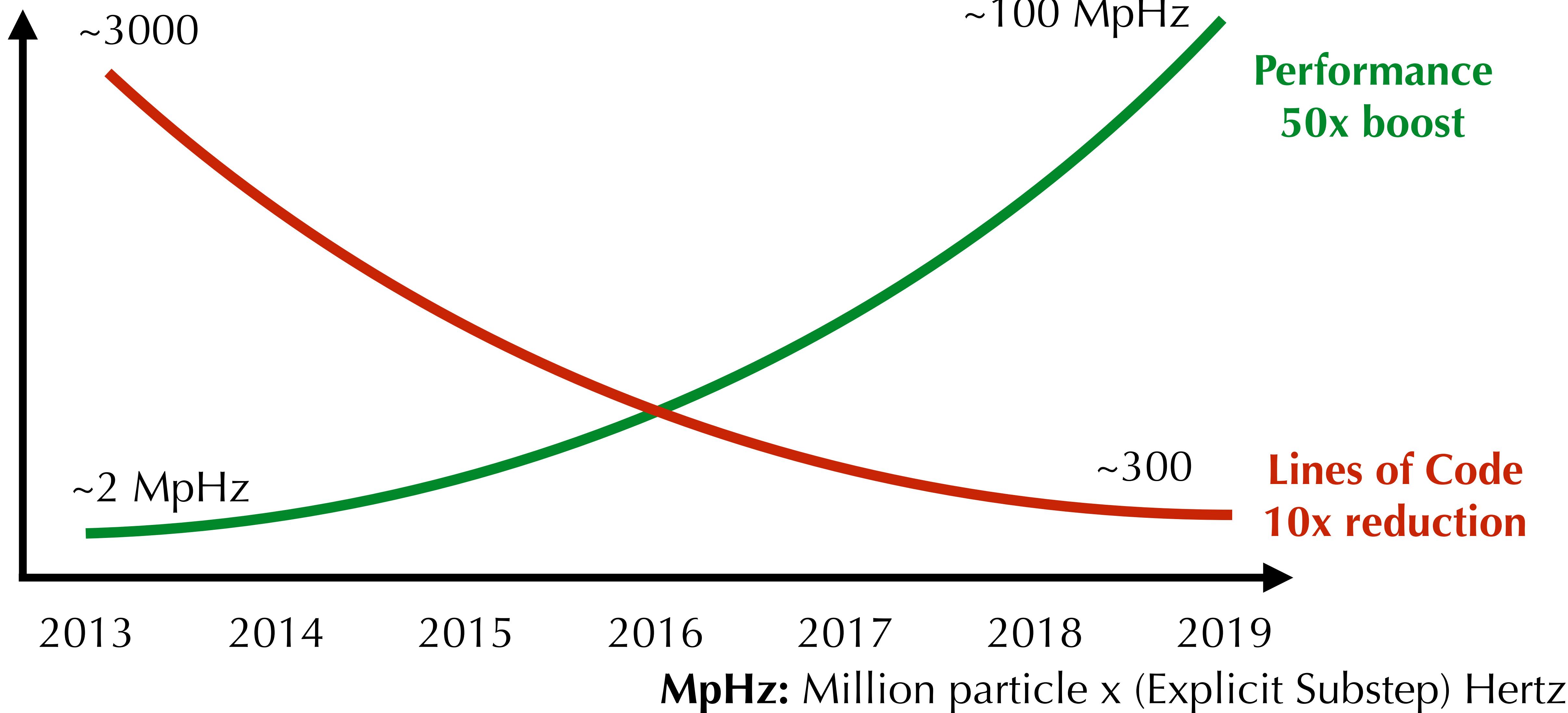
1. **[Architecture-aware programming]** will become increasingly important in the future since processors and memory are stopping getting faster.
2. Processors are more capable than you thought.  
**[Parallelism: Computation is cheap]**
3. Memory bandwidth is a more scarce resource nowadays.  
**[Locality: Communication is expensive]**

# Takeaways:

1. **[Architecture-aware programming]** will become increasingly important in the future since processors and memory are stopping getting faster.
2. Processors are more capable than you thought.  
**[Parallelism: Computation is cheap]**
3. Memory bandwidth is a more scarce resource nowadays.  
**[Locality: Communication is expensive]**

**Same rules apply to GPUs**

# The “Moore’s Law” of MPM







# The Design Space for High Performance

## ♦ Data structures

- For particles:
  - array of structure (AOS)/ structure of arrays (SOA), sorting/reordering
- For grid:
  - Dense/sparse (VDB/SPGrid), dynamic/fixed hierarchy, leaf block data layout, Z-indexing...

## ♦ Parallelization:

- what does each vector lane/thread/core/warp/block/streaming multiprocessor do?
- How to avoid data race and cacheline sharing?

# Organizing Particle Data

# AOS v.s. SOA Layout

## ◆ Array of Structures (AOS)

```
struct Particle {float x, y, z};  
  
Particle particles[8192];
```

## ◆ Structure of Arrays (SOA)

```
struct particles {  
    float particle_x[8192];  
    float particle_y[8192];  
    float particle_z[8192];  
};
```

# Array of Structures

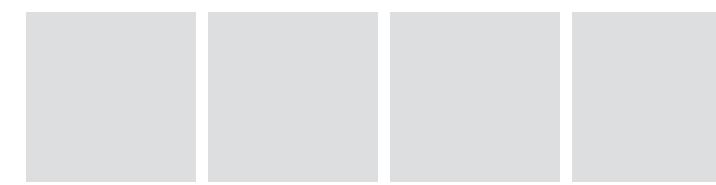
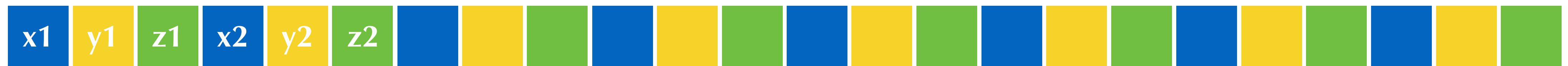
## Linear Memory



Each particle's fields are continuous in memory

# Array of Structures: Sequential Access

## Linear Memory

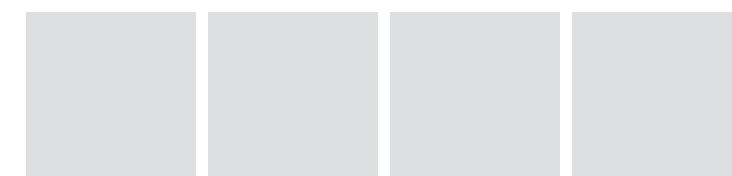
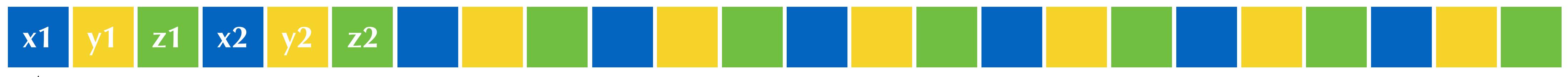


Cacheline

**Cacheline size: x86\_64: 64B; NVIDIA GPU: 128B**

# Array of Structures: Sequential Access

**Linear Memory**

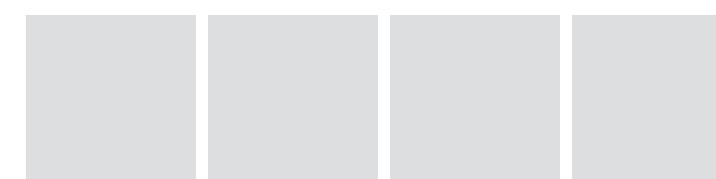
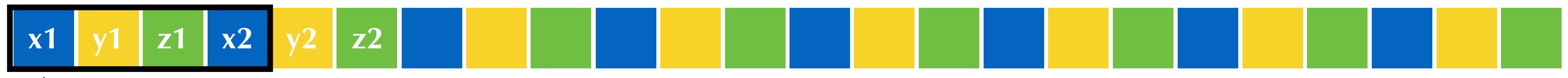


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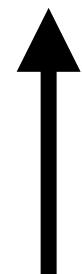


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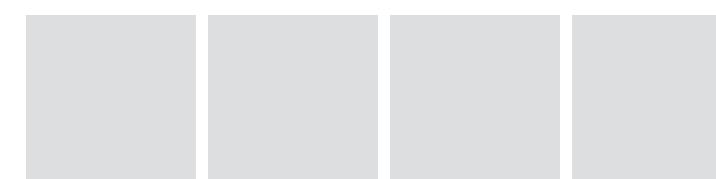


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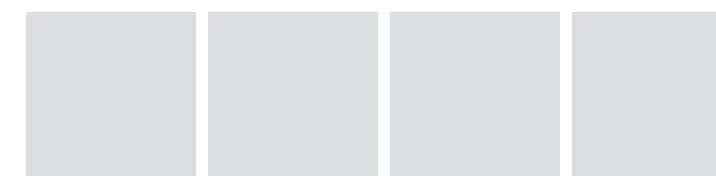
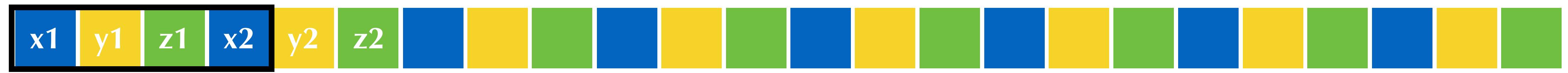


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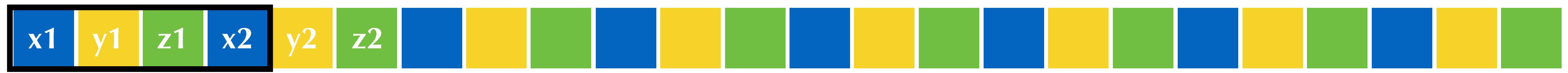


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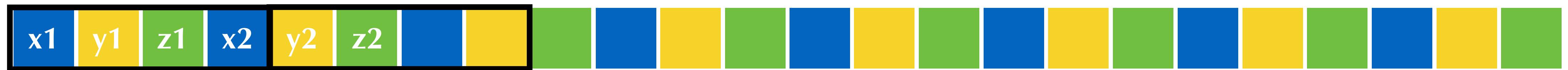


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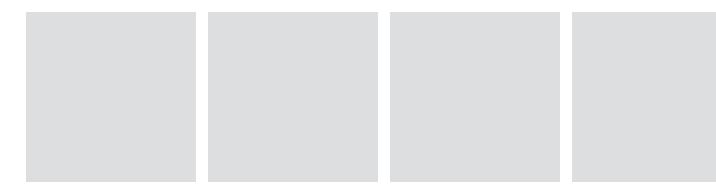


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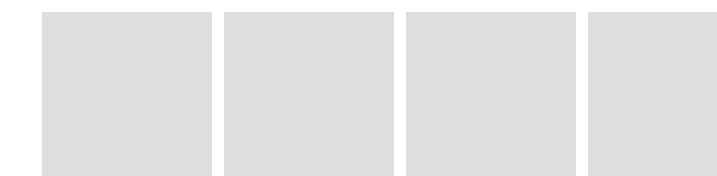


**Cacheline**

**Cacheline size: x86\_64: 64B; NVIDIA GPU: 128B**

# Array of Structures: Sequential Access

**Linear Memory**



**Cacheline**

**Cacheline size: x86\_64: 64B; NVIDIA GPU: 128B**

**Cacheline Utilization: 100%**

# Array of Structures: Random Access

## Linear Memory



Cacheline

# Array of Structures: Random Access

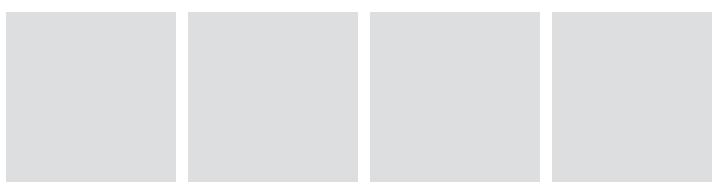
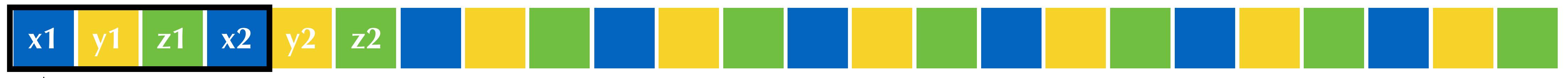
**Linear Memory**



**Cacheline**

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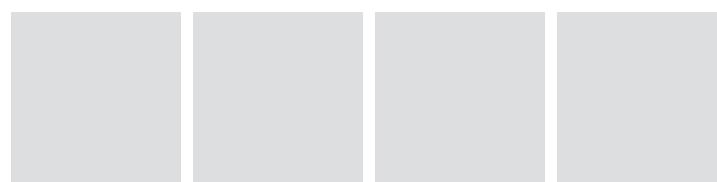
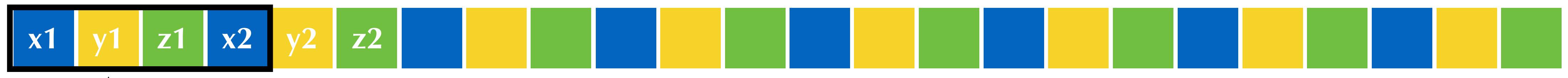
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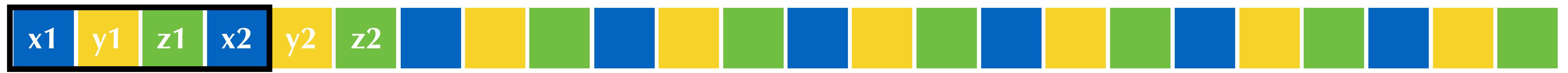
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**Cacheline**

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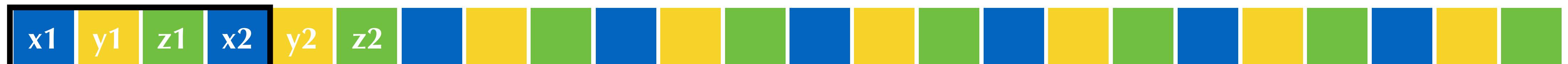
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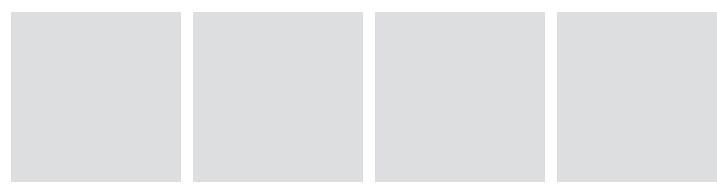
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**Cacheline**

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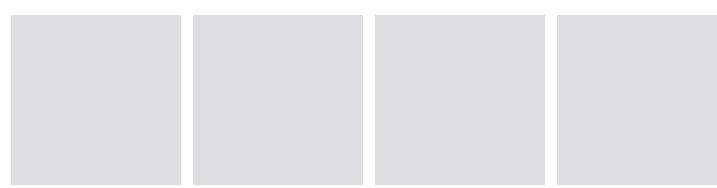
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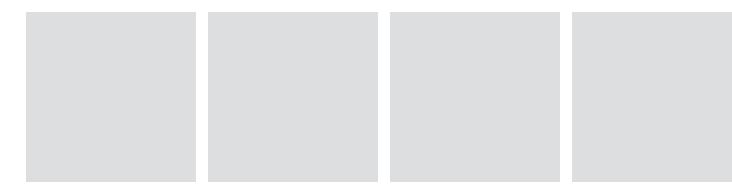
**Linear Memory**



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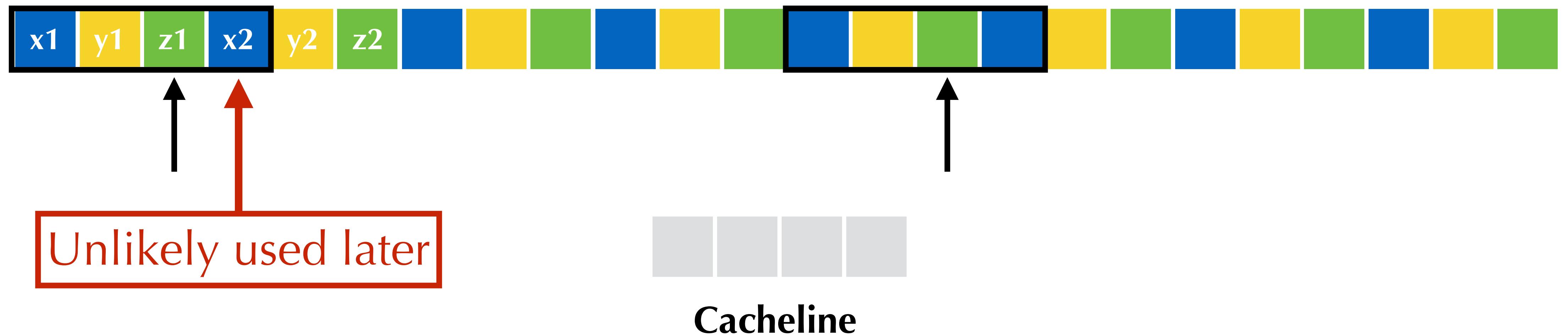
**Linear Memory**



**Cacheline**

# Array of Structures: Random Access

## Linear Memory



# Array of Structures: Random Access

Linear Memory



Cacheline Utilization: 75%

# Array of Structures

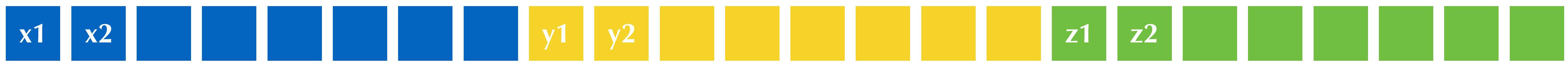
## Linear Memory



Each particle's fields are continuous in memory

# Structure of Arrays

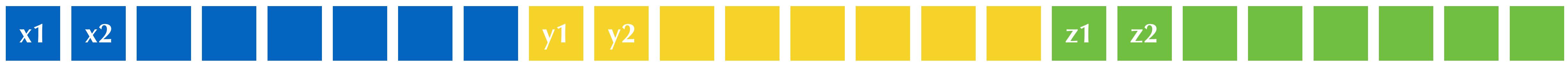
## Linear Memory



Each field's particle instances are continuous in memory

# Structure of Arrays: Sequential Access

## Linear Memory



# Structure of Arrays: Sequential Access

**Linear Memory**



# Structure of Arrays: Sequential Access

**Linear Memory**



# Structure of Arrays: Sequential Access

**Linear Memory**



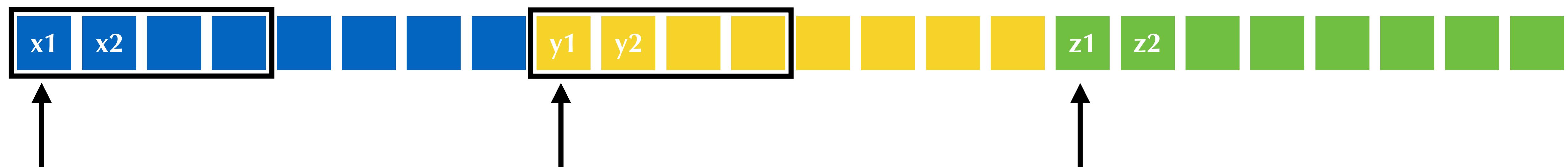
# Structure of Arrays: Sequential Access

**Linear Memory**



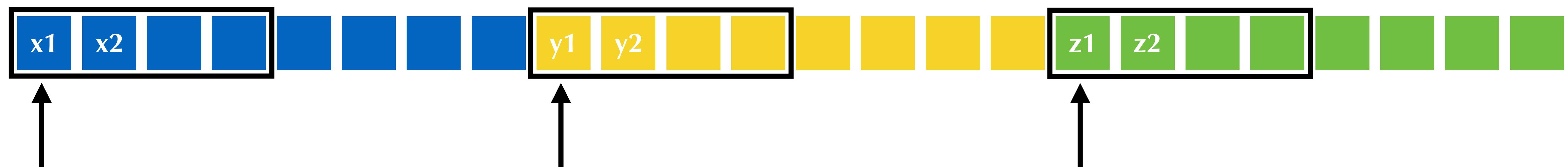
# Structure of Arrays: Sequential Access

**Linear Memory**



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**Linear Memory**



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**Linear Memory**



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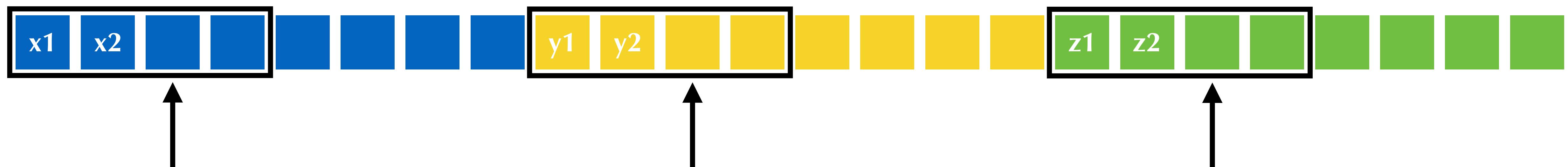
# Structure of Arrays: Sequential Access

**Linear Memory**



# Structure of Arrays: Sequential Access

Linear Memory



Cacheline Utilization: 100%

# Structure of Arrays: Random Access

**Linear Memory**



**Assuming cache size=3**

# Structure of Arrays: Random Access

**Linear Memory**



**Assuming cache size=3**

# Structure of Arrays: Random Access

**Linear Memory**



**Assuming cache size=3**

# Structure of Arrays: Random Access

**Linear Memory**



**Assuming cache size=3**

# Structure of Arrays: Random Access

**Linear Memory**



**Assuming cache size=3**

# Structure of Arrays: Random Access

**Linear Memory**



**Assuming cache size=3**

# Structure of Arrays: Random Access

**Linear Memory**



**Assuming cache size=3**

# Structure of Arrays: Random Access

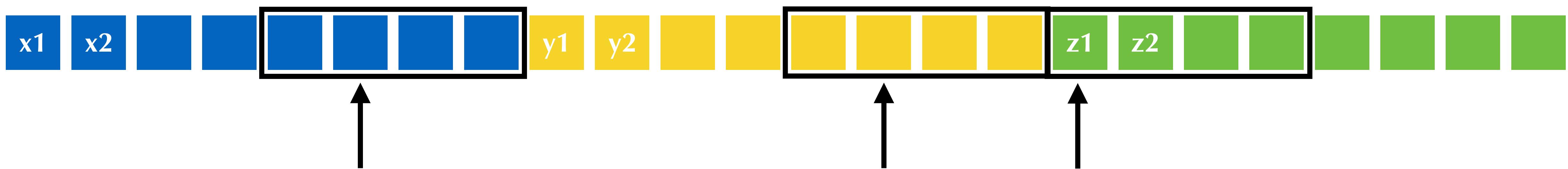
**Linear Memory**



**Assuming cache size=3**

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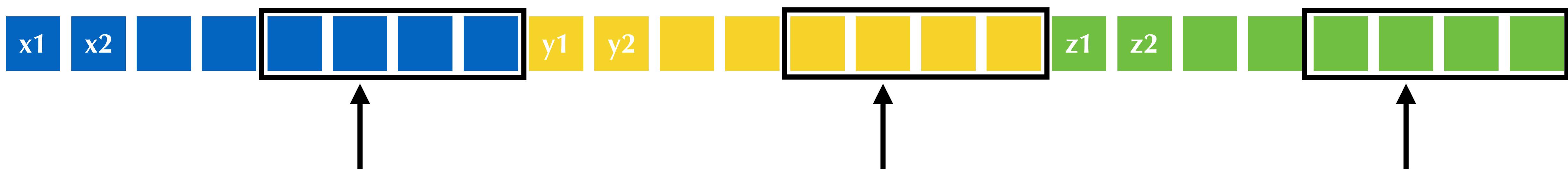
**Linear Memory**



**Assuming cache size=3**

# Structure of Arrays: Random Access

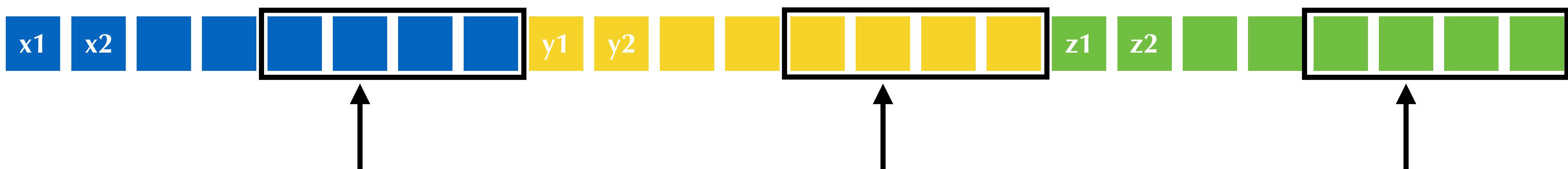
**Linear Memory**



**Assuming cache size=3**

# Structure of Arrays: Random Access

Linear Memory



Assuming cache size=3

Cacheline Utilization: 25 %

# Data Structures for MPM Particles

## ♦ SOA: very efficient when sorted

- Coalesced access on GPUs
- Large number of streams (e.g. 20): may invalidate prefetchers on CPU
  - not a problem for GPU - GPUs are designed for streaming and have no prefetching
- Random access: low cacheline utilization

## ♦ AOS: efficient even unsorted

- Random access: much better than SOA but should still be avoided if possible (cache/TLB misses)
- Sequential access: Slightly inferior than AOS
  - Vector lane shuffling on CPUs
  - Non-coalesced access on GPUs
- No sorting needed

# Real world 3D MPM: $\mathbf{x}$ (3 floats), $\mathbf{v}$ (3 floats), $\mathbf{F}$ (9 floats), $\mathbf{C}$ (9 floats)...

Particle Layout	Ordered	Randomly Shuffled
SOA	3.52ms	21.23 ms
AOS	3.15ms	4.28 ms

- ♦ SOA 6x slower when random shuffled
  - Periodic reordering is key to high performance for SOA
- ♦ AOS is less sensitive to particle order

# Data Structures for MPM Grids

- ♦ **Multi-Level Hierarchical Sparse Grids**
  - e.g. VDB, SPGrid
- ♦ **Dense blocks (e.g. 4x4x4 grid nodes) organized in tree structures**
  - Grid nodes store velocity (momentum) and mass

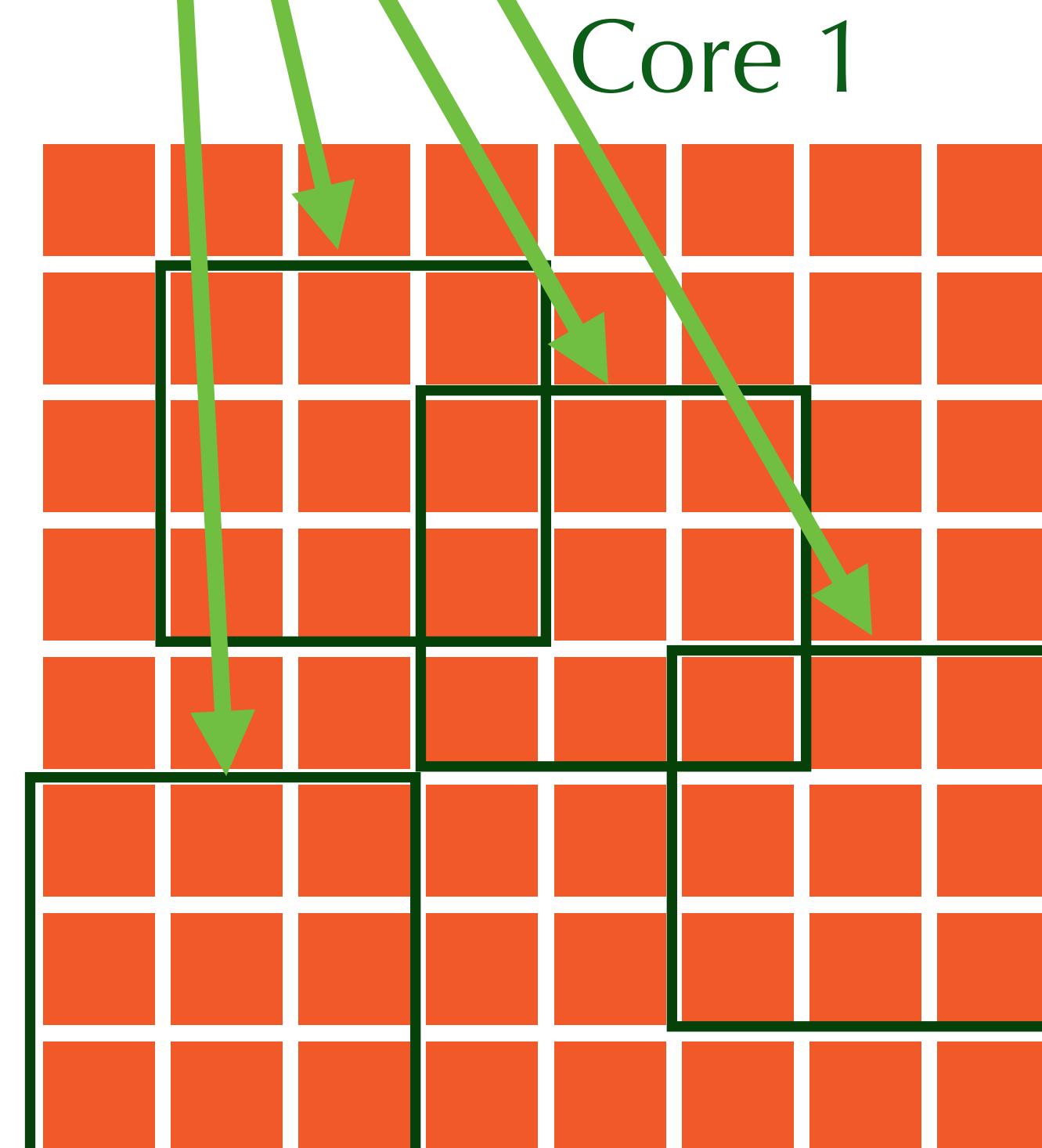
# **Organizing Grid Data & Parallelization based on Grid Blocks**

# Partition Particle for Parallelization

Particle data



Naive Partition



Each core touches all grid nodes:  
**Poor locality!**

# Partition Particle for Parallelization

Particle data

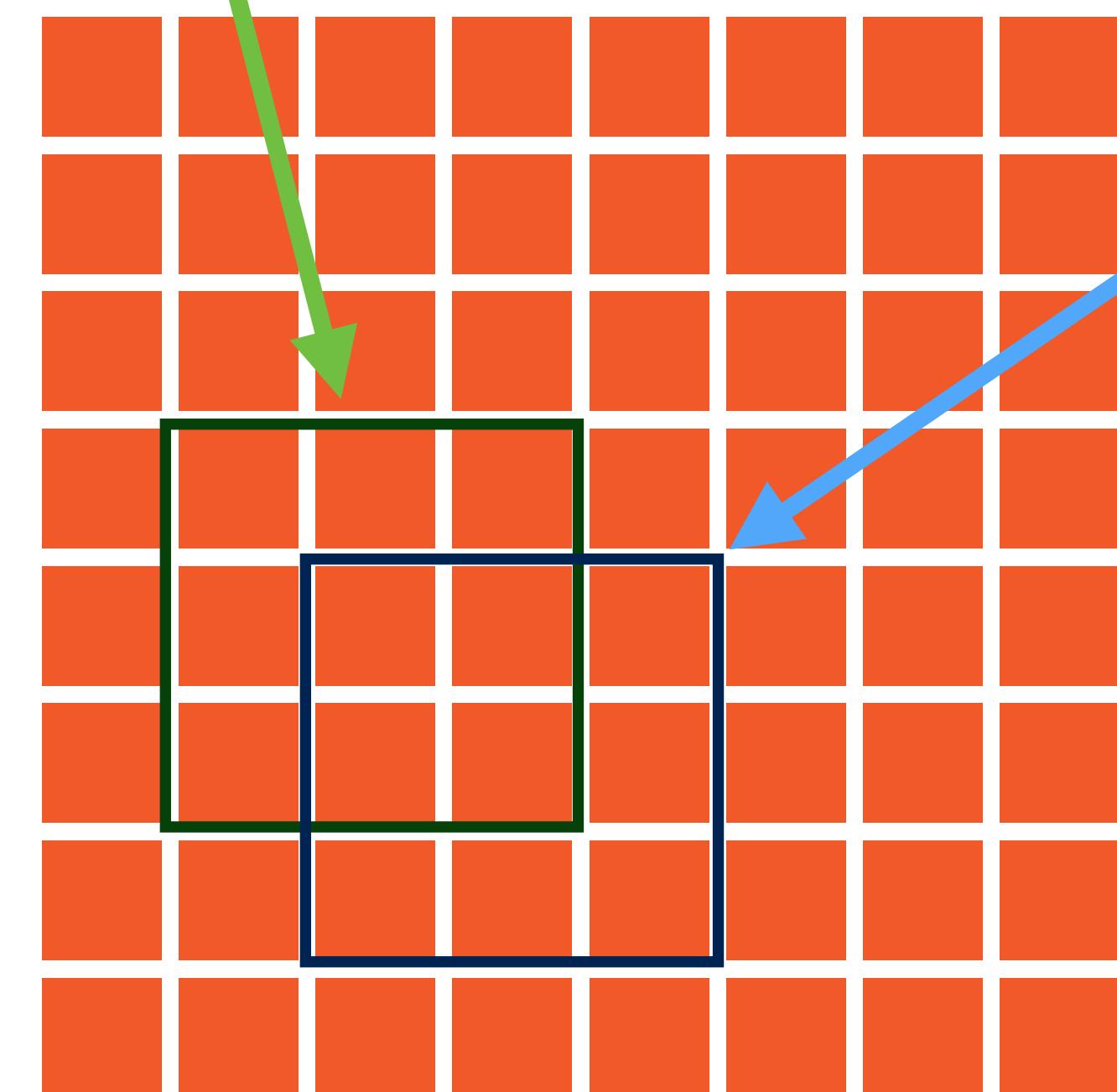


Naive Partition



Core 1

Core 2



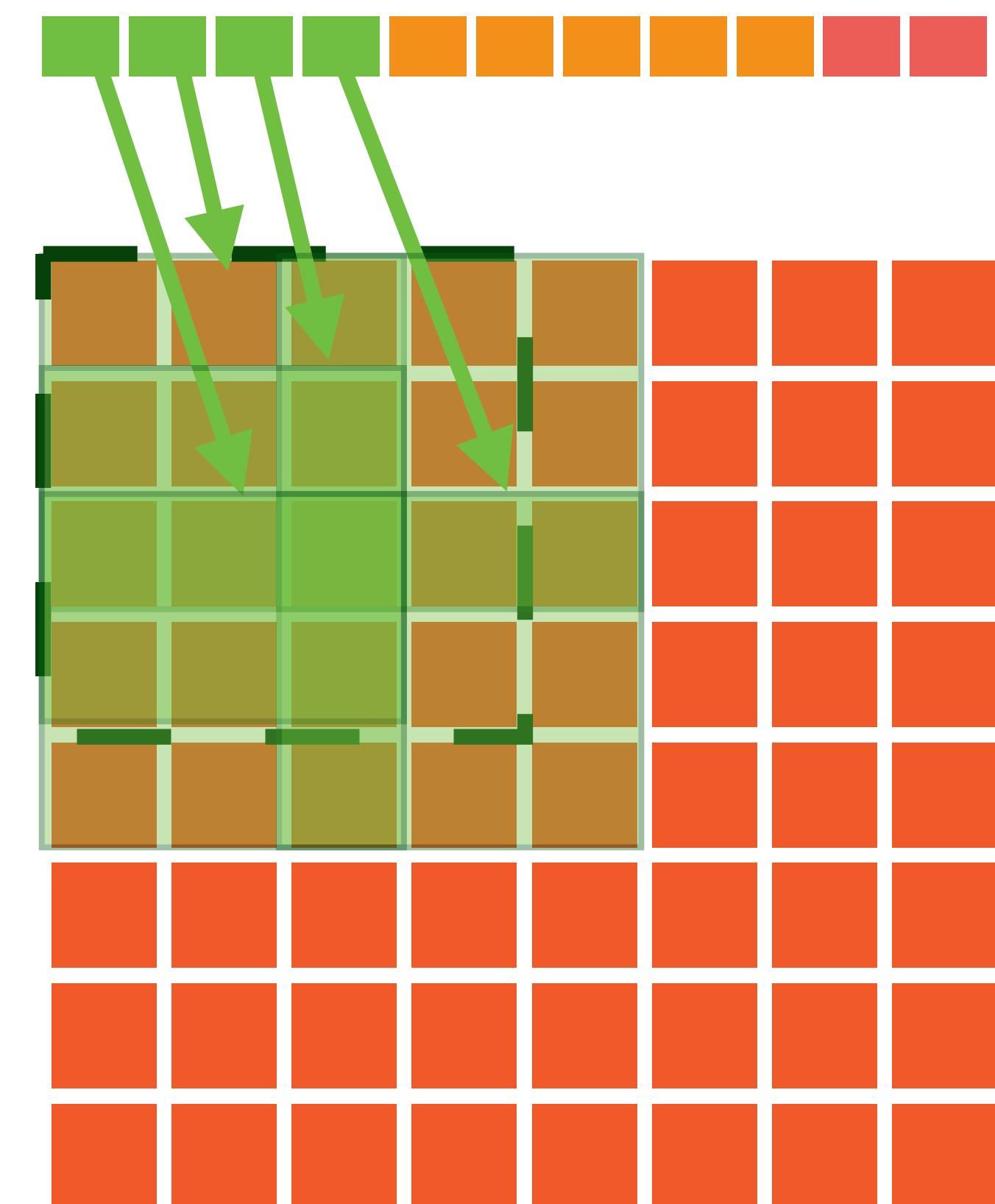
Data race! Needs locks on CPUs:  
**Poor parallelism!**

# Partition Particle for Parallelization

Particle data



Blockwise  
Partition



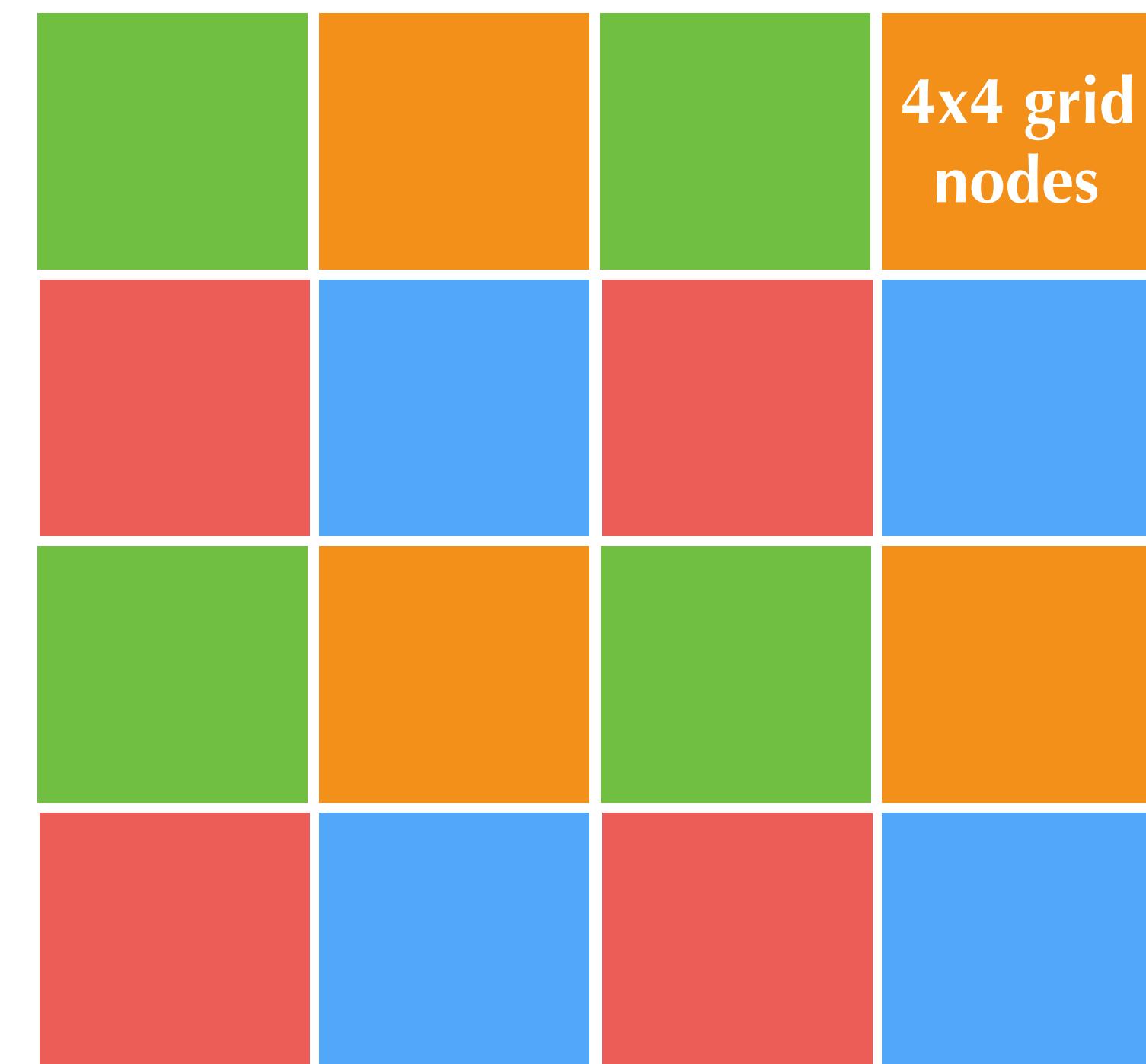
Particles in each block touches only  
a small number of grid nodes:  
**Good locality!**

# Partition Particle for Parallelization

# Particle data



# Blockwise Partition

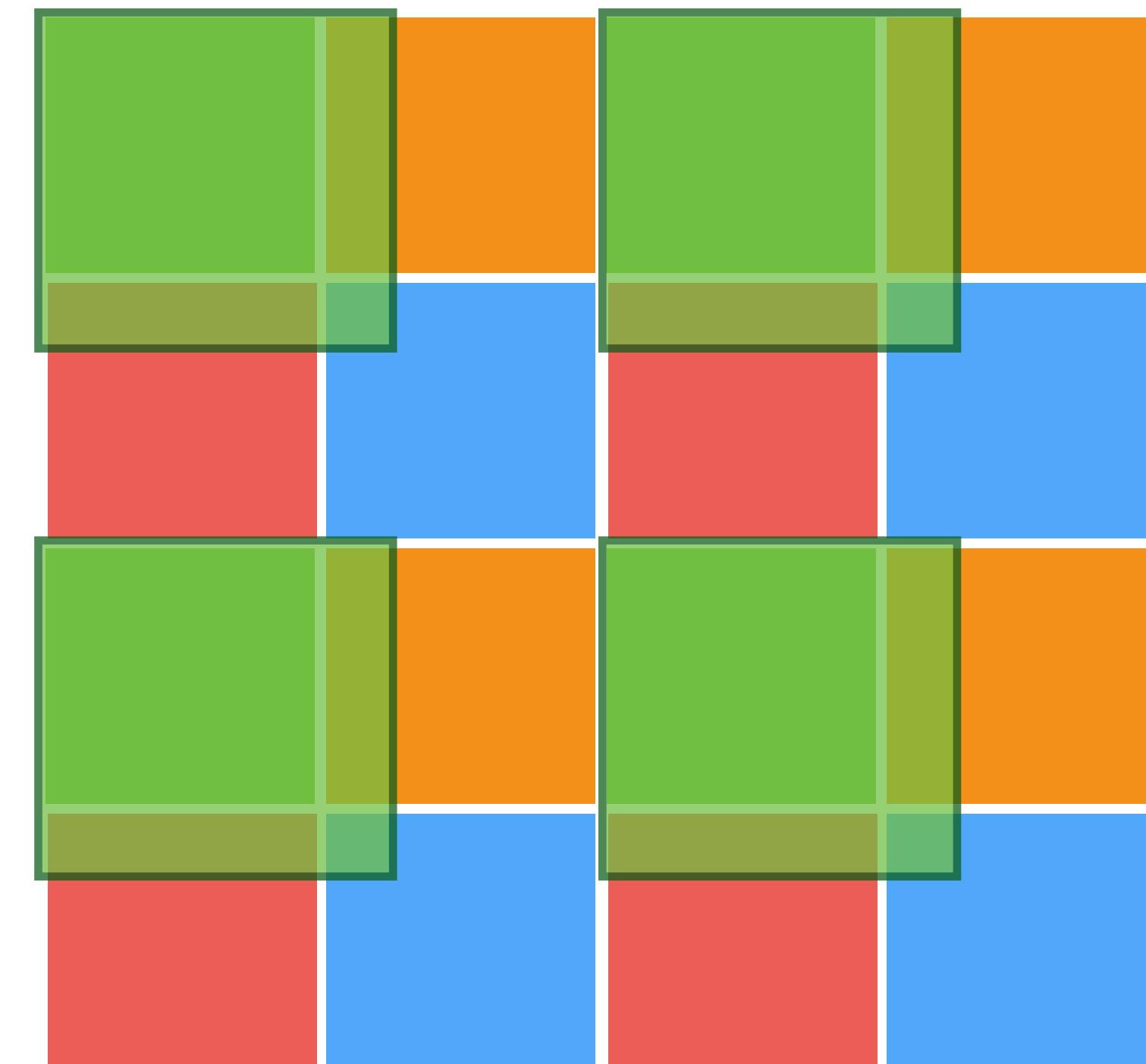


# Partition Particle for Parallelization

Particle data



Blockwise  
Partition

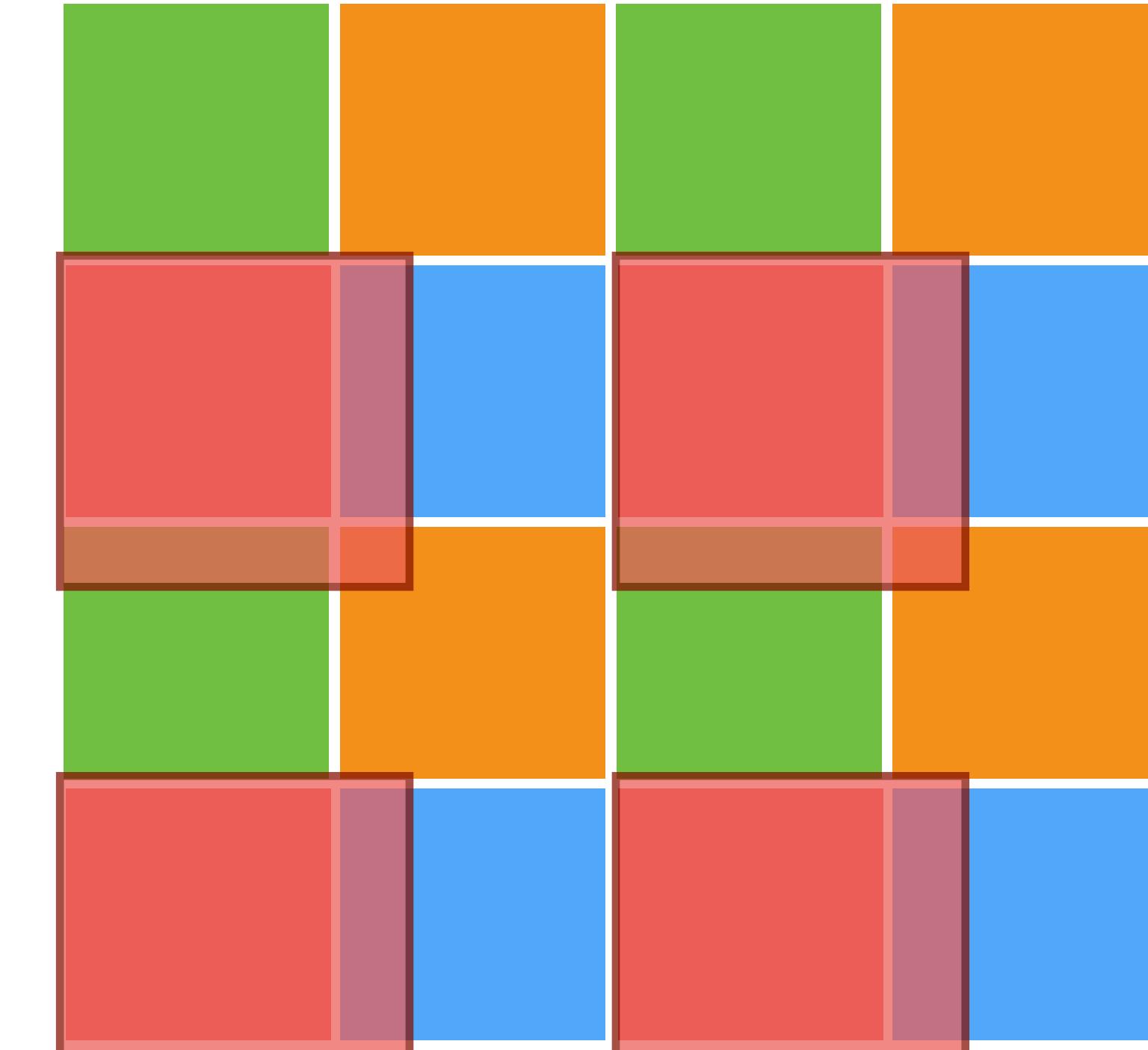


# Partition Particle for Parallelization

Particle data



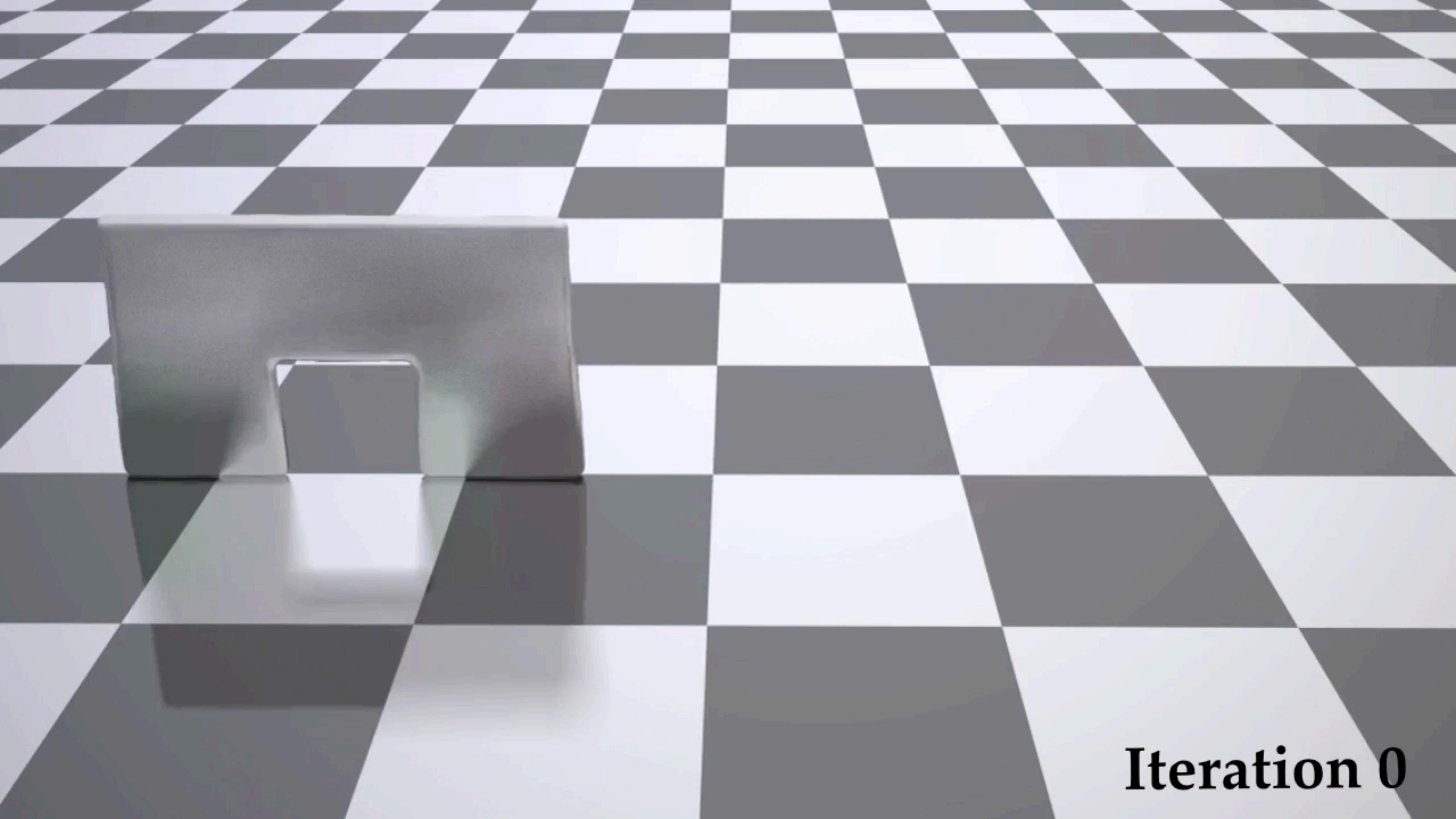
Blockwise  
Partition



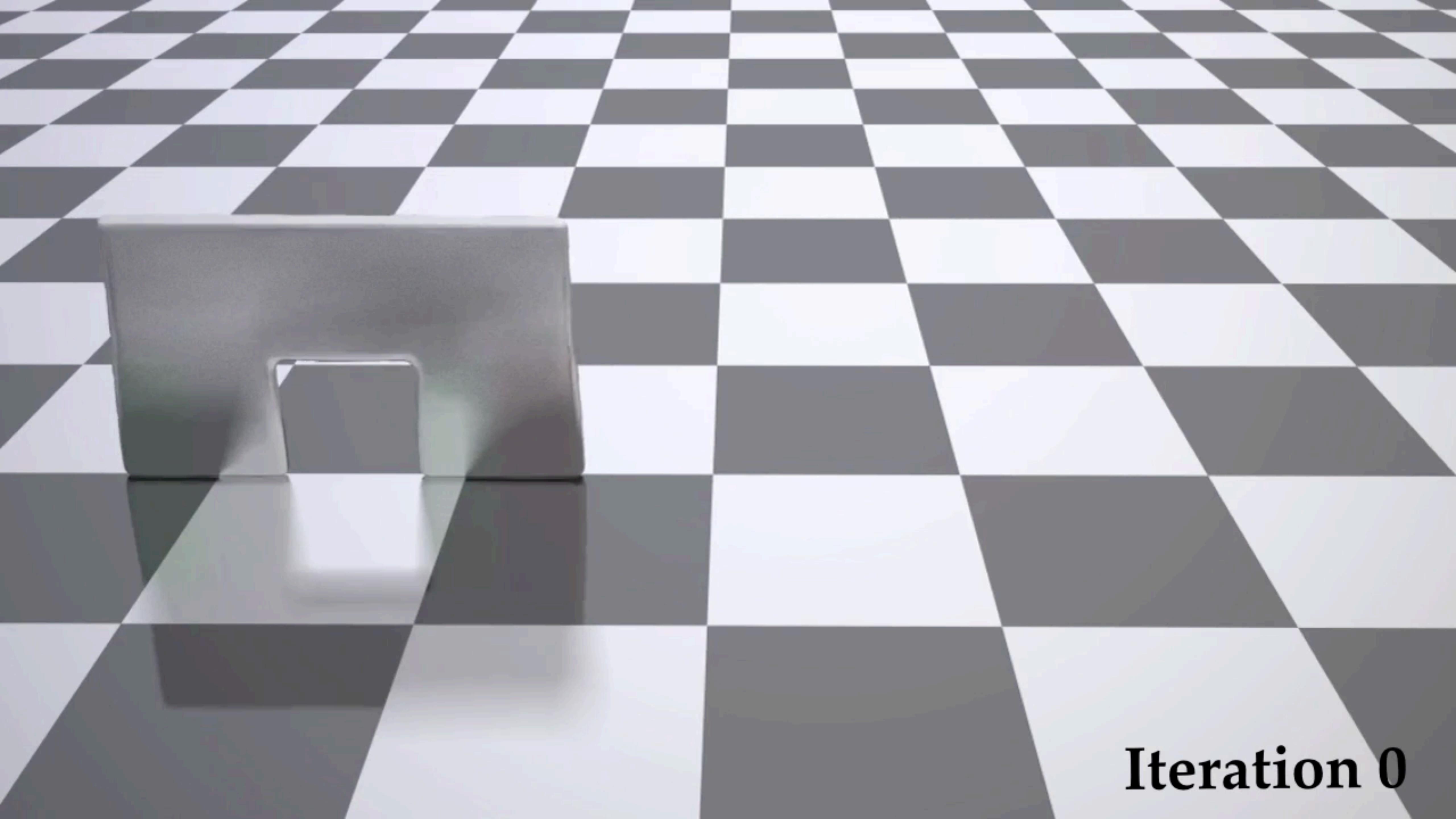
One color at a time, in parallel  
No data race - **good parallelism!**

# Advertisement: ChainQueen 乾坤

- ♦ **Differentiable MLS-MPM Solver for Soft Robotics [Hu et al., ICRA 2019]**
- ♦ Direct gradient-based optimization of robots and their controllers
  - By the “Chain” rule, hence the name “ChainQueen”
  - Orders of magnitude faster than reinforcement learning!

A 3D rendering of a metallic door handle on a checkered floor. The door handle is rectangular with rounded corners and a small slot in the center. It is mounted on a dark, reflective surface. The floor is a black and white checkered pattern. The lighting creates strong highlights and shadows, giving the scene a realistic appearance.

**Iteration 0**

A 3D rendering of a metallic door handle on a checkered floor. The door handle is rectangular with rounded corners and a small slot in the center. It is mounted on a dark, reflective surface. The floor is a black and white checkered pattern. The lighting creates strong highlights and shadows, giving the scene a realistic appearance.

**Iteration 0**

---

# On Hybrid Lagrangian-Eulerian Simulation Methods: Practical Notes and High-Performance Aspects

---

Yuanming Hu, Xinxin Zhang, **Ming Gao\***, Chenfanfu Jiang

Tencent America & University of Pennsylvania

---

# On Hybrid Lagrangian-Eulerian Simulation Methods: Practical Notes and High-Performance Aspects

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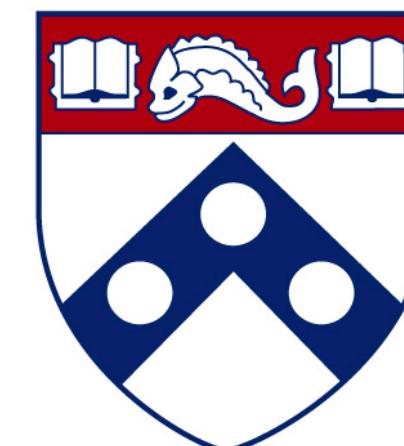
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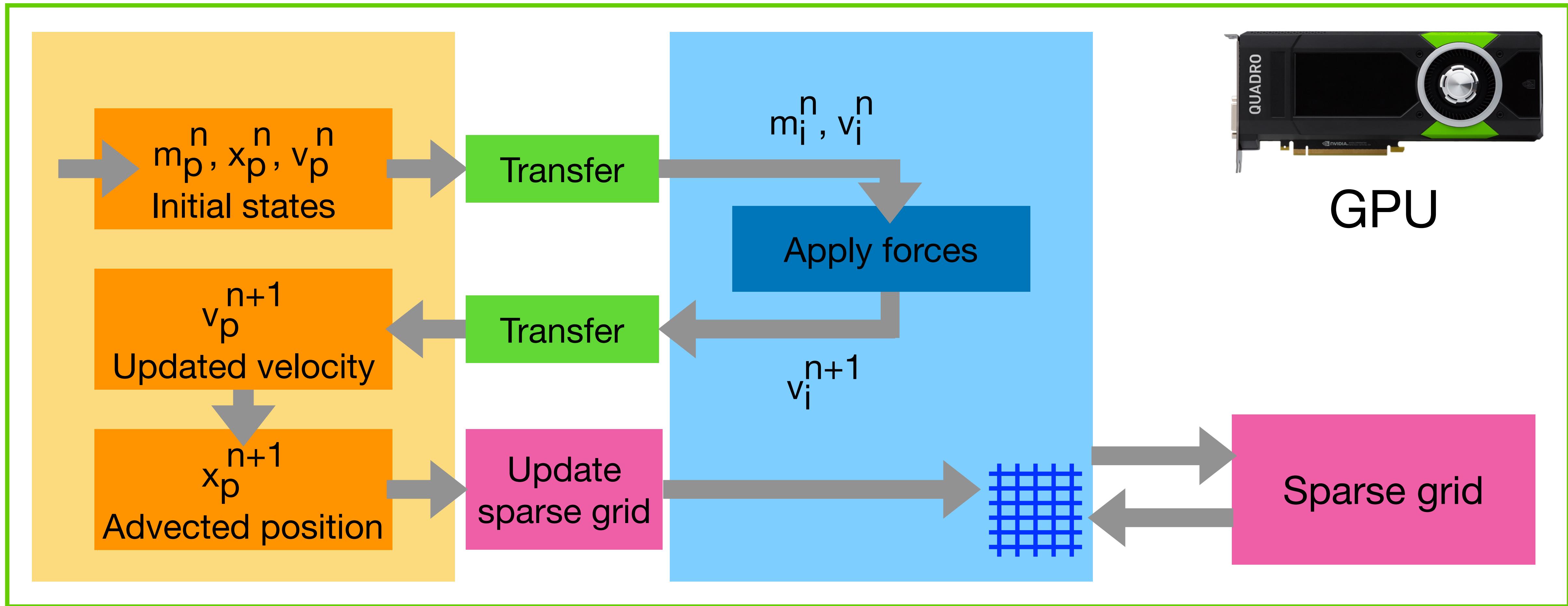
---

Yuanming Hu, Xinxin Zhang, **Ming Gao\***, Chenfanfu Jiang

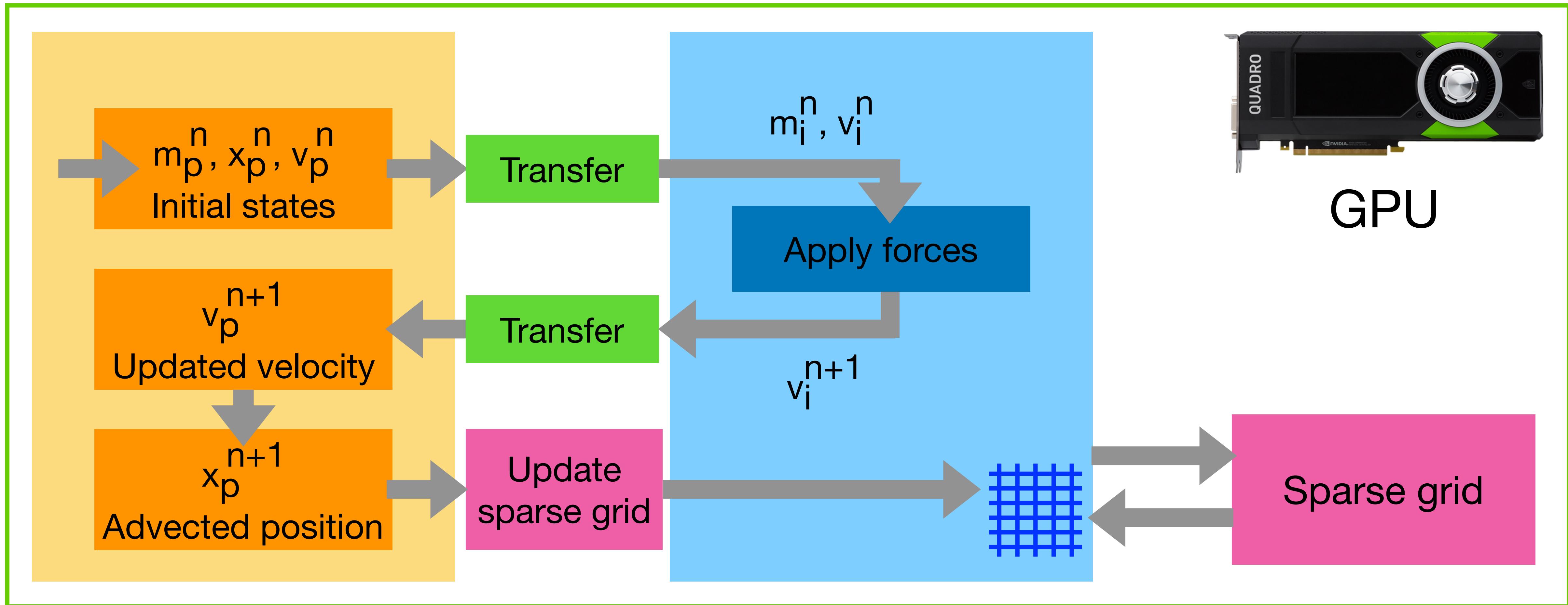
Tencent America & University of Pennsylvania



# GPU MPM - explicit time integration



# GPU MPM - explicit time integration



# Pipeline

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1: procedure GPUMPM( )
2:     P  $\leftarrow$  Initialize particle positions
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4:     for each time step do
5:         dt  $\leftarrow$  Compute dt (P)
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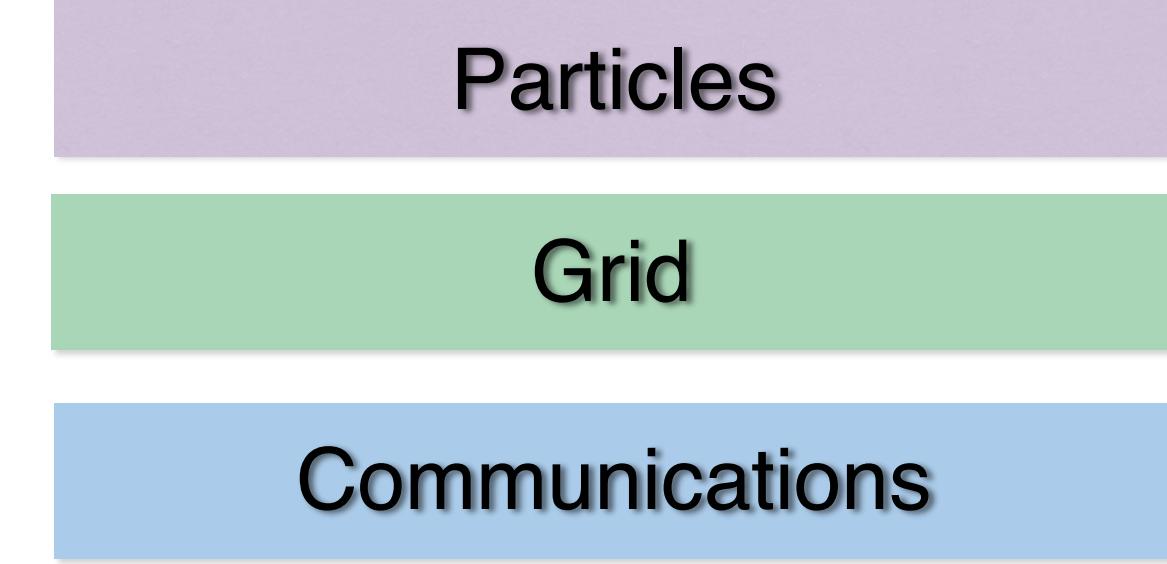
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# Pure particle operations

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5:     dt  $\leftarrow$  Compute dt (P)          2. Max dt  
6:     G  $\leftarrow$  Refresh GSPGrid (P)  
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# SVD computation

**Computing the Singular Value Decomposition of 3x3 matrices with minimal branching  
and elementary floating point operations**

**A. McAdams, A. Selle, R. Tamstorf, J. Teran and E. Sifakis**

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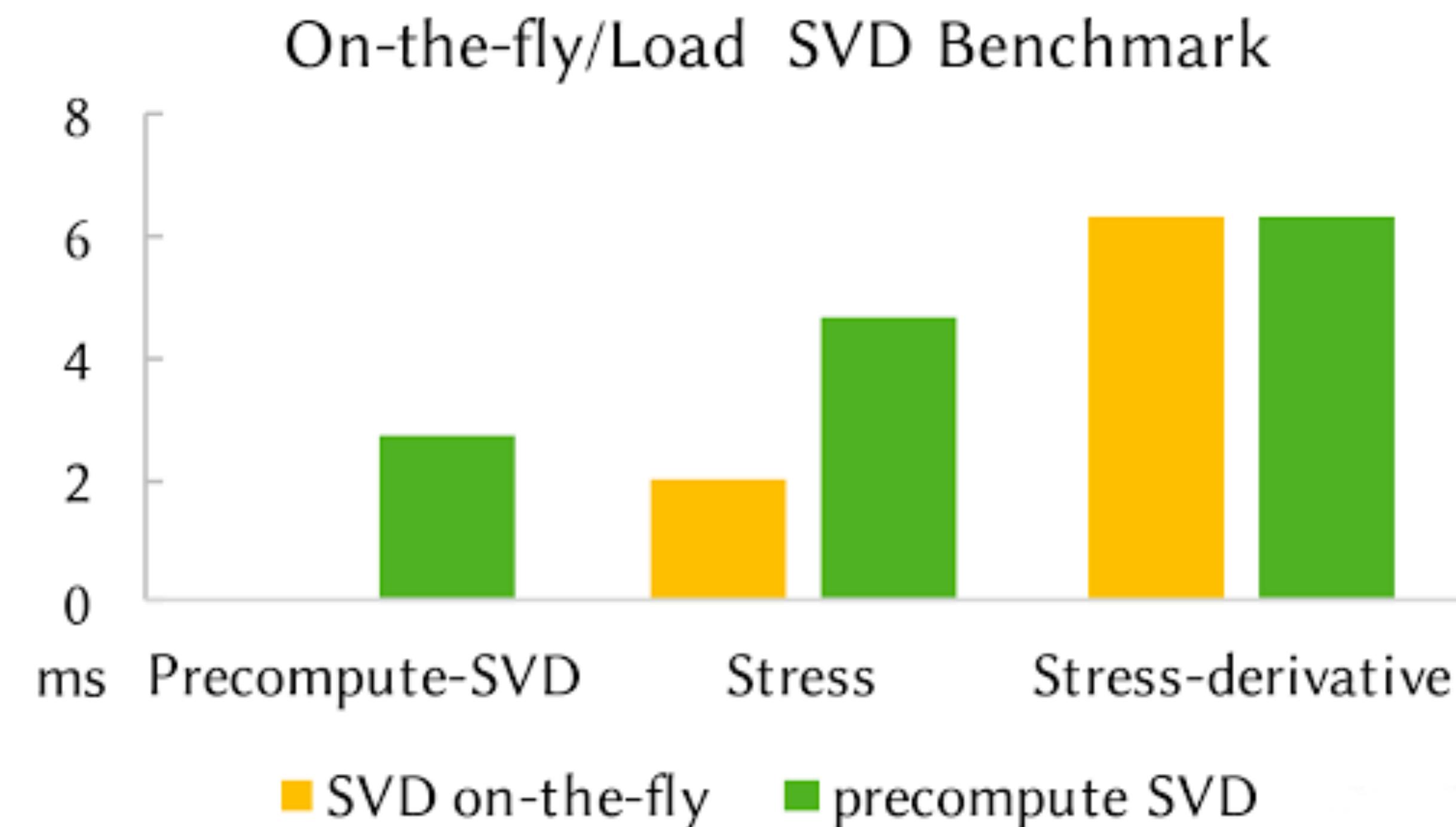
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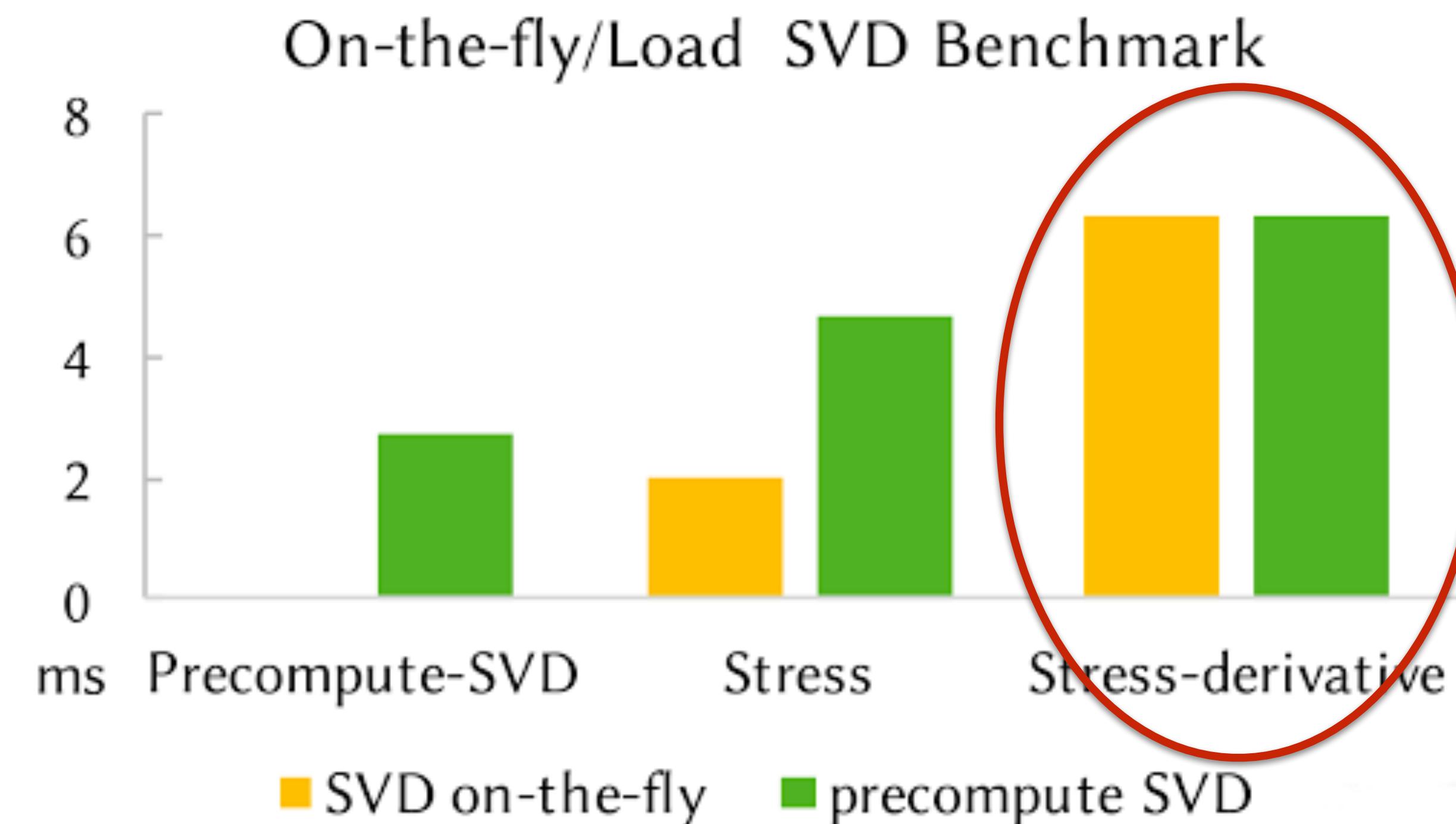
$$U \Sigma V^T$$

Store them in  
memory???

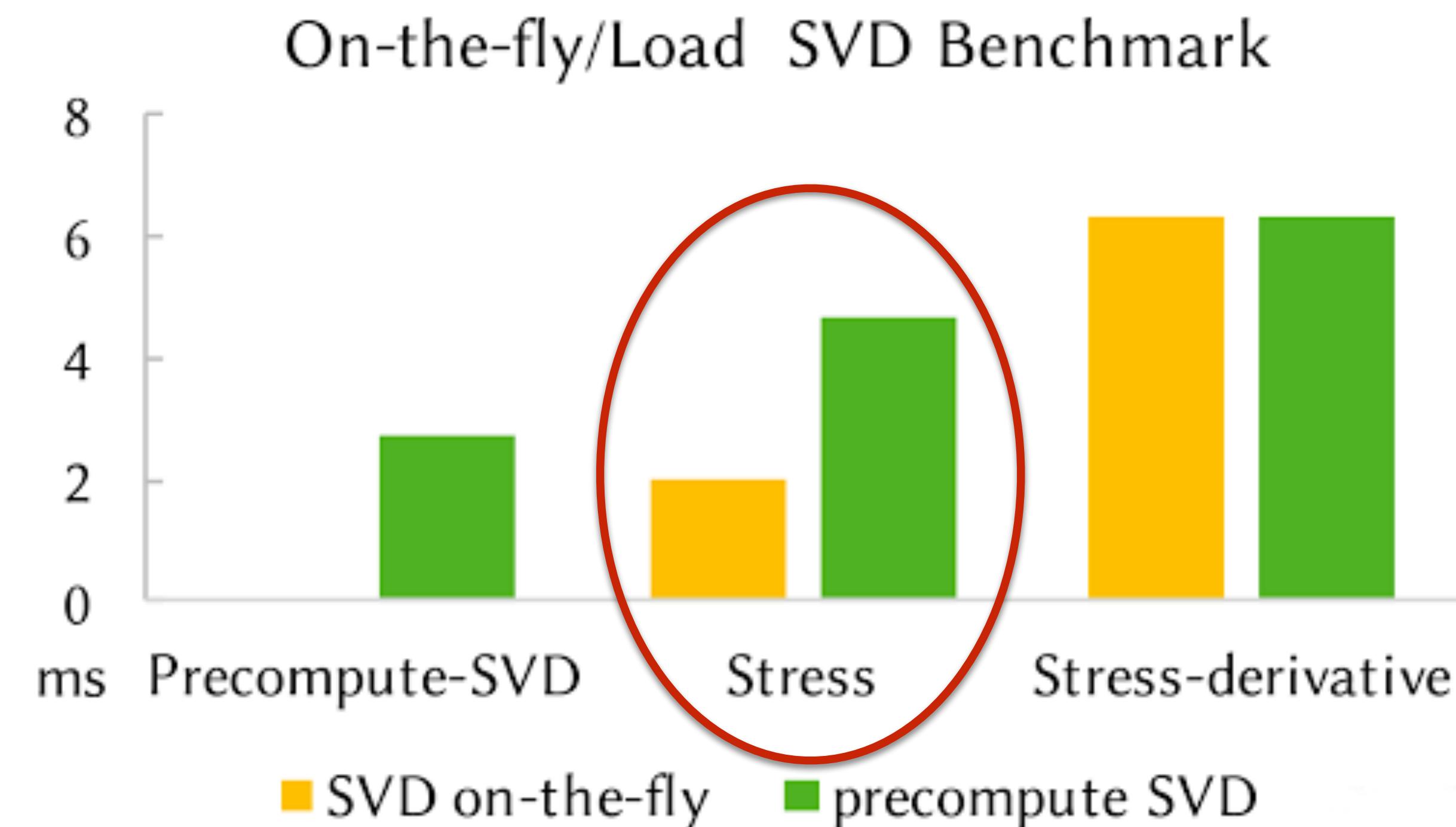
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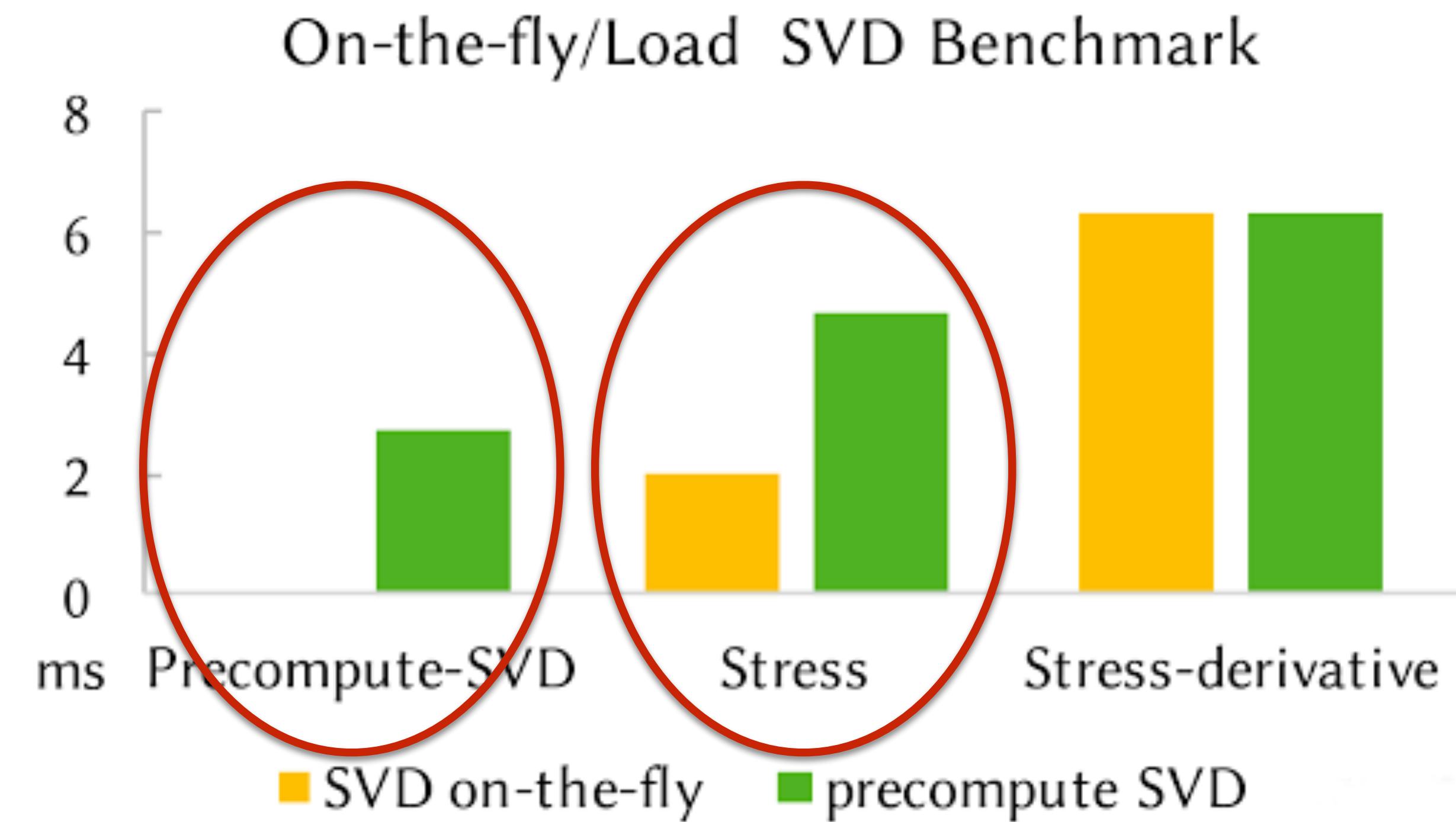
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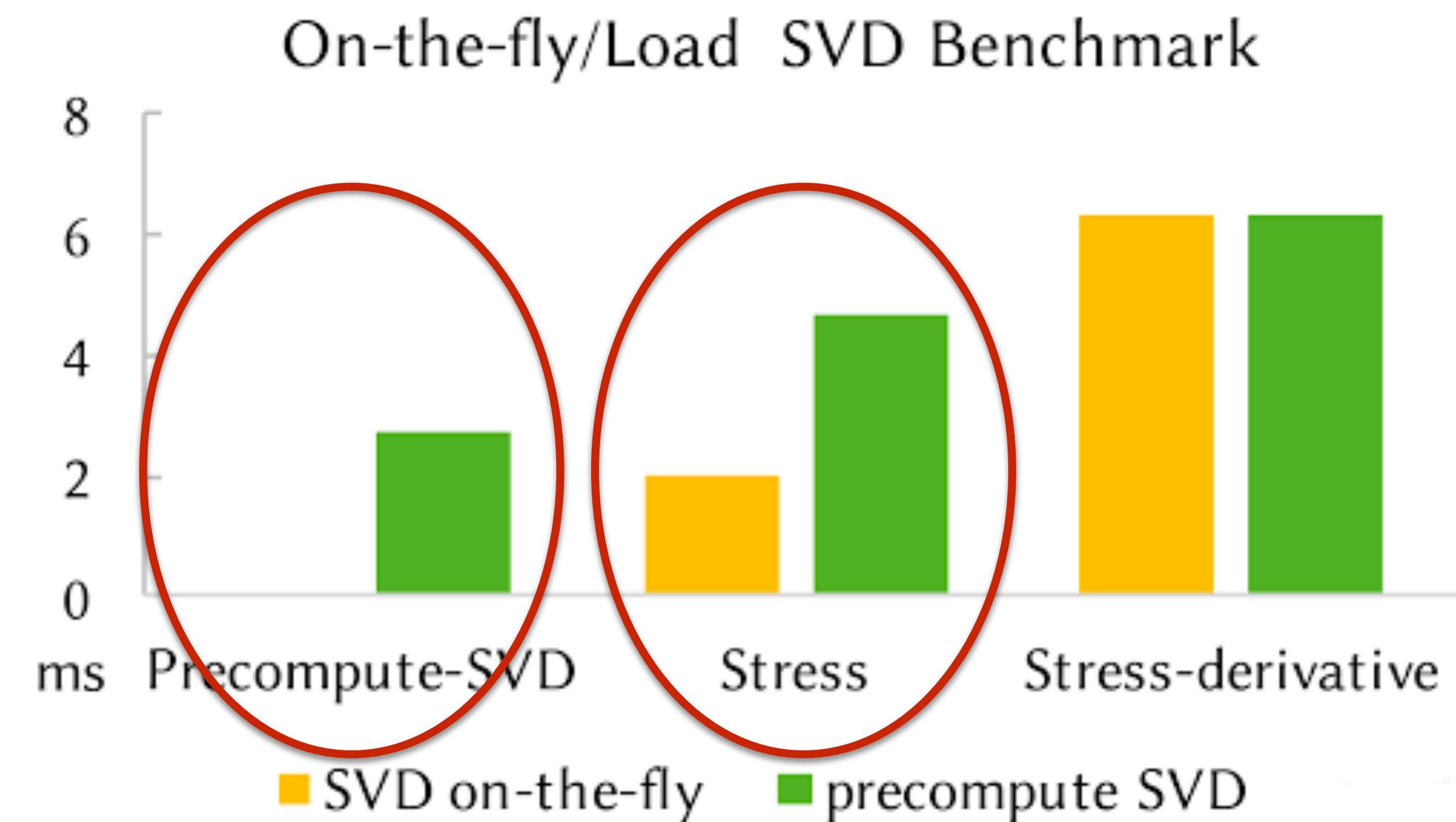
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# SVD computation



# SVD computation

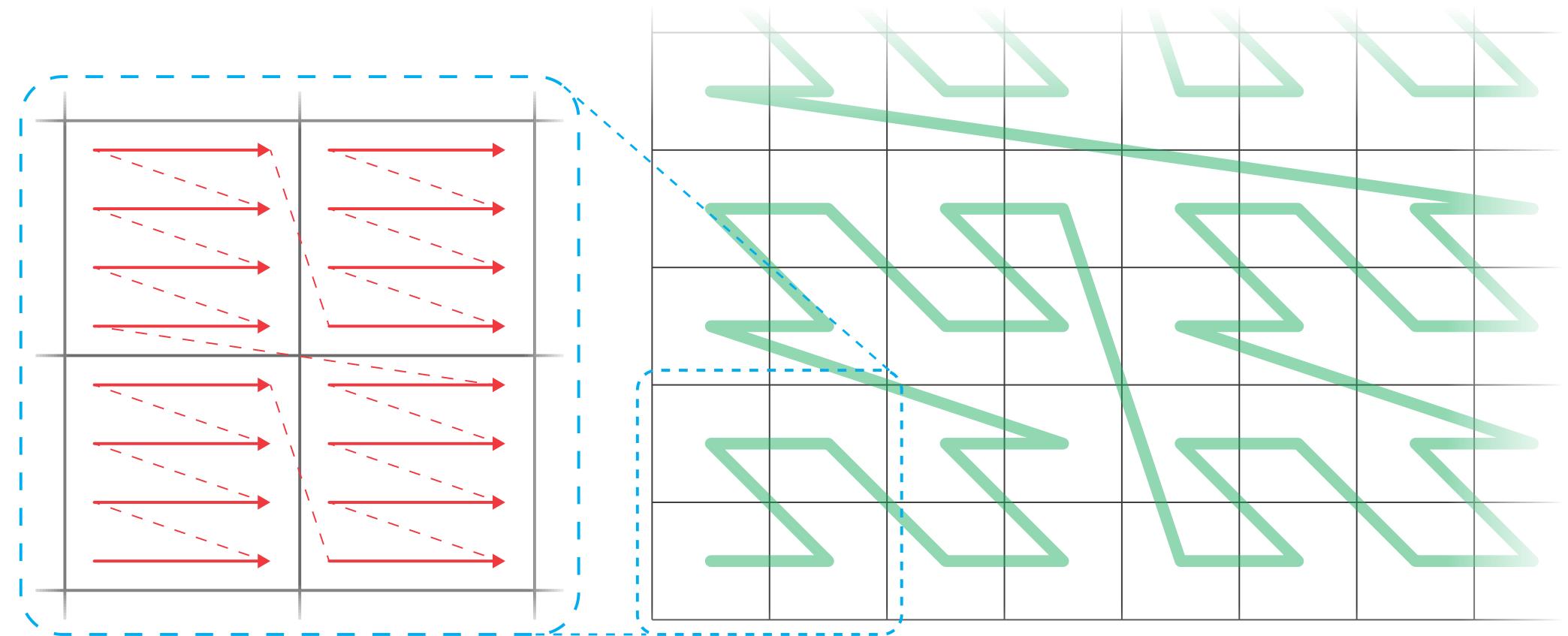


# Resorting && reordering

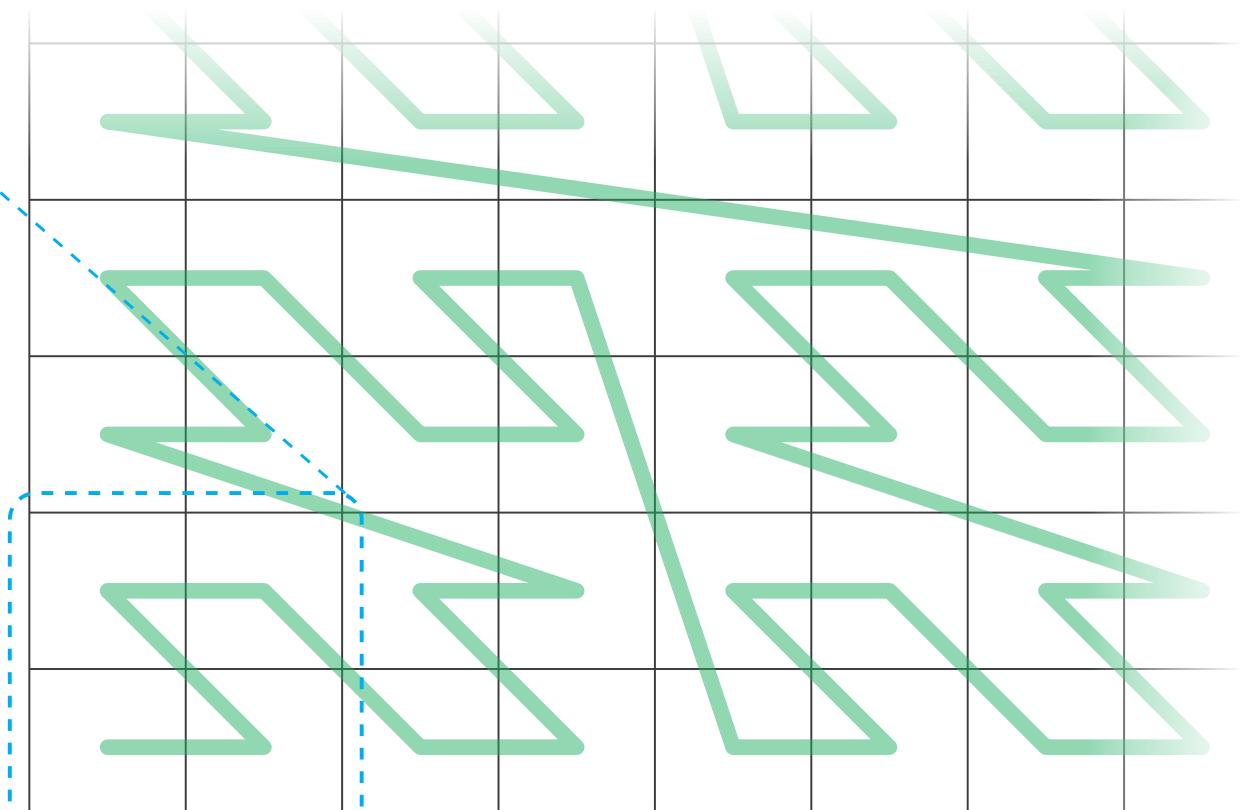
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# Particle storage

Lexicographical  
curve



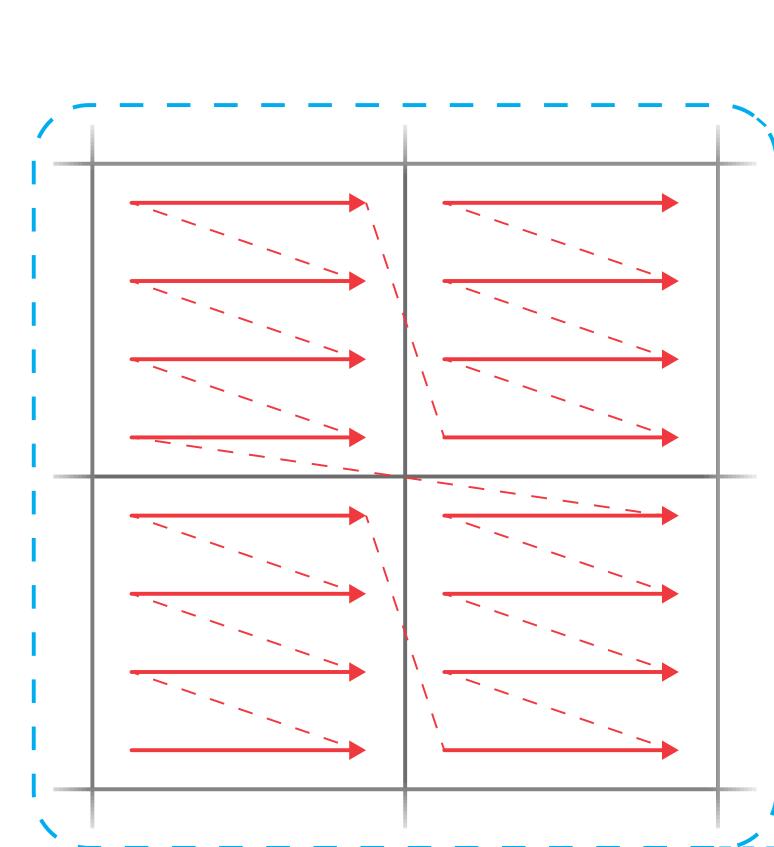
Morton coding  
curve



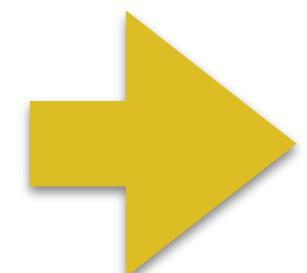
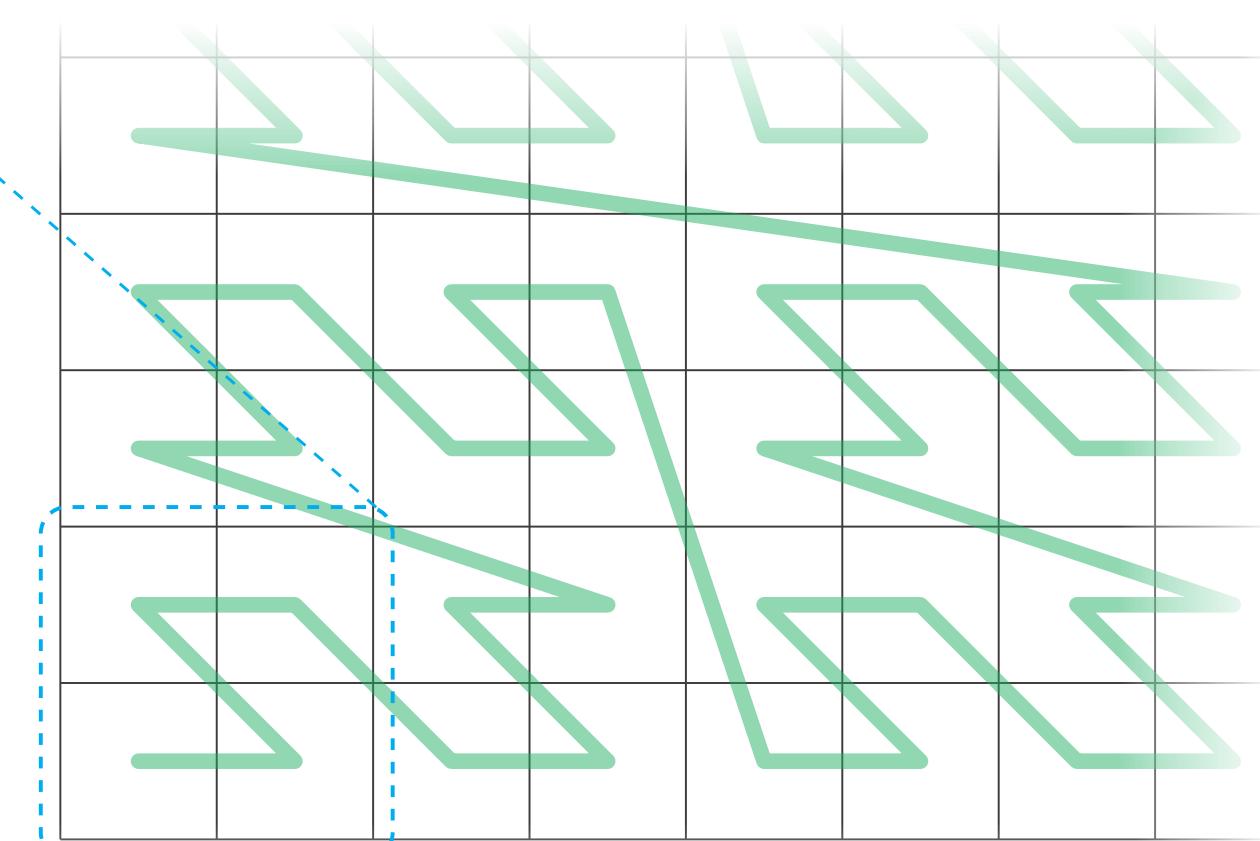
SPGrid  
Setaluri et al 2014

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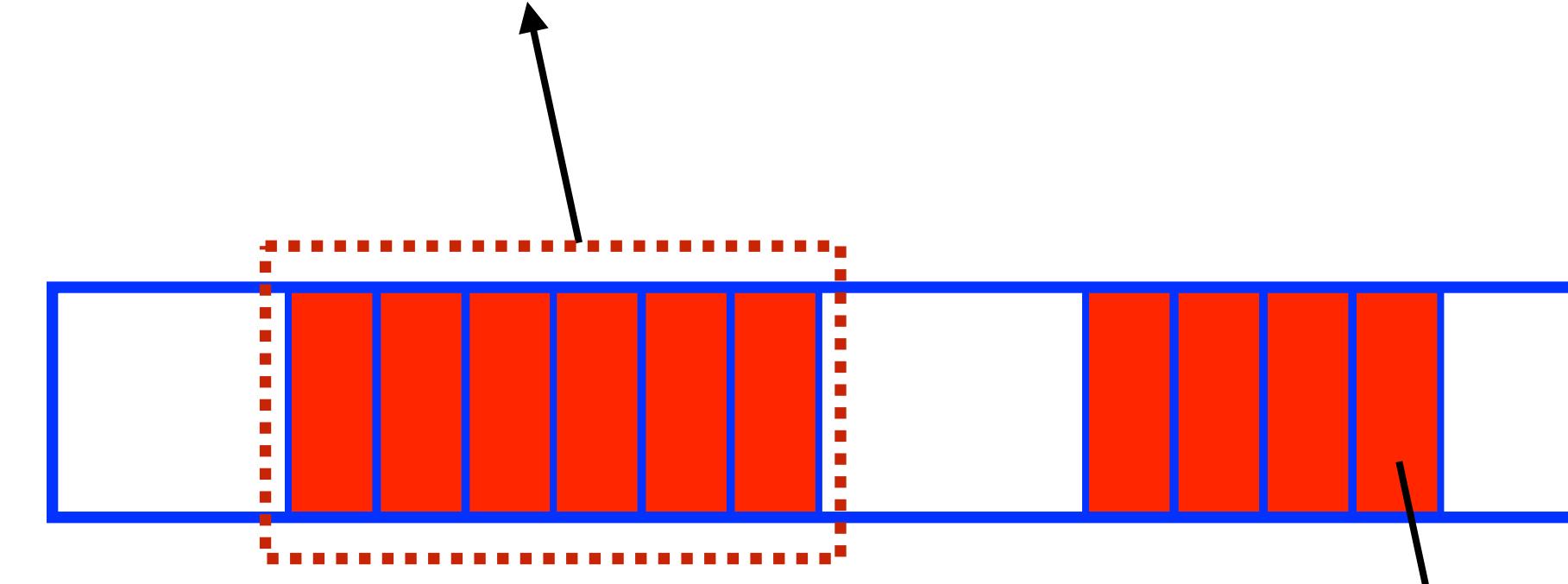


SPGrid

Setaluri et al 2014

Particles in one block

GPU memory



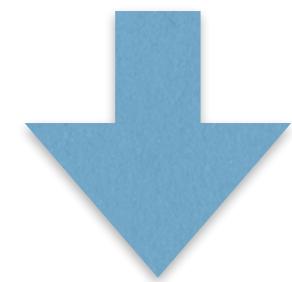
Particles in one cell

# Radix vs histogram

$(x,y,z) \longrightarrow (i,j,k) \longrightarrow$  64-bit offset

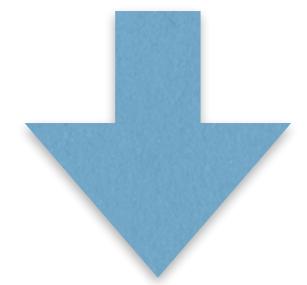
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$(x,y,z) \longrightarrow (i,j,k) \longrightarrow$  64-bit offset



# Radix vs histogram

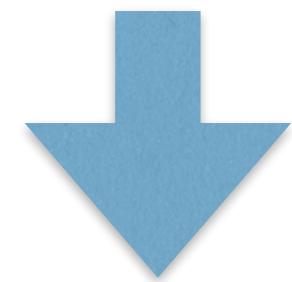
$(x,y,z) \longrightarrow (i,j,k) \longrightarrow$  64-bit offset



52 bits + 12 bits

# Radix vs histogram

$(x,y,z) \longrightarrow (i,j,k) \longrightarrow$  64-bit offset

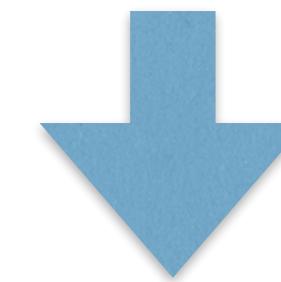


52 bits + 12 bits

Continuous bins + 12 bits

# Radix vs histogram

$(x,y,z) \longrightarrow (i,j,k) \longrightarrow$  64-bit offset

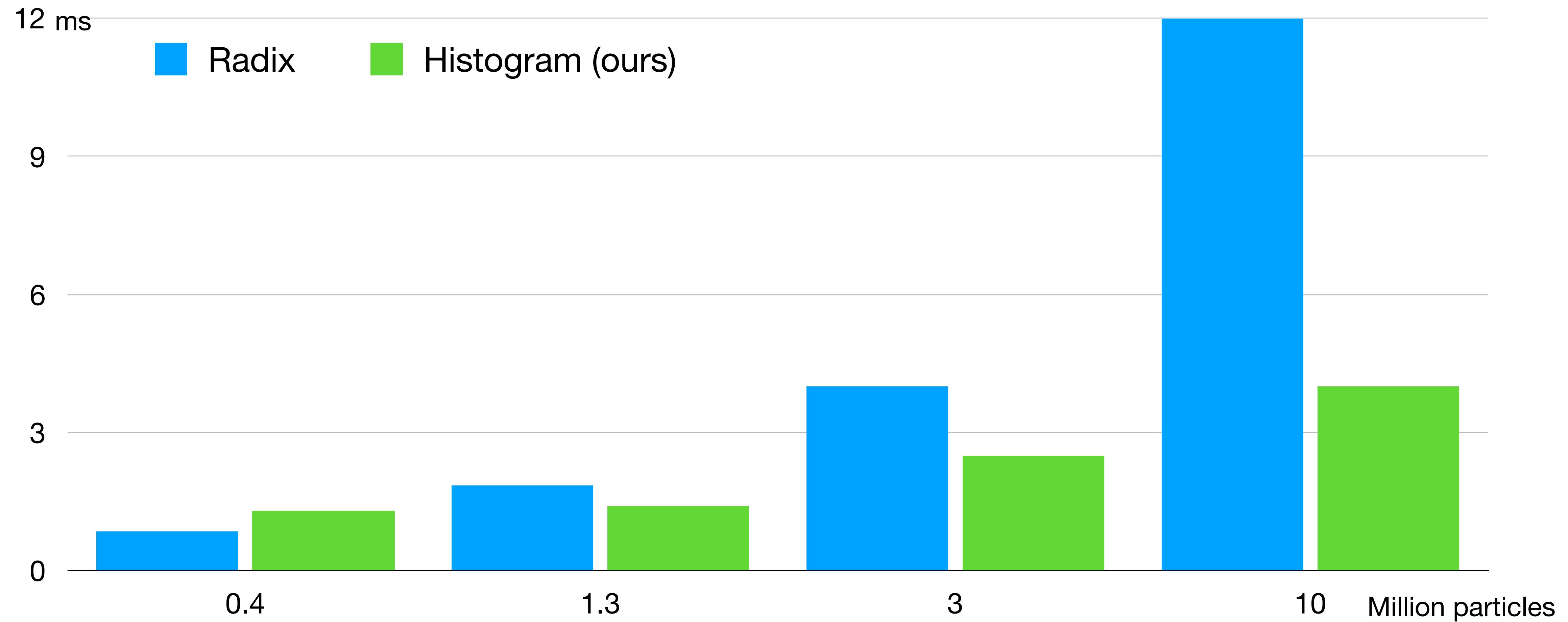


52 bits + 12 bits

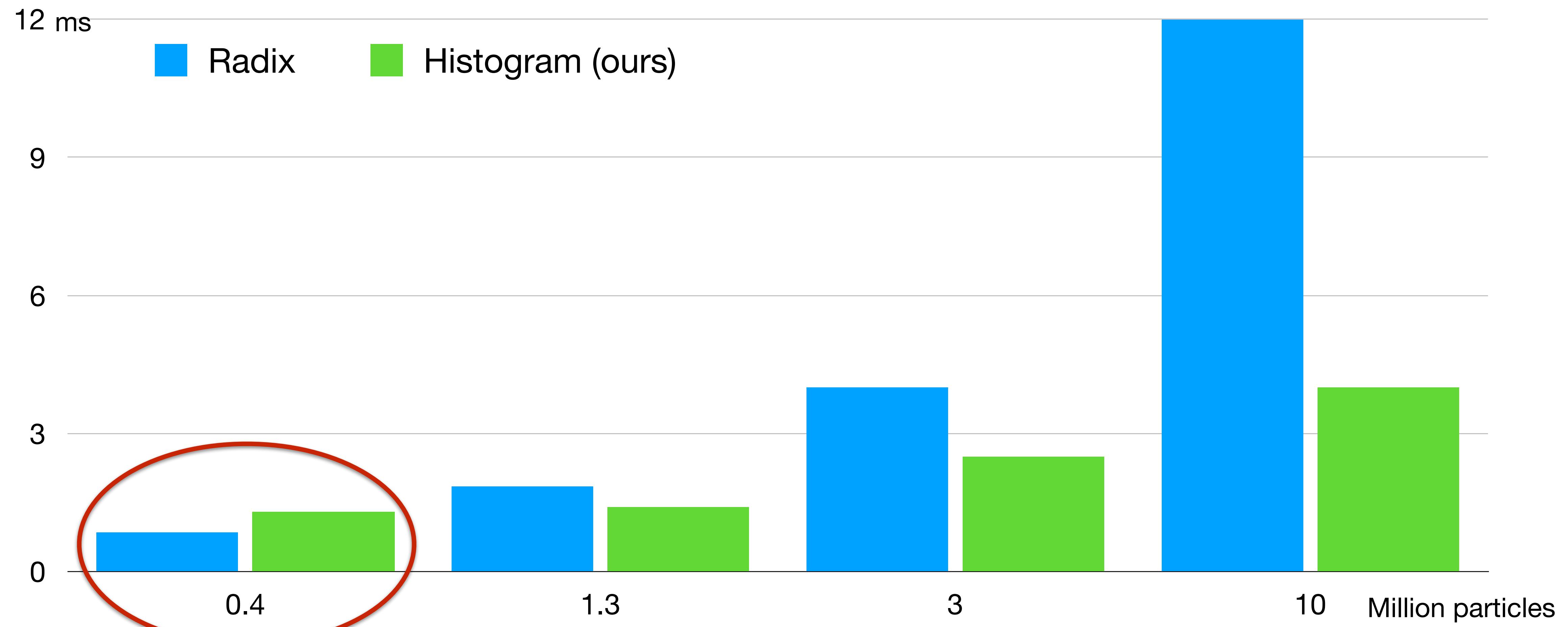
Sparsely occupied

Continuous bins + 12 bits

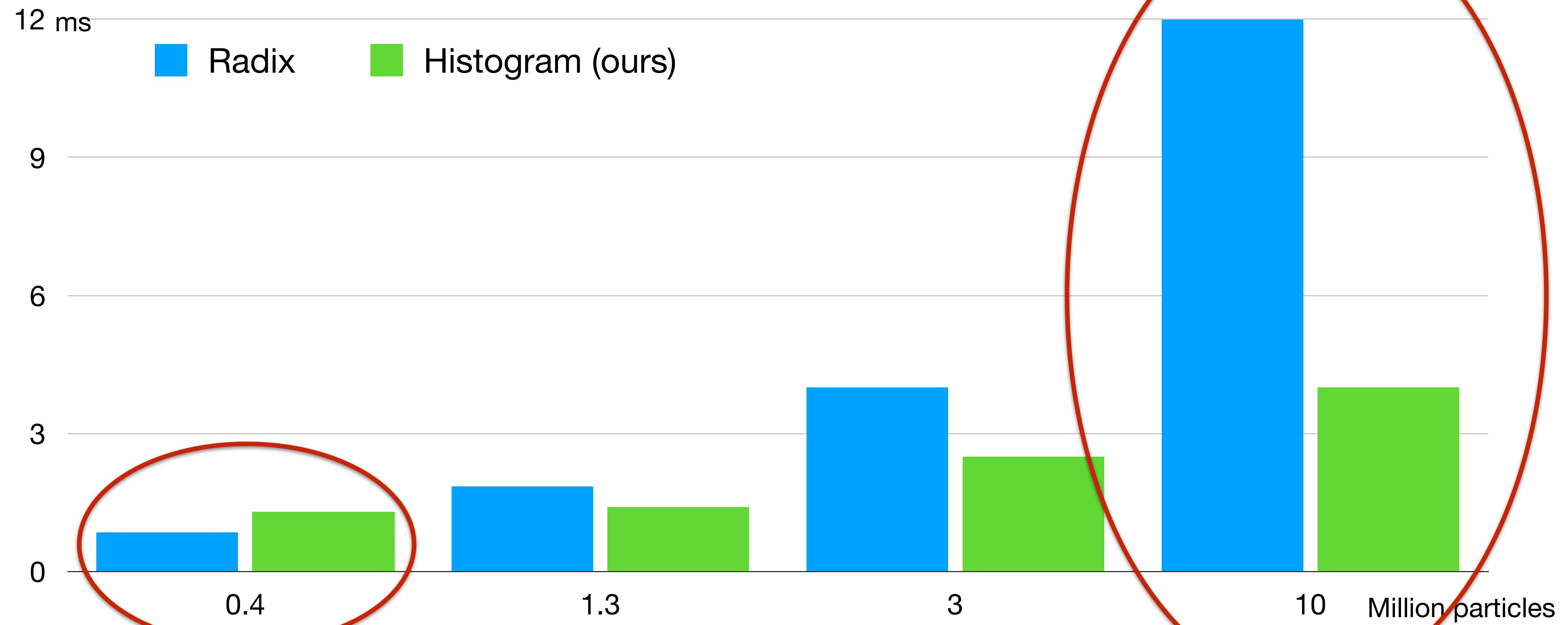
# Radix vs histogram



# Radix vs histogram



# Radix vs histogram

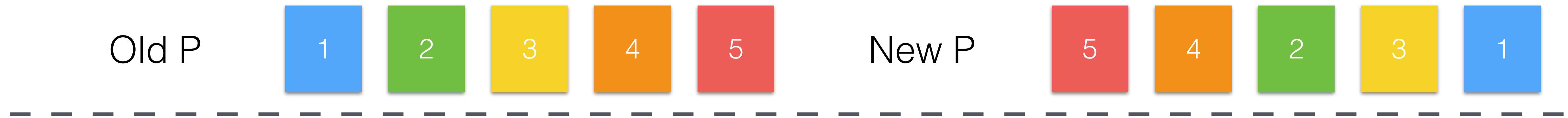


# Reordering - memory movement

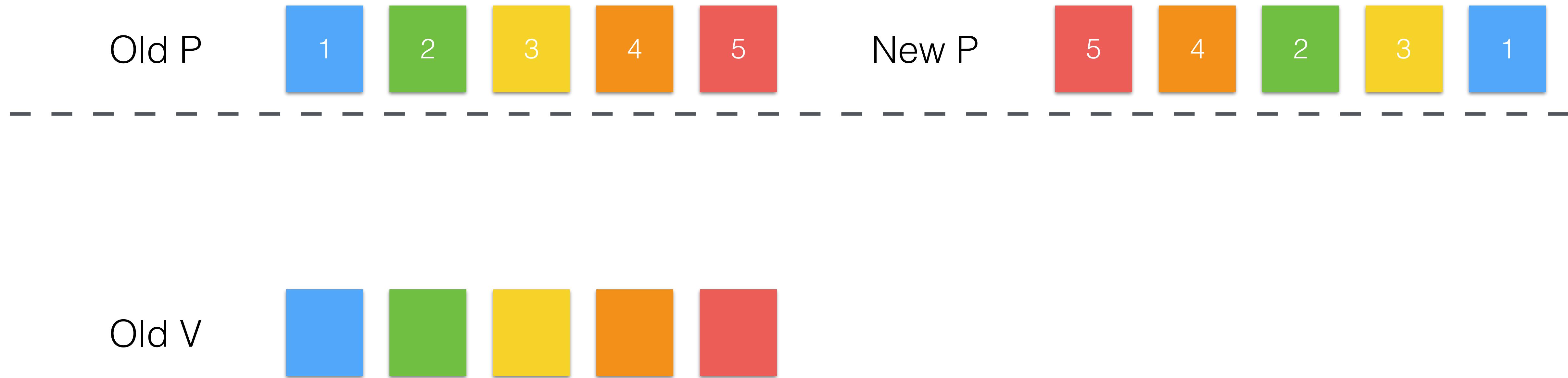
# Reordering - memory movement



# Reordering - memory movement



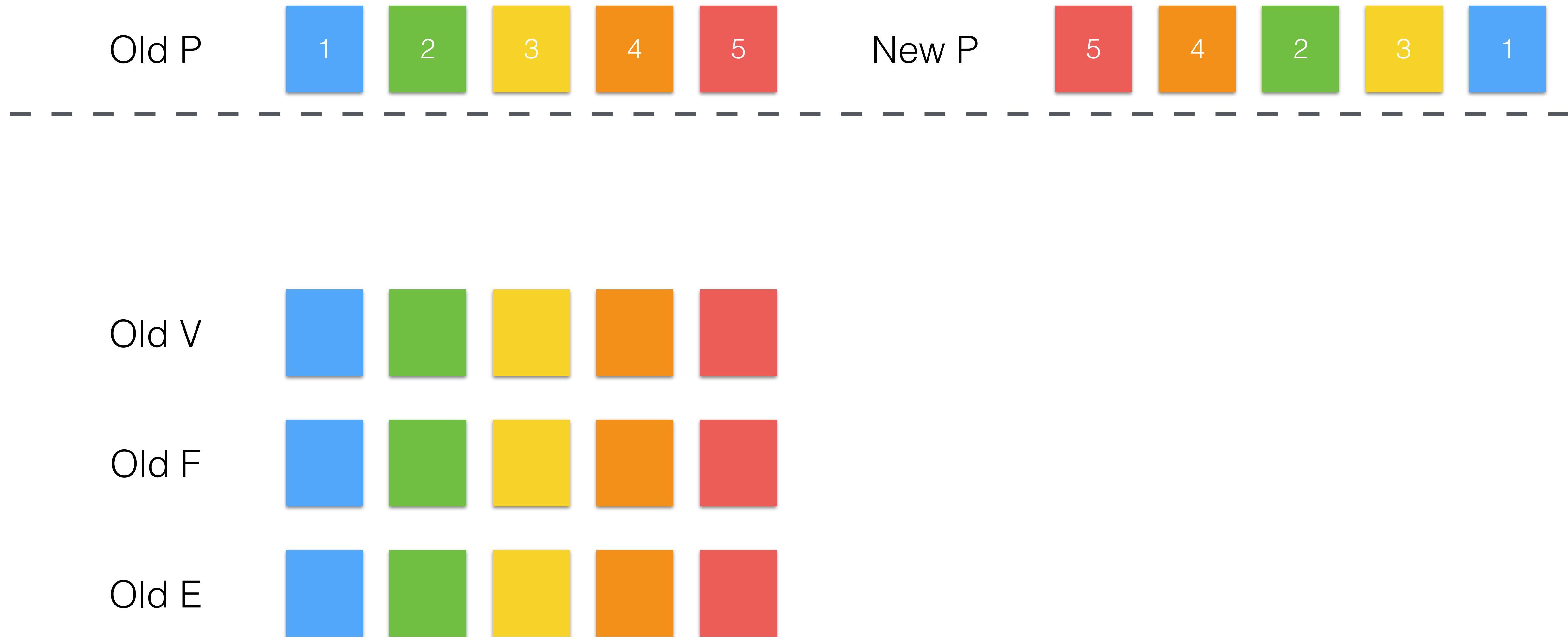
# Reordering - memory movement



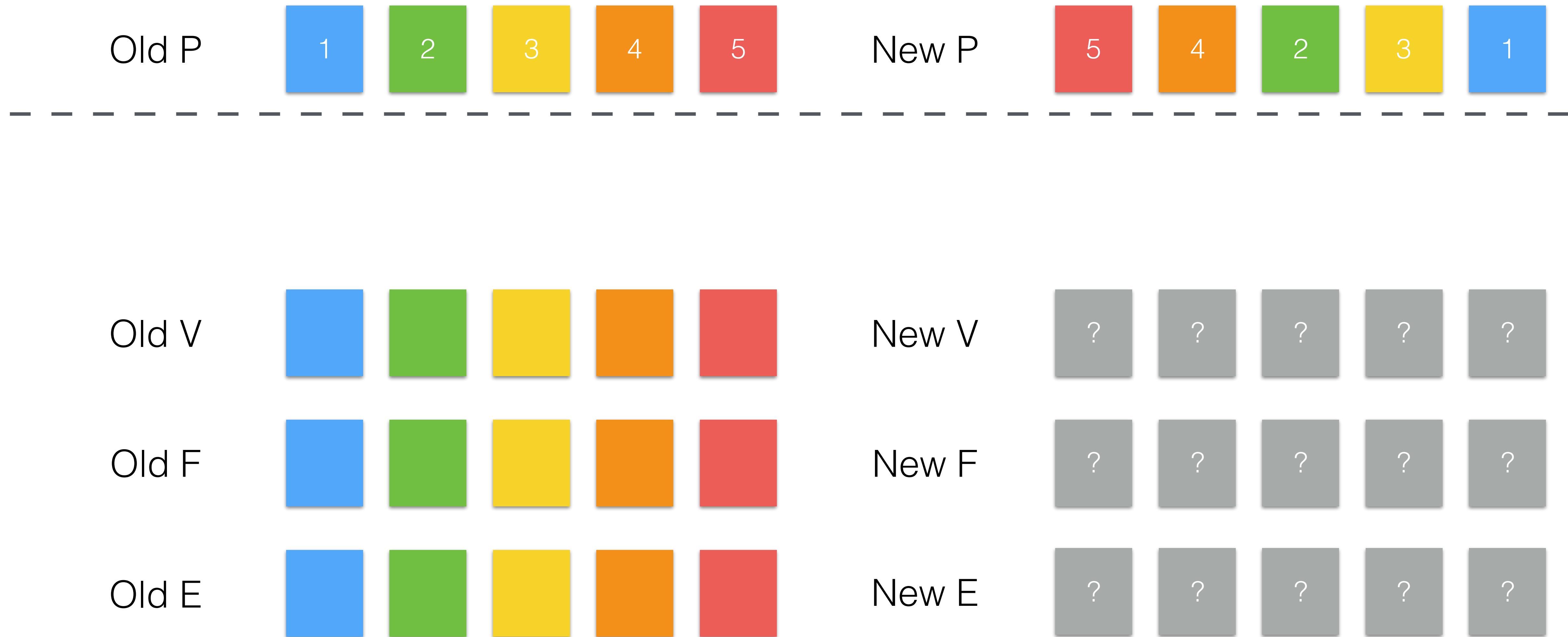
# Reordering - memory movement



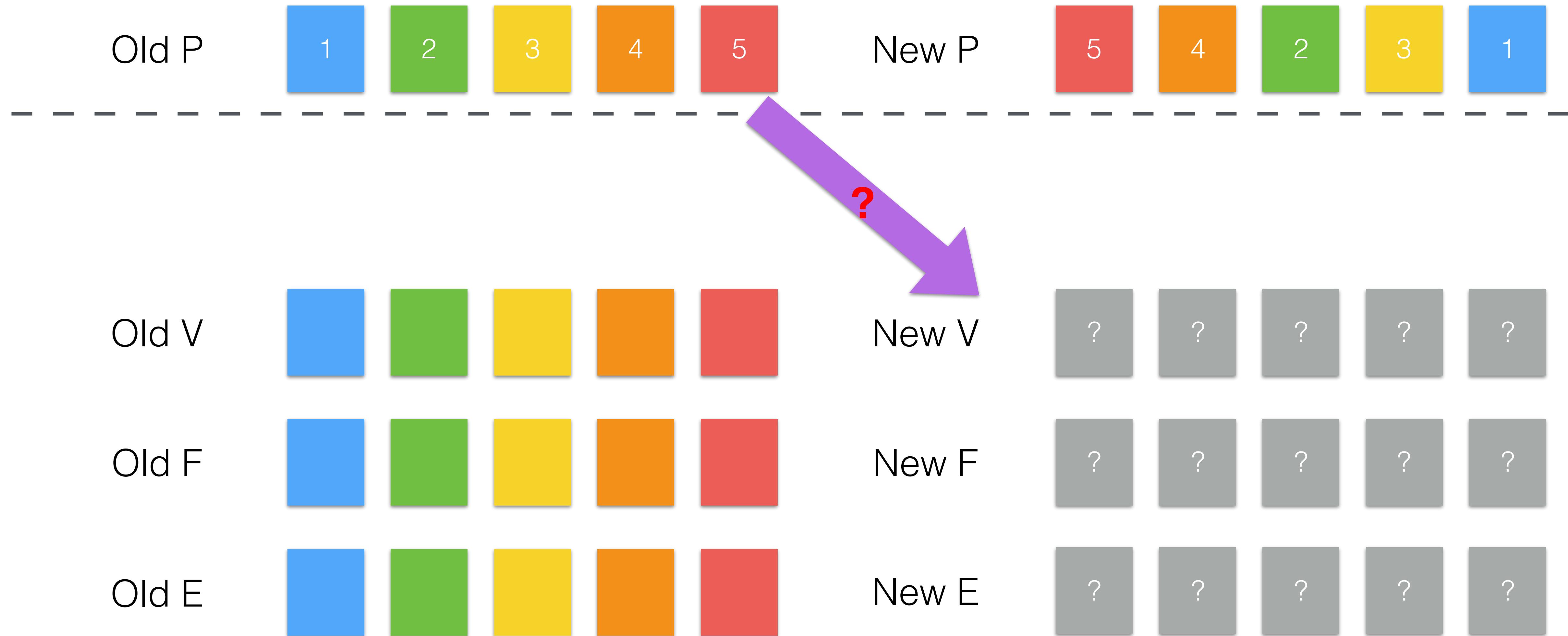
# Reordering - memory movement



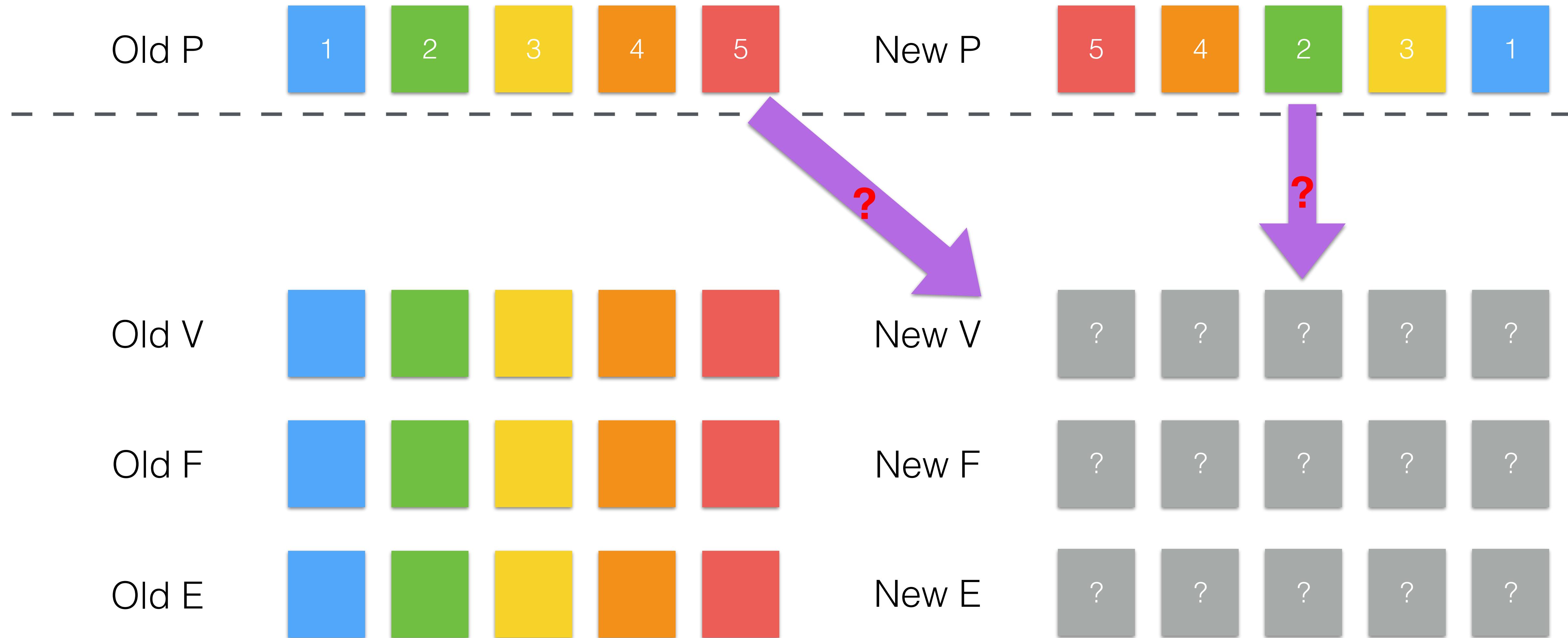
# Reordering - memory movement



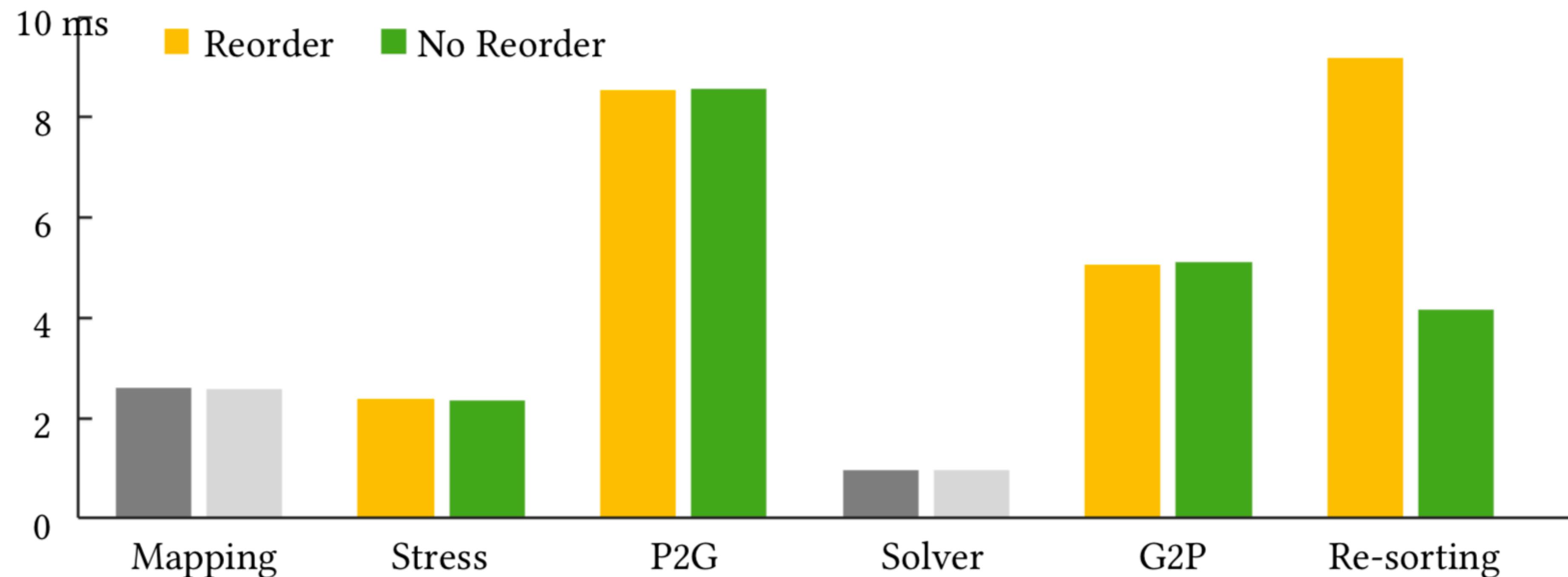
# Reordering - memory movement



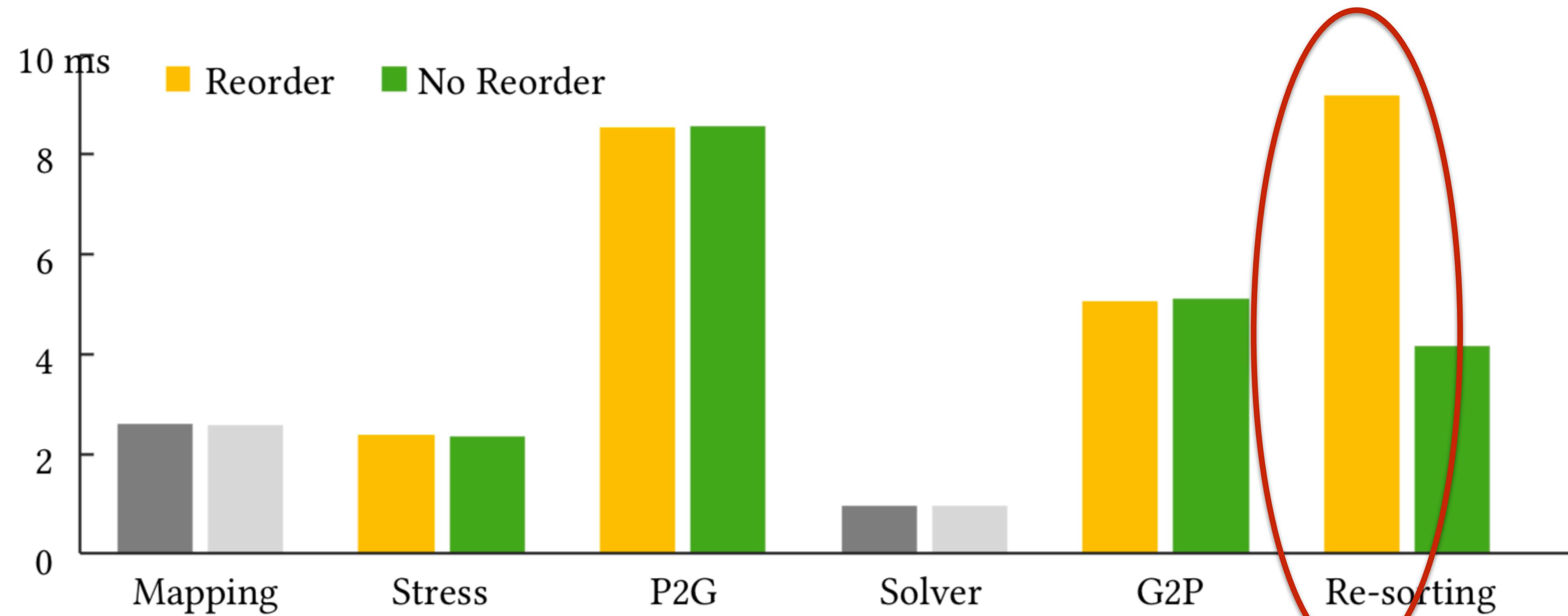
# Reordering - memory movement



# Pure memory operation - slow



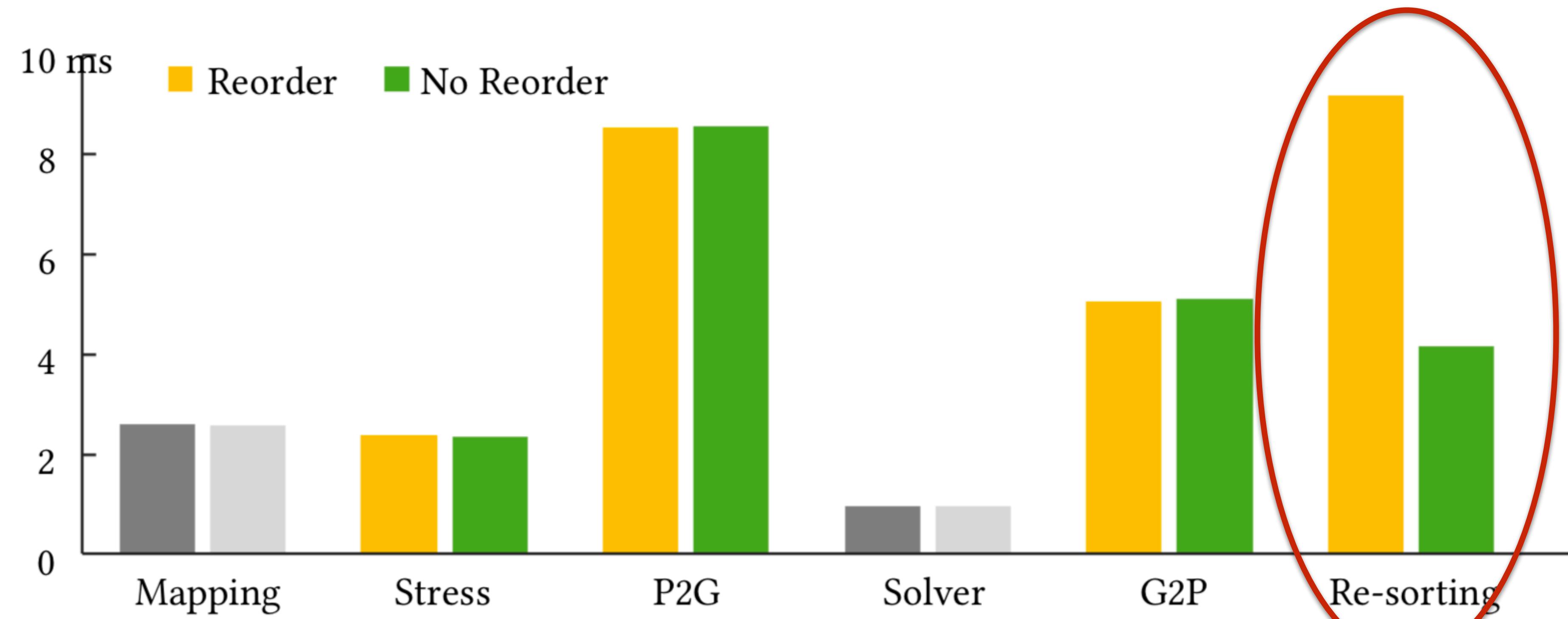
# Pure memory operation - slow



# Delayed reordering



# Delayed reordering



# Pure grid operations

```
1: procedure GPUMPM( )
2:   P  $\leftarrow$  Initialize particle positions
3:   P  $\leftarrow$  Sort and reorder (P)
4:   for each time step do
5:     dt  $\leftarrow$  Compute dt (P)
6:     G  $\leftarrow$  Refresh GSPGrid (P)
7:     M  $\leftarrow$  Build particle-grid mapping (P, G)
8:     G  $\leftarrow$  Transfer from particles to grid (P, M)
9:     G  $\leftarrow$  Apply external forces (G)
10:    G  $\leftarrow$  Solve on the grid (G, dt)
11:    P  $\leftarrow$  Transfer from grid to particles (G, M)
12:    P  $\leftarrow$  Update particle attributes (P, dt)
13:    P  $\leftarrow$  Resort and reorder (P)
```

# Pure grid operations

```
1: procedure GPUMPM( )  
2:   P  $\leftarrow$  Initialize particle positions  
3:   P  $\leftarrow$  Sort and reorder (P)  
4:   for each time step do  
5:     dt  $\leftarrow$  Compute dt (P)  
6:     G  $\leftarrow$  Refresh GSPGrid (P)  
7:     M  $\leftarrow$  Build particle-grid mapping (P, G)  
8:     G  $\leftarrow$  Transfer from particles to grid (P, M)  
9:     G  $\leftarrow$  Apply external forces (G)  
10:    G  $\leftarrow$  Solve on the grid (G, dt)  
11:    P  $\leftarrow$  Transfer from grid to particles (G, M)  
12:    P  $\leftarrow$  Update particle attributes (P, dt)  
13:    P  $\leftarrow$  Resort and reorder (P)
```

Boundary condition

# Particle grid communications

```
1: procedure GPUMPM( )
2:   P  $\leftarrow$  Initialize particle positions
3:   P  $\leftarrow$  Sort and reorder (P)
4:   for each time step do
5:     dt  $\leftarrow$  Compute dt (P)
6:     G  $\leftarrow$  Refresh GSPGrid (P)
7:     M  $\leftarrow$  Build particle-grid mapping (P, G)
8:     G  $\leftarrow$  Transfer from particles to grid (P, M)
9:     G  $\leftarrow$  Apply external forces (G)
10:    G  $\leftarrow$  Solve on the grid (G, dt)
11:    P  $\leftarrow$  Transfer from grid to particles (G, M)
12:    P  $\leftarrow$  Update particle attributes (P, dt)
13:    P  $\leftarrow$  Resort and reorder (P)
```

# Particle grid communications

```
1: procedure GPUMPM( )
2:   P  $\leftarrow$  Initialize particle positions
3:   P  $\leftarrow$  Sort and reorder (P)
4:   for each time step do
5:     dt  $\leftarrow$  Compute dt (P)
6:     G  $\leftarrow$  Refresh GSPGrid (P) (highlighted)
7:     M  $\leftarrow$  Build particle-grid mapping (P, G) (highlighted)
8:     G  $\leftarrow$  Transfer from particles to grid (P, M) (highlighted)
9:     G  $\leftarrow$  Apply external forces (G)
10:    G  $\leftarrow$  Solve on the grid (G, dt)
11:    P  $\leftarrow$  Transfer from grid to particles (G, M) (highlighted)
12:    P  $\leftarrow$  Update particle attributes (P, dt)
13:    P  $\leftarrow$  Resort and reorder (P)
```

# Build particle-grid mapping

```
1: procedure GPUMPM( )
2:   P  $\leftarrow$  Initialize particle positions
3:   P  $\leftarrow$  Sort and reorder (P)
4:   for each time step do
5:     dt  $\leftarrow$  Compute dt (P)
6:     G  $\leftarrow$  Refresh GSPGrid (P)
7:     M  $\leftarrow$  Build particle-grid mapping (P, G)
8:     G  $\leftarrow$  Transfer from particles to grid (P, M)
9:     G  $\leftarrow$  Apply external forces (G)
10:    G  $\leftarrow$  Solve on the grid (G, dt)
11:    P  $\leftarrow$  Transfer from grid to particles (G, M)
12:    P  $\leftarrow$  Update particle attributes (P, dt)
13:    P  $\leftarrow$  Resort and reorder (P)
```

# Build particle-grid mapping

```
1: procedure GPUMPM( )
2:   P  $\leftarrow$  Initialize particle positions
3:   P  $\leftarrow$  Sort and reorder (P)
4:   for each time step do
5:     dt  $\leftarrow$  Compute dt (P)
6:     G  $\leftarrow$  Refresh GSPGrid (P)
7:     M  $\leftarrow$  Build particle-grid mapping (P, G)
8:     G  $\leftarrow$  Transfer from particles to grid (P, M)
9:     G  $\leftarrow$  Apply external forces (G)
10:    G  $\leftarrow$  Solve on the grid (G, dt)
11:    P  $\leftarrow$  Transfer from grid to particles (G, M)
12:    P  $\leftarrow$  Update particle attributes (P, dt)
13:    P  $\leftarrow$  Resort and reorder (P)
```

Particles <->  
nodes

# Build particle-grid mapping

```
1: procedure GPUMPM( )  
2:   P  $\leftarrow$  Initialize particle positions  
3:   P  $\leftarrow$  Sort and reorder (P)  
4:   for each time step do  
5:     dt  $\leftarrow$  Compute dt (P)  
6:     G  $\leftarrow$  Refresh GSPGrid (P) Particles <-> nodes  
7:     M  $\leftarrow$  Build particle-grid mapping (P, G) Particles <-> blocks  
8:     G  $\leftarrow$  Transfer from particles to grid (P, M)  
9:     G  $\leftarrow$  Apply external forces (G)  
10:    G  $\leftarrow$  Solve on the grid (G, dt)  
11:    P  $\leftarrow$  Transfer from grid to particles (G, M)  
12:    P  $\leftarrow$  Update particle attributes (P, dt)  
13:    P  $\leftarrow$  Resort and reorder (P)
```

# Particle to grid (P2G)

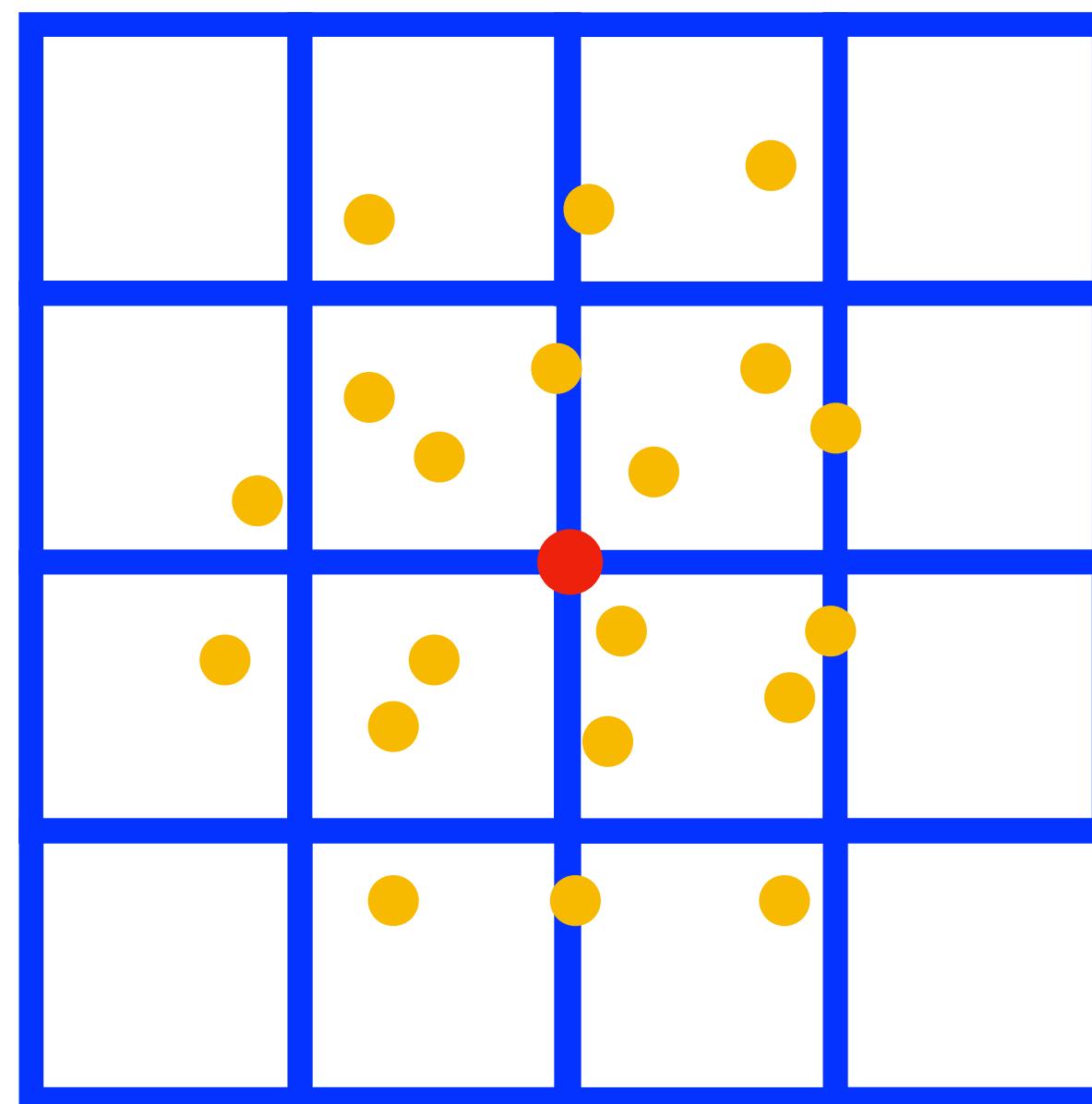
```
1: procedure GPUMPM( )
2:   P  $\leftarrow$  Initialize particle positions
3:   P  $\leftarrow$  Sort and reorder (P)
4:   for each time step do
5:     dt  $\leftarrow$  Compute dt (P)
6:     G  $\leftarrow$  Refresh GSPGrid (P)
7:     M  $\leftarrow$  Build particle-grid mapping (P, G)
8:     G  $\leftarrow$  Transfer from particles to grid (P, M)
9:     G  $\leftarrow$  Apply external forces (G)
10:    G  $\leftarrow$  Solve on the grid (G, dt)
11:    P  $\leftarrow$  Transfer from grid to particles (G, M)
12:    P  $\leftarrow$  Update particle attributes (P, dt)
13:    P  $\leftarrow$  Resort and reorder (P)
```

# Particle to grid (P2G)

```
1: procedure GPUMPM( )
2:   P  $\leftarrow$  Initialize particle positions
3:   P  $\leftarrow$  Sort and reorder (P)
4:   for each time step do
5:     dt  $\leftarrow$  Compute dt (P)
6:     G  $\leftarrow$  Refresh GSPGrid (P)
7:     M  $\leftarrow$  Build particle-grid mapping (P, G)
8:     G  $\leftarrow$  Transfer from particles to grid (P, M)
9:     G  $\leftarrow$  Apply external forces (G)
10:    G  $\leftarrow$  Solve on the grid (G, dt)
11:    P  $\leftarrow$  Transfer from grid to particles (G, M)
12:    P  $\leftarrow$  Update particle attributes (P, dt)
13:    P  $\leftarrow$  Resort and reorder (P)
```

B-Spline

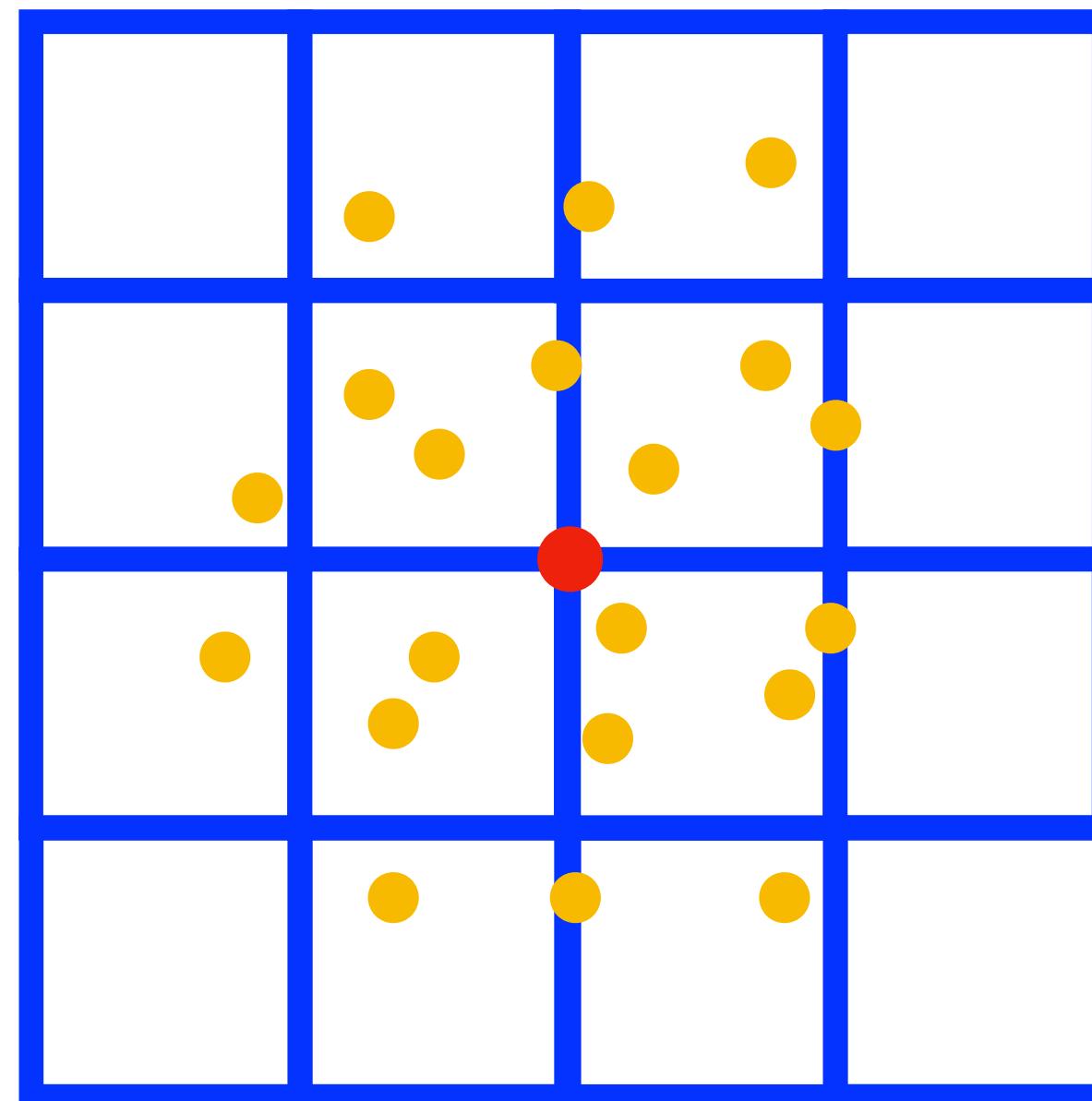
# Particle V.S. node per thread



CUDA thread - grid node



# Particle V.S. node per thread

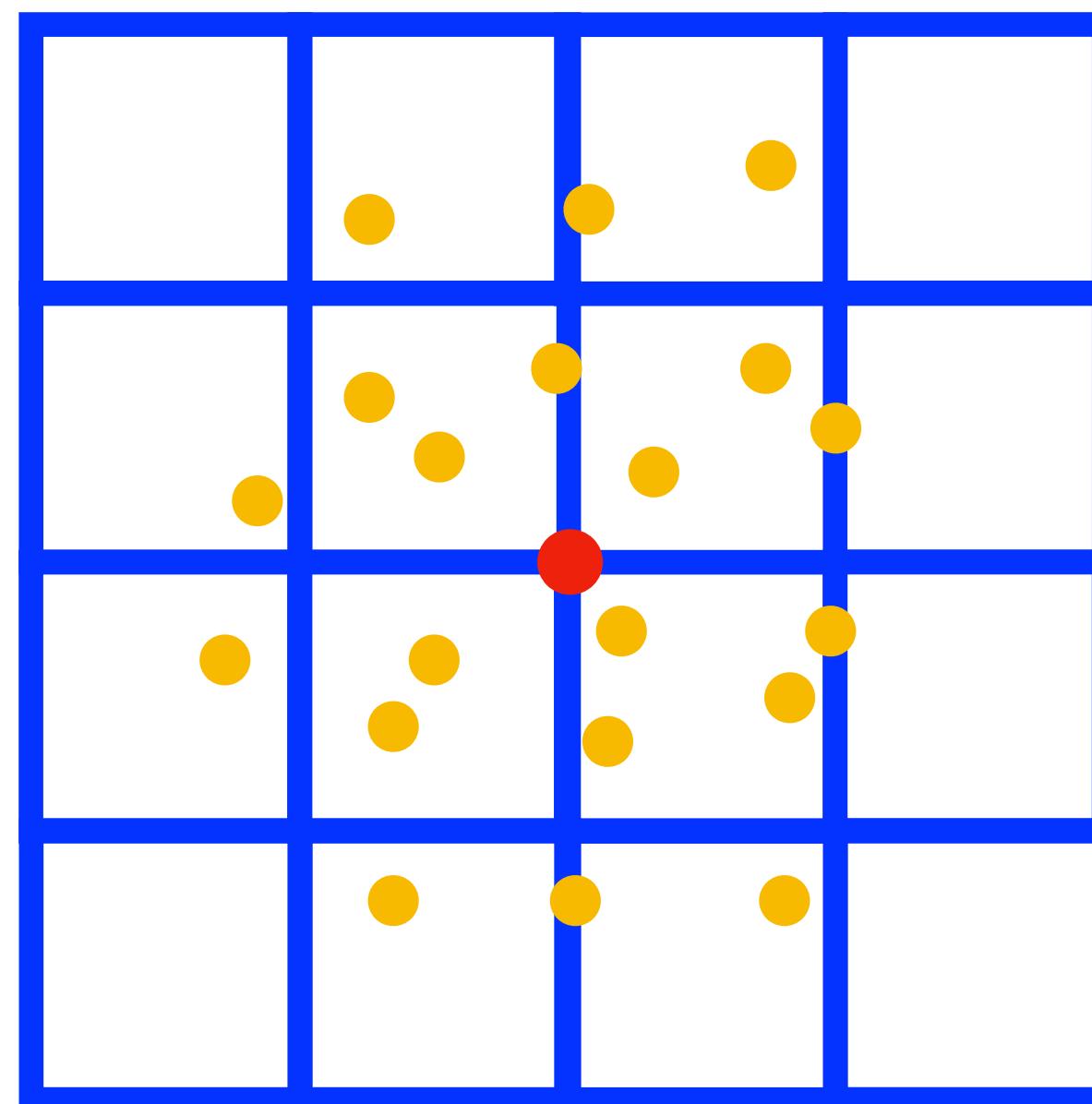


CUDA thread - grid node

v.s.



# Particle V.S. node per thread



CUDA thread - grid node



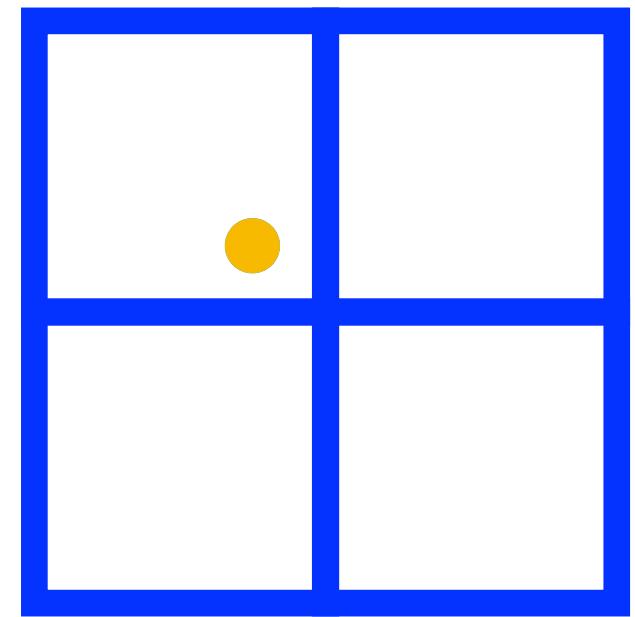
v.s.

CUDA thread - particle



# Scattering V.S. gathering

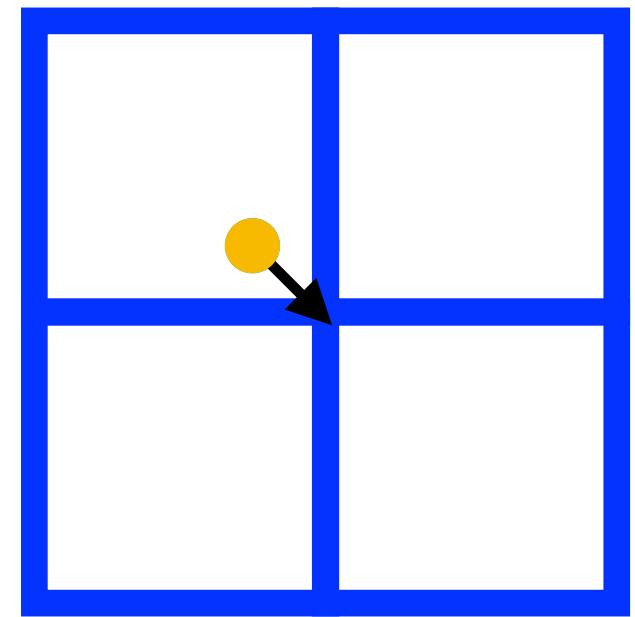
Particle  
Grid node



CUDA thread - ●

# Scattering V.S. gathering

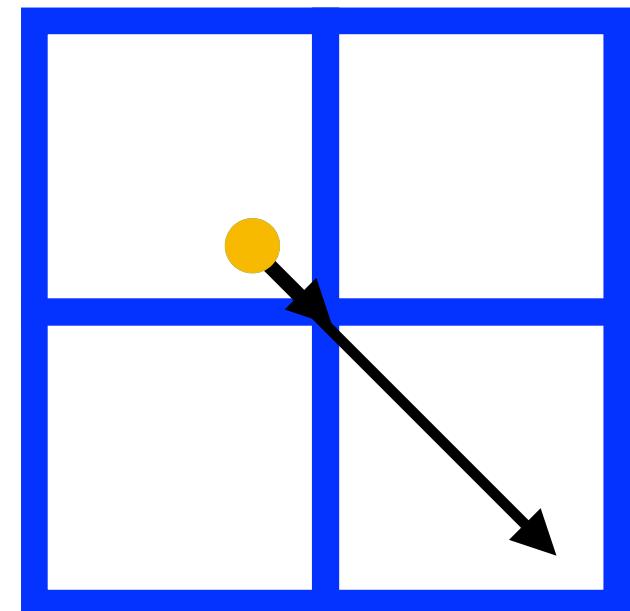
Particle  
Grid node



CUDA thread - ●

# Scattering V.S. gathering

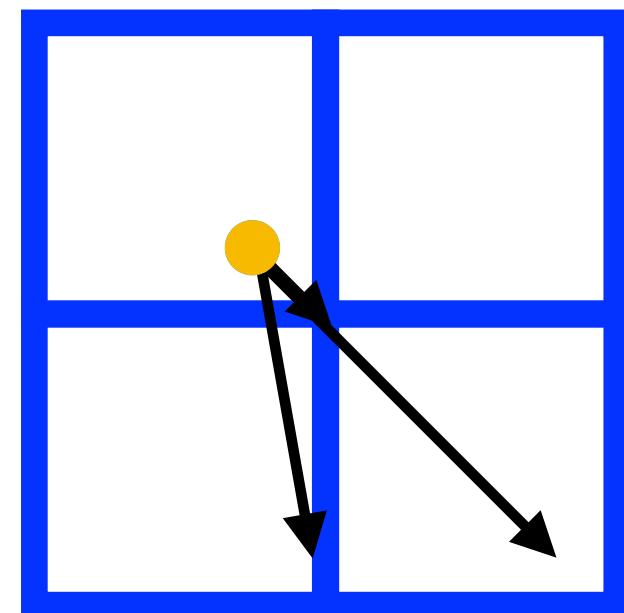
Particle  
Grid node



CUDA thread - ●

# Scattering V.S. gathering

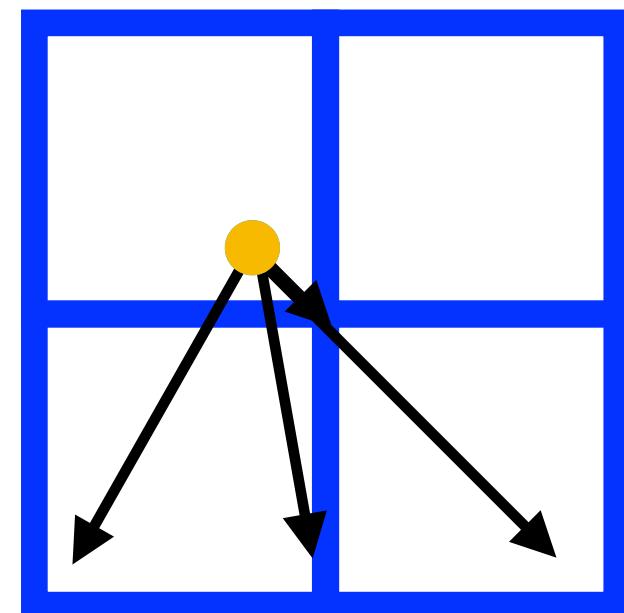
Particle  
Grid node



CUDA thread - ●

# Scattering V.S. gathering

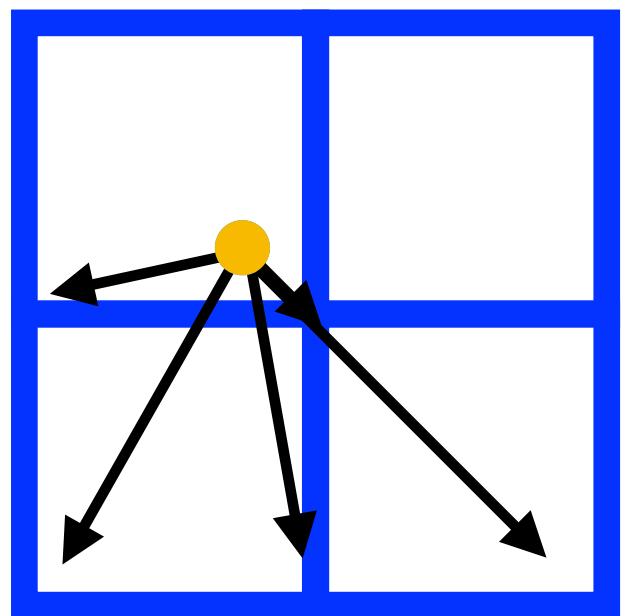
Particle  
Grid node



CUDA thread - ●

# Scattering V.S. gathering

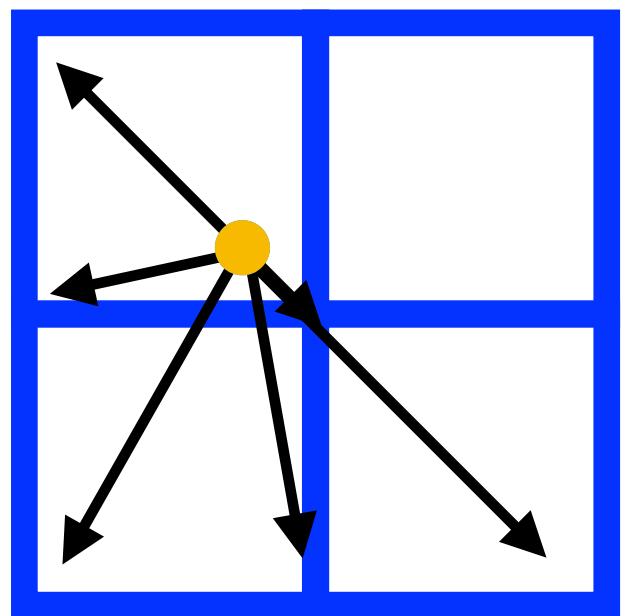
Particle  
Grid node



CUDA thread - ●

# Scattering V.S. gathering

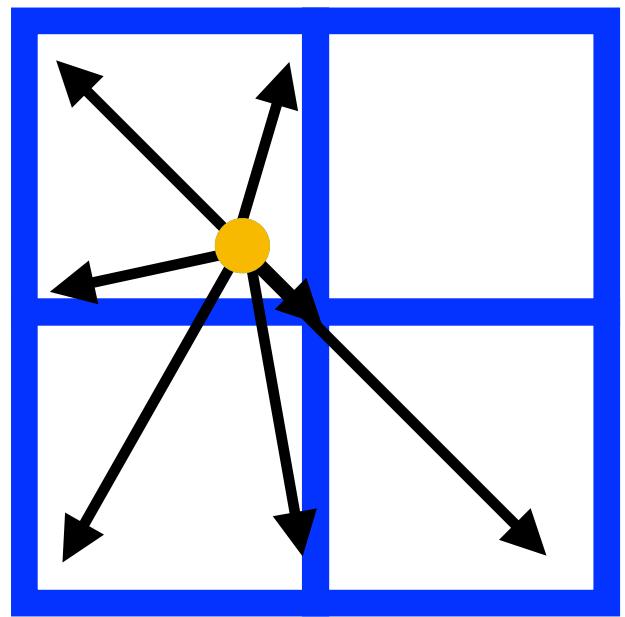
Particle  
Grid node



CUDA thread - ●

# Scattering V.S. gathering

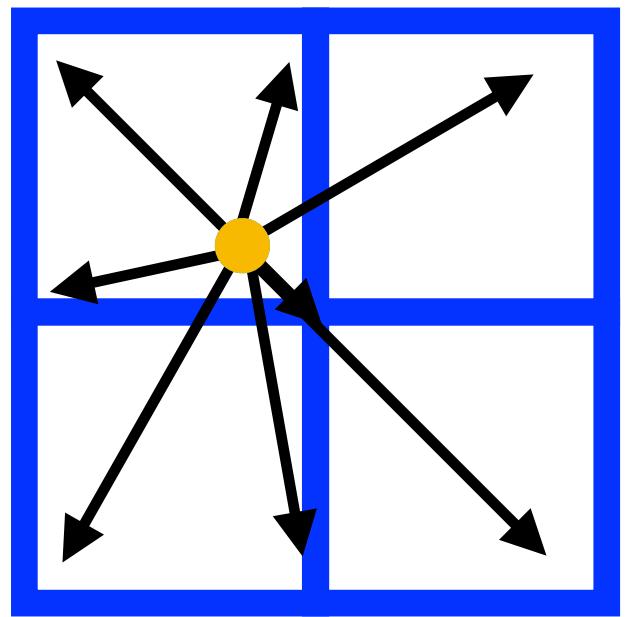
Particle  
Grid node



CUDA thread - ●

# Scattering V.S. gathering

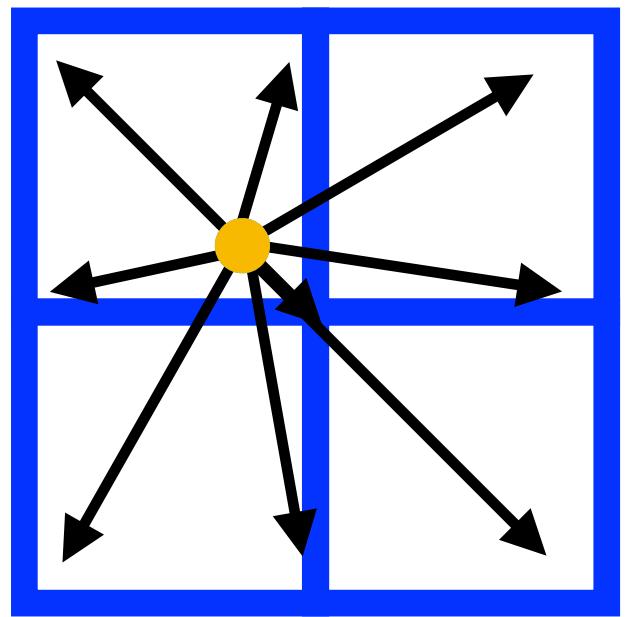
Particle  
Grid node



CUDA thread - ●

# Scattering V.S. gathering

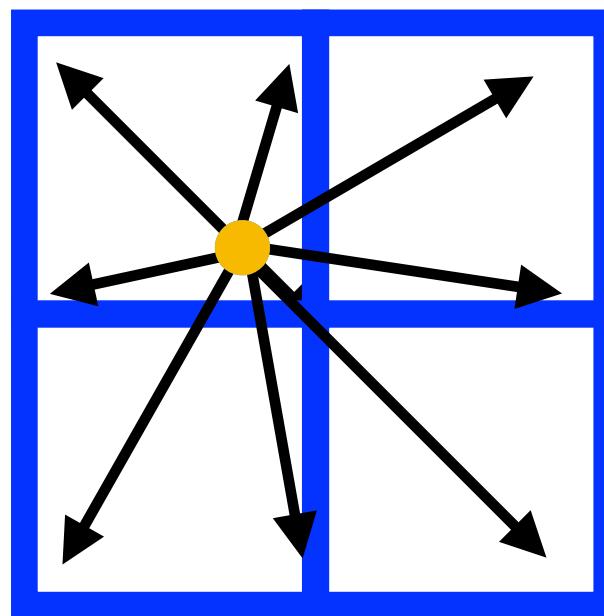
Particle  
Grid node



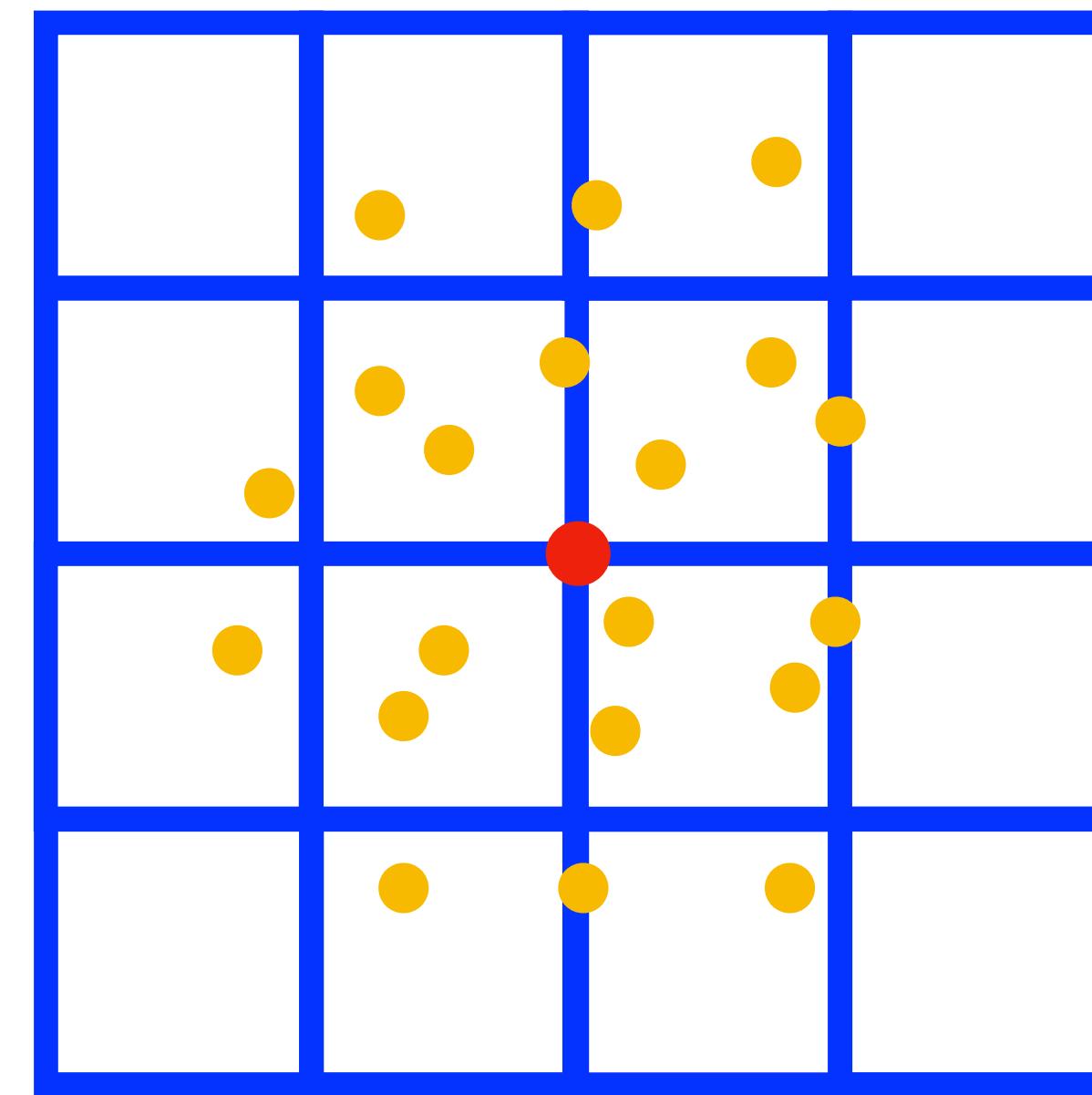
CUDA thread - ●

# Scattering V.S. gathering

Particle  
Grid node



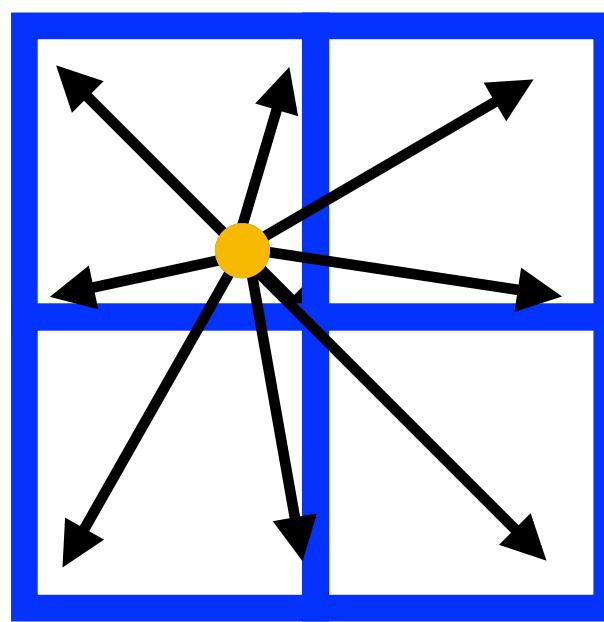
CUDA thread - ●



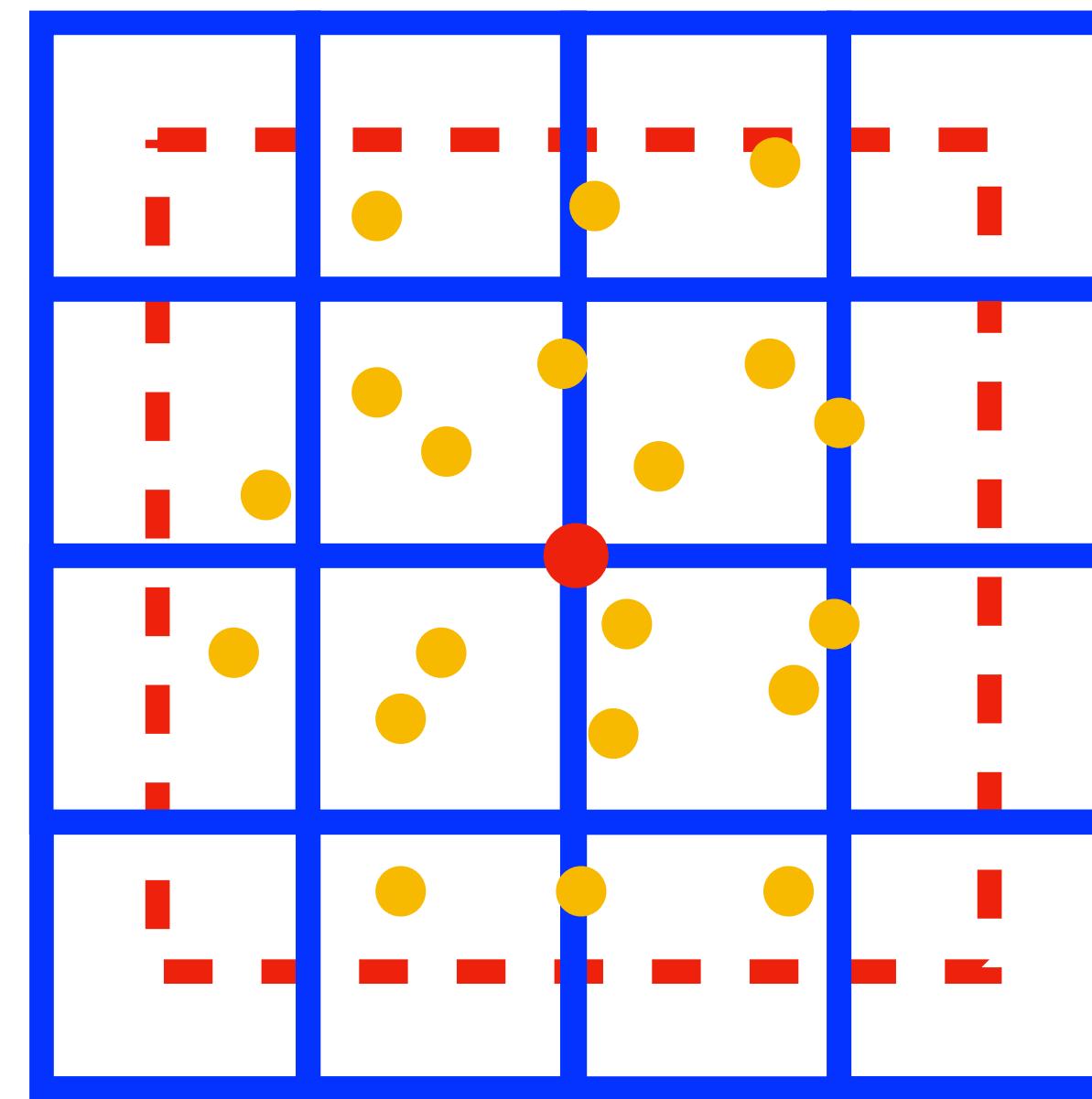
CUDA thread - ●

# Scattering V.S. gathering

Particle  
Grid node



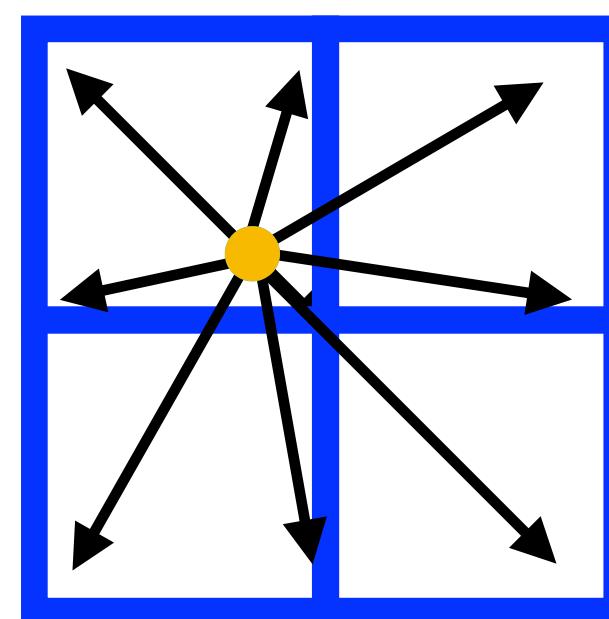
CUDA thread - ●



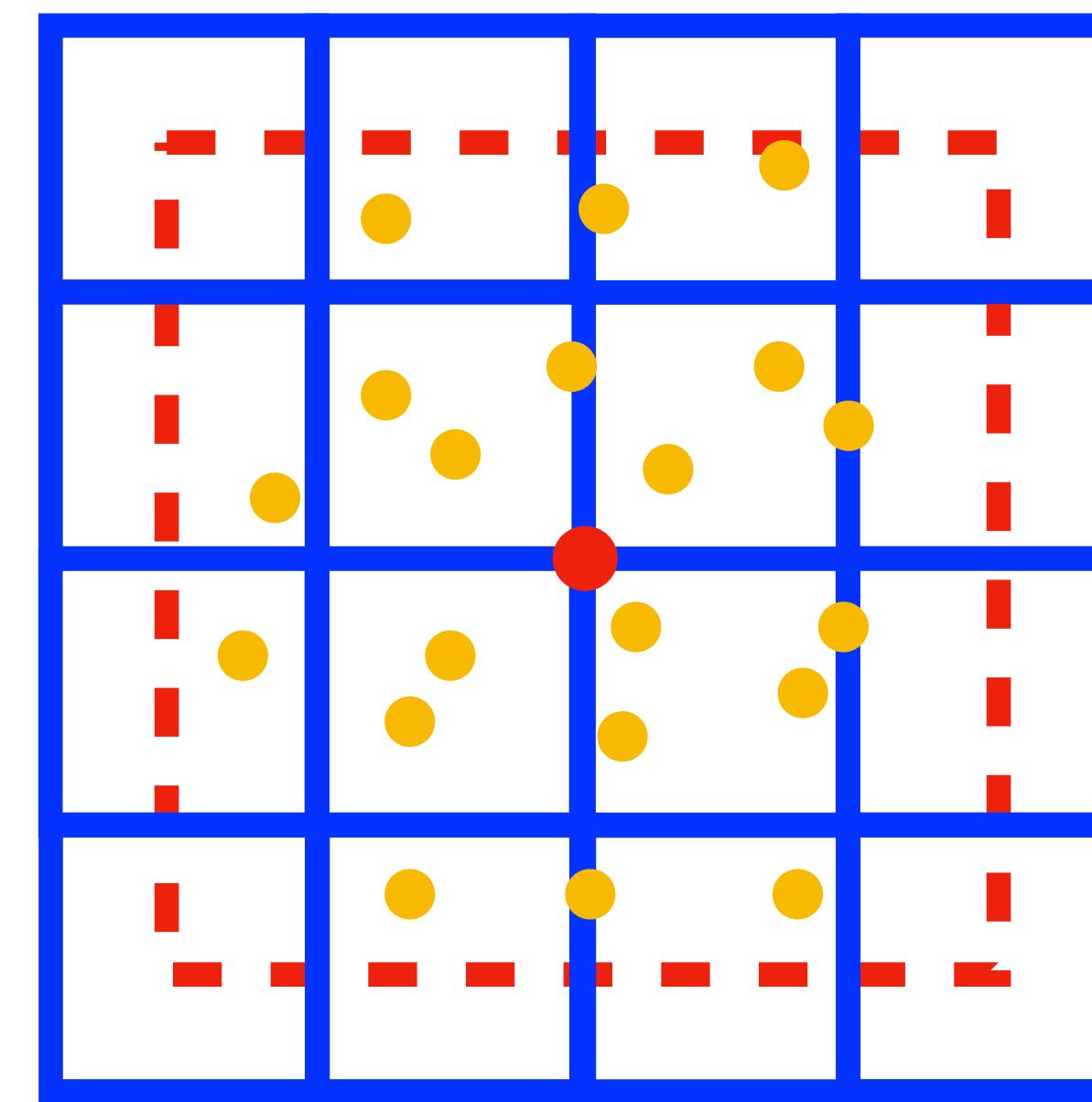
CUDA thread - ●

# Scattering V.S. gathering

Particle  
Grid node



CUDA thread - ●



CUDA thread - ●

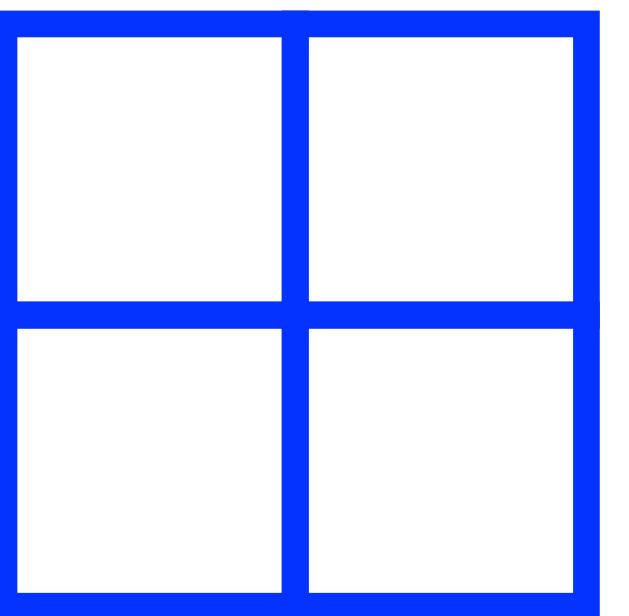
Particle list for a node - ● ● ● ● ● ● ● ● ● ● ● ●

# Gathering - thread divergence



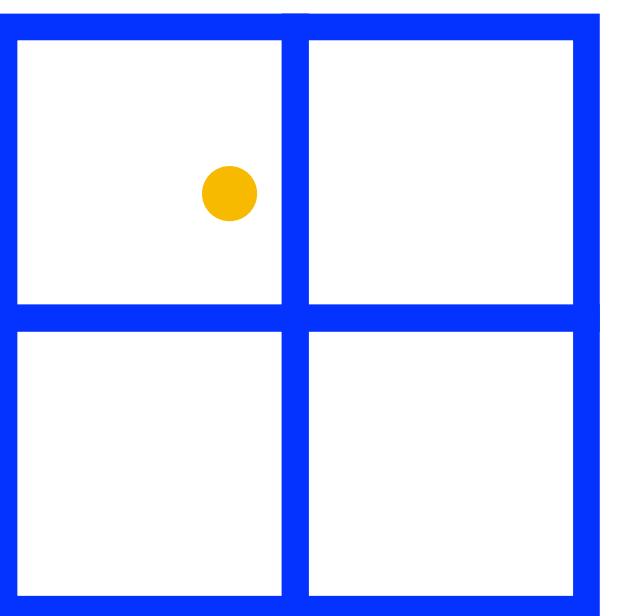
# Write hazard

Particle  
Grid node



# Write hazard

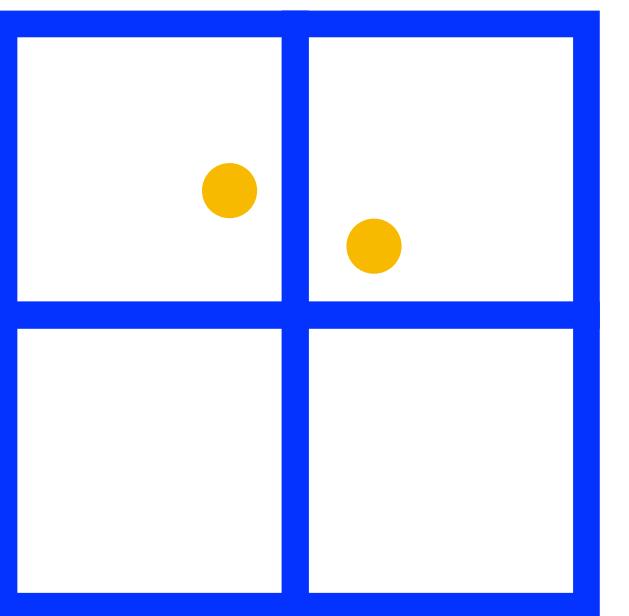
Particle  
Grid node



Thread 1 •

# Write hazard

Particle  
Grid node

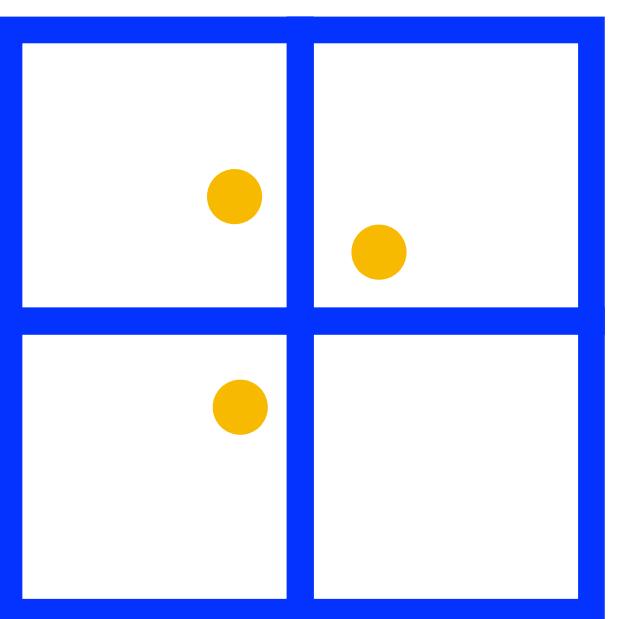


Thread 1 •

Thread 2 •

# Write hazard

Particle  
Grid node



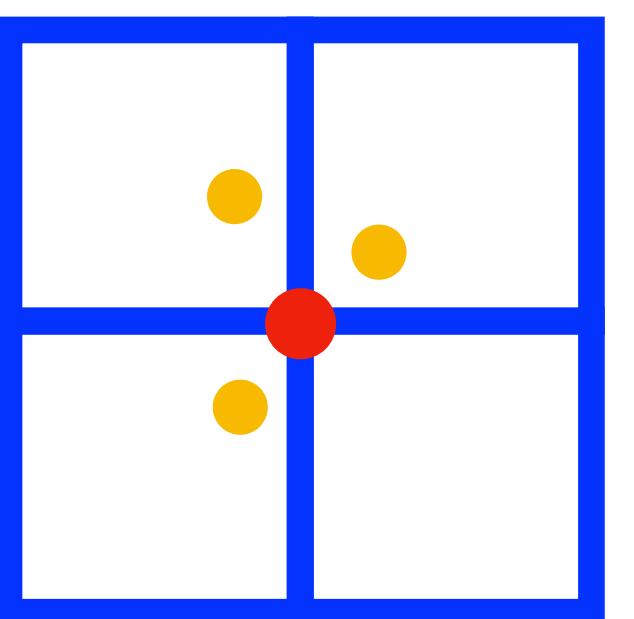
Thread 1 •

Thread 2 •

Thread 3 •

# Write hazard

Particle  
Grid node



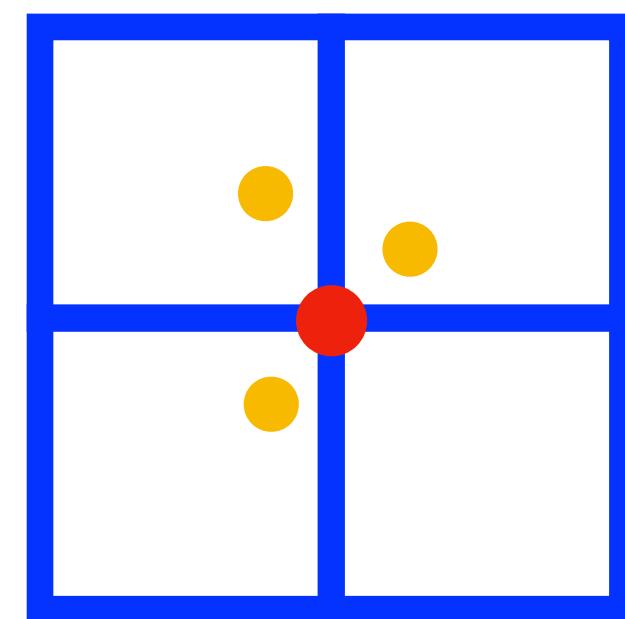
Thread 1 •

Thread 2 •

Thread 3 •

# Write hazard

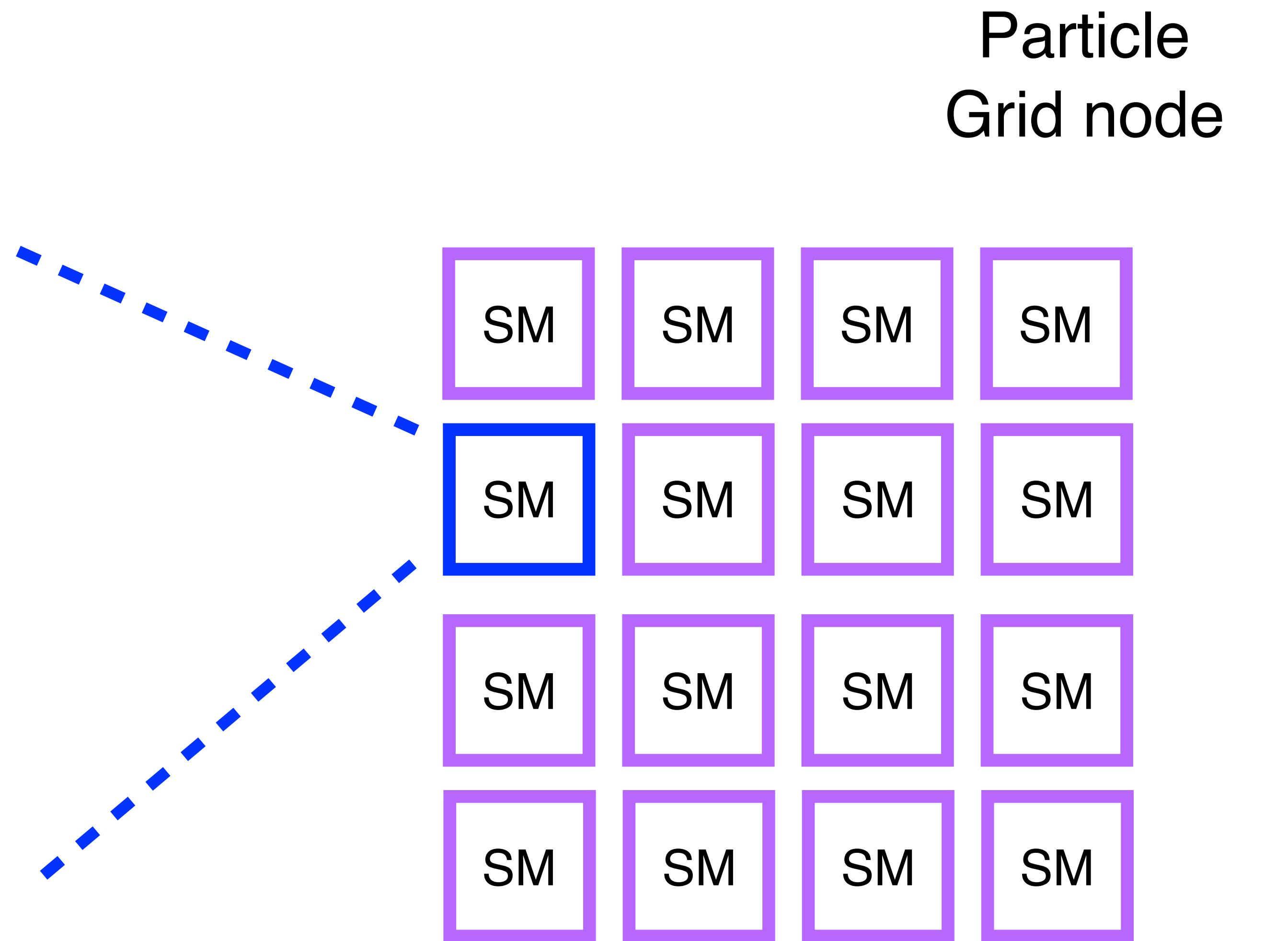
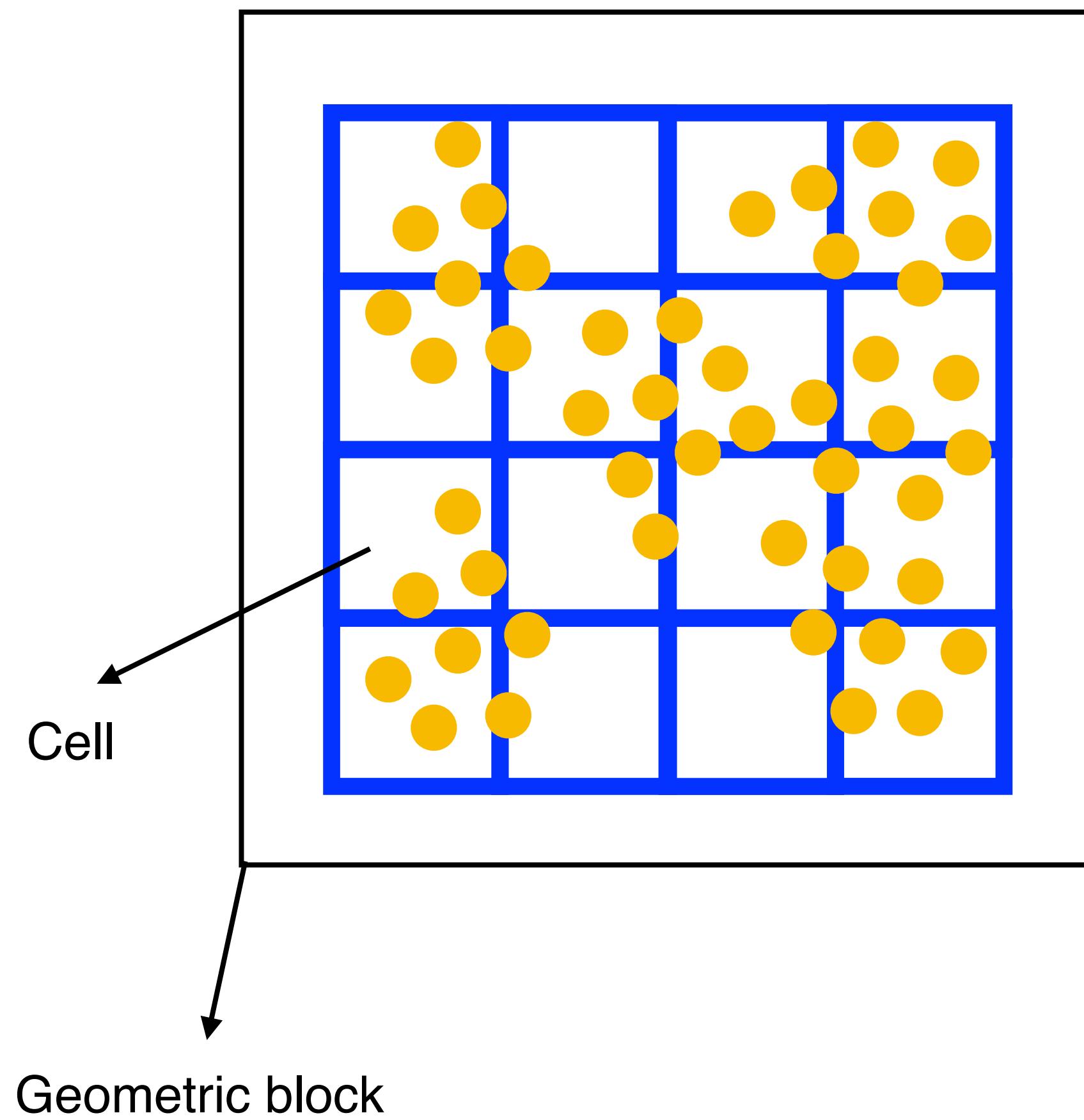
Particle  
Grid node



Thread 1  
Thread 2  
Thread 3

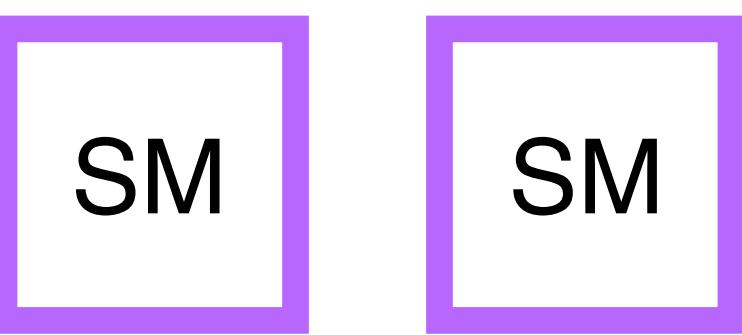
**Write hazard!!!**

# Hierarchy

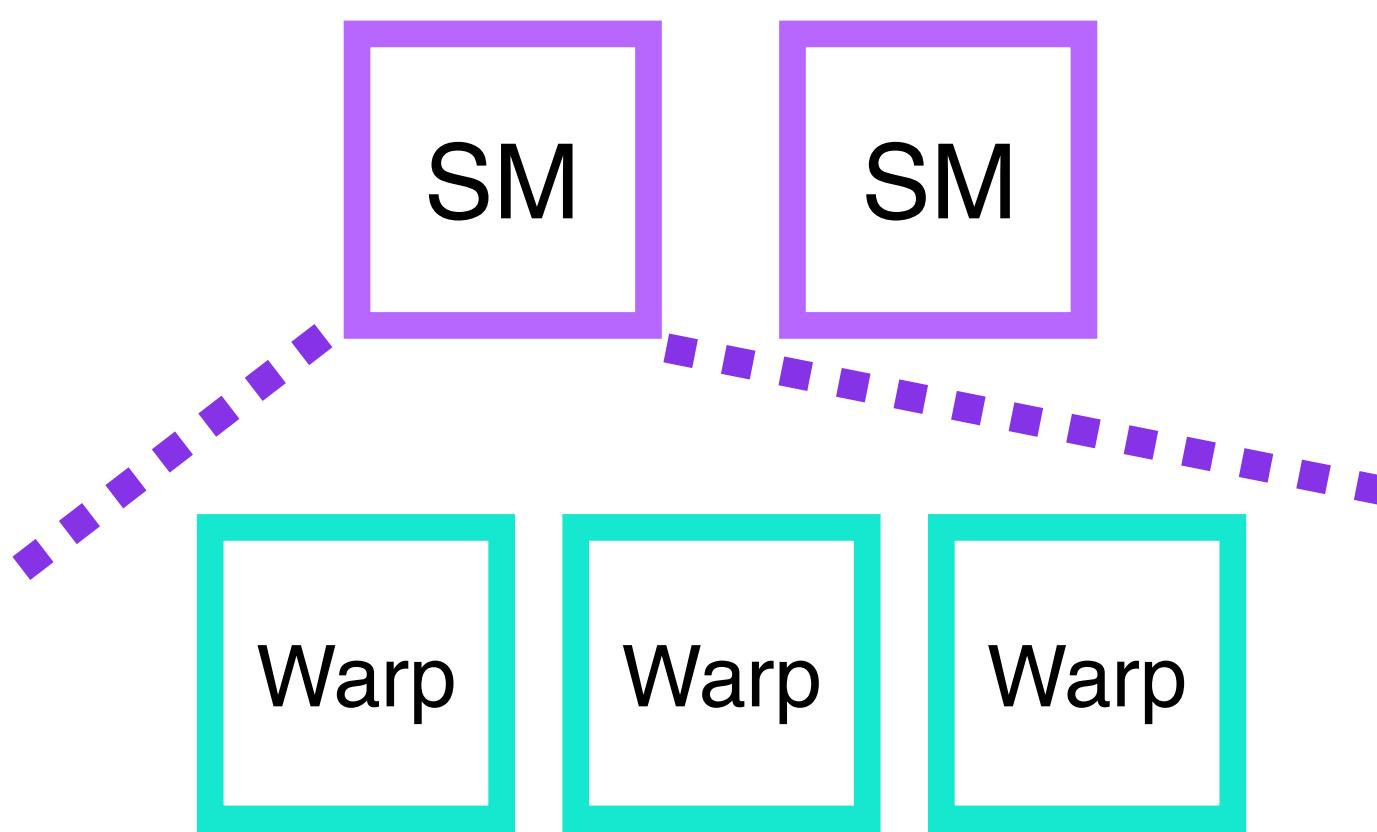


# Hierarchy

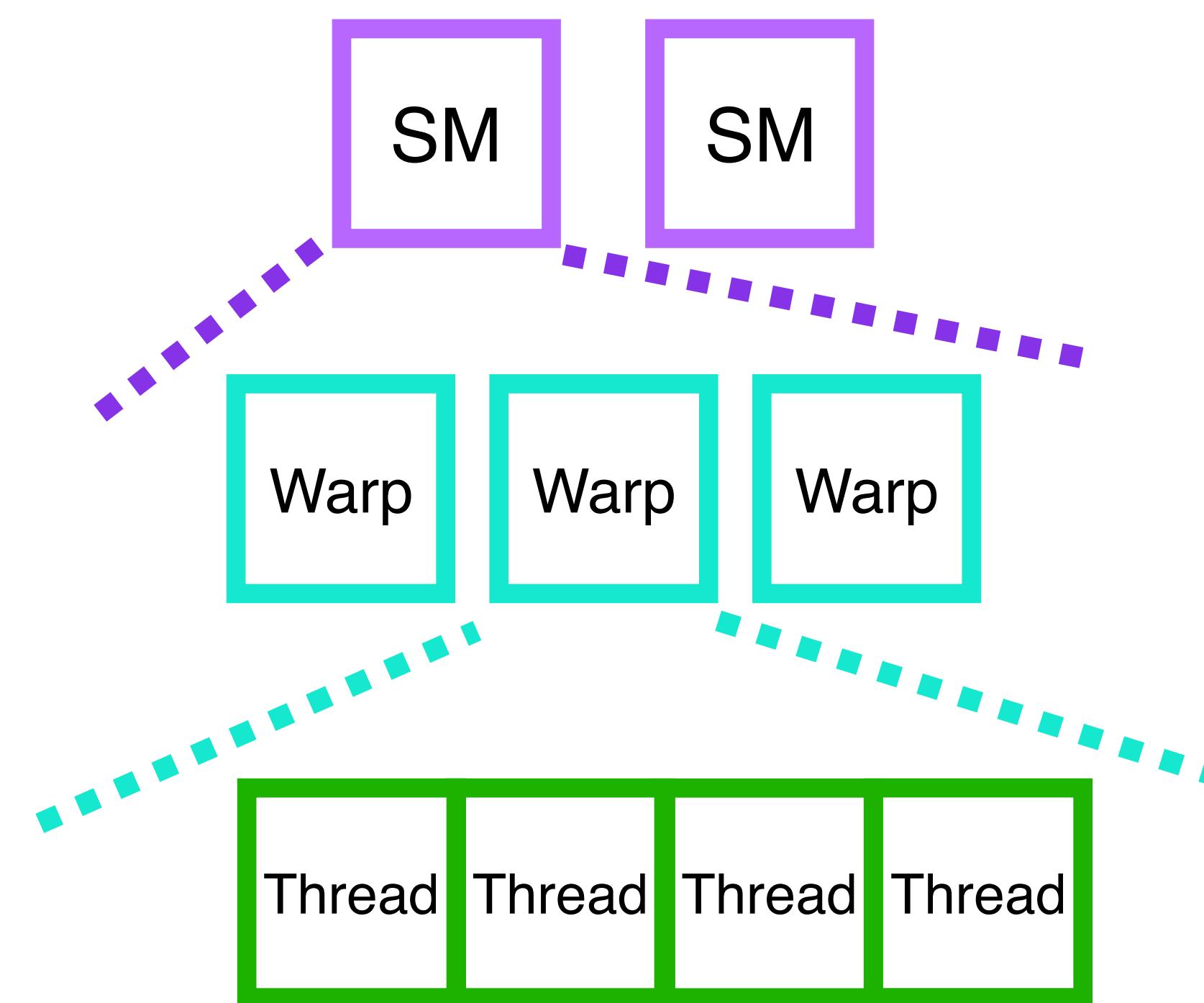
# Hierarchy



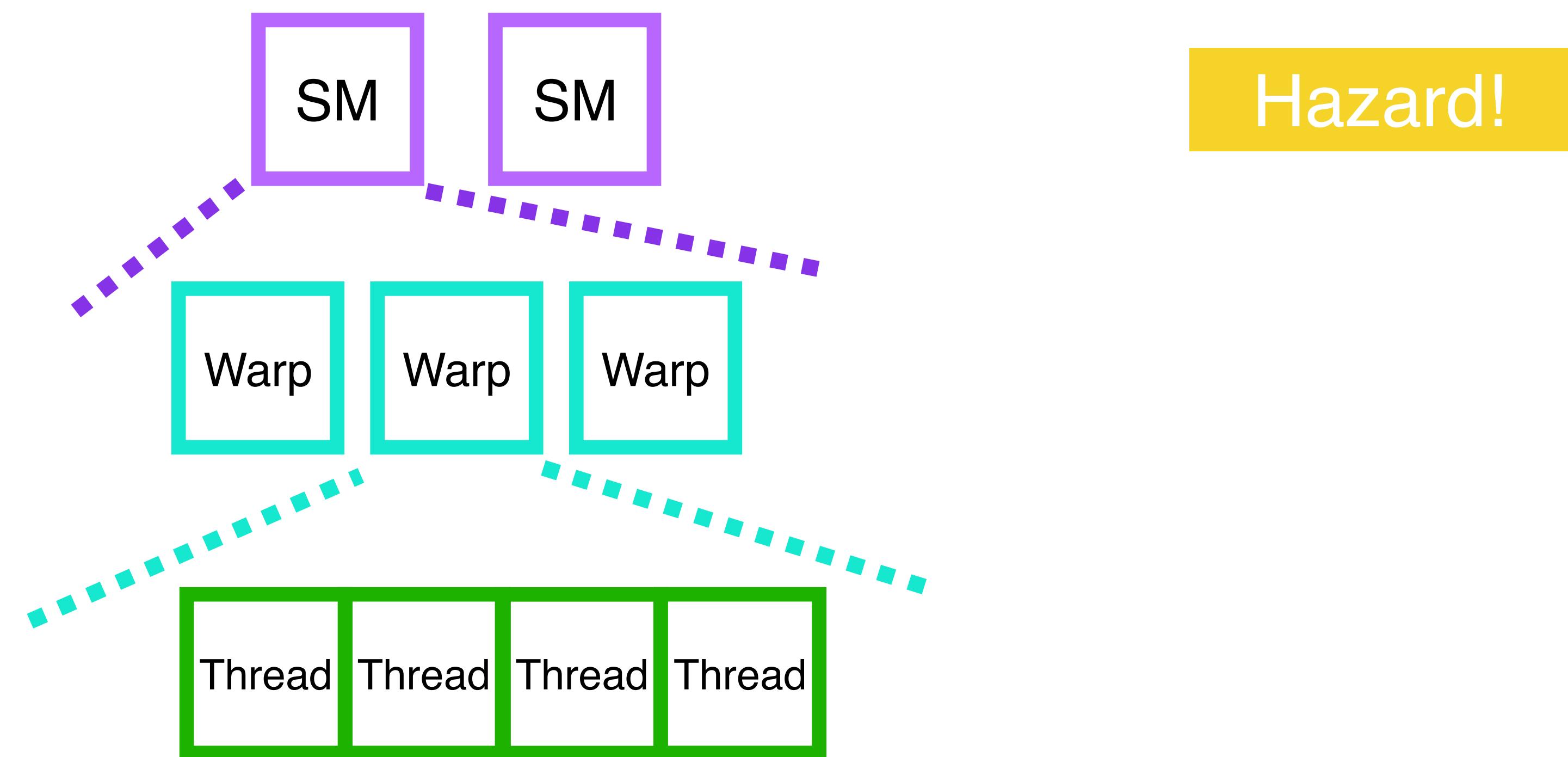
# Hierarchy



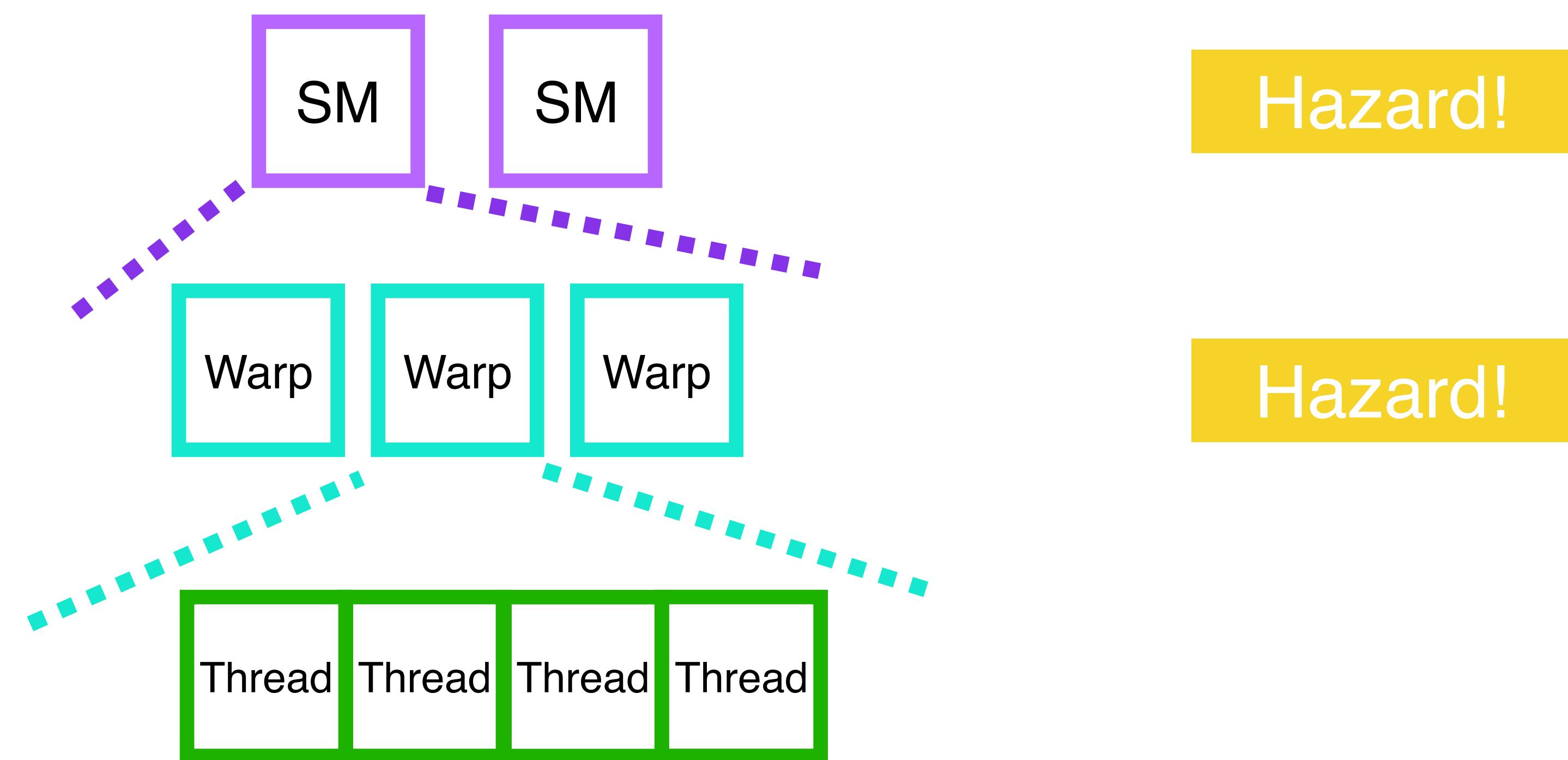
# Hierarchy



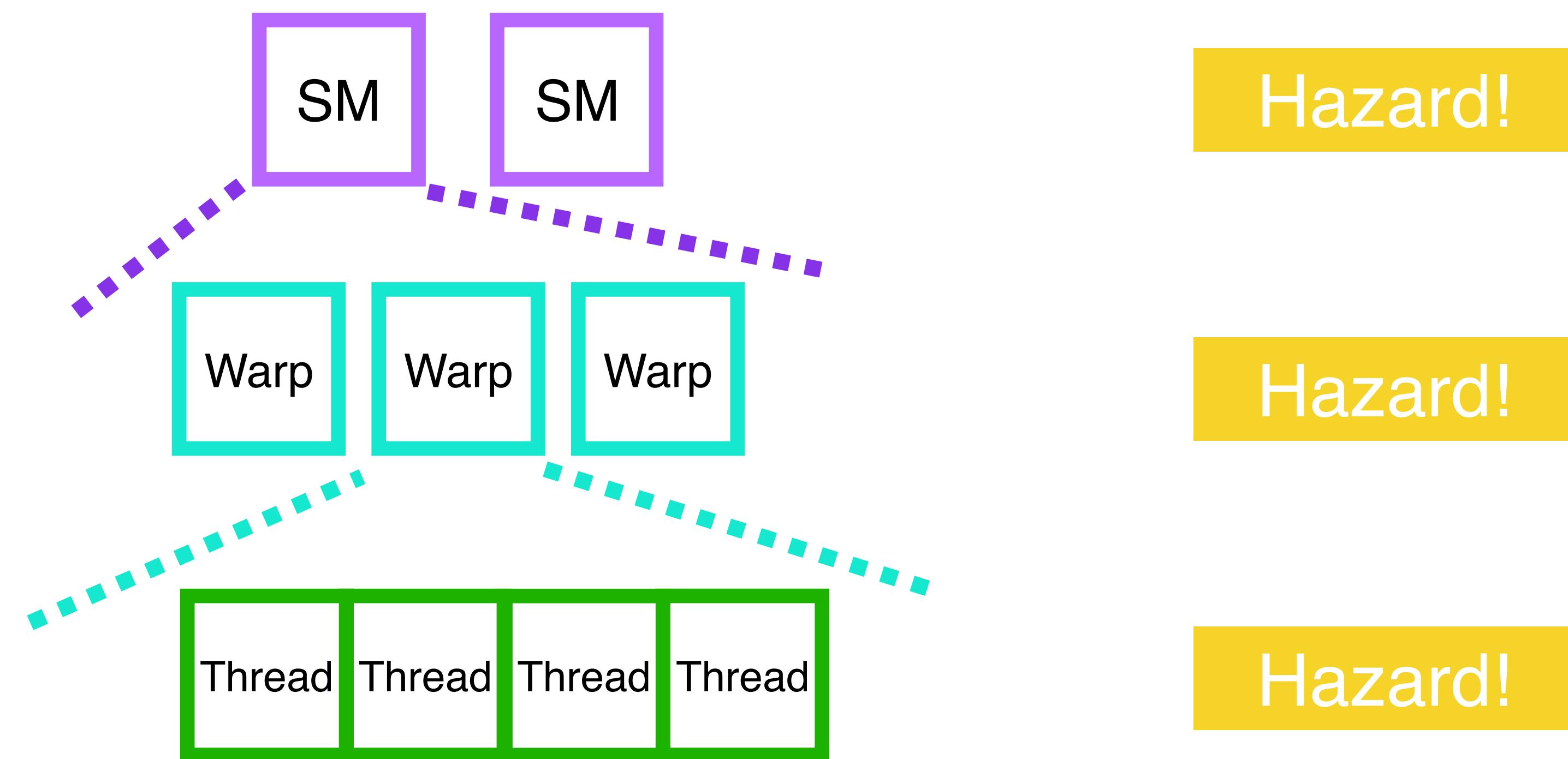
# Hierarchy



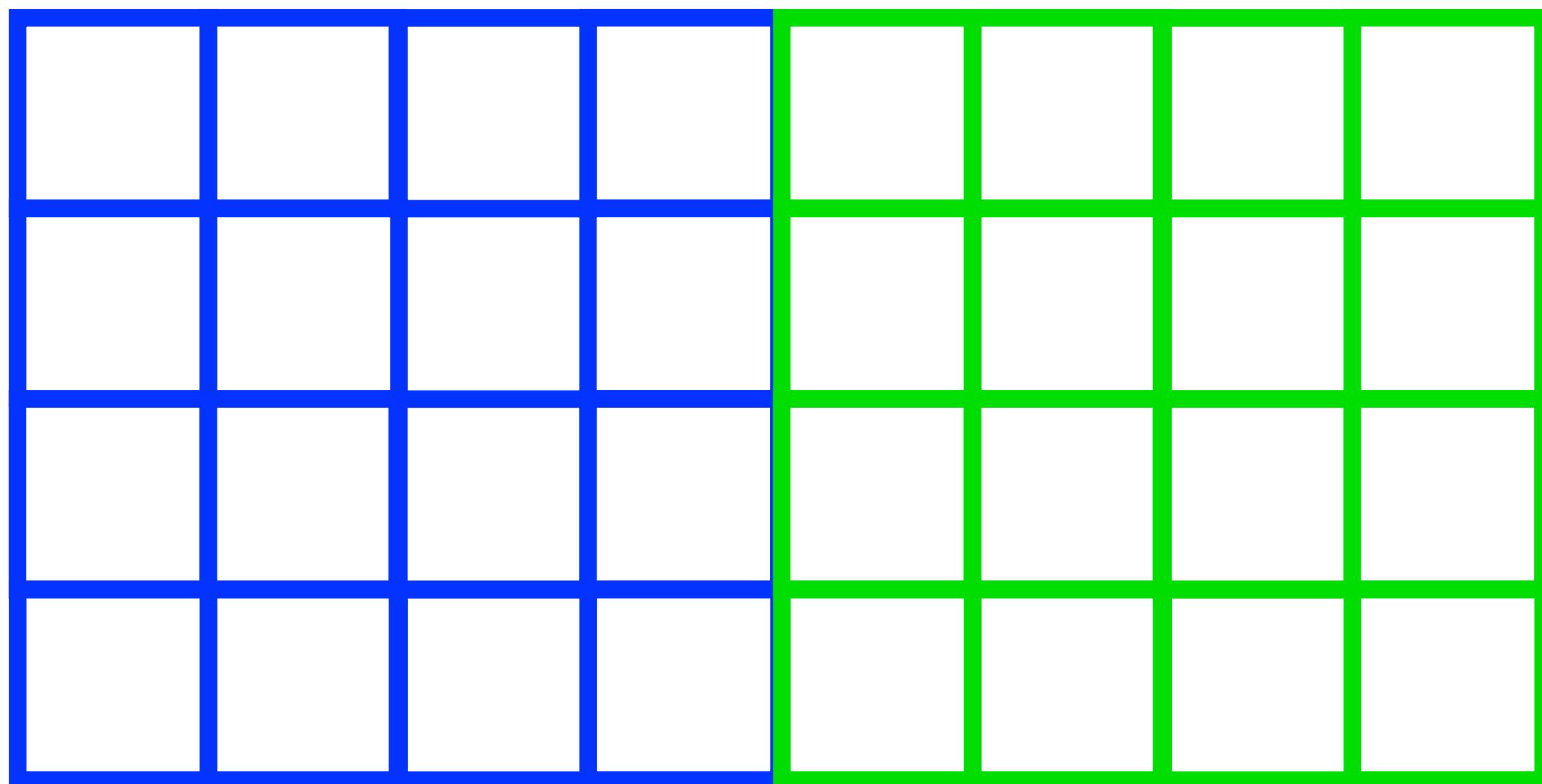
# Hierarchy



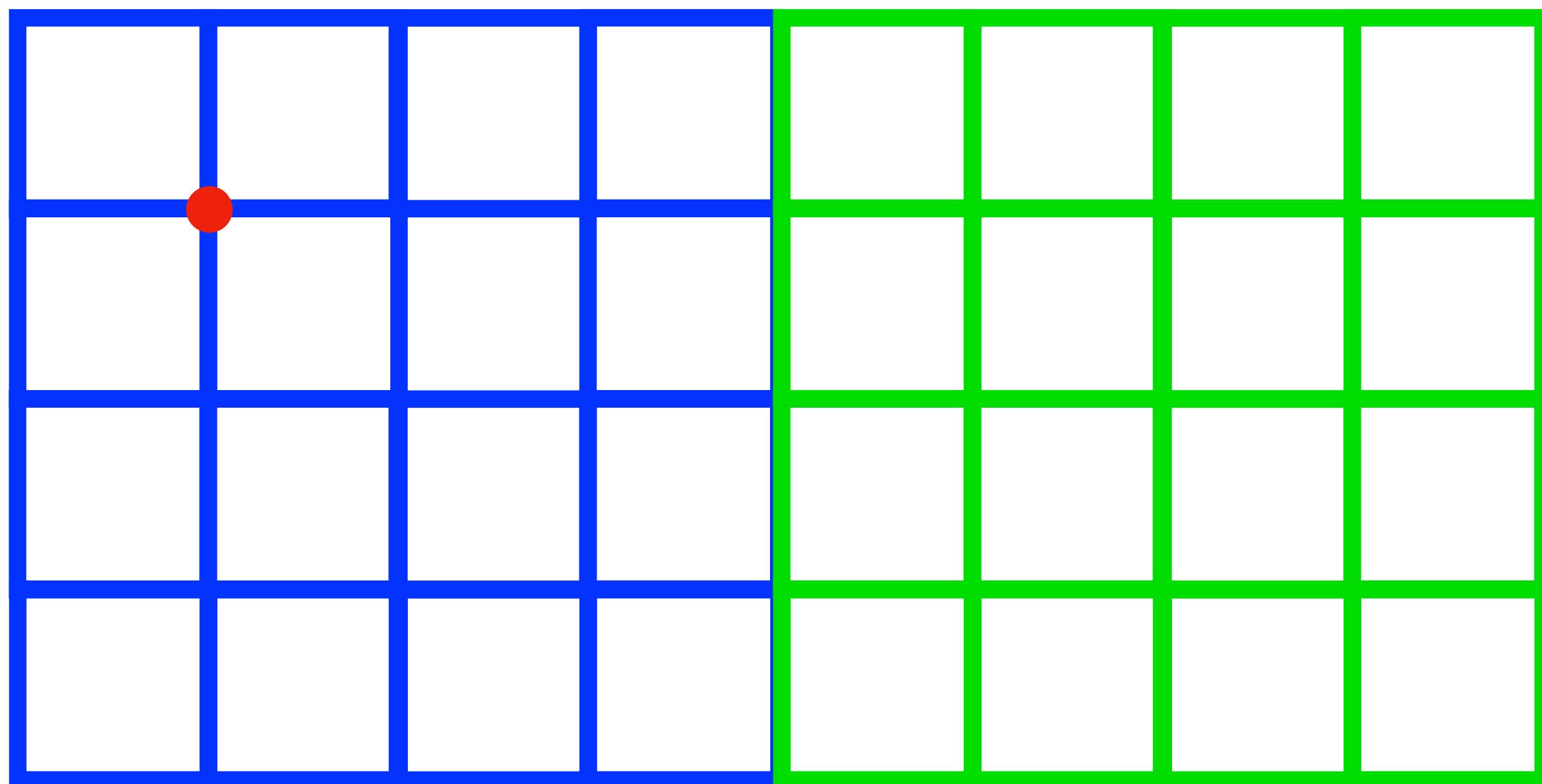
# Hierarchy



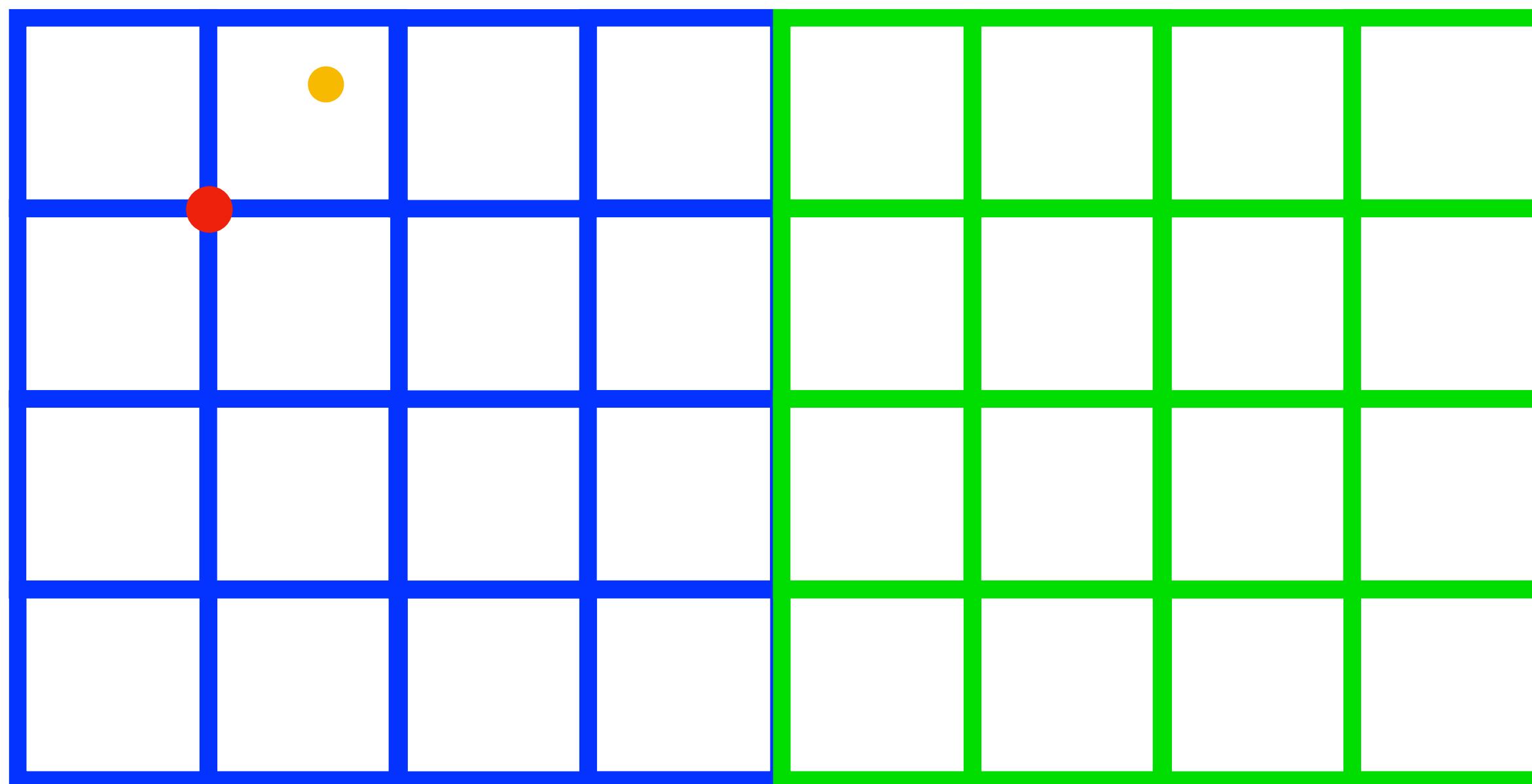
# Naive solution



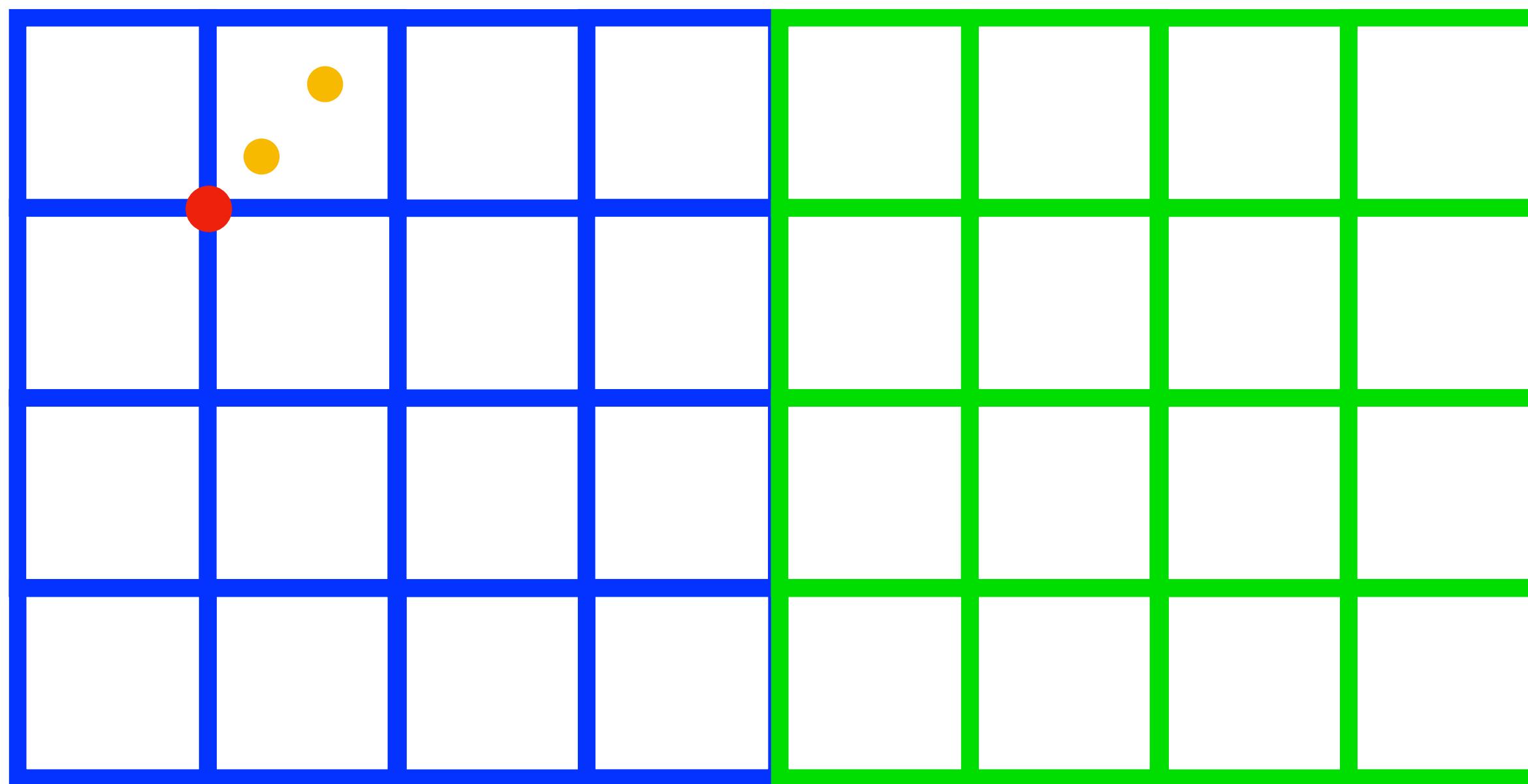
# Naive solution



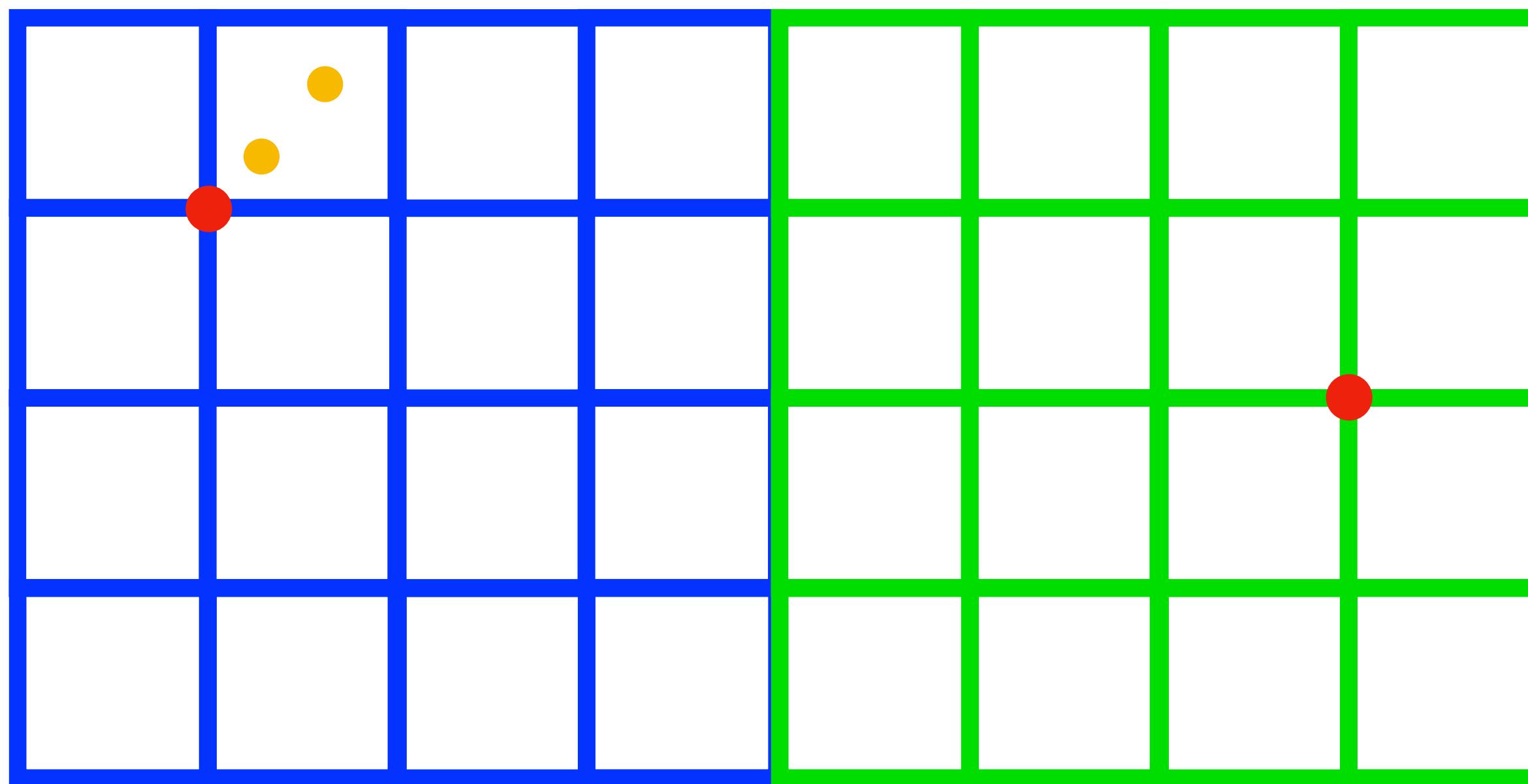
# Naive solution



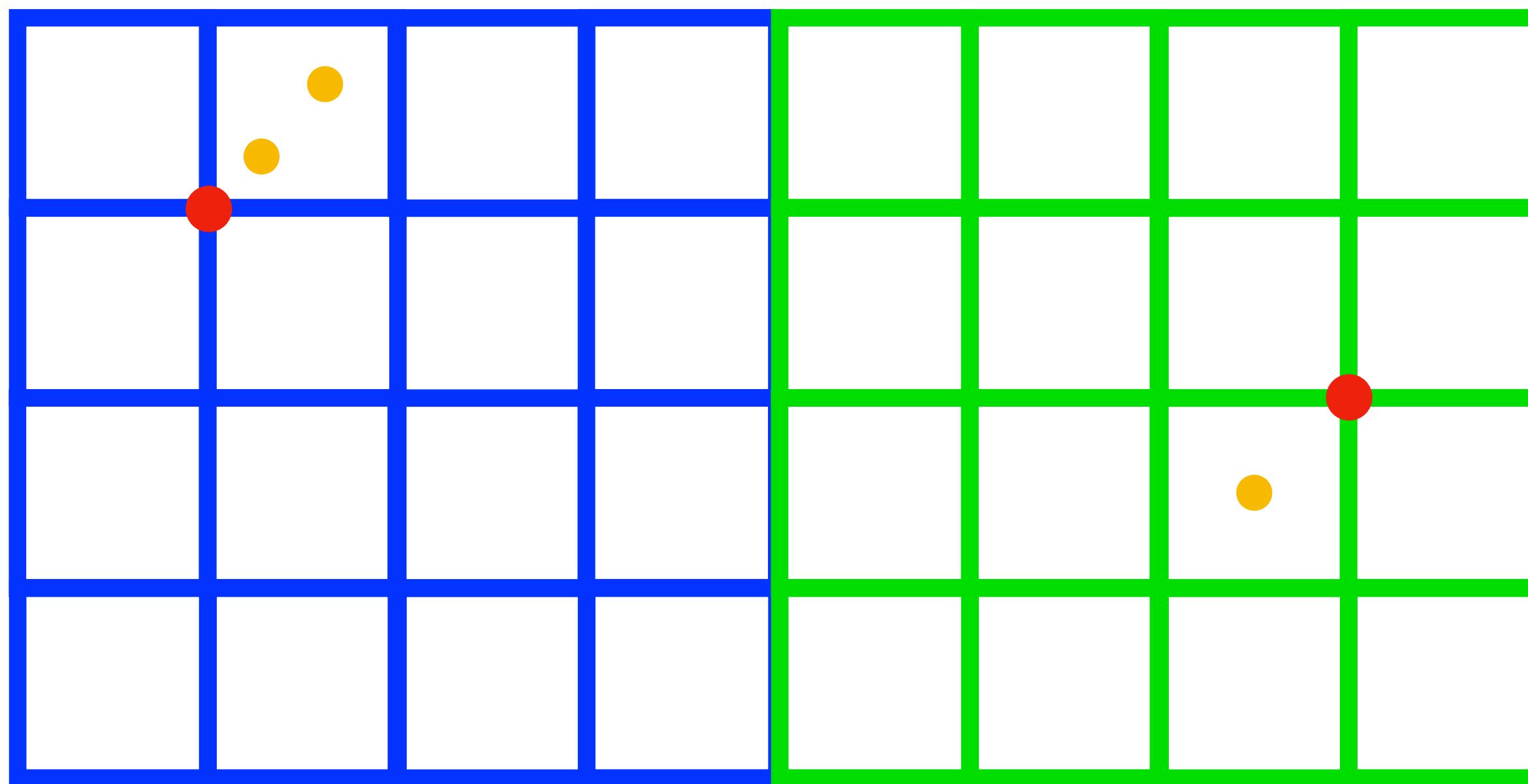
# Naive solution



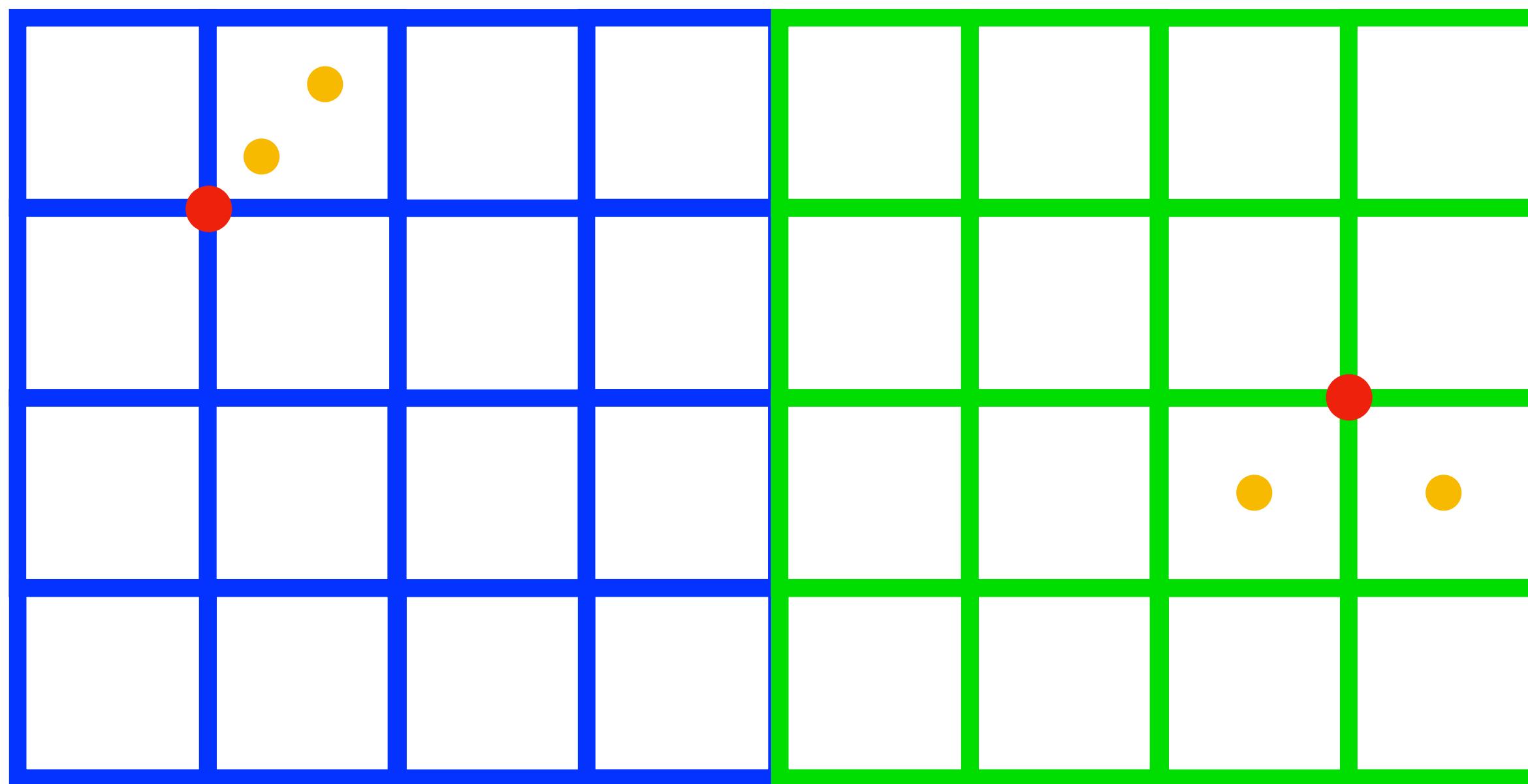
# Naive solution



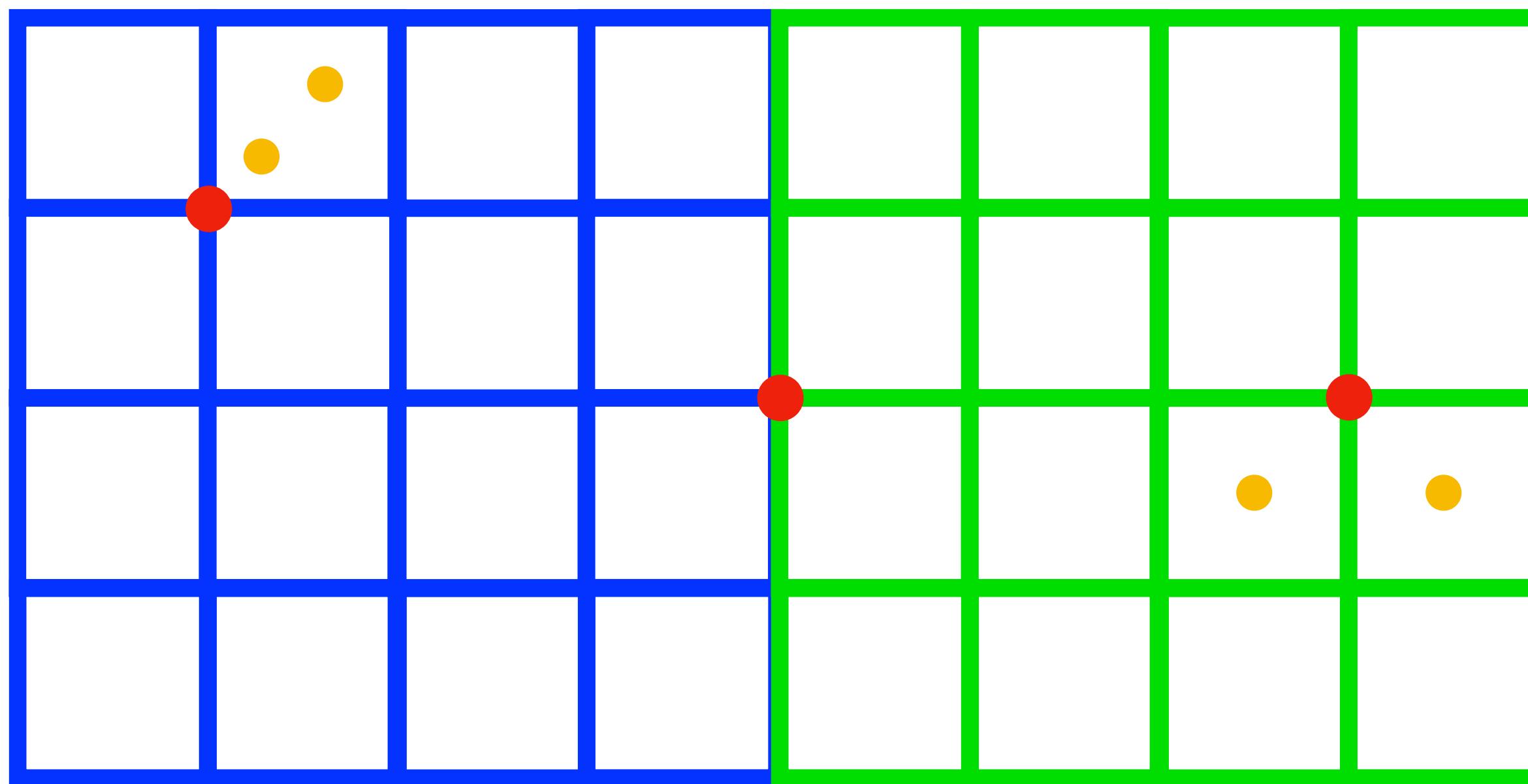
# Naive solution



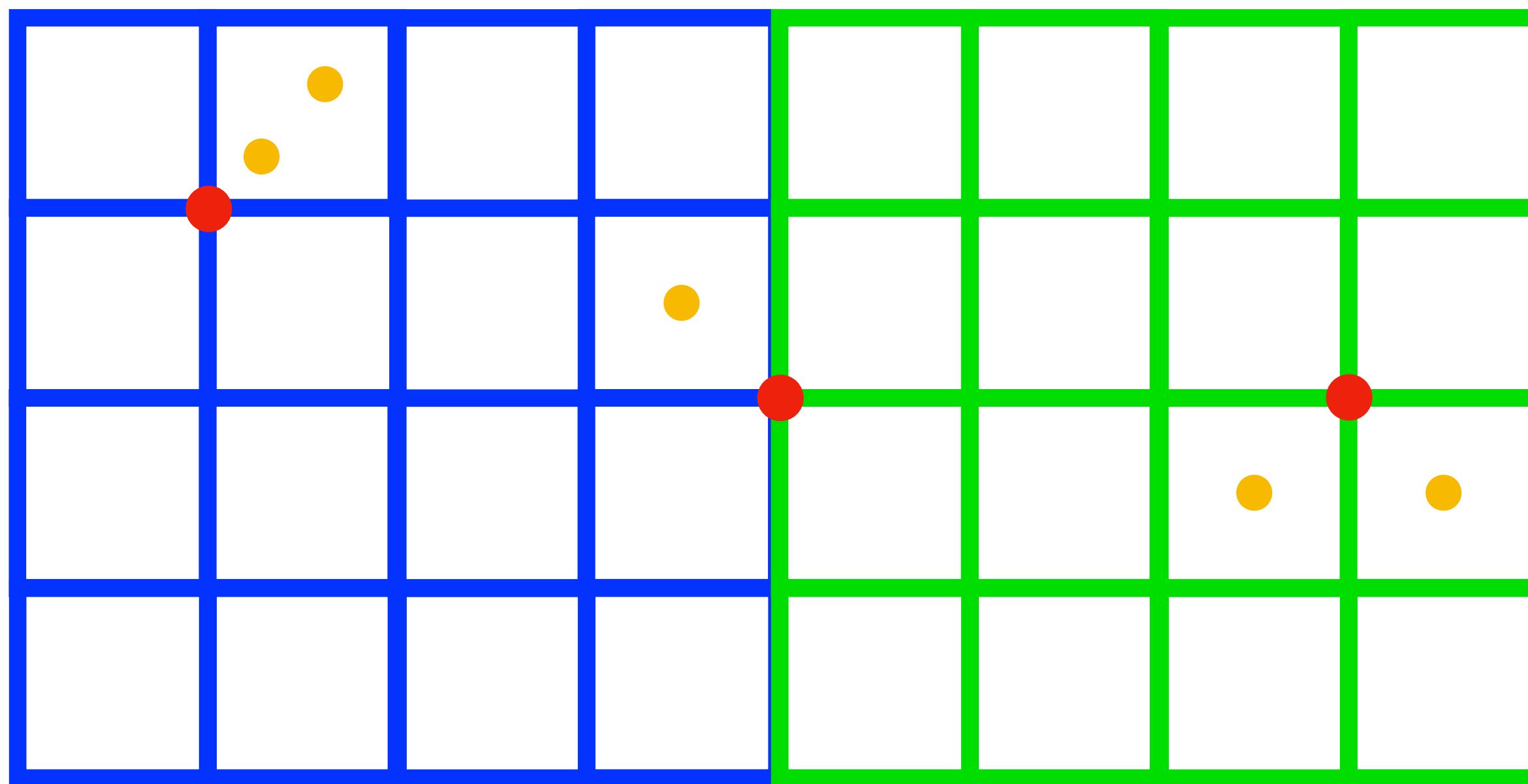
# Naive solution



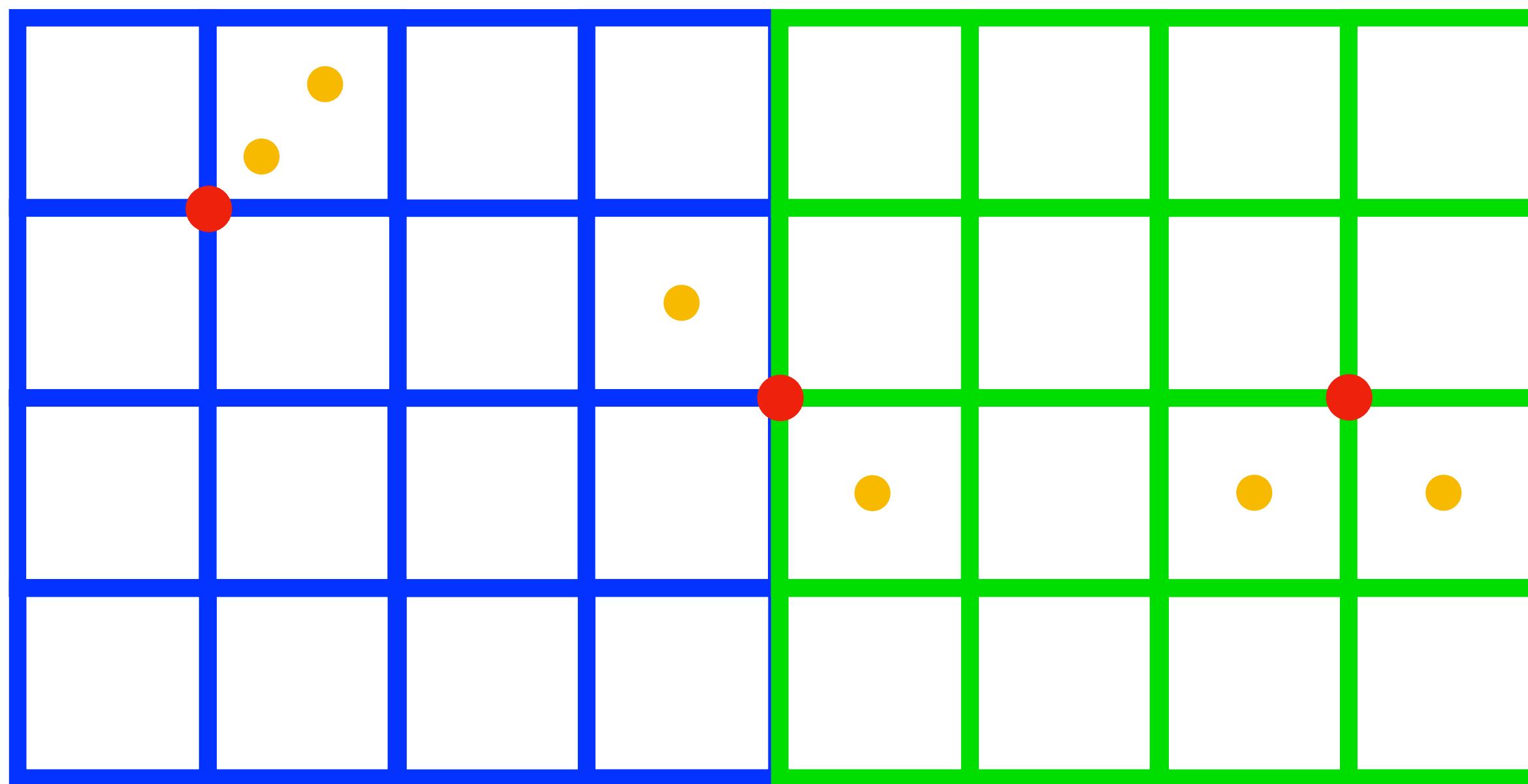
# Naive solution



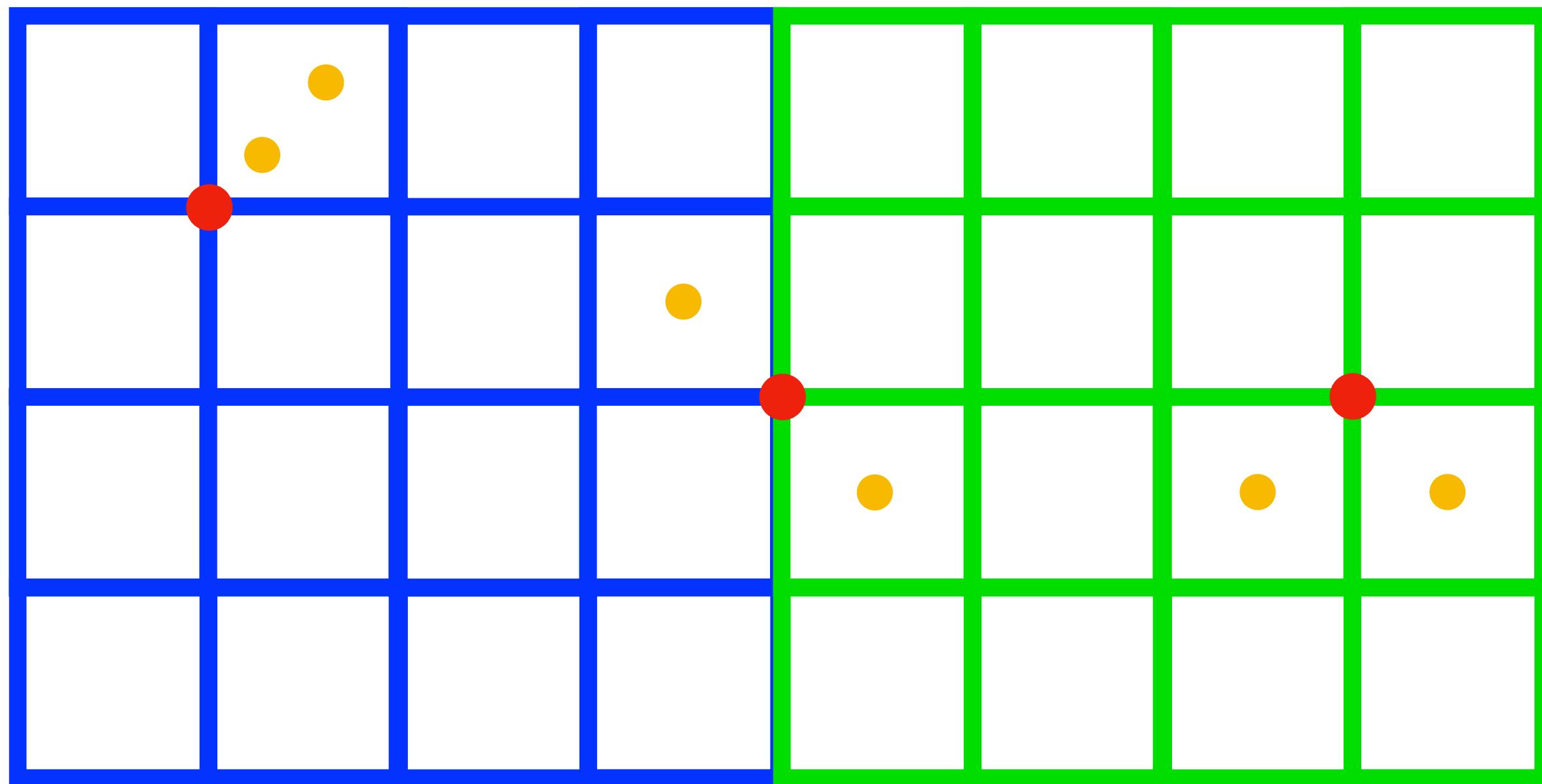
# Naive solution



# Naive solution

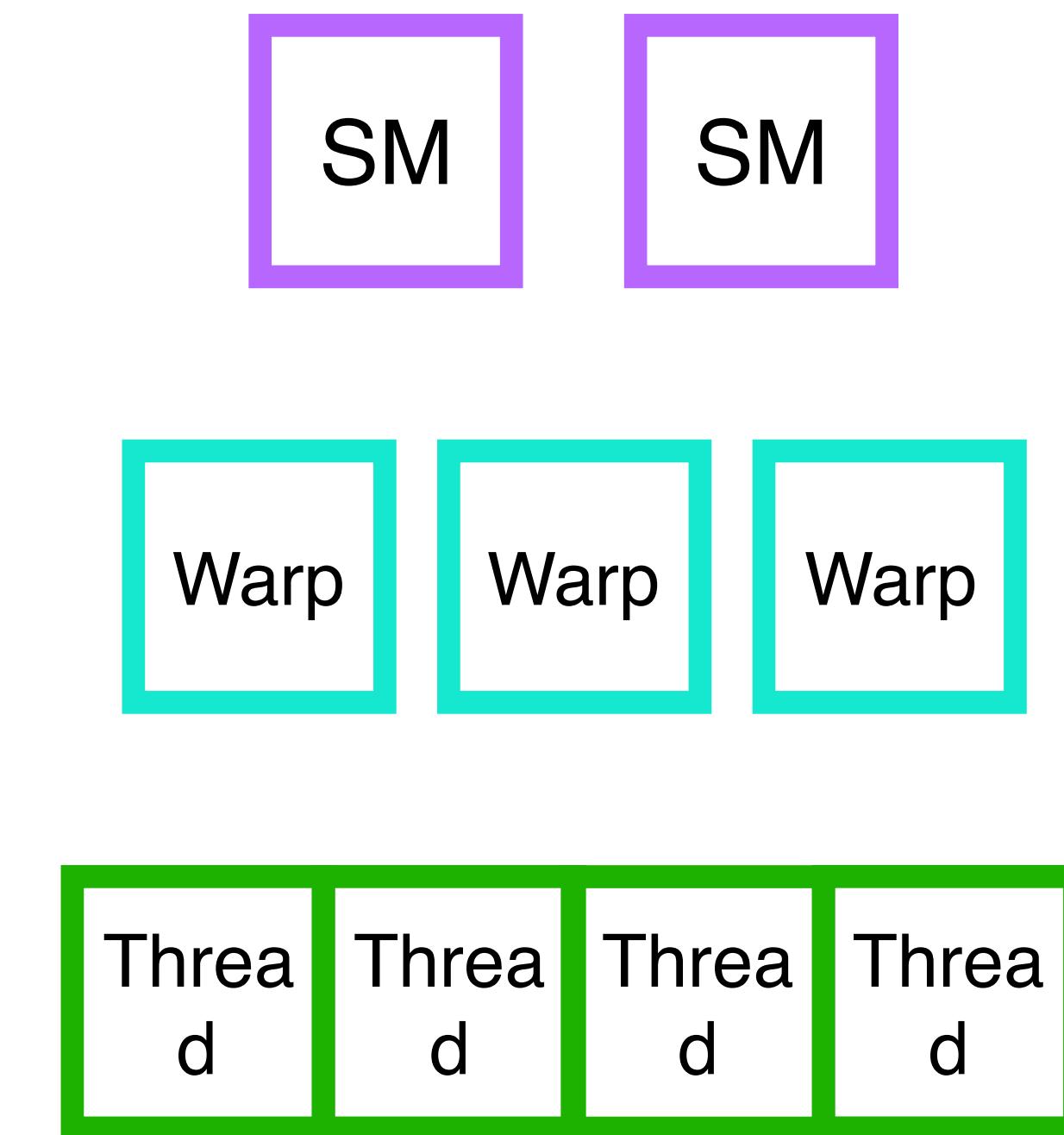
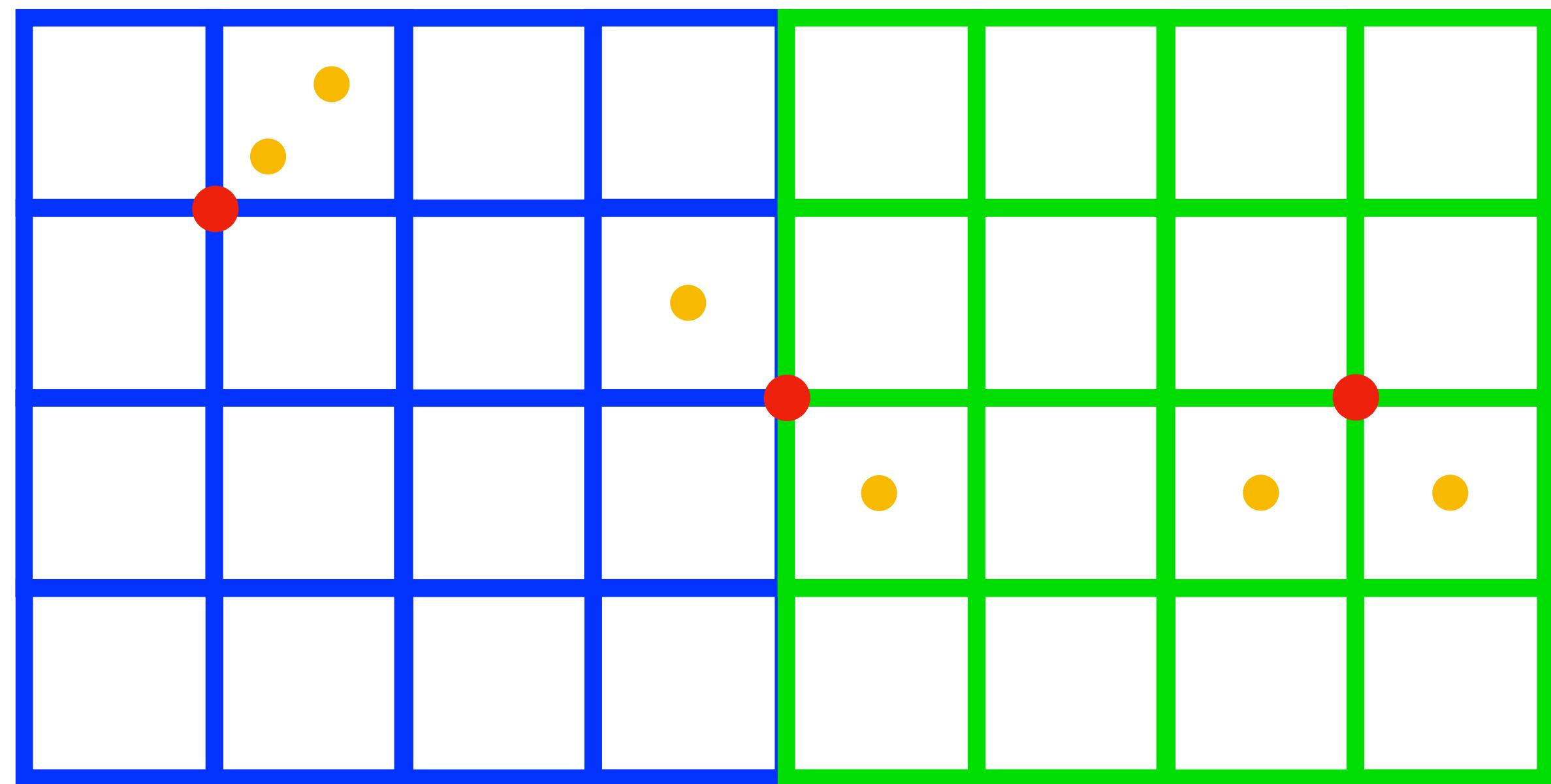


# Naive solution



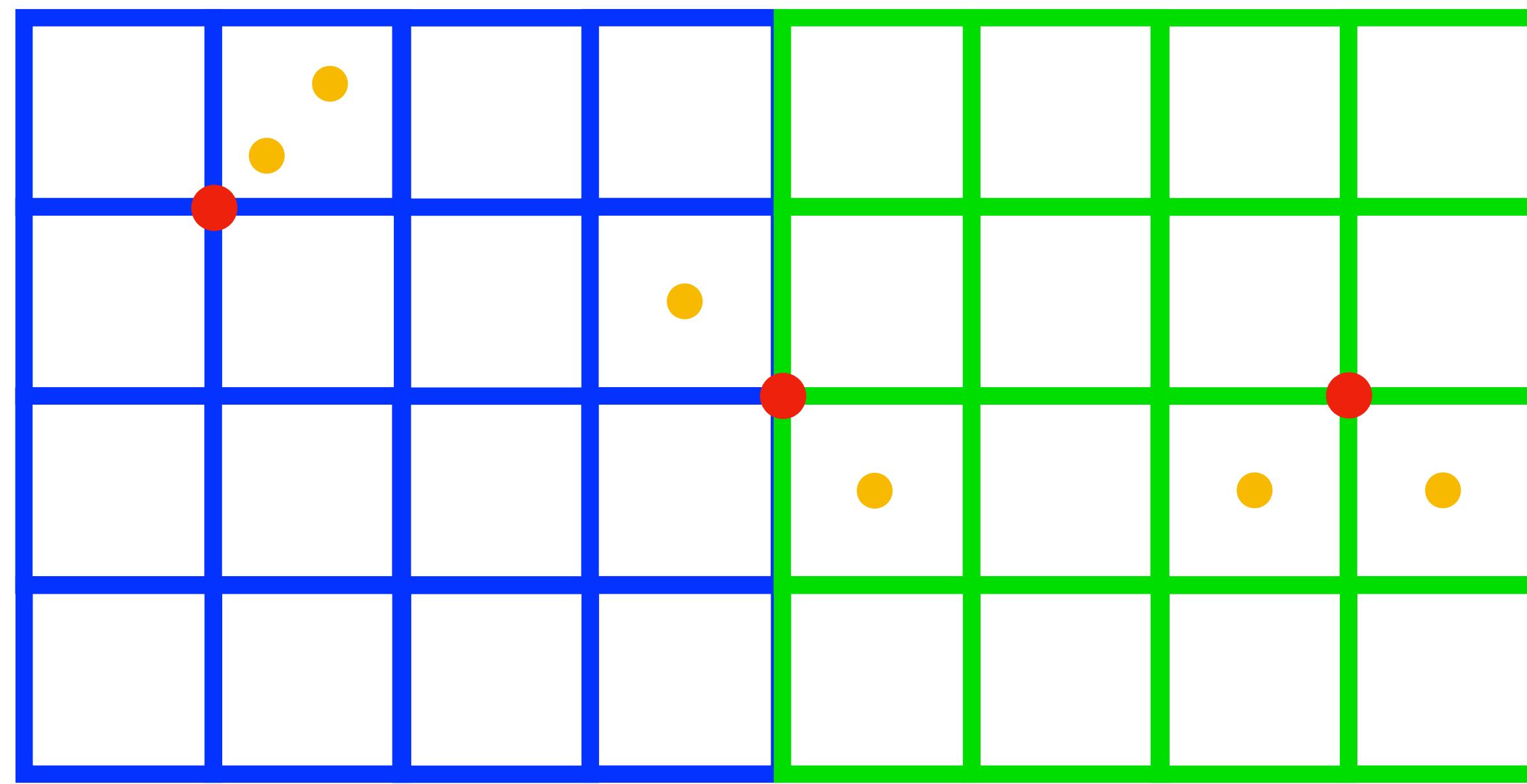
**Naive scattering**  
**P2G - 90%**

# Naive solution

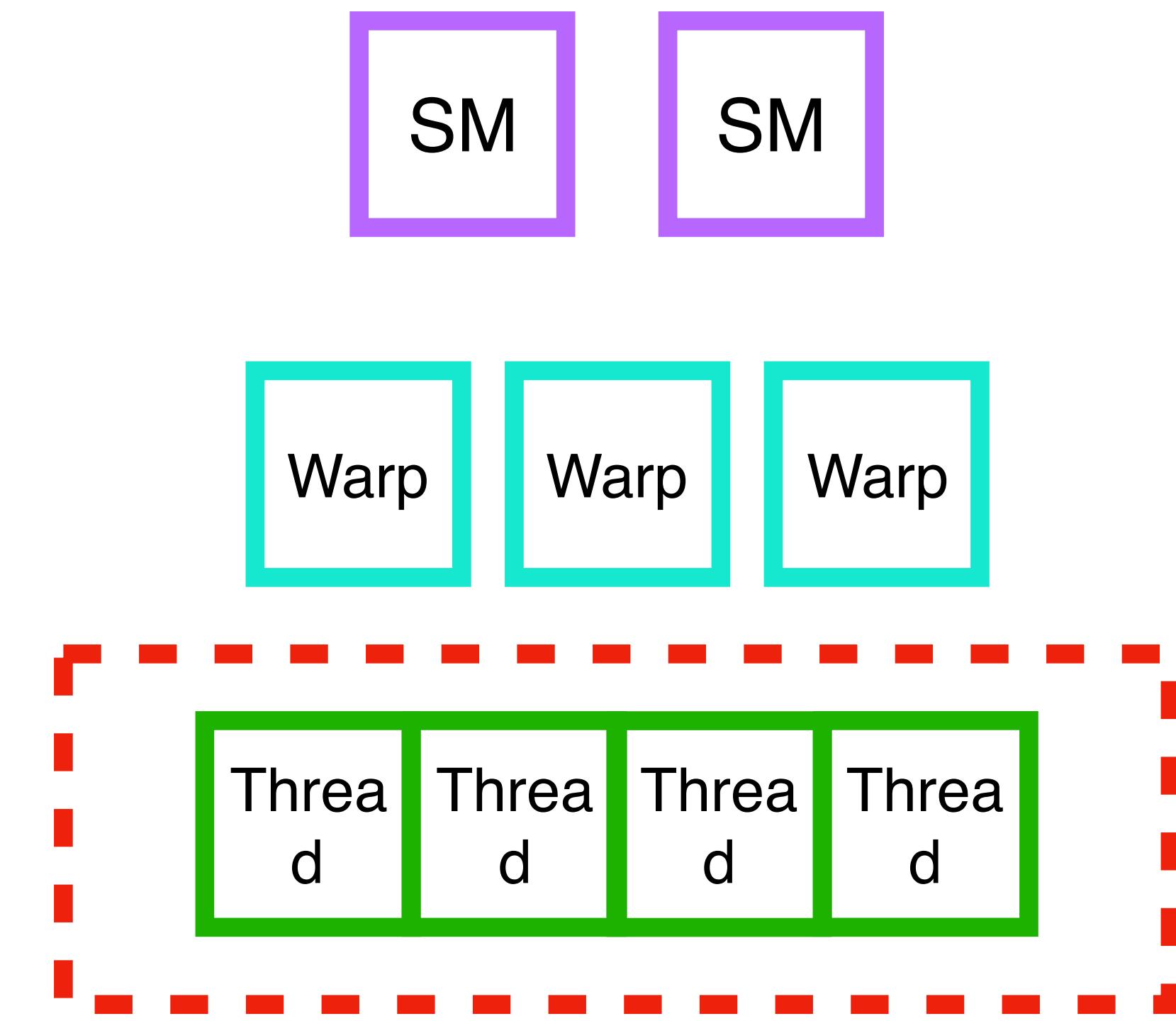


**Naive scattering**  
**P2G - 90%**

# Naive solution



**Naive scattering**  
**P2G - 90%**



lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3

lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3

lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3

lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3

lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3

lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3
boundary mark	1	1	0	0	0	1	0	1

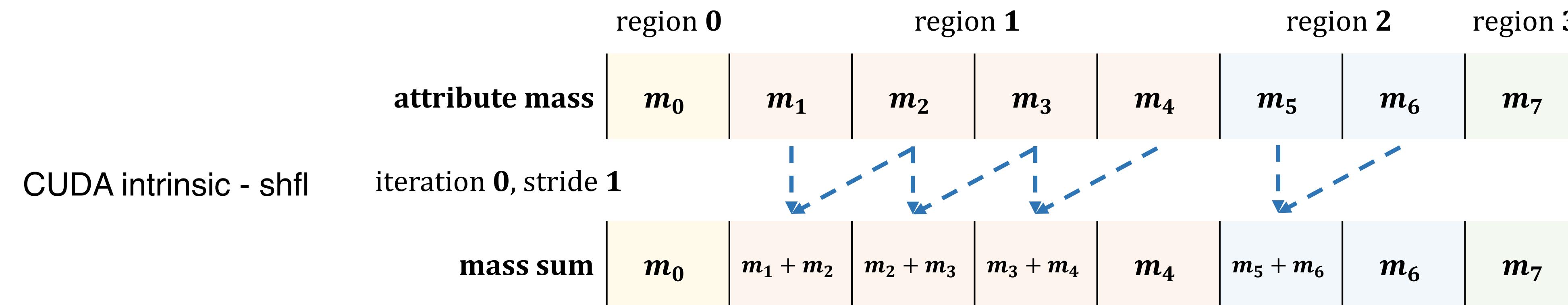
CUDA intrinsic - ballot

lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3
boundary mark	1	1	0	0	0	1	0	1
region interval	0	3	2	1	0	1	0	0

region 0                          region 1                          region 2                          region 3

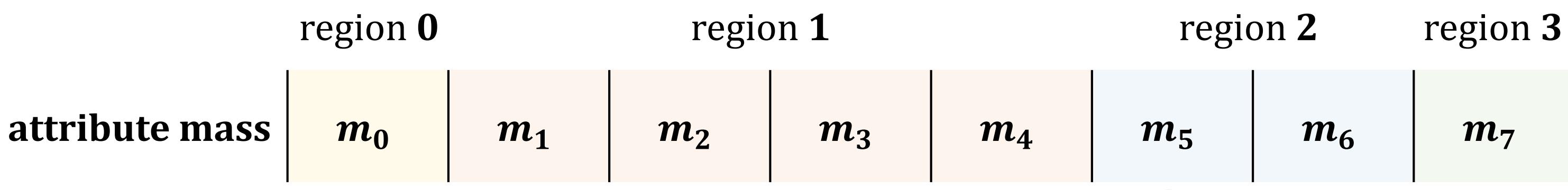
lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3
boundary mark	1	1	0	0	0	1	0	1
region interval	0	3	2	1	0	1	0	0

# CUDA intrinsic - ballot

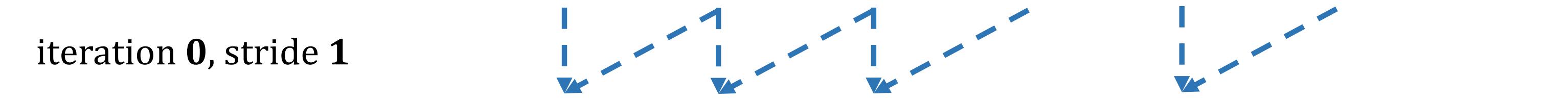


lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3
boundary mark	1	1	0	0	0	1	0	1
region interval	0	3	2	1	0	1	0	0

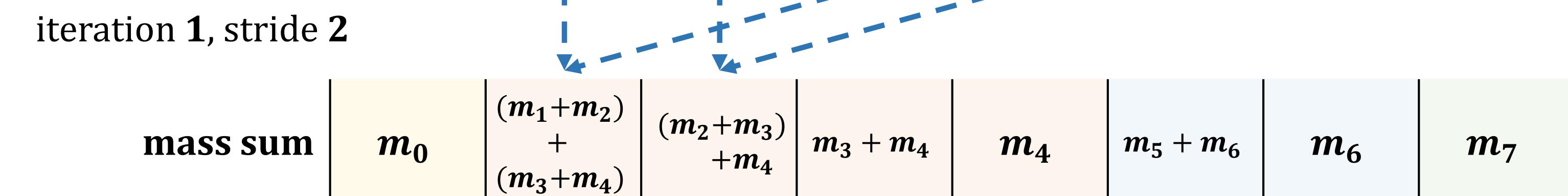
# CUDA intrinsic - ballot



## CUDA intrinsic - shfl



## CUDA intrinsic - shfl



CUDA intrinsic - ballot

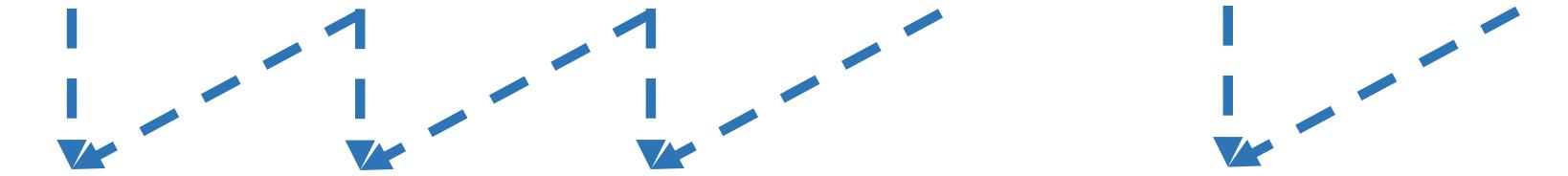
lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3
boundary mark	1	1	0	0	0	1	0	1
region interval	0	3	2	1	0	1	0	0

region 0                          region 1                          region 2                          region 3

attribute mass	$m_0$	$m_1$	$m_2$	$m_3$	$m_4$	$m_5$	$m_6$	$m_7$
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CUDA intrinsic - shfl

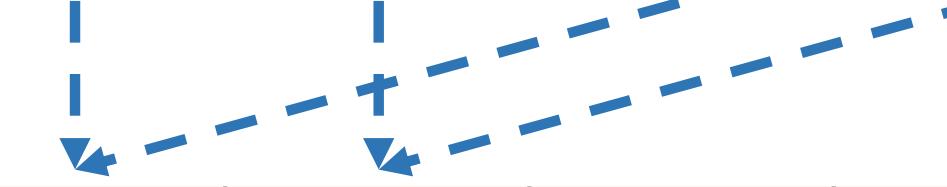
iteration 0, stride 1



mass sum	$m_0$	$m_1 + m_2$	$m_2 + m_3$	$m_3 + m_4$	$m_4$	$m_5 + m_6$	$m_6$	$m_7$
----------	-------	-------------	-------------	-------------	-------	-------------	-------	-------

CUDA intrinsic - shfl

iteration 1, stride 2



mass sum	$m_0$	$(m_1+m_2) + (m_3+m_4)$	$(m_2+m_3) + m_4$	$m_3 + m_4$	$m_4$	$m_5 + m_6$	$m_6$	$m_7$
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CUDA intrinsic - ballot

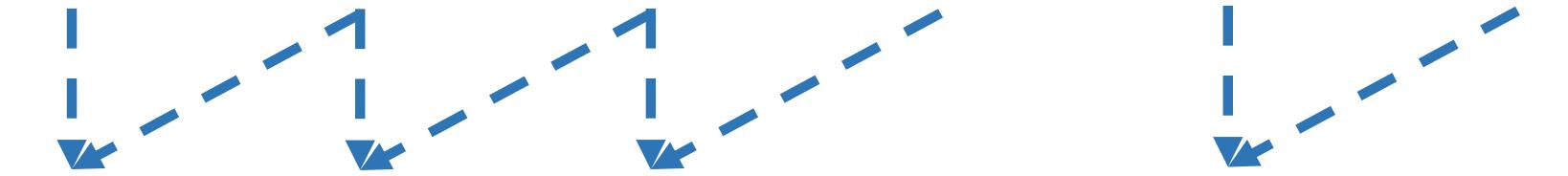
lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3
boundary mark	1	1	0	0	0	1	0	1
region interval	0	3	2	1	0	1	0	0

region 0                          region 1                          region 2                          region 3

attribute mass	$m_0$	$m_1$	$m_2$	$m_3$	$m_4$	$m_5$	$m_6$	$m_7$
----------------	-------	-------	-------	-------	-------	-------	-------	-------

CUDA intrinsic - shfl

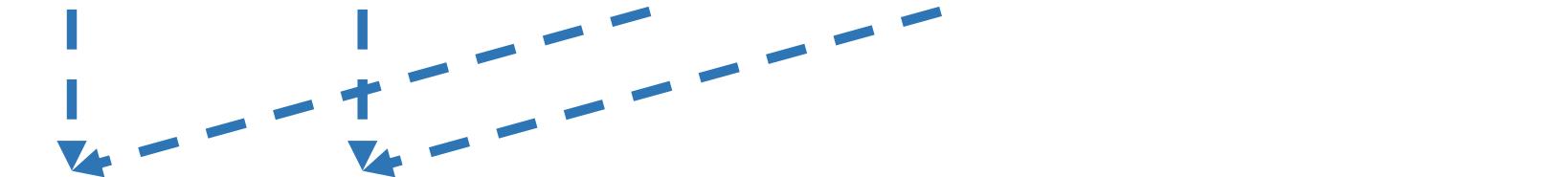
iteration 0, stride 1



mass sum	$m_0$	$m_1 + m_2$	$m_2 + m_3$	$m_3 + m_4$	$m_4$	$m_5 + m_6$	$m_6$	$m_7$
----------	-------	-------------	-------------	-------------	-------	-------------	-------	-------

CUDA intrinsic - shfl

iteration 1, stride 2



mass sum	$m_0$	$(m_1+m_2) + (m_3+m_4)$	$(m_2+m_3) + m_4$	$m_3 + m_4$	$m_4$	$m_5 + m_6$	$m_6$	$m_7$
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CUDA intrinsic - ballot

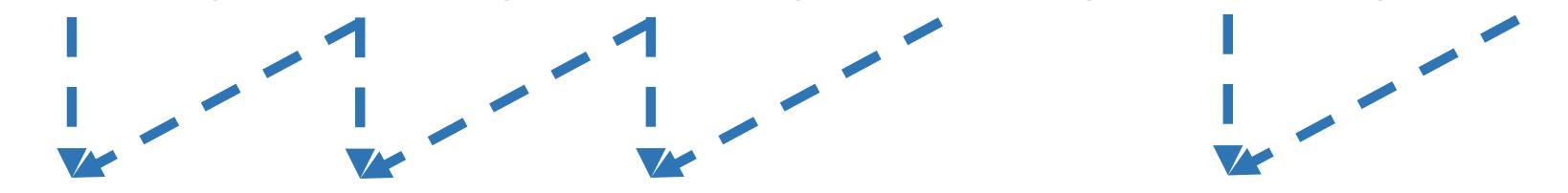
lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3
boundary mark	1	1	0	0	0	1	0	1
region interval	0	3	2	1	0	1	0	0

region 0                          region 1                          region 2                          region 3

attribute mass	$m_0$	$m_1$	$m_2$	$m_3$	$m_4$	$m_5$	$m_6$	$m_7$
----------------	-------	-------	-------	-------	-------	-------	-------	-------

CUDA intrinsic - shfl

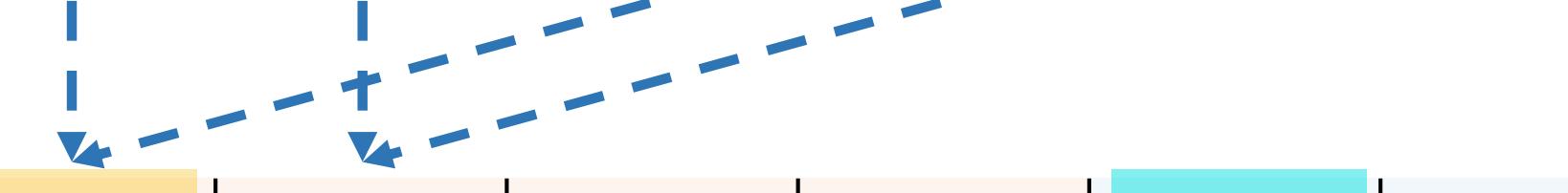
iteration 0, stride 1



mass sum	$m_0$	$m_1 + m_2$	$m_2 + m_3$	$m_3 + m_4$	$m_4$	$m_5 + m_6$	$m_6$	$m_7$
----------	-------	-------------	-------------	-------------	-------	-------------	-------	-------

CUDA intrinsic - shfl

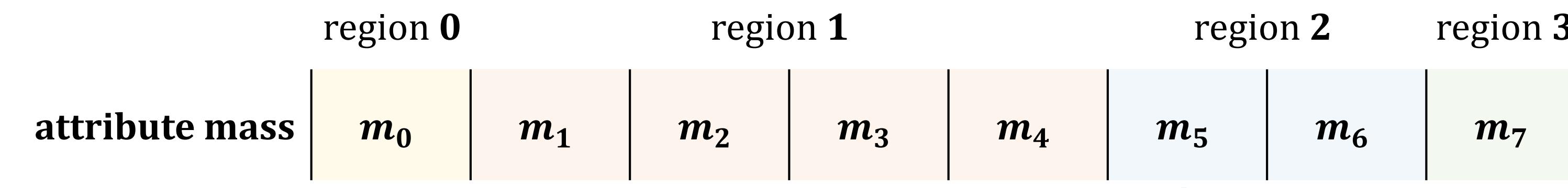
iteration 1, stride 2



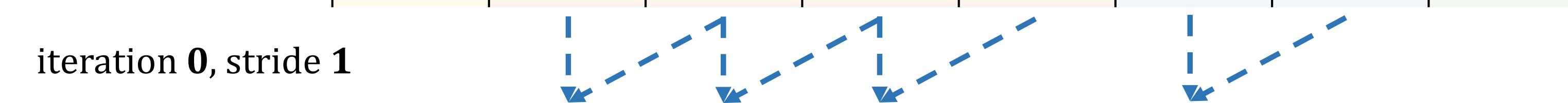
mass sum	$m_0$	$(m_1+m_2) + (m_3+m_4)$	$(m_2+m_3) + m_4$	$m_3 + m_4$	$m_4$	$m_5 + m_6$	$m_6$	$m_7$
----------	-------	-------------------------	-------------------	-------------	-------	-------------	-------	-------

lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3
boundary mark	1	1	0	0	0	1	0	1
region interval	0	3	2	1	0	1	0	0

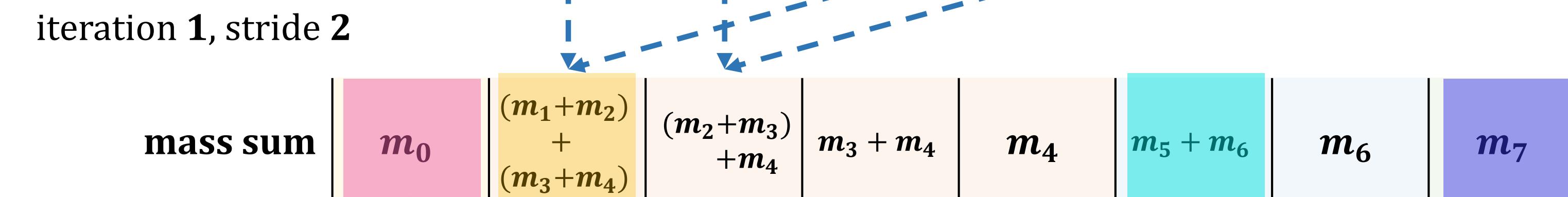
# CUDA intrinsic - ballot



# CUDA intrinsic - shfl

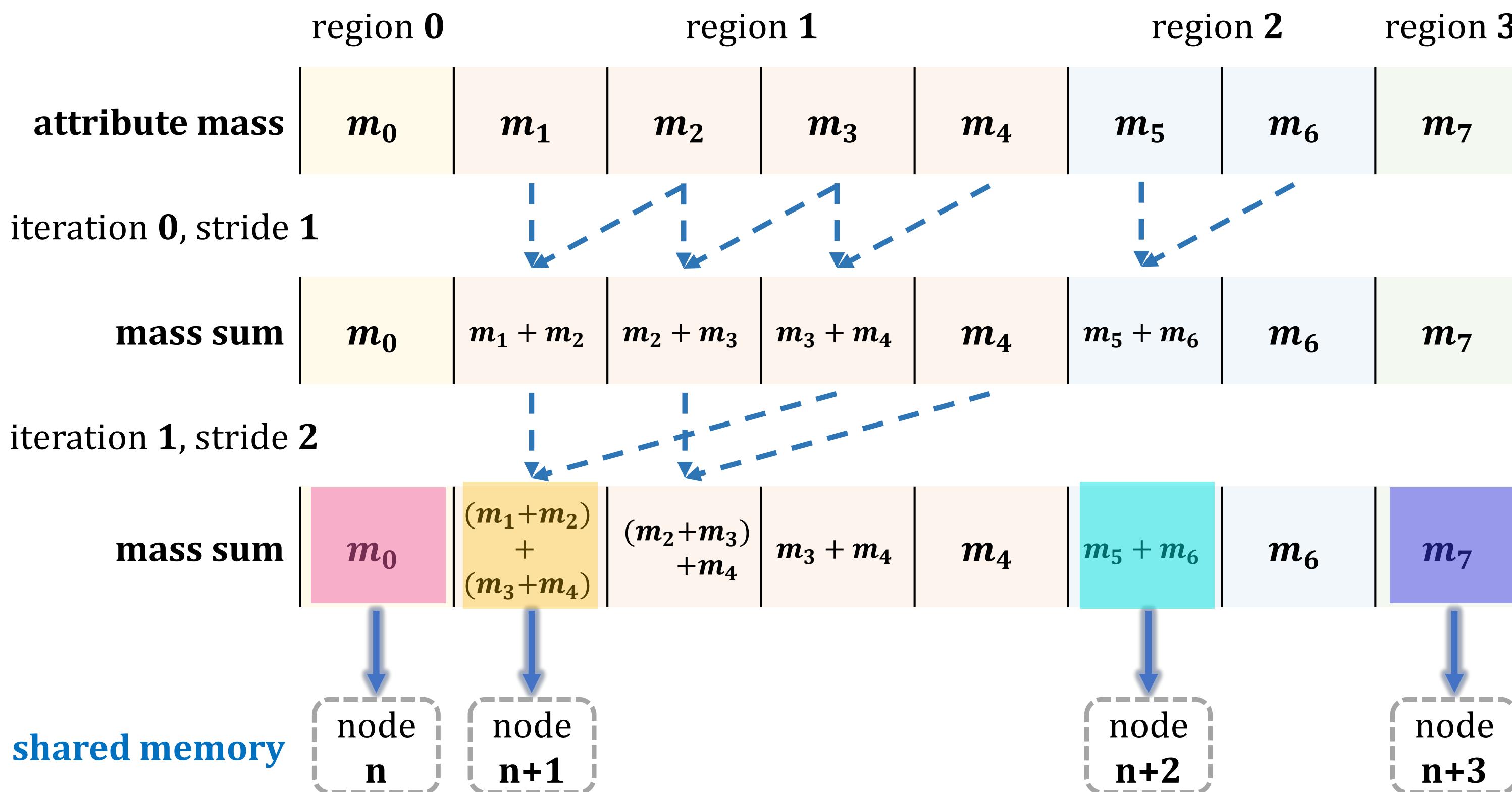


## CUDA intrinsic - shfl



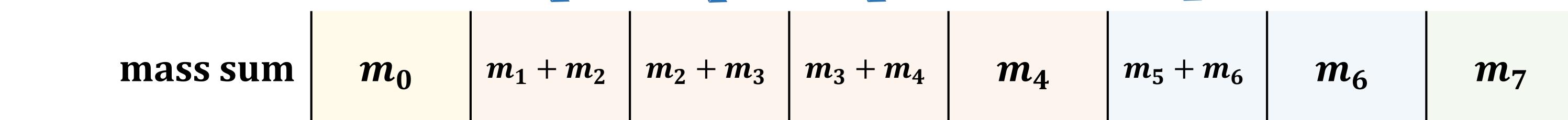
lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3
boundary mark	1	1	0	0	0	1	0	1
region interval	0	3	2	1	0	1	0	0

# CUDA intrinsic - ballot



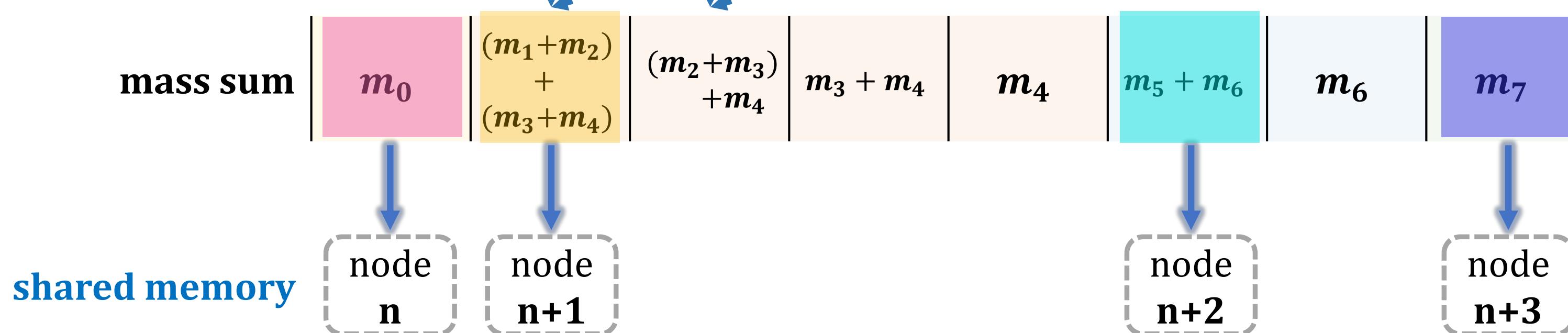
# CUDA intrinsic - shfl

## iteration 0, stride 1



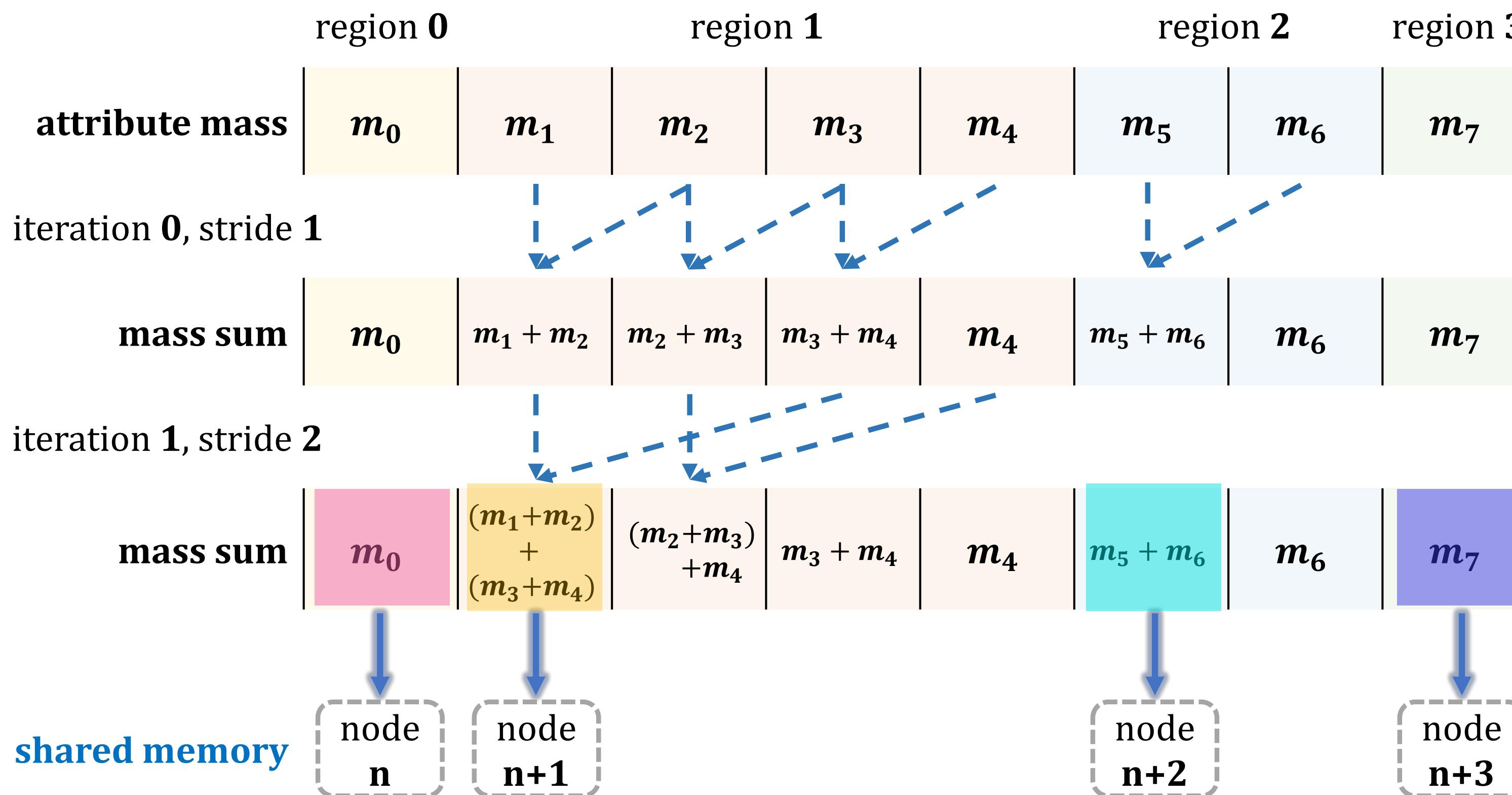
## CUDA intrinsic - shfl

## iteration 1, stride 2



lane id	0	1	2	3	4	5	6	7
node id	n	n+1	n+1	n+1	n+1	n+2	n+2	n+3
boundary mark	1	1	0	0	0	1	0	1
region interval	0	3	2	1	0	1	0	0

# CUDA intrinsic - ballot

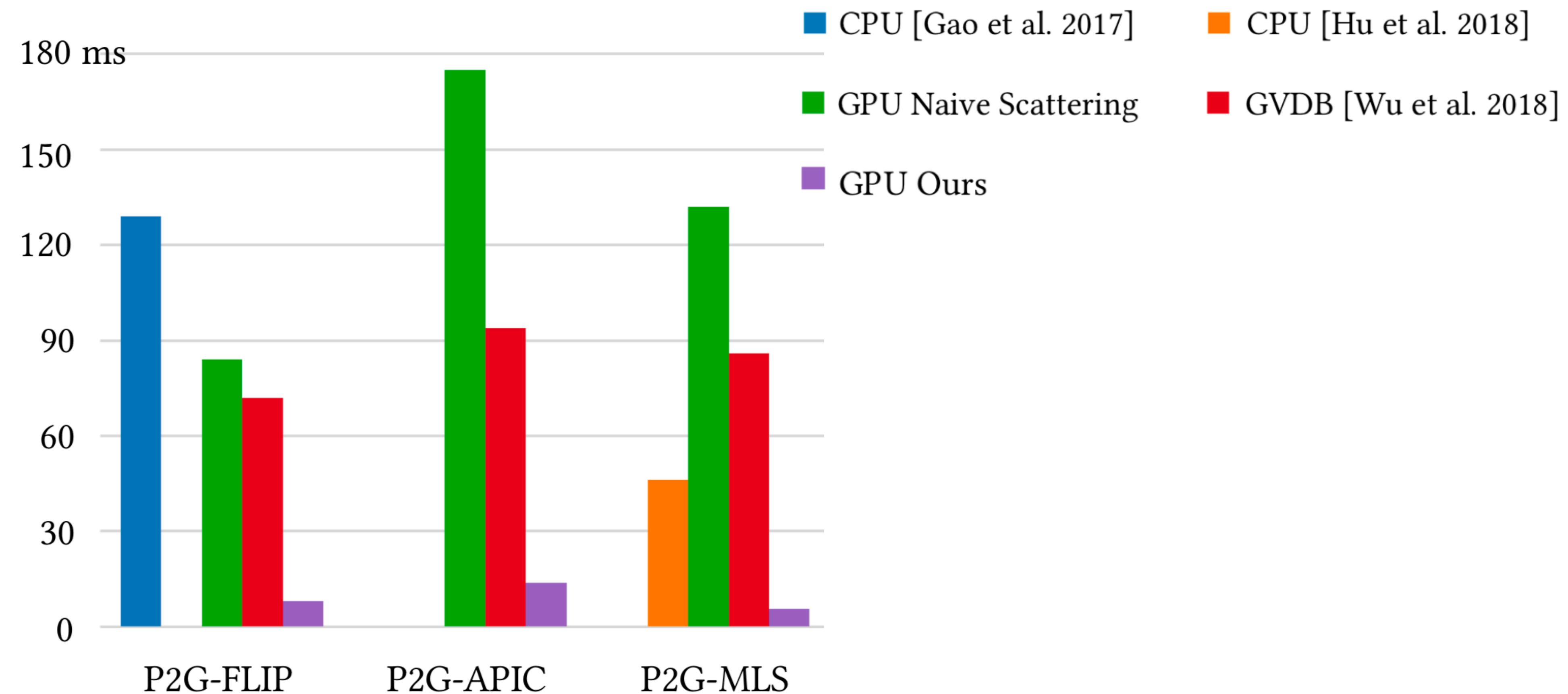


# CUDA intrinsic - shfl

# CUDA intrinsic - shfl

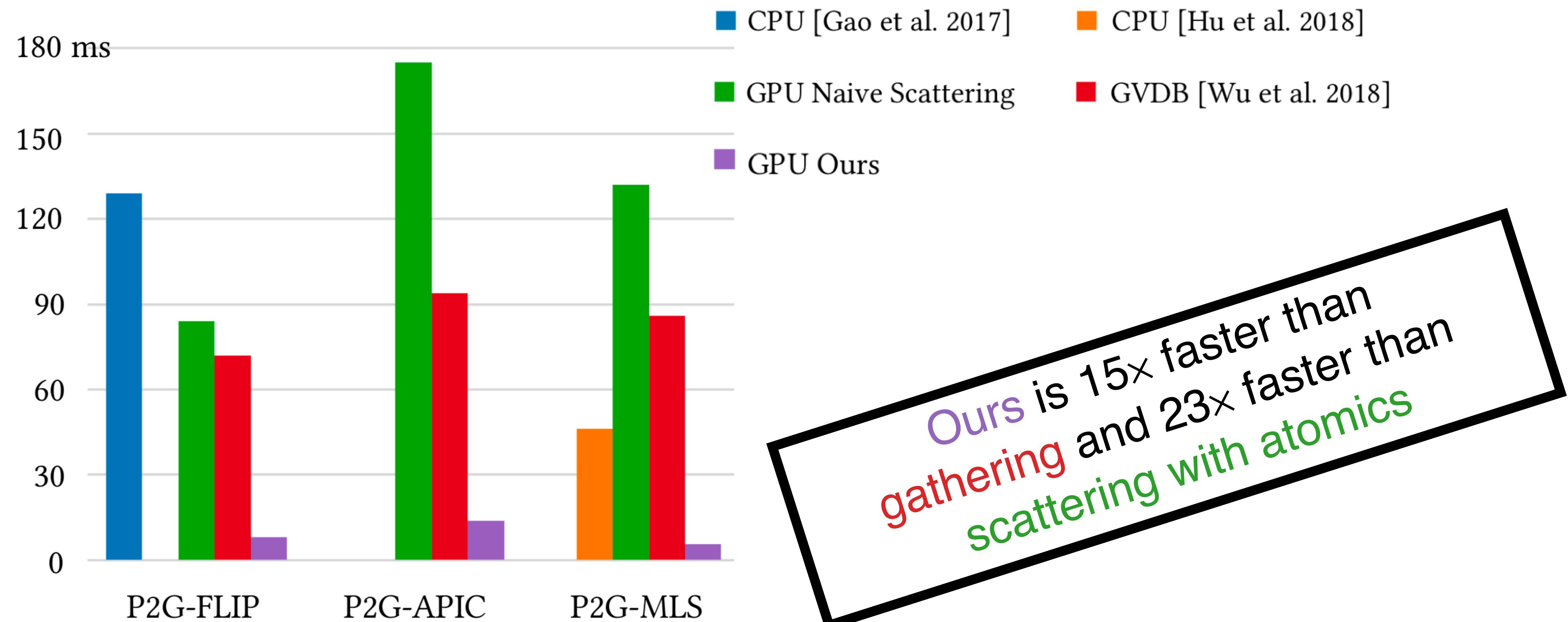
# Benchmark

NVIDIA TITAN Xp  
Particles #: 7M  
Grid res: 128<sup>3</sup>



# Benchmark

NVIDIA TITAN Xp  
Particles #: 7M  
Grid res: 128<sup>3</sup>



# Grid to particle (G2P)

```
1: procedure GPUMPM( )
2:   P  $\leftarrow$  Initialize particle positions
3:   P  $\leftarrow$  Sort and reorder (P)
4:   for each time step do
5:     dt  $\leftarrow$  Compute dt (P)
6:     G  $\leftarrow$  Refresh GSPGrid (P)
7:     M  $\leftarrow$  Build particle-grid mapping (P, G)
8:     G  $\leftarrow$  Transfer from particles to grid (P, M)
9:     G  $\leftarrow$  Apply external forces (G)
10:    G  $\leftarrow$  Solve on the grid (G, dt)
11:    P  $\leftarrow$  Transfer from grid to particles (G, M)
12:    P  $\leftarrow$  Update particle attributes (P, dt)
13:    P  $\leftarrow$  Resort and reorder (P)
```





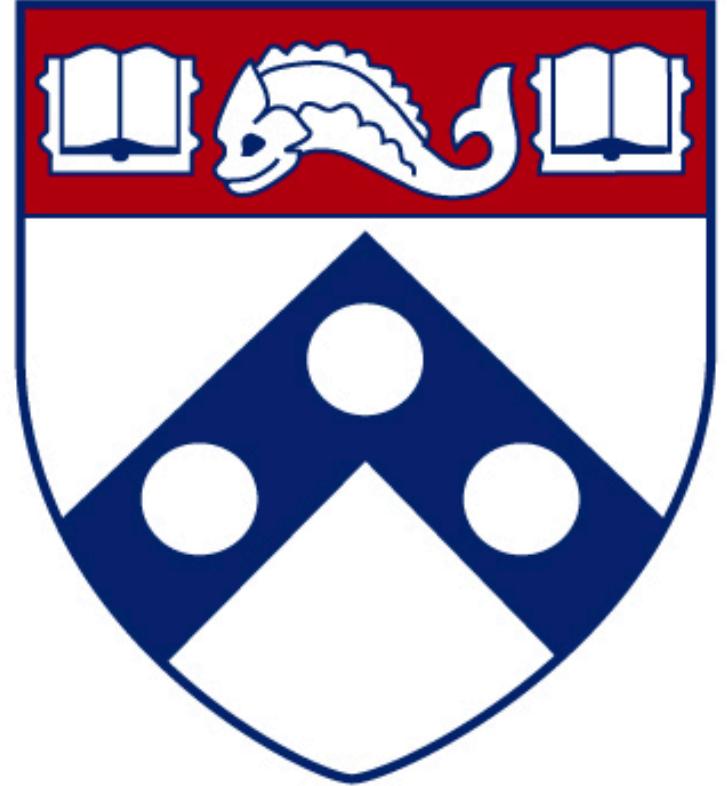
Particles: 4.2 M  
Grid resolution:  $256^3$   
Simulation: 10.48 secs/frame



Particles: 4.2 M  
Grid resolution:  $256^3$   
Simulation: 10.48 secs/frame



# Thank you!



Source code - <https://github.com/kuiwuchn/GPUMPM>

Contact - [ming.gao07@gmail.com](mailto:ming.gao07@gmail.com)