Scalable Simulation of Realistic Volume Fraction Red Blood Cell Flows through Vascular Networks

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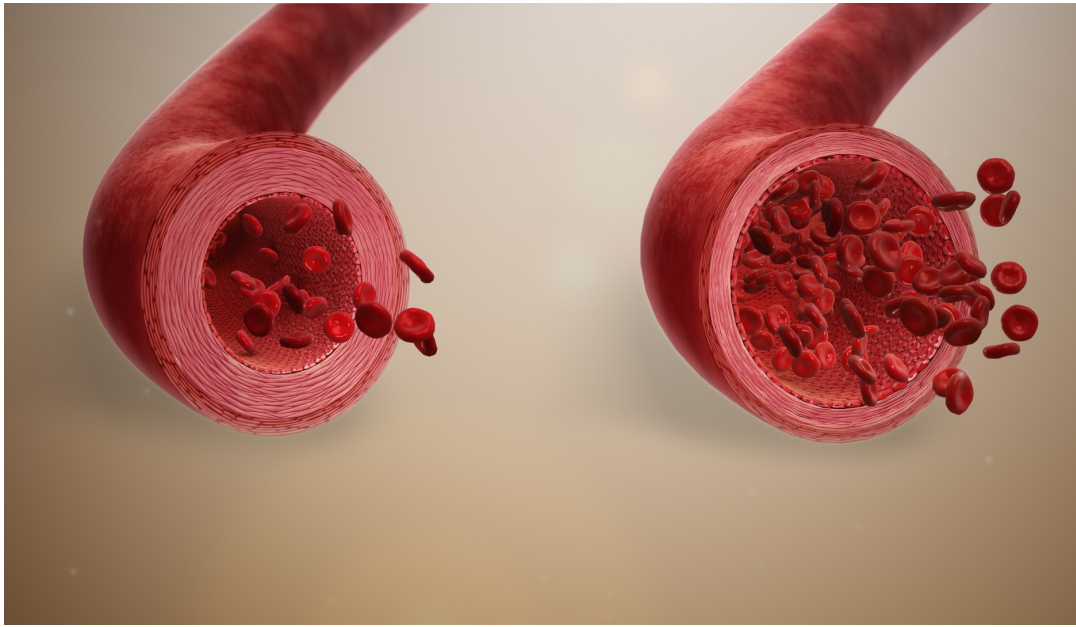
Joint work with Libin Lu, Abtin Rahimian, Georg Stadler, Denis Zorin

Outline

- **Motivation**
- Formulation, Numerics, Algorithms
- Results

Goal: Simulate red blood cell flow in capillaries

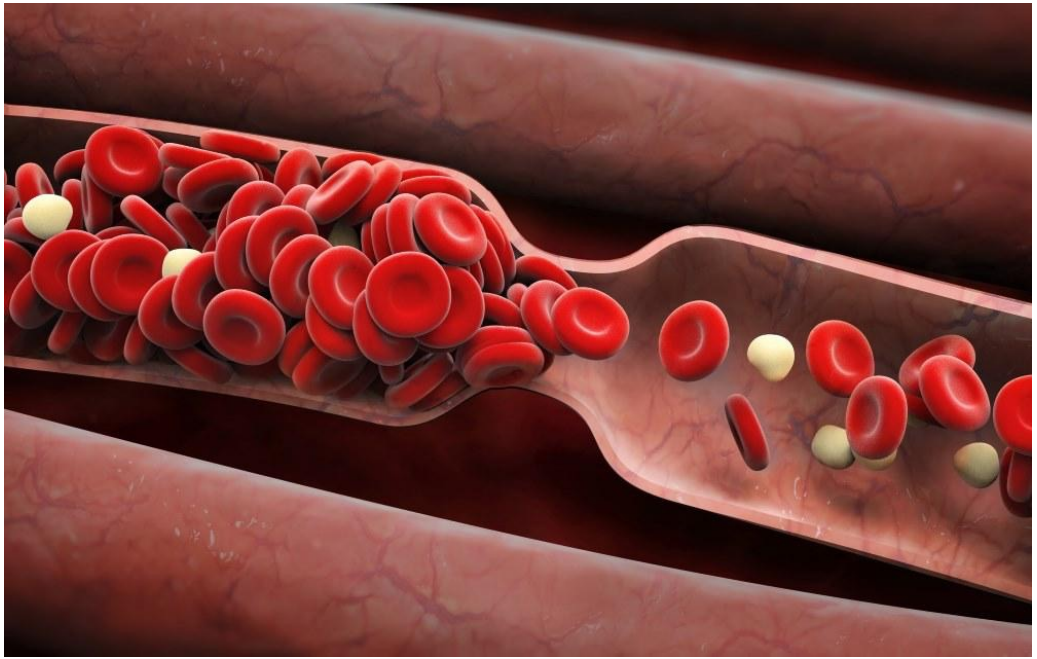
- Important biophysical phenomena:
  - vasoconstriction
  - vasodilation



https://en.wikipedia.org/wiki/Vasodilation

Goal: Simulate red blood cell flow in capillaries

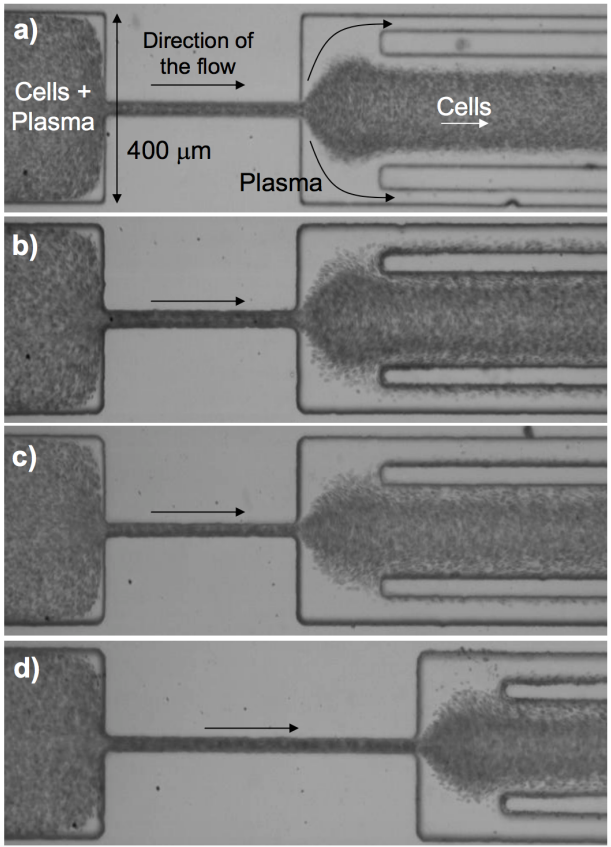
- Important biophysical phenomena:
  - vasoconstriction
  - vasodilation
  - blood clotting



shutterstock.com

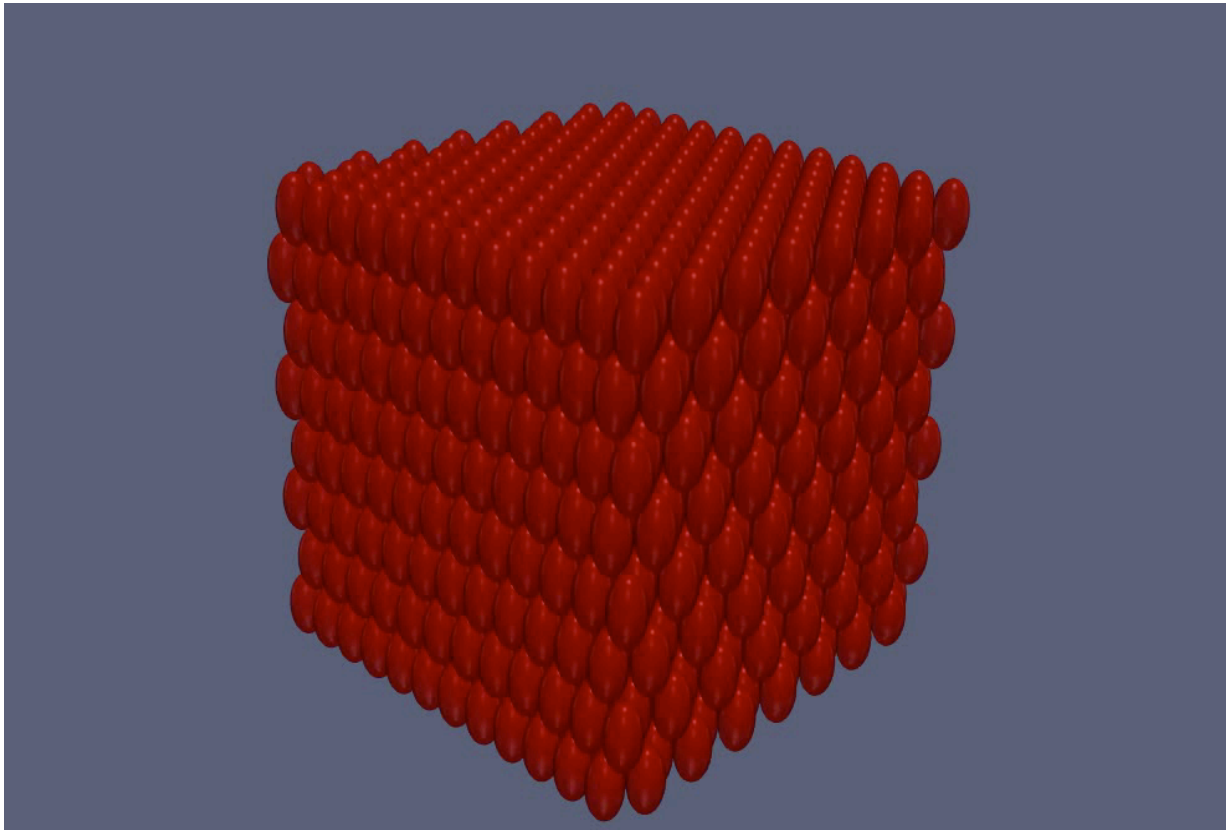
Goal: Simulate red blood cell flow in capillaries

- Important biophysical phenomena:
  - vasoconstriction
  - vasodilation
  - blood clotting
  - microfluidic device design



Drops, vesicles and red blood cells: Deformability and behavior under flow - Magalie Faivre, Thesis 2006

There are many free space codes...



Parallel contact-aware simulations of deformable particles in 3D Stokes flow, L. Lu et. al., arxiv 2018

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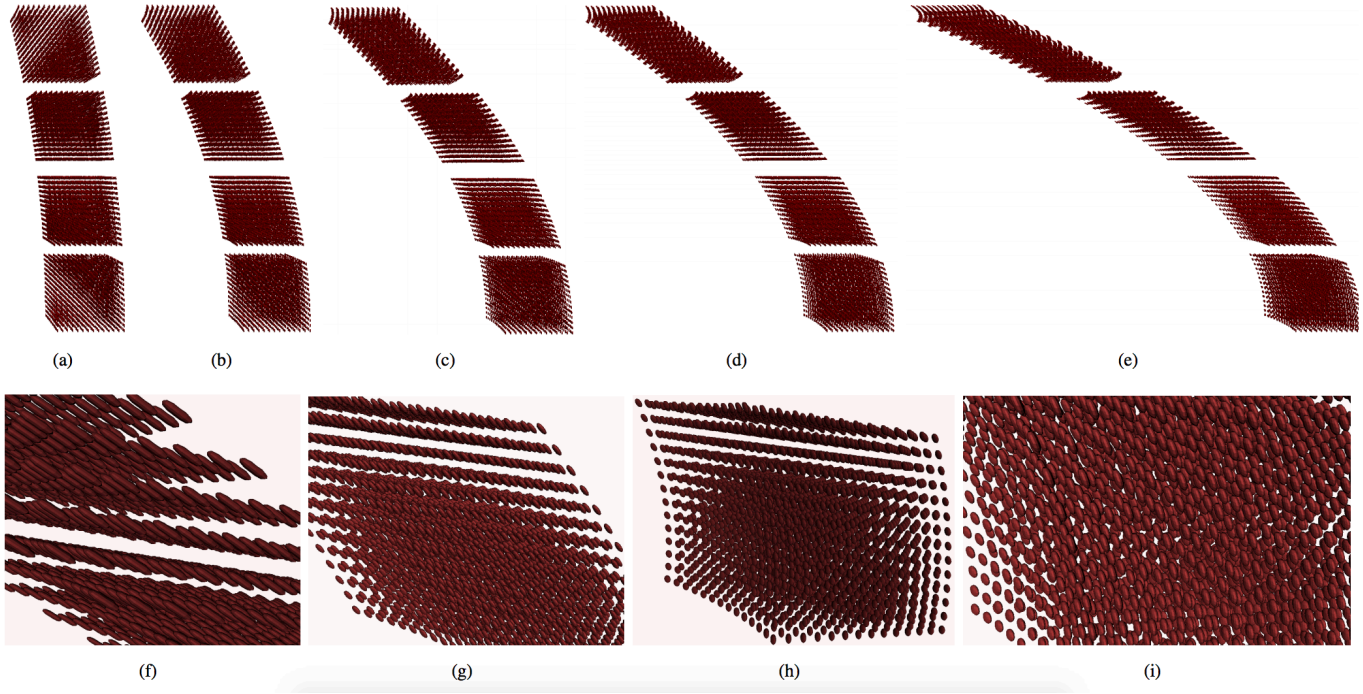
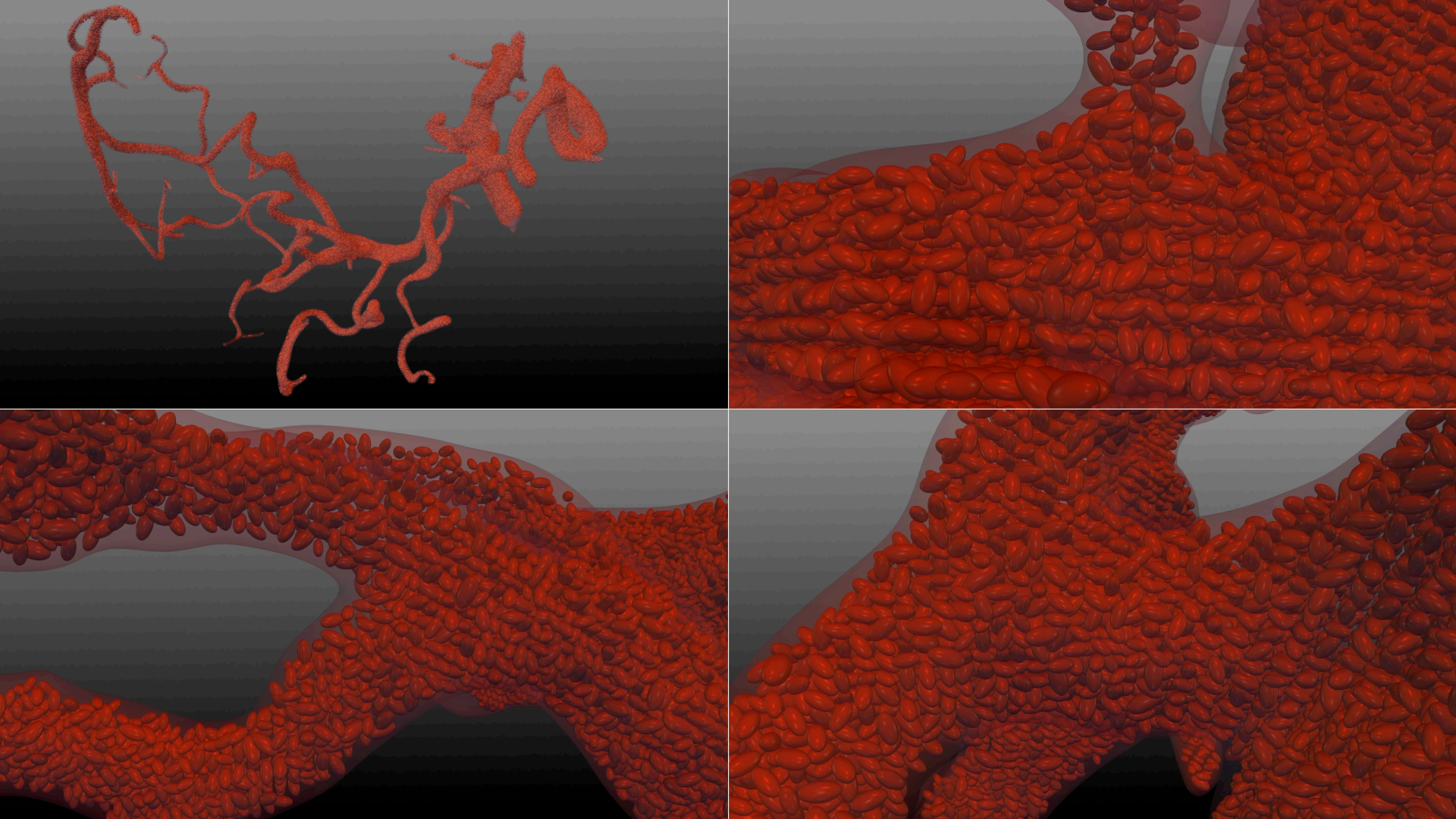


"Petascale direct numerical simulation of blood flow on 200k cores and heterogeneous architectures." Rahimian et. al., SC 2010

… but few with boundaries

- Either:
  - Large scale, low-order accurate
  - Small scale, high-order accurate



Contribution

- Parallel Stokes boundary solver on complex geometry
- Parallel collision handling between RBCs + blood vessel
- Scaled to ~35k cores (resource limited)

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Stokes flow on RBCs

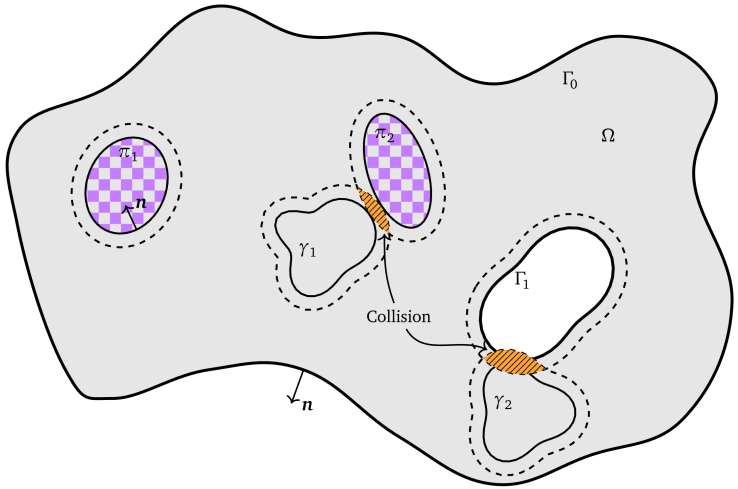
$$\mu\Delta\mathbf{u}(\mathbf{x}) + \nabla p(\mathbf{x}) = \mathbf{F}(\mathbf{x}), \quad \Delta \cdot \mathbf{u} = 0, \quad \mathbf{x} \in \Omega$$

$$\mathbf{u}(\mathbf{x}) = \mathbf{g}(\mathbf{x}), \quad \mathbf{x} \in \partial\Omega$$

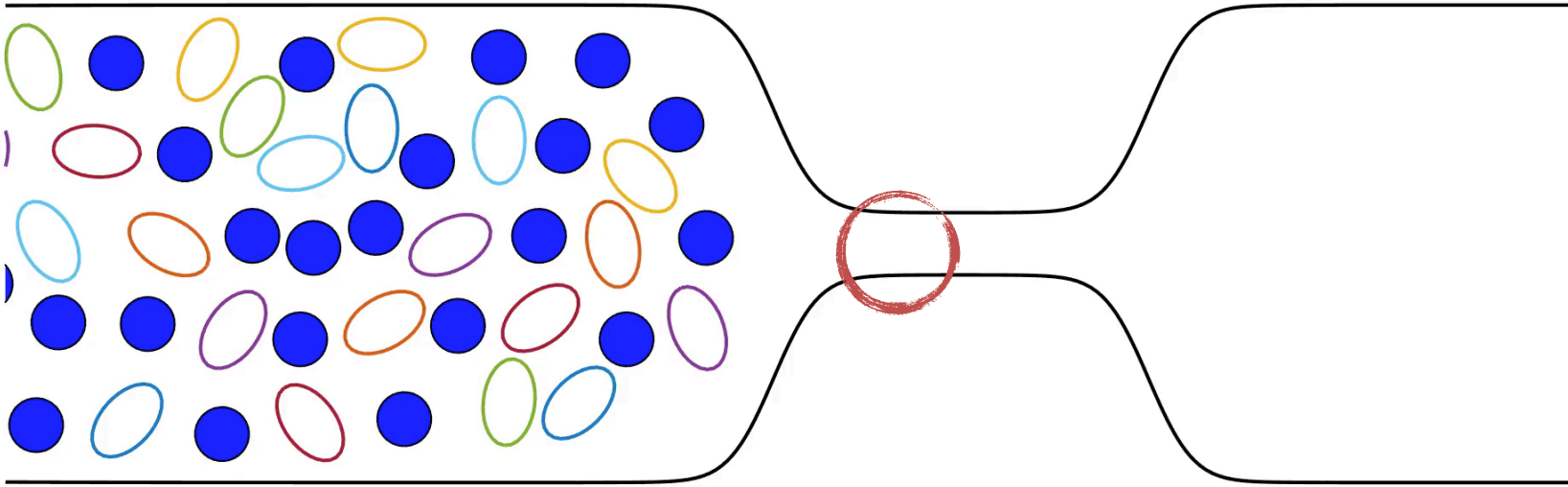
$$\mathbf{X}_t = \mathbf{u}(\mathbf{X}), \quad \mathbf{X} \in \gamma_i$$

$$\mathbf{F}(\mathbf{x}) = \sum_i \int_{\gamma_i} \mathbf{f}(\mathbf{y})\delta(\mathbf{x}-\mathbf{y})d\mathbf{y}$$

$$\mathbf{f}(\mathbf{y}) = \mathbf{f}_\sigma + \mathbf{f}_b$$



Collision handling is hard!



Collision handling is hard!

- Small time steps
- Fine spatial discretization
  - Too expensive
- Maintain accurate physics?
  - requires solving non-linear complementarity problem (NCP)

Collision handling is harder in parallel!

- Need to detect colliding geometry on other processors
- Need scalable algorithms to solve resulting non-linear complementarity problem

Stokes flow on RBCs

$$\mu\Delta\mathbf{u}(\mathbf{x}) + \nabla p(\mathbf{x}) = \mathbf{F}(\mathbf{x}), \quad \Delta \cdot \mathbf{u} = 0, \quad \mathbf{x} \in \Omega$$

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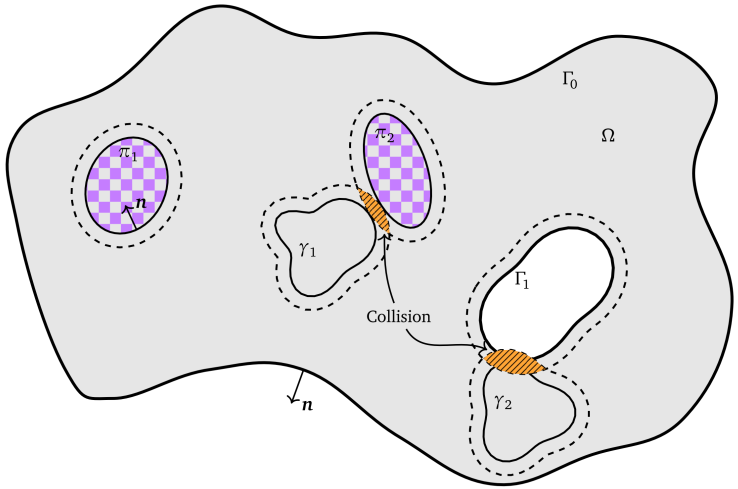
$$\mathbf{f}(\mathbf{y}) = \mathbf{f}_\sigma + \mathbf{f}_b + \mathbf{f}_c$$

$\mathbf{f}_c$: [Harmon et. al. 2011]: space-time interference volume



Boundary Integral Formulation

$$\mathbf{u} = \sum_i \mathbf{u}^{\gamma_i} + \mathbf{u}^{\Gamma}$$

- RBCs:

$$\mathbf{u}^{\gamma_i}(\mathbf{x}) = \int_{\gamma_i} \mathcal{S}(\mathbf{x}-\mathbf{y})\mathbf{f}(\mathbf{y})d\mathbf{y}, \quad \mathcal{S}(\mathbf{r}) = \frac{1}{8\mu\pi}\left(\frac{1}{\mathbf{r}} + \frac{\mathbf{r}\otimes\mathbf{r}}{\mathbf{r}^3}\right)$$

- Existing methods: [Veerapeneni et. al. JCP 2011], [Malhotra et. al. arxiv 2017, Lu et. al. arxiv 2018]

Boundary Integral Formulation

$$\mathbf{u} = \sum_i \mathbf{u}^{\gamma_i} + \mathbf{u}^{\Gamma}$$

- Vessel:

$$\mathbf{u}^{\Gamma}(\mathbf{x}) = \int_{\Gamma} \mathcal{D}(\mathbf{x}-\mathbf{y})\phi(\mathbf{y})d\mathbf{y}, \quad \mathcal{D}(\mathbf{r}) = \frac{\partial \mathcal{S}(\mathbf{r})}{\partial n}$$

$$\left(\frac{1}{2}I + D + N\right)\phi = \mathbf{g} - \sum_i \mathbf{u}^{\gamma_i}, \quad \mathbf{x} \in \Gamma$$

BIE Representation + Discretization

- RBCs:
  - Spherical harmonic representation
  - Semi-implicit time stepping
- Vessel:
  - Bezier polynomial patches
- Nyström discretization with spectrally accurate quadrature rules

Evaluating velocity

$$\mathbf{u}^{\Gamma}(\mathbf{x}) = \int_{\Gamma} \mathcal{D}(\mathbf{x}-\mathbf{y})\phi(\mathbf{y})d\mathbf{y}$$

$$\mathbf{u}^{\Gamma}(\mathbf{x}) = \sum_{i=1}^{N} \int_{P_i} \mathcal{D}(\mathbf{x}-\mathbf{y})\phi(\mathbf{y})d\mathbf{y}$$

$$\mathbf{u}^{\Gamma}(\mathbf{x}) \approx \sum_{i=1}^{N} \sum_{j=1}^{q} \mathcal{D}(\mathbf{x}-\mathbf{y}_i)\phi(\mathbf{y}_i)w_i$$

N-body sum

N-body sum —> FMM

- Accelerate with fast multipole method (FMM)
- All hydrodynamic interaction through FMMs
- Many high performance parallel FMMs exist; we choose PVFMM [Malhotra et. al., CCP 2015]

BIE: Pros and Cons

Pros:

- Linear Complexity
- High-order accuracy
- Dimension reduction
- No volume mesh
- Parallel scalability

Cons:

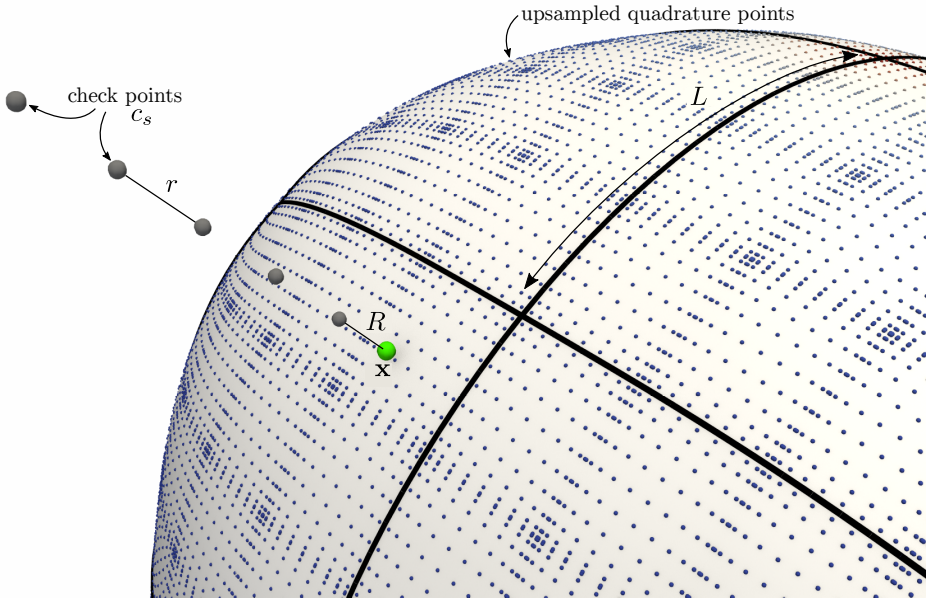
- Requires singular integration
- Only valid for Re << 1 (i.e. Stokes)

Challenges for Parallel RBC Simulation

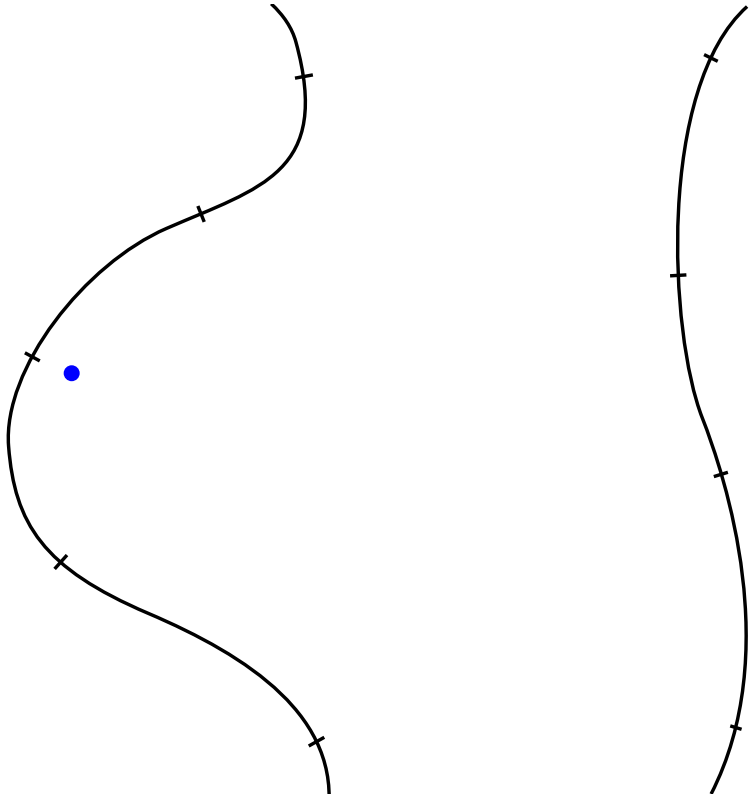
- Evaluate fluid velocity in parallel (FMM)
- Parallel singular quadrature
- Guarantee collision-free state across non-local geometry

Singular quadrature

- Upsample boundary data
- Find closest point
- Construct check points
- Evaluate velocity at check points
- Extrapolate velocity

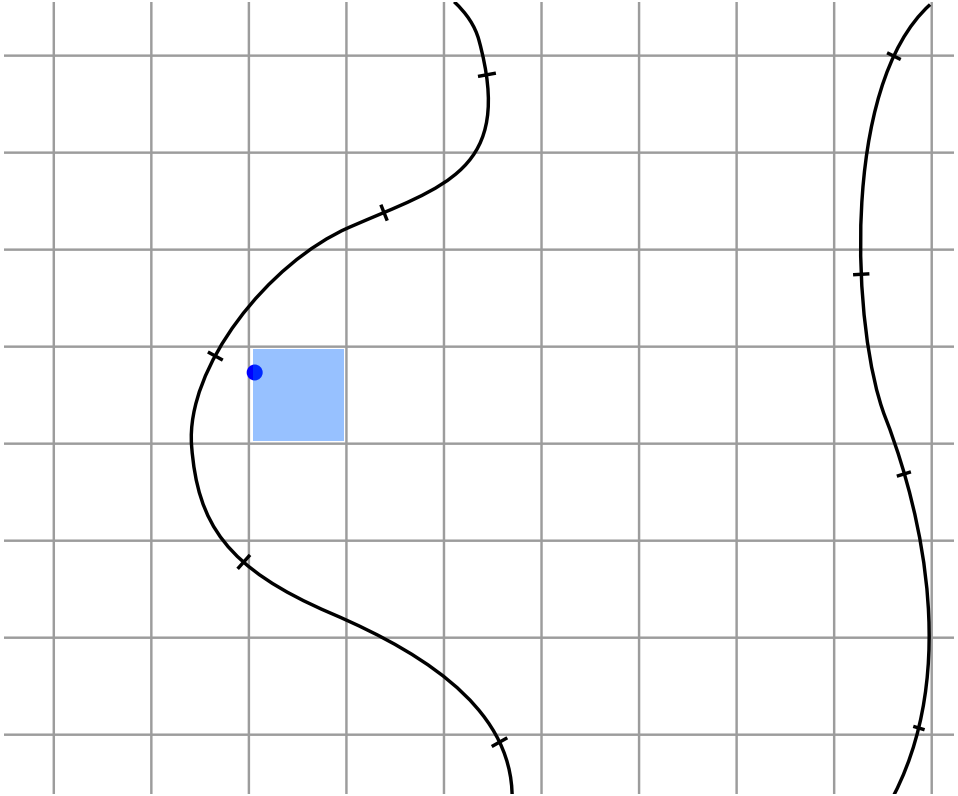


Closest point

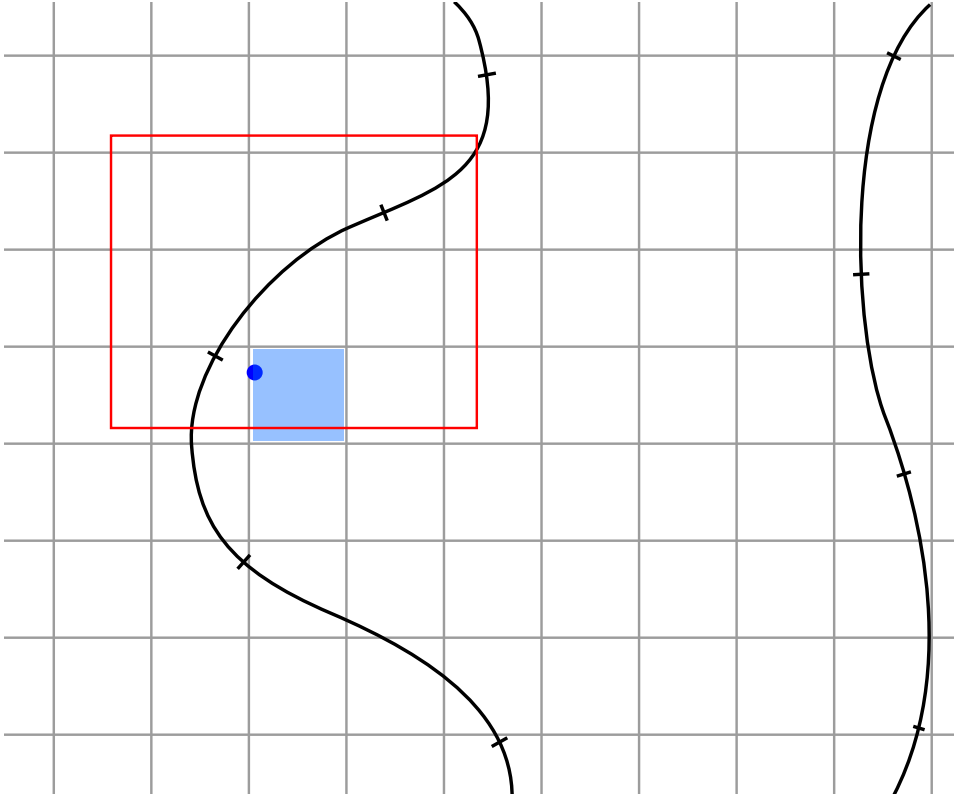


Parallel contact-aware simulations of deformable particles in 3D Stokes flow, Lu et. al., arxiv 2018

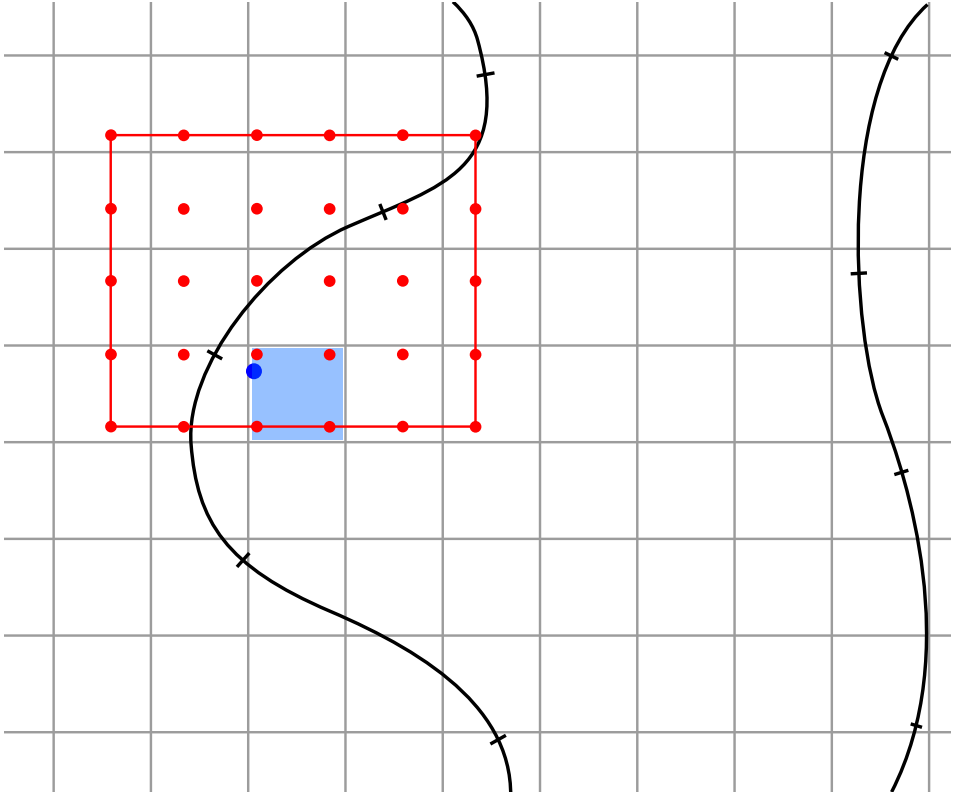
Step 1: Form spatial hash



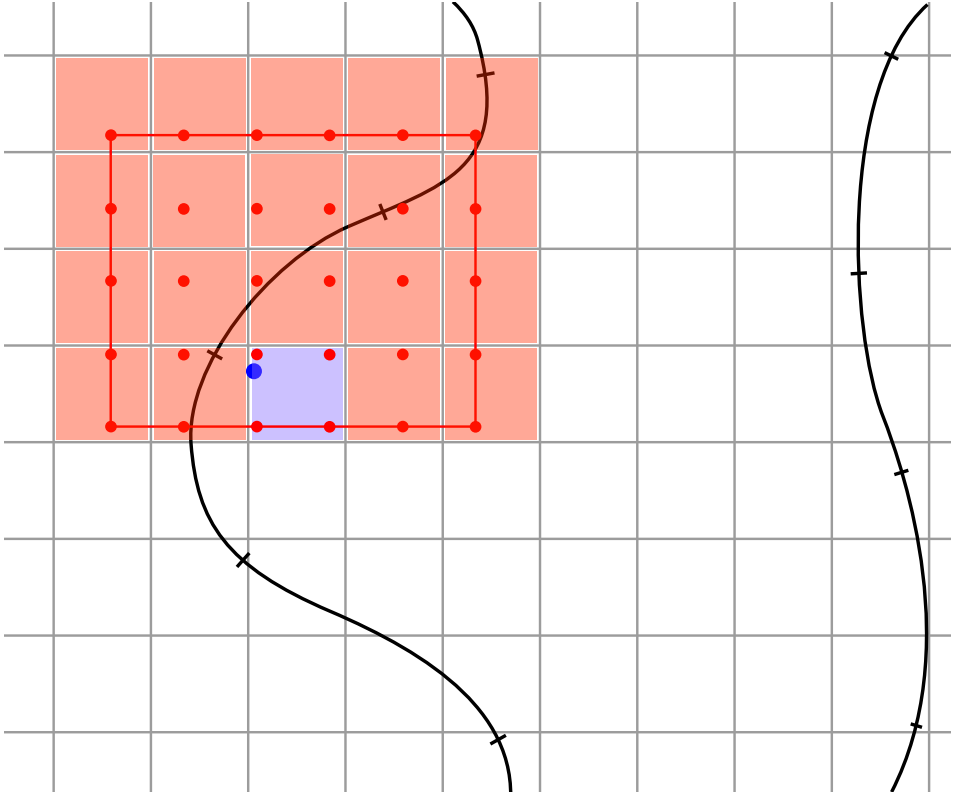
Step 2: Compute bounding box



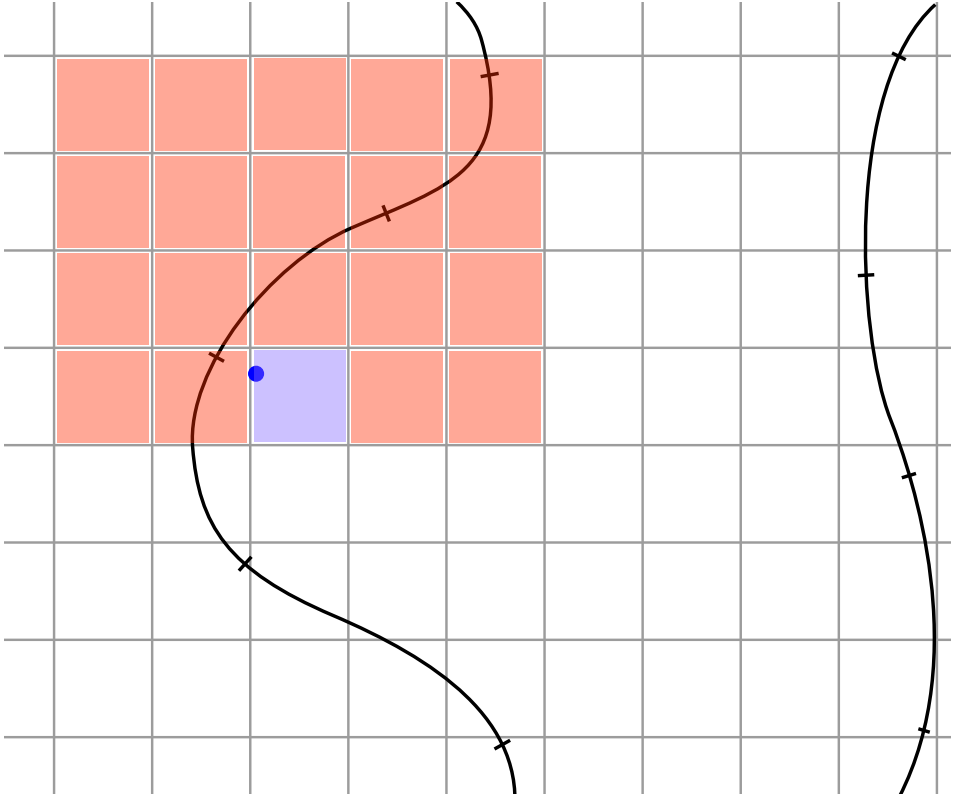
Step 3: Sample bounding box



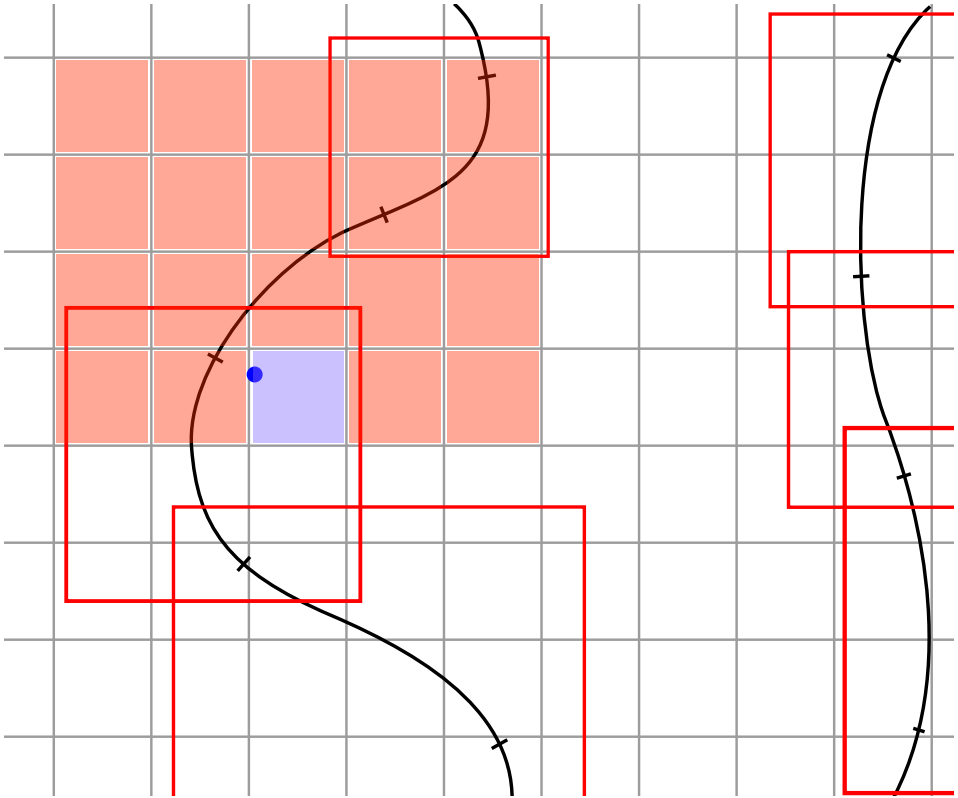
Step 4: Hash bounding box samples



Step 5: Parallel sort + scatter



Repeat for all patches…



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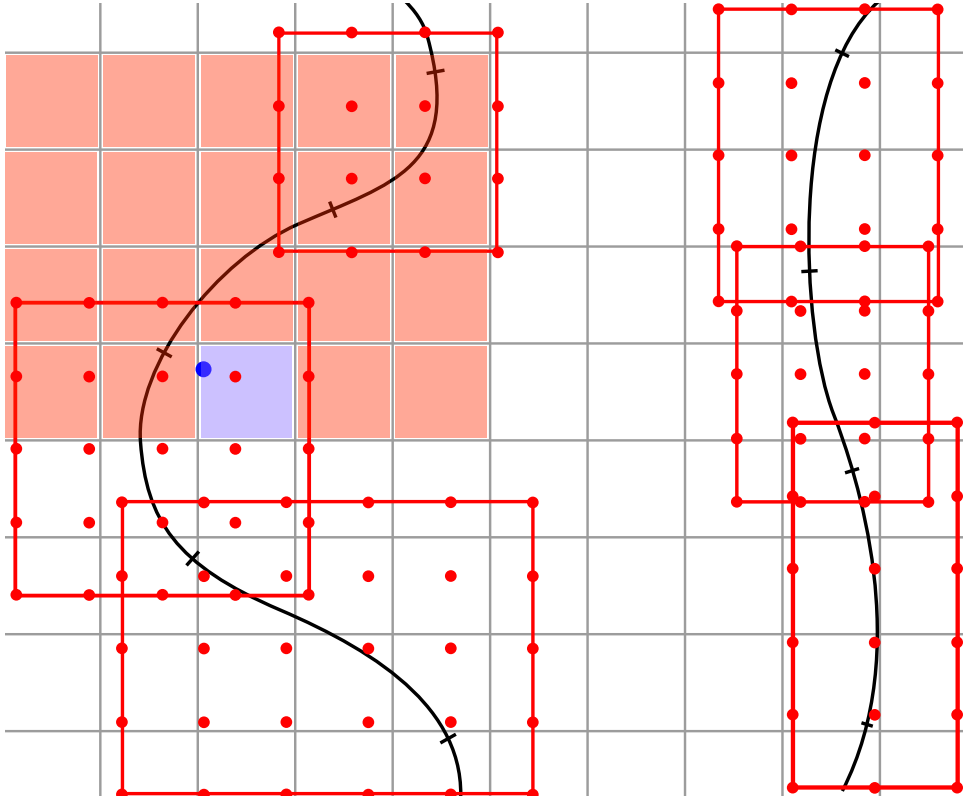

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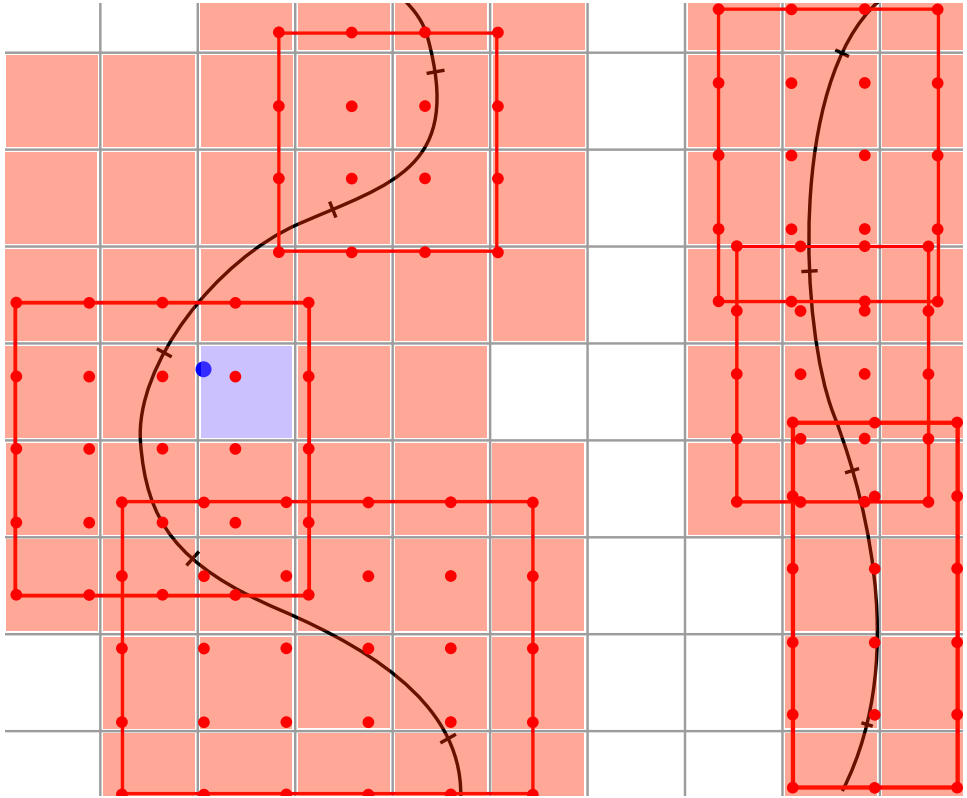

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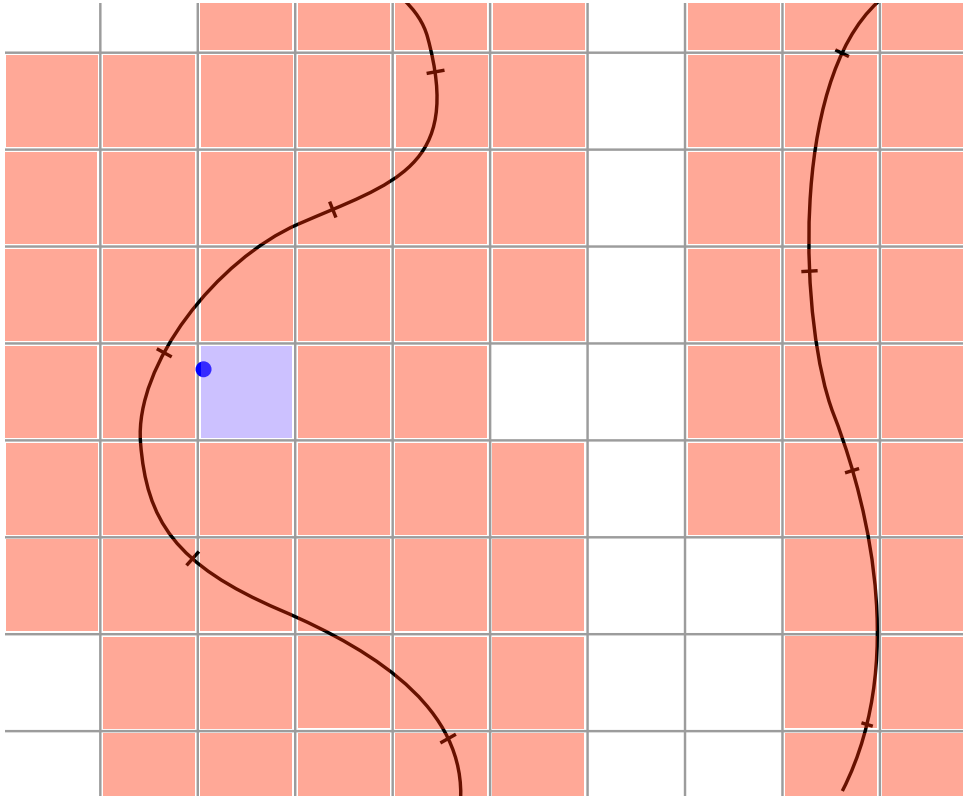
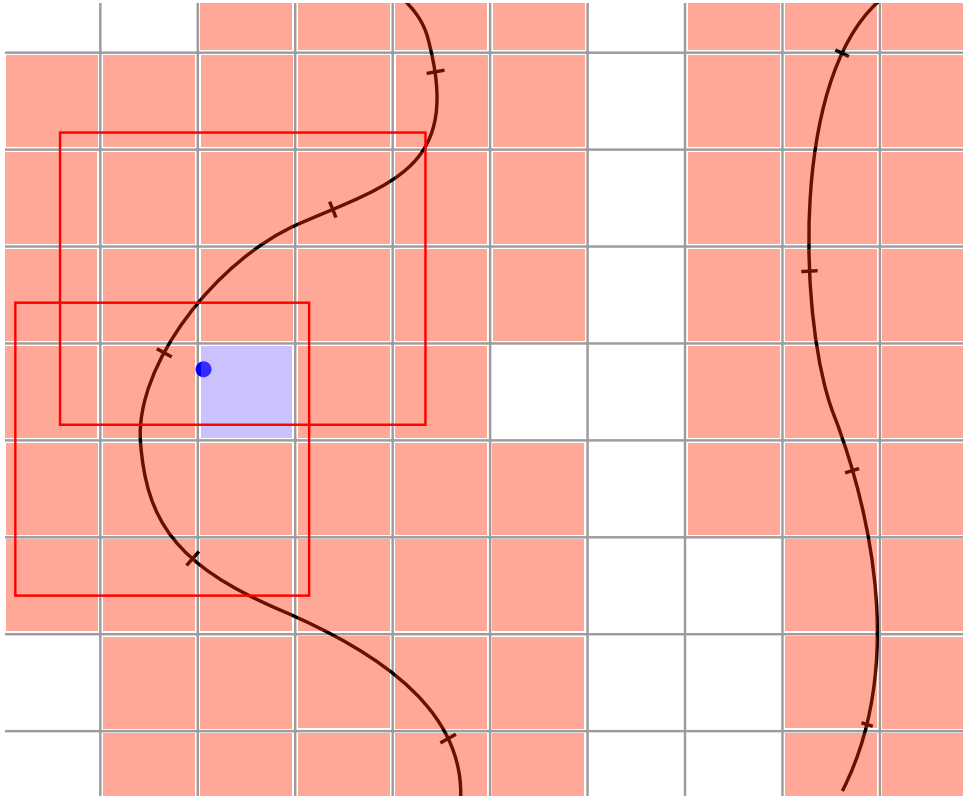
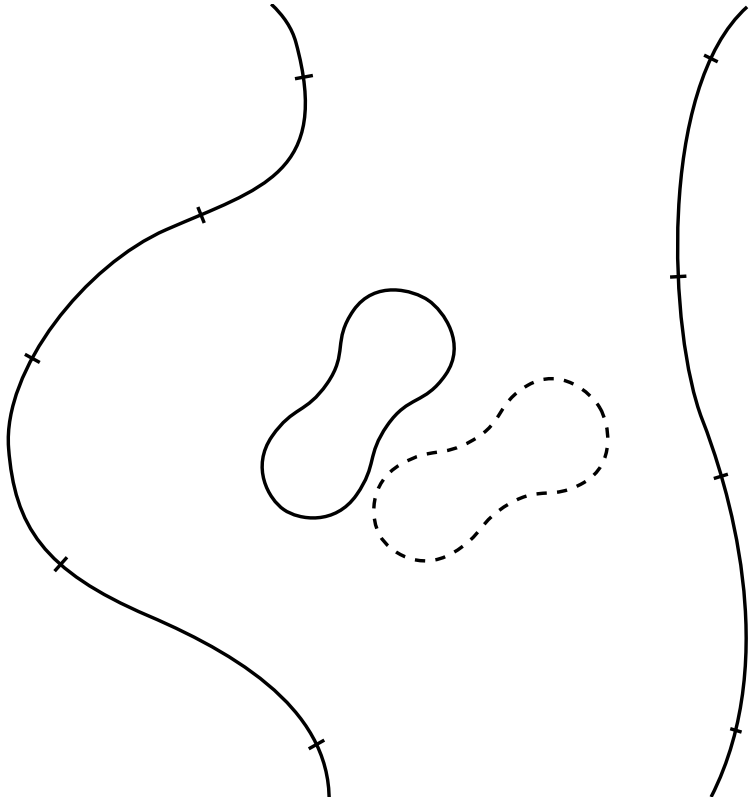


Hyksort: a new variant of hypercube quicksort on distributed memory architectures, H. Sundar et. al.; ICS 2016

Step 6: Compute distance locally



Collision handling



L. Lu et. al. Parallel contact-aware simulations of deformable particles in 3D Stokes flow, arxiv 2018

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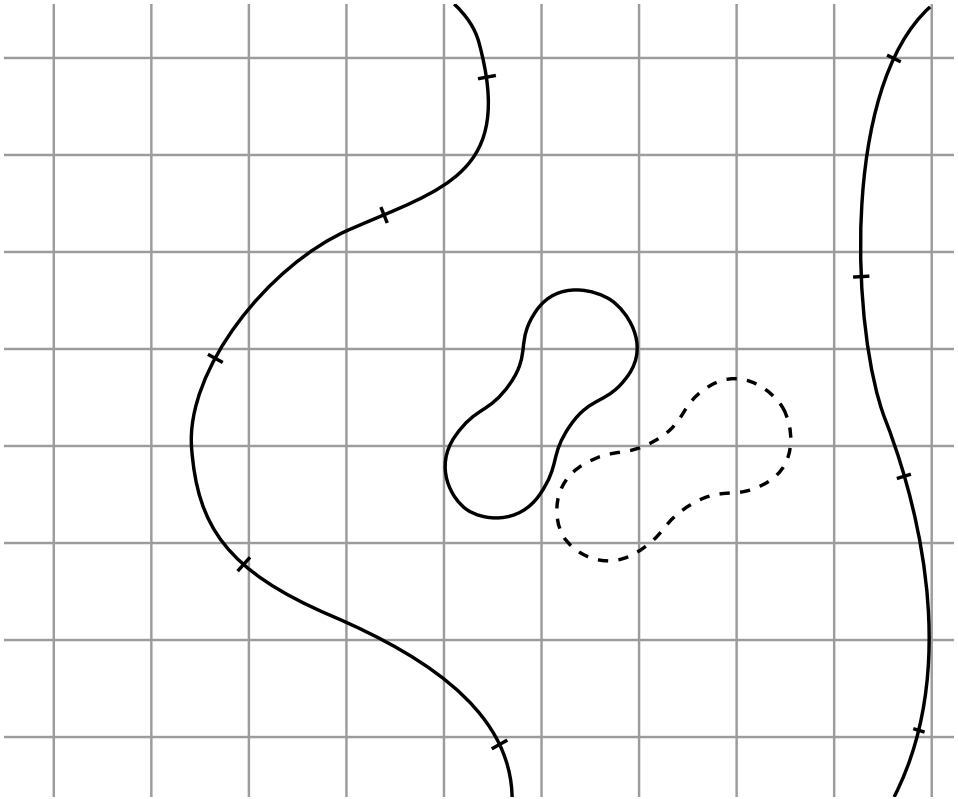
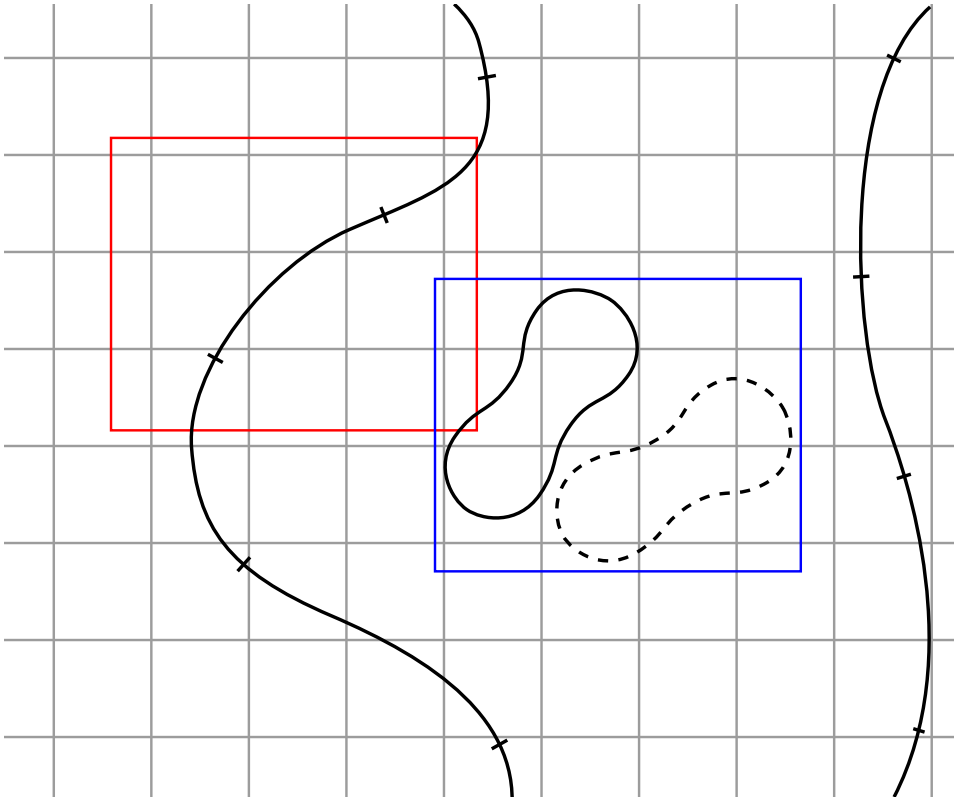
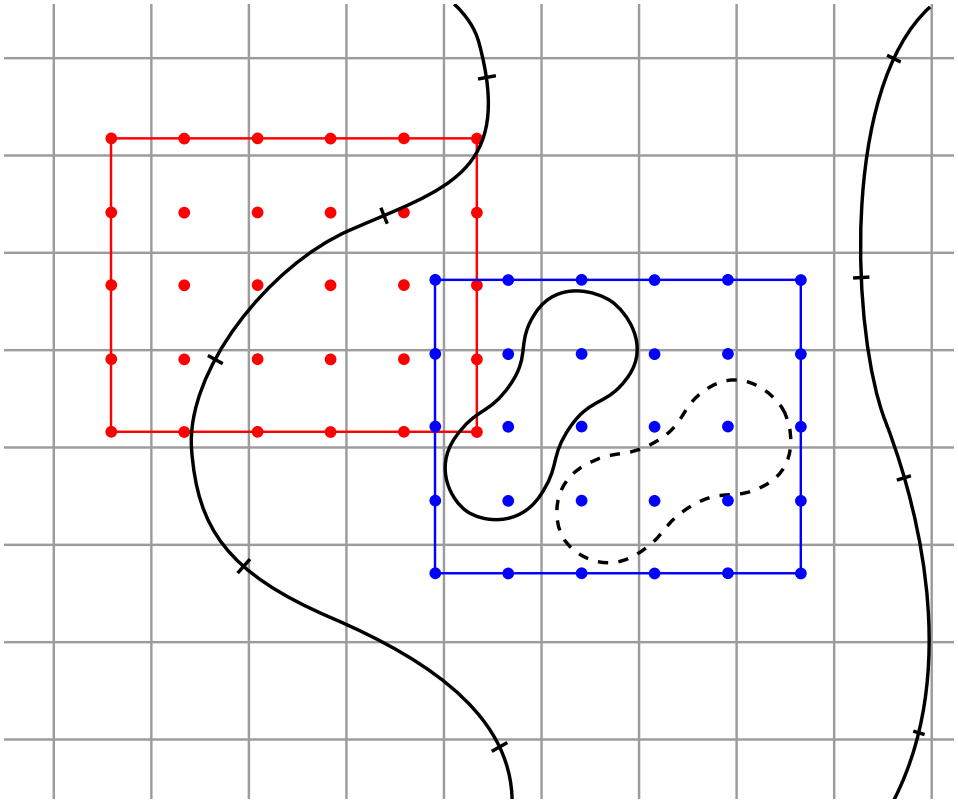


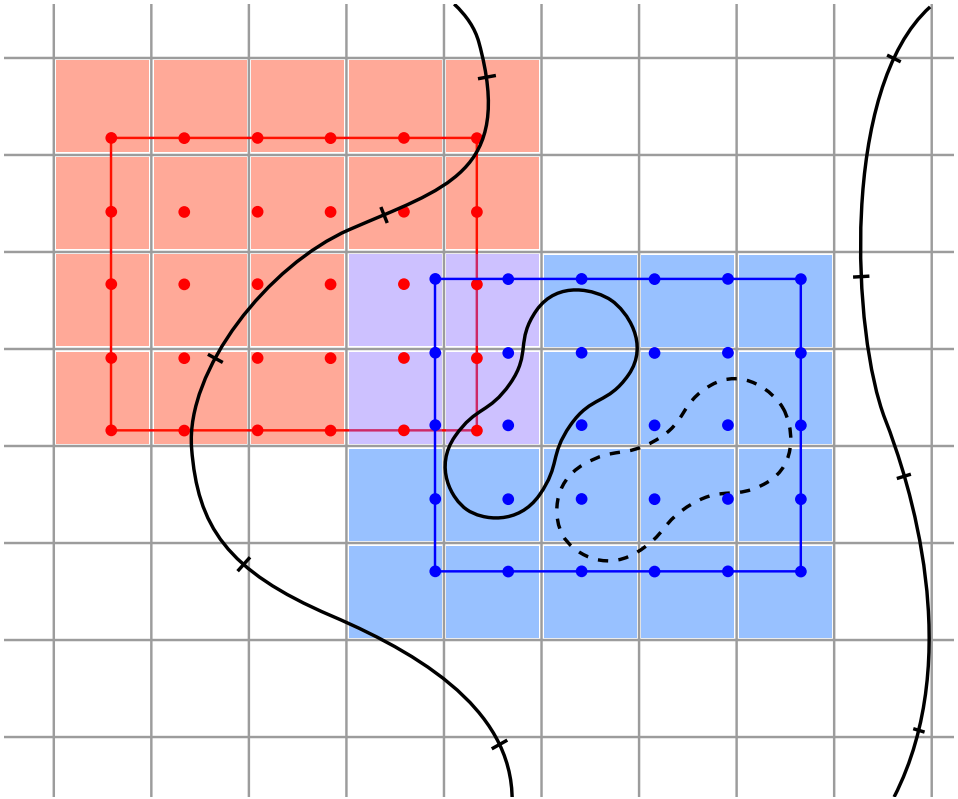
Step 2: Compute space-time bounding boxes



Step 3: Sample bounding boxes

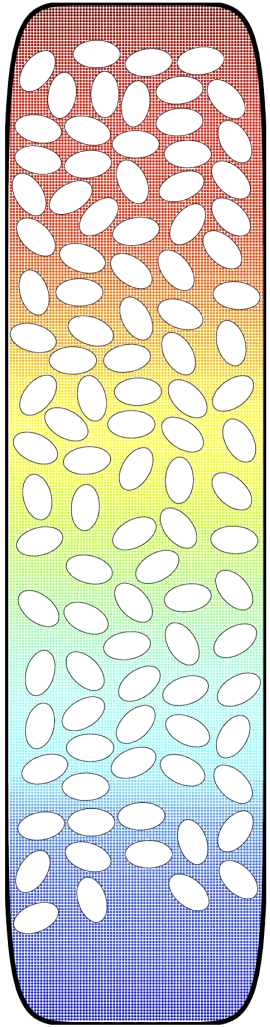


Step 4: Hash samples and parallel sort



Step 5: Iteratively solve NCP; repeat until collision-free

- Follow [Lu et. al. arxiv 2018]
- Solve NCP by a sequence of parallel linear complementarity problems (LCPs)



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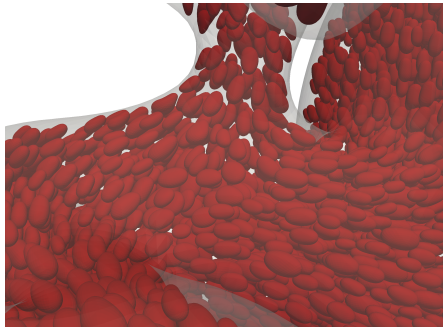
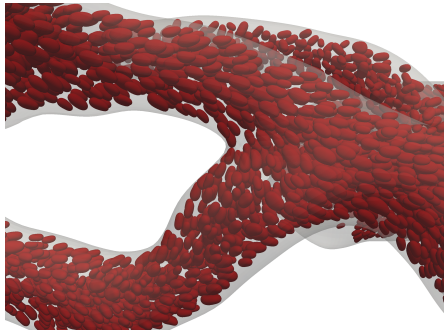
- **Results**

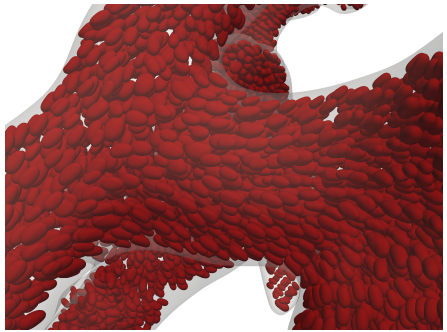
Setup

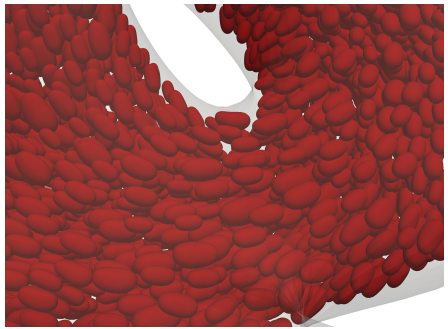
- Stampede2 at TACC
- Skylake (SKX): dual socket 24 core 2.1 GHz CPU, 192GB RAM
- Knights Landing (KNL): 68 core 1.4 GHz CPU, 96 GB RAM + 16 GB high-speed MCDRAM

Strong scaling



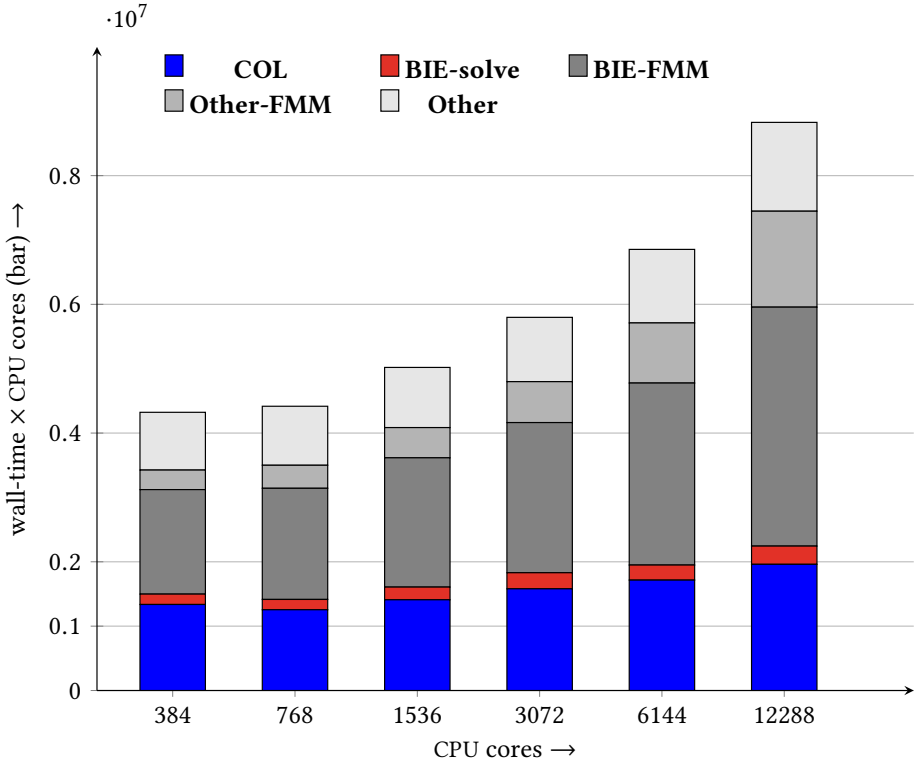




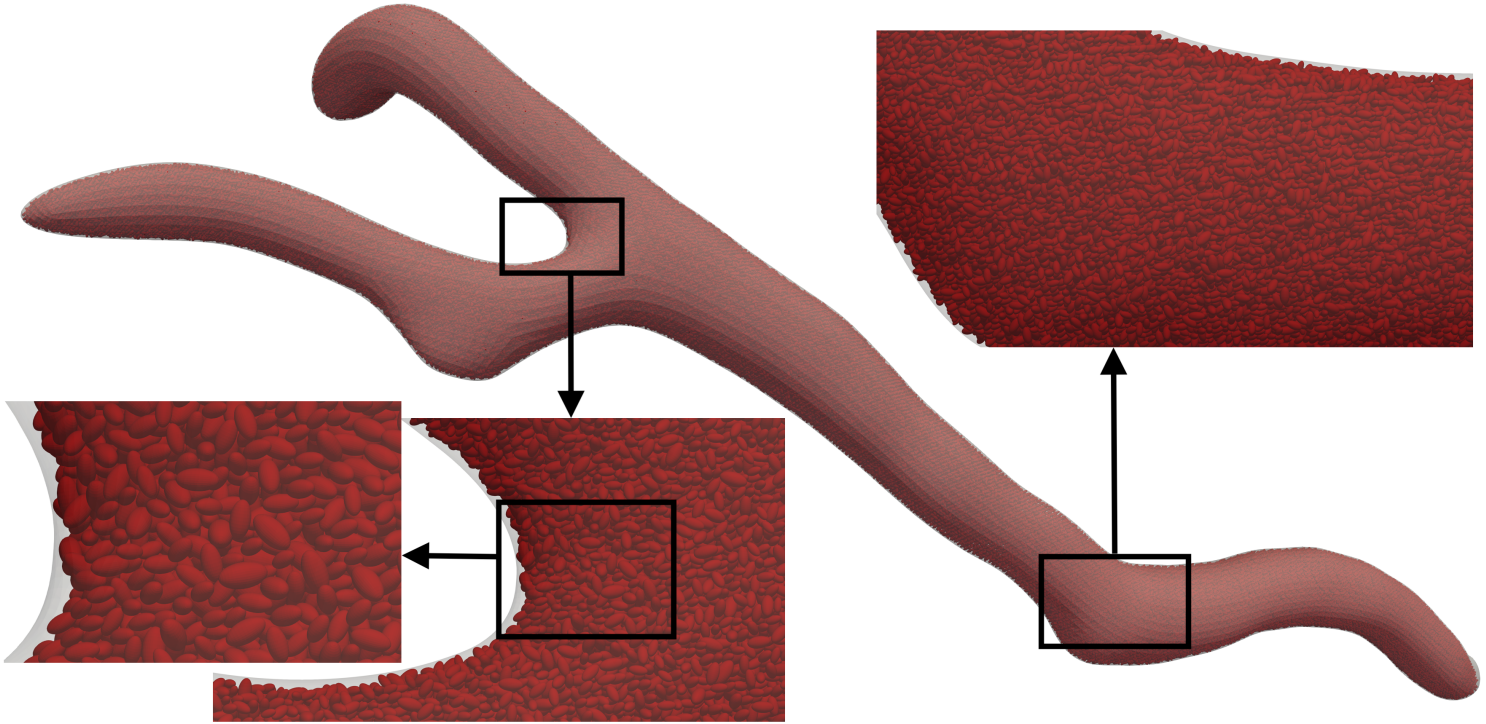


Strong scaling

- Skylake
- 40,960 RBCs with 40,960 patch blood vessel
- ~89 million DOF for RBCs
- ~15 million DOF for vessel
- 15.7x speed-up from 384 to 12288 cores
- 49% overall parallel efficiency
- 66% efficiency of collision handling + singular integration

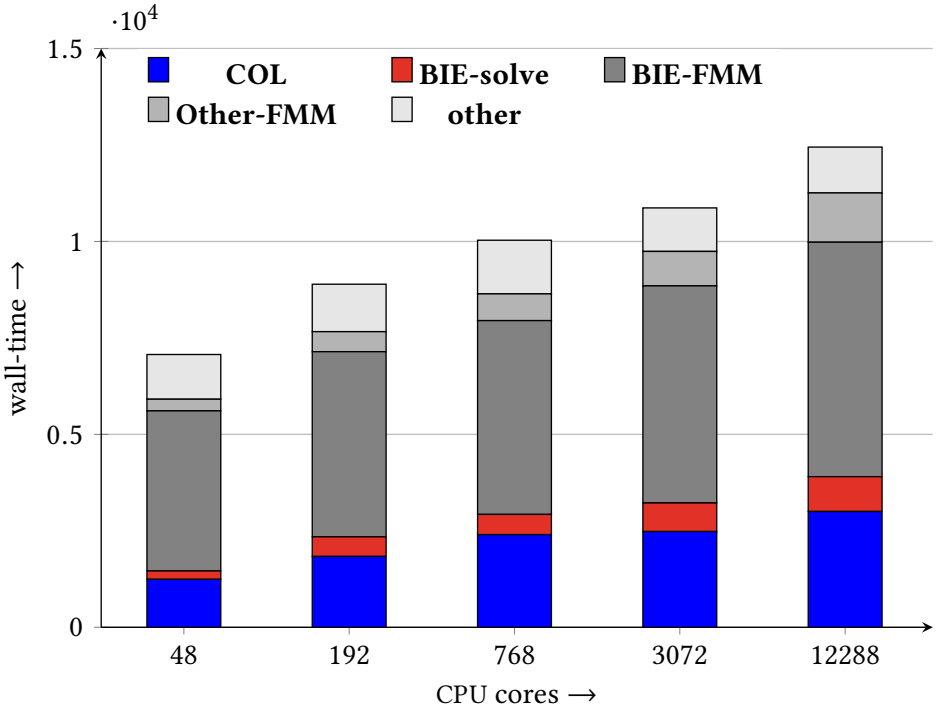


Weak scaling



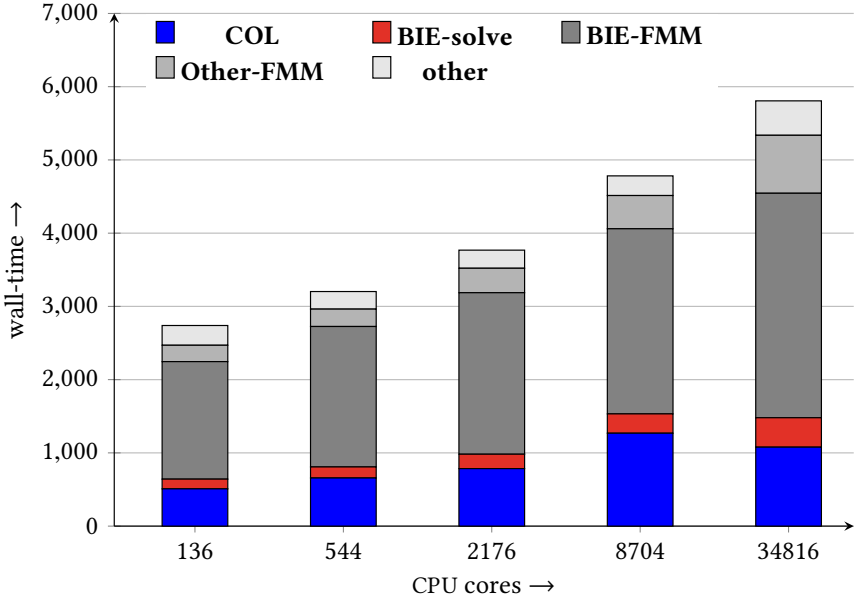
Weak Scaling: SKX

- Skylake
- 71% overall parallel efficiency
- 60% efficiency of collision handling + singular integration



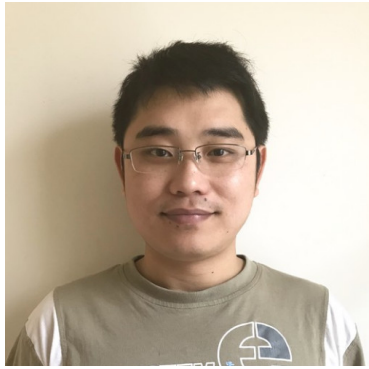
Weak Scaling: KNL

- Skylake
- 47% overall parallel efficiency
- 43% efficiency of collision handling + singular integration
- Largest simulation: 1 million RBCs and 2 million patches on vessel
- 3 billion total DOF
- Maintain collision-free state among 4.1 billion surface elements



Credits

Abtin Rahimian



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Denis Zorin

Dhairya Malhotra

Michael Shelley

Georg Stadler

Thanks!