Interpolated compressed inverse preconditioning

Fast and accurate simulation of close-to-touching discs in Stokes flow

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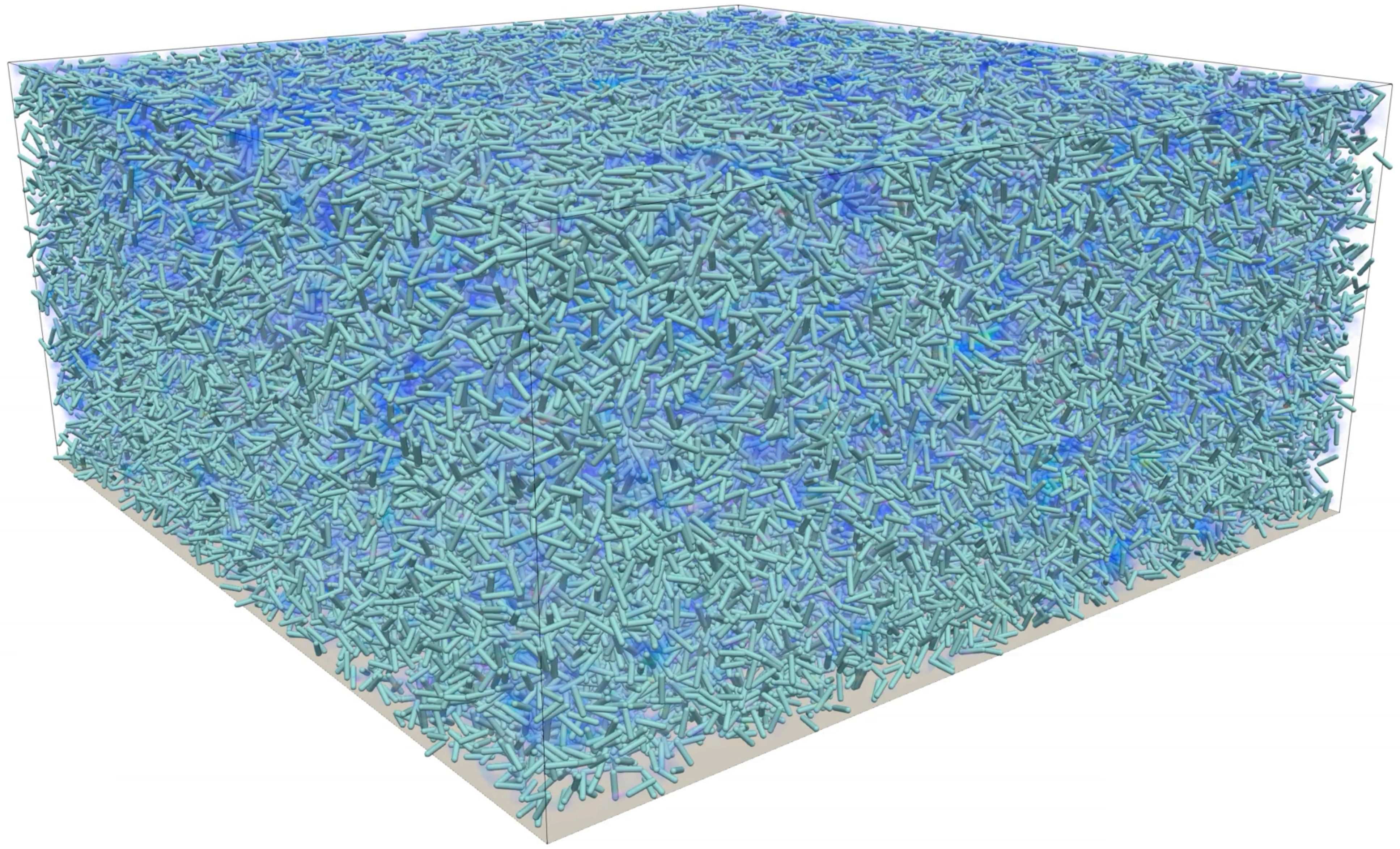
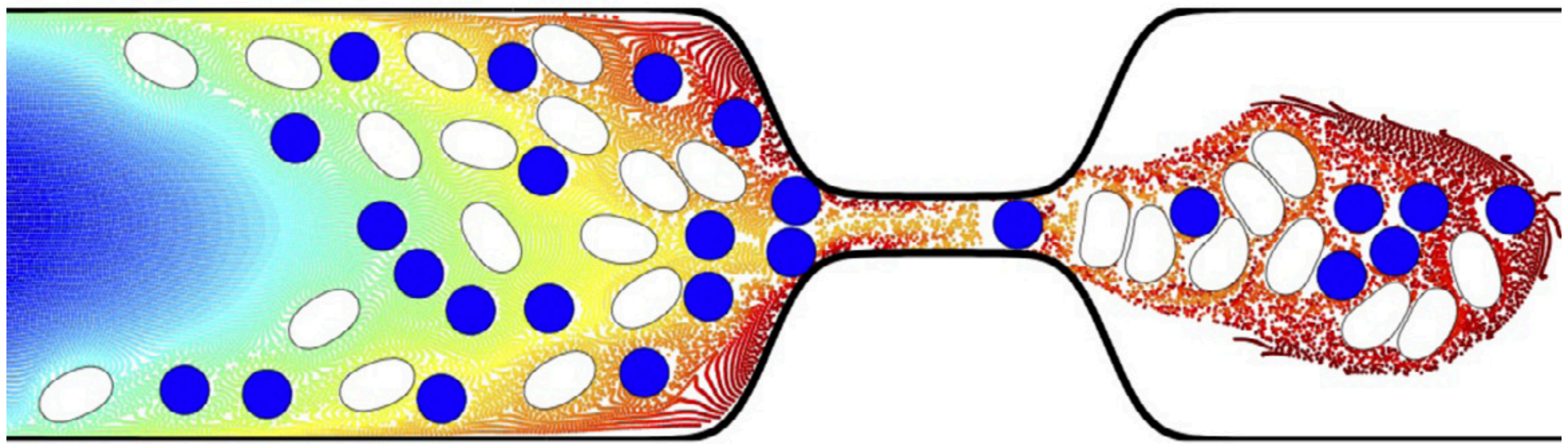
Introduction
Particulate flows

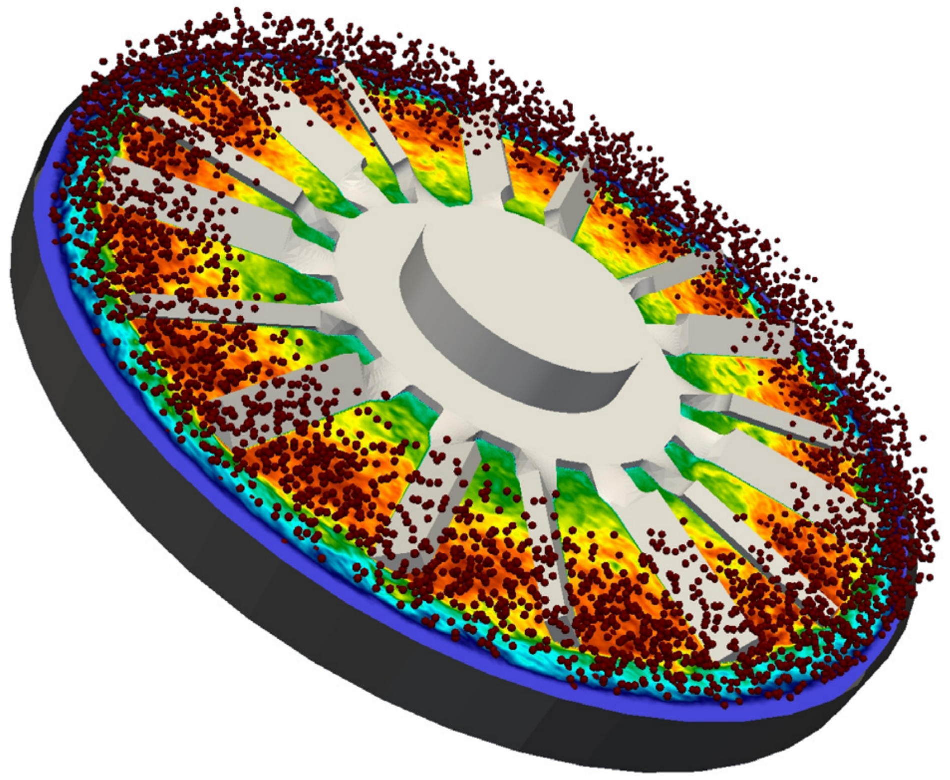
Active swimmers [Yan et al, 2020]



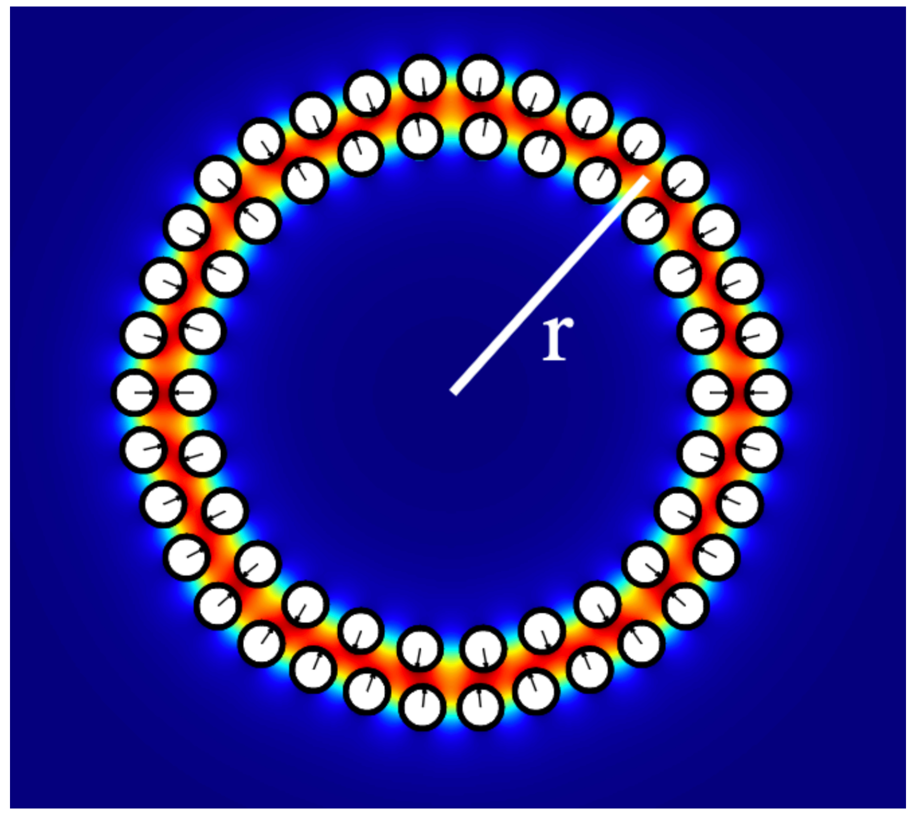
Vesicle flows [Lu et al, 2017]



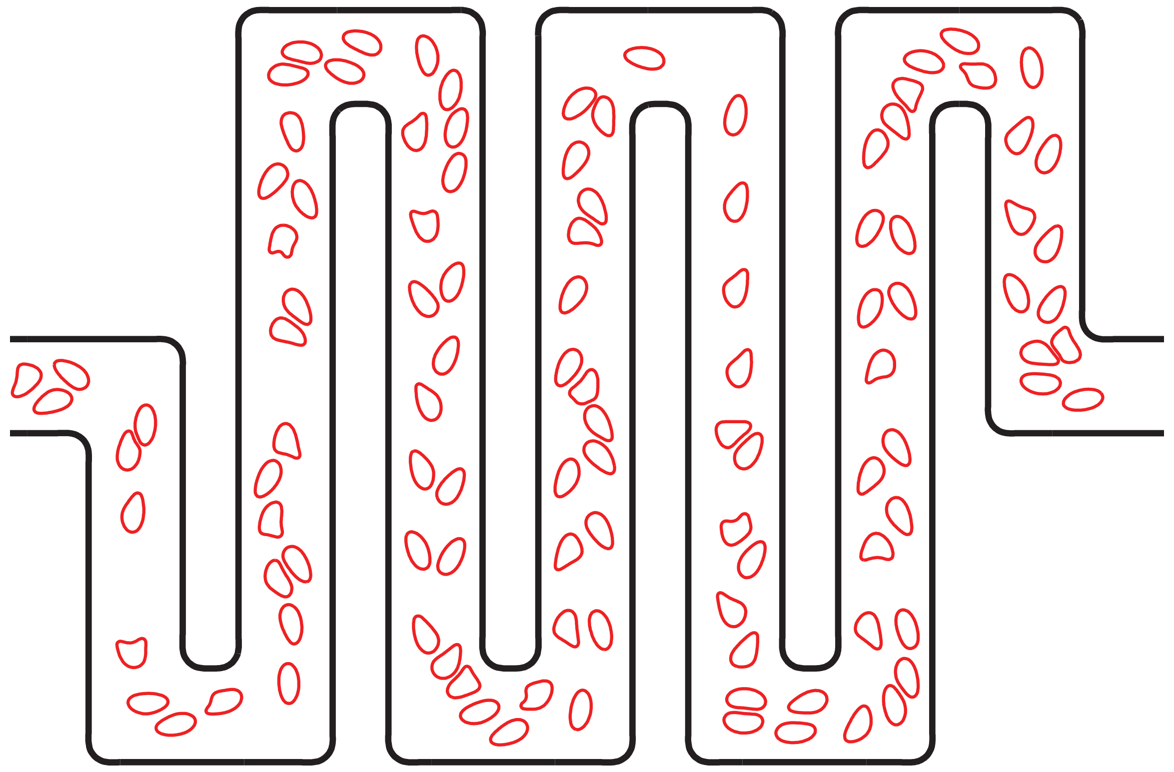
Industrial processes [Krause et al, 2021]



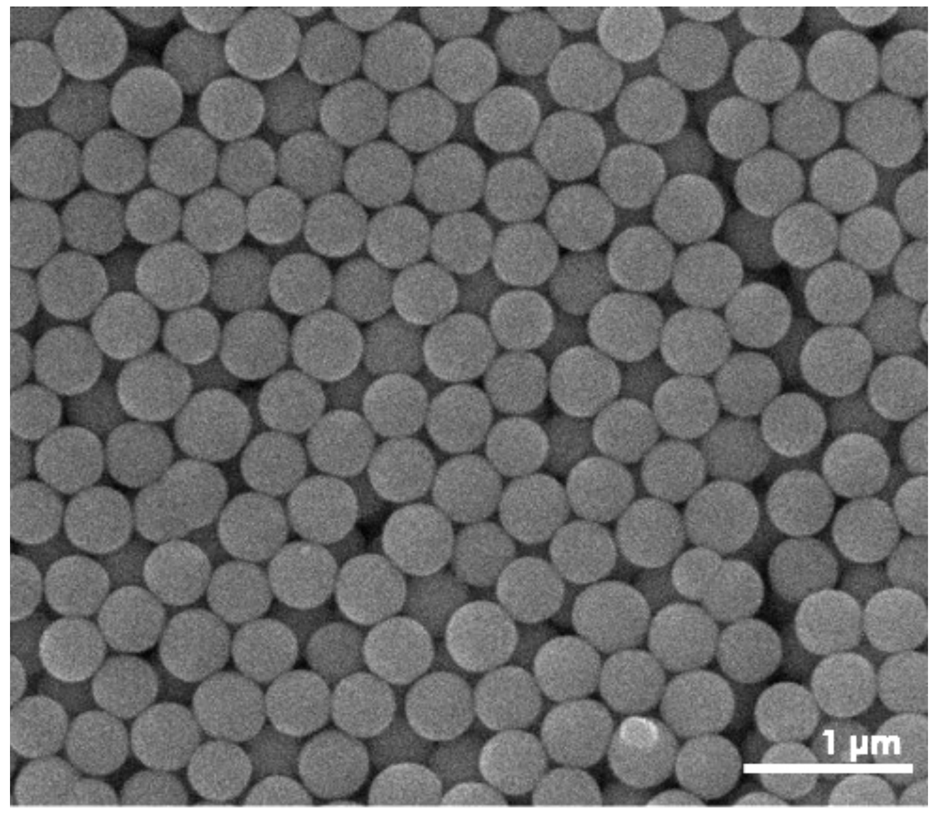
Janus particles [Fu et al, 2021]



Microfluidics [Marple et al, 2015]



Colloidal suspensions [Wikipedia]



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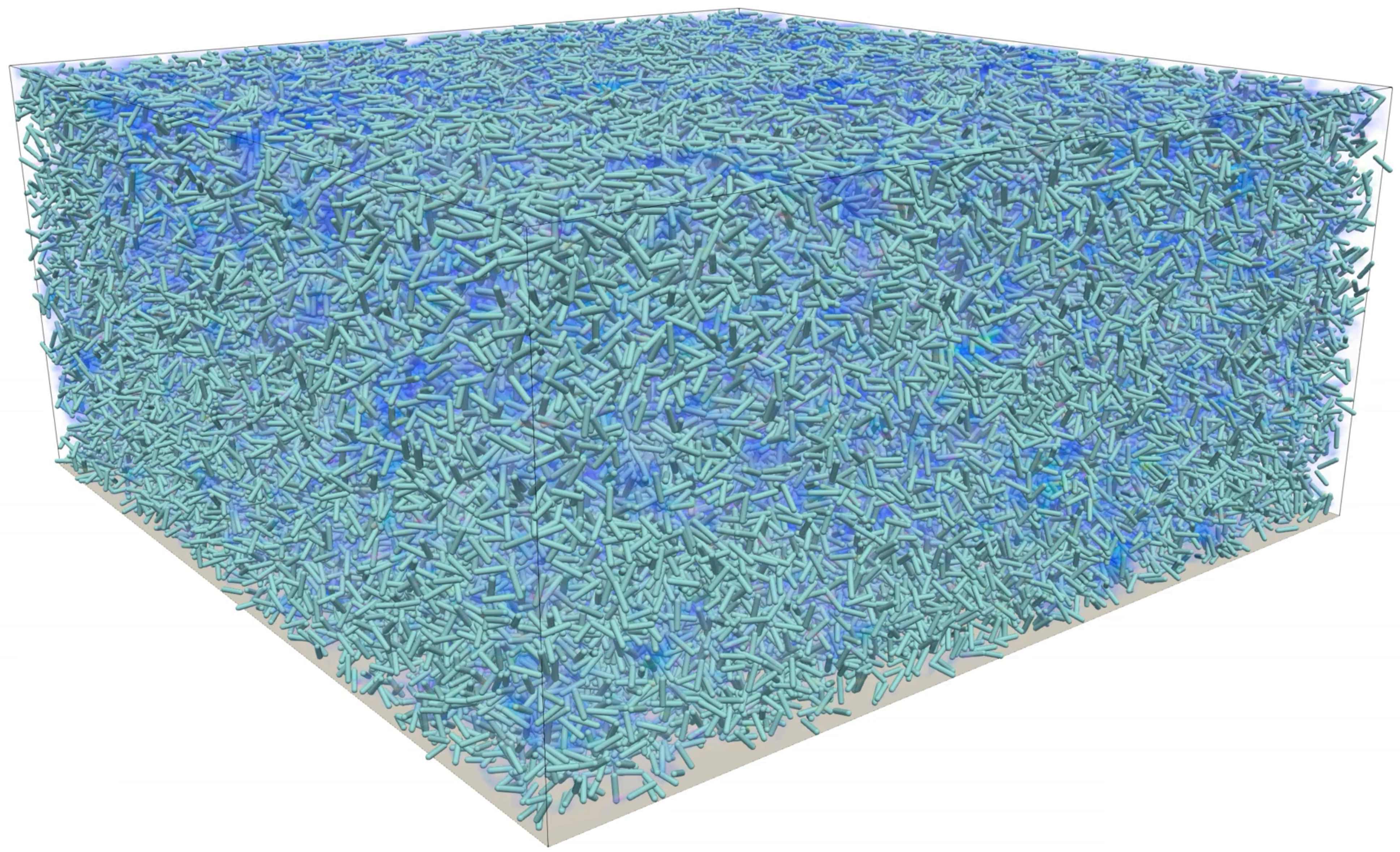

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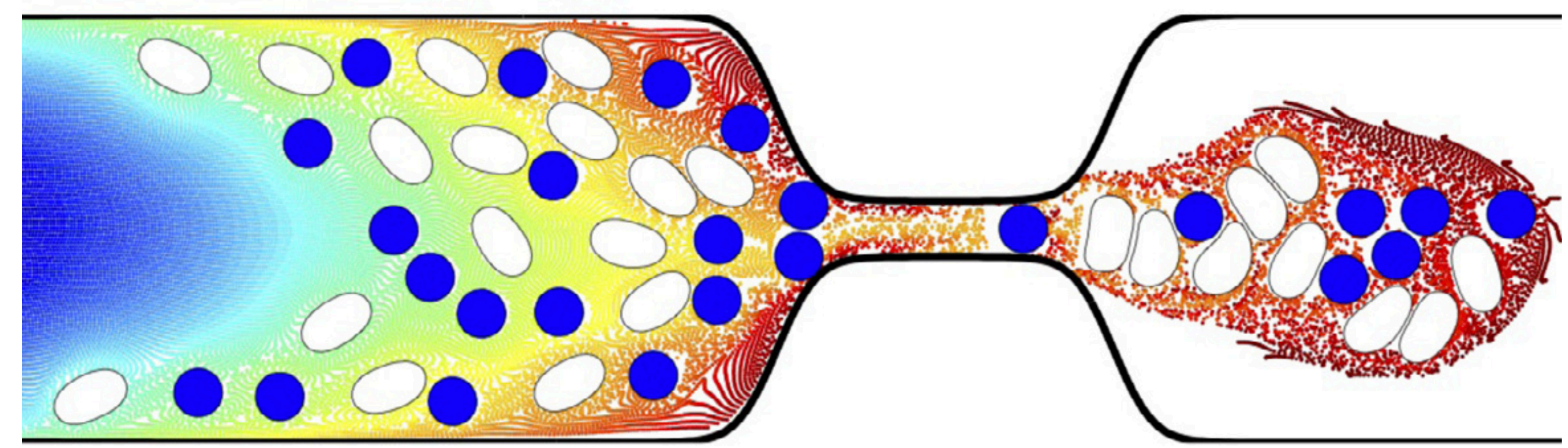

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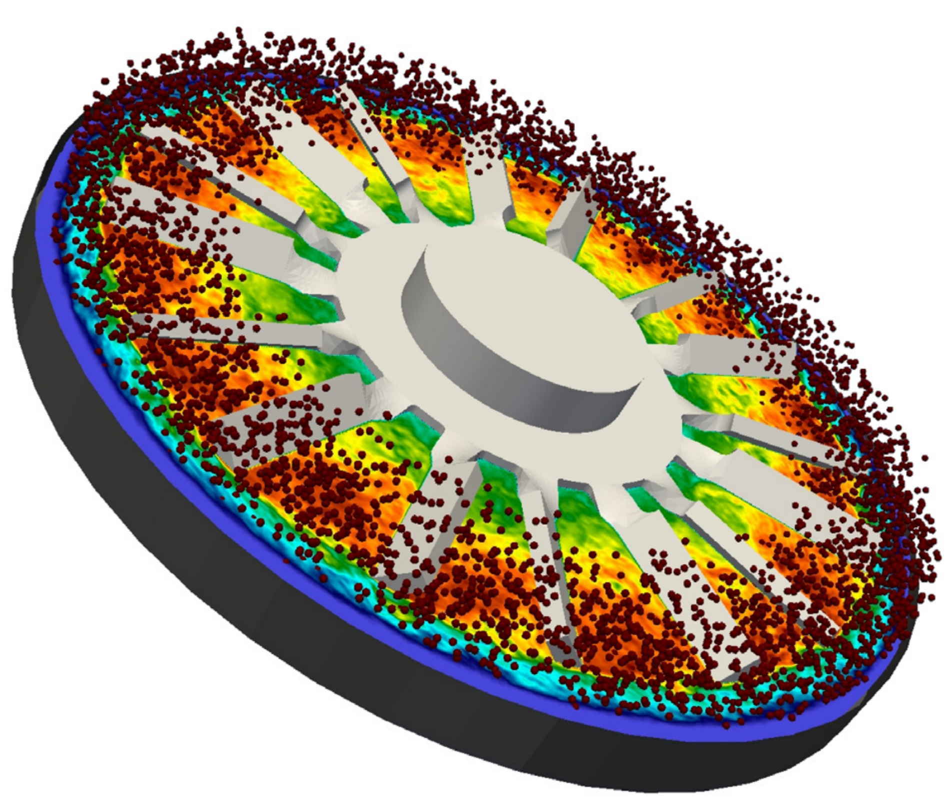

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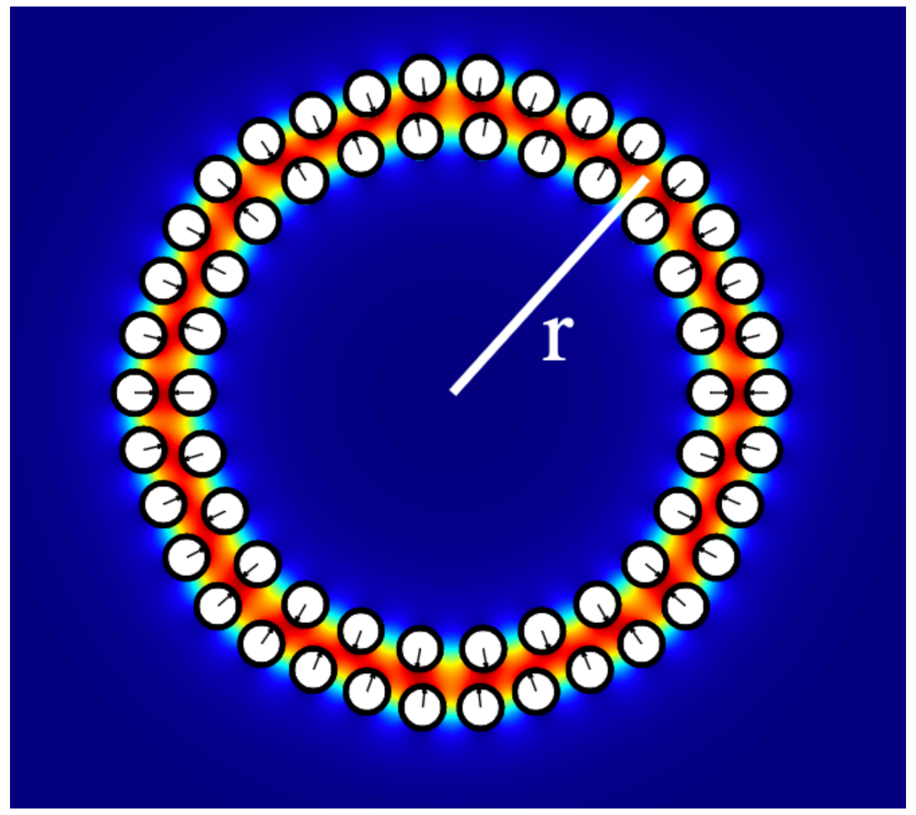

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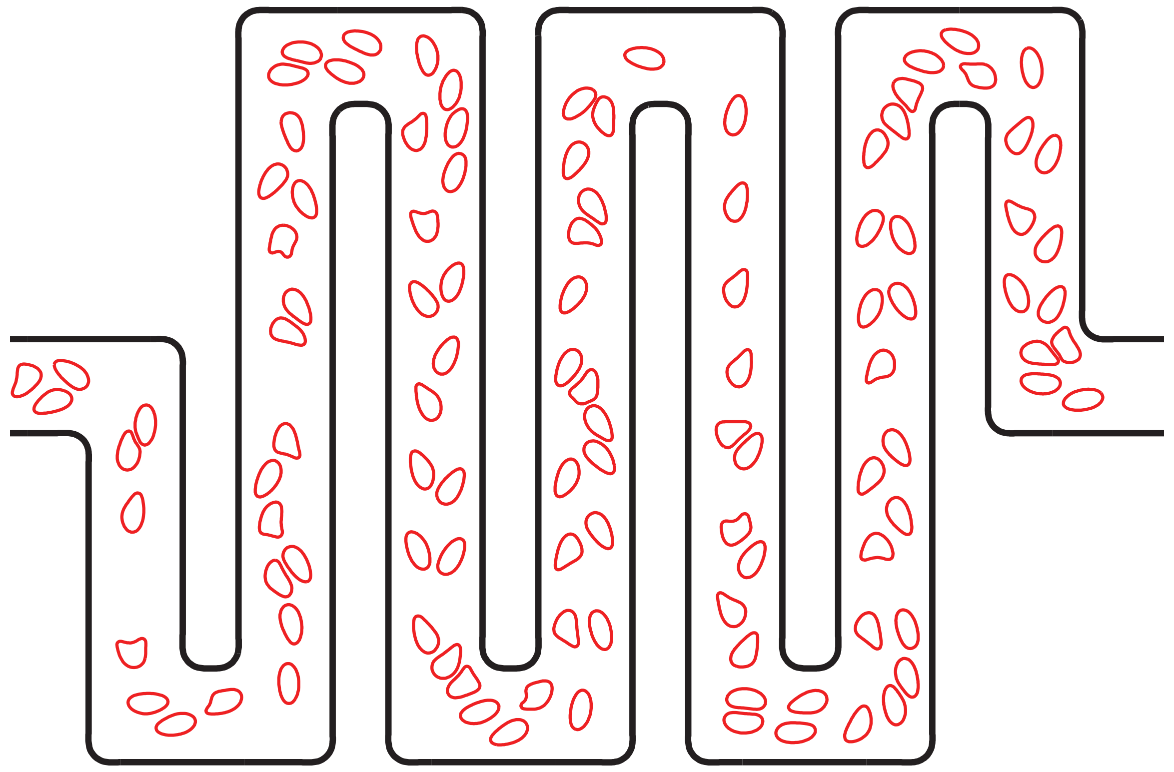

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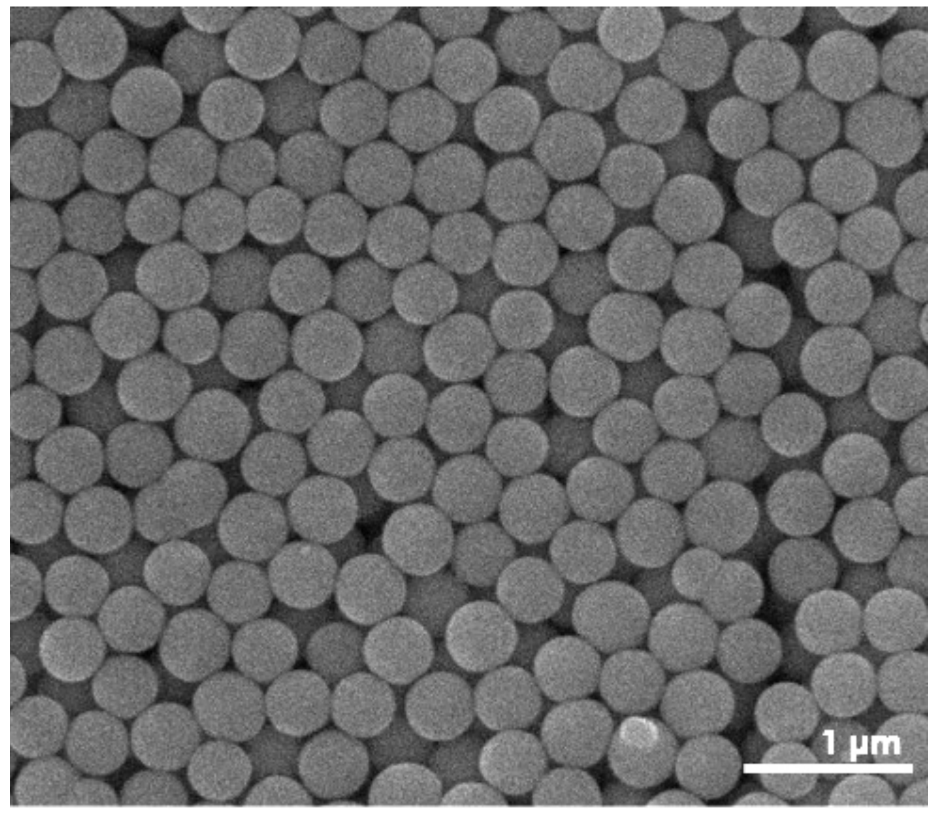
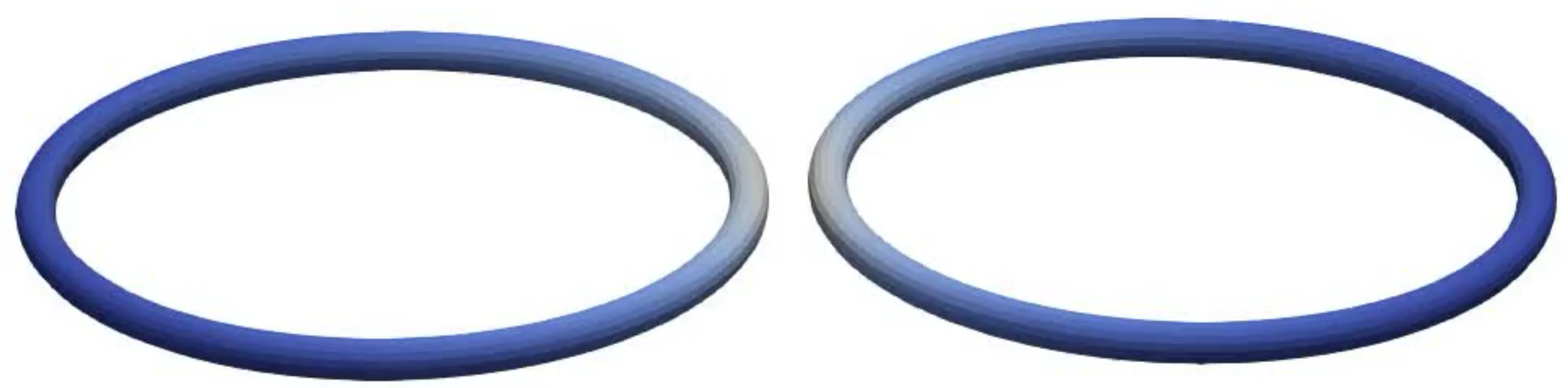
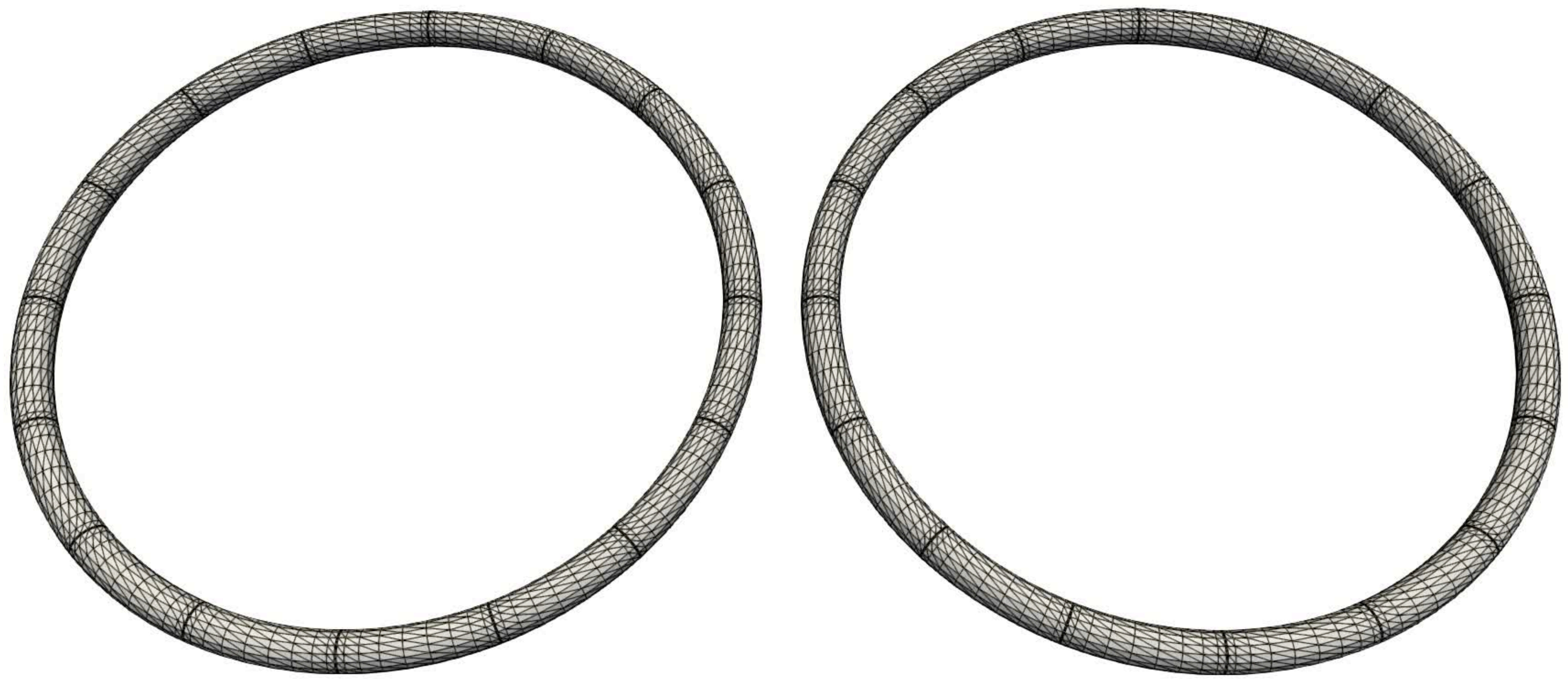


Example: Sedimenting rings in Stokes flow [Malhotra & Barnett, 2024]





Figures from [Malhotra & Barnett, 2024]

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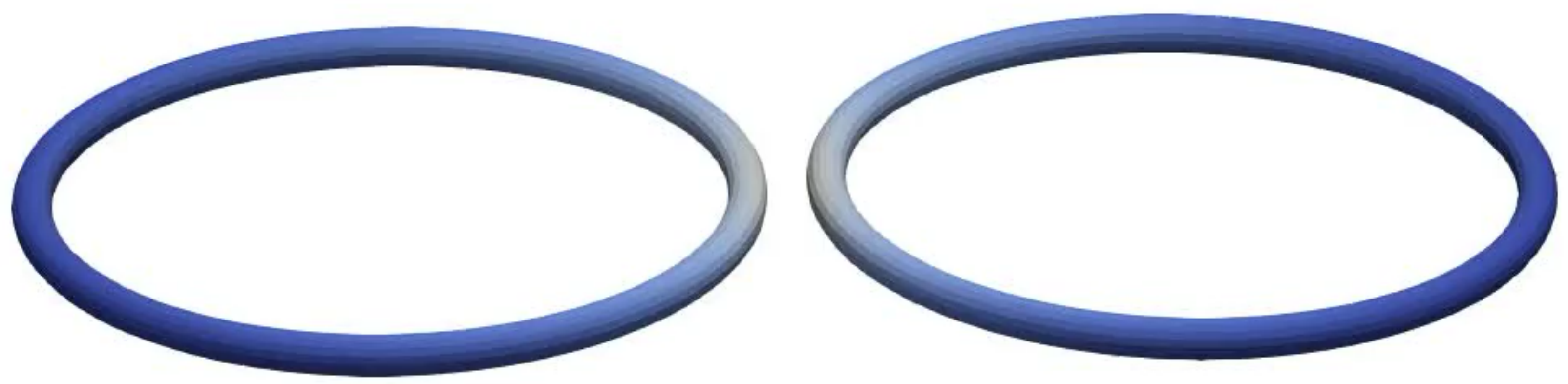

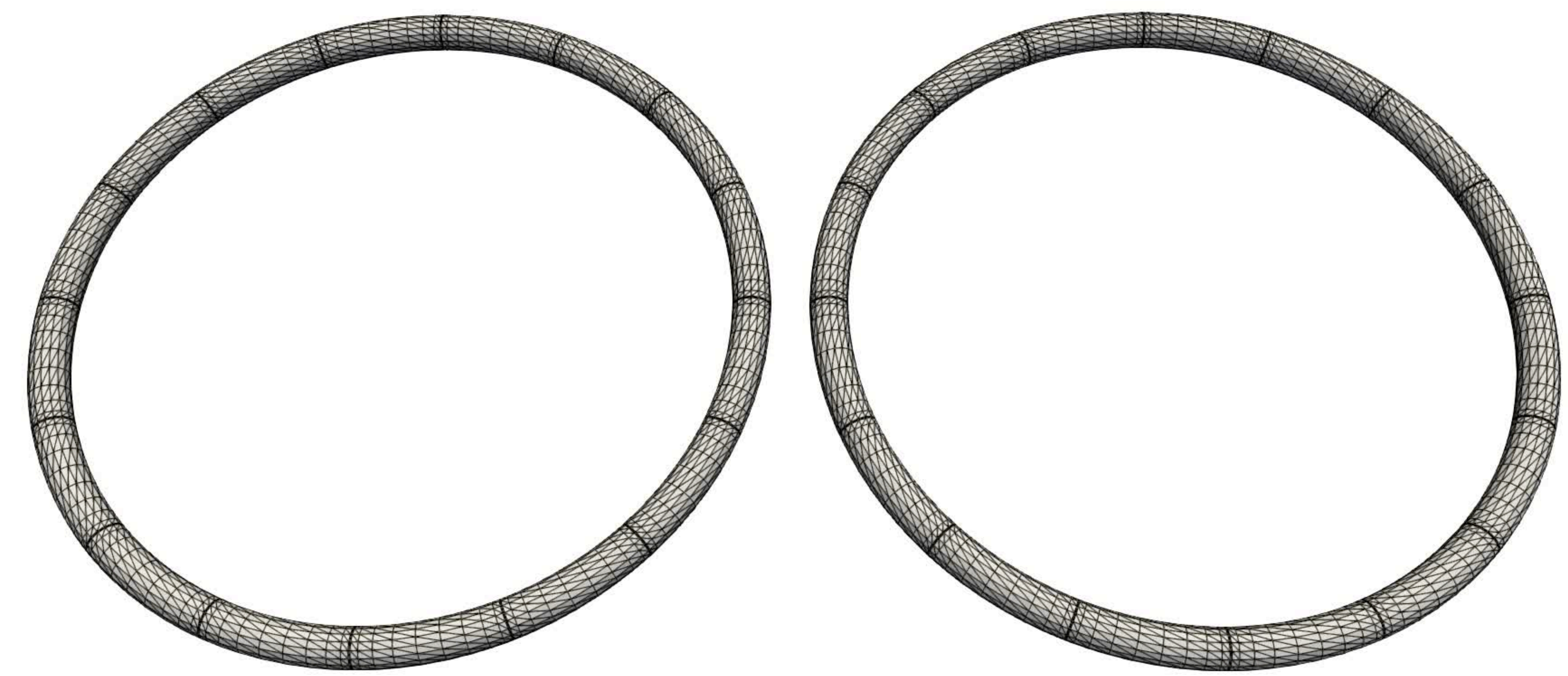

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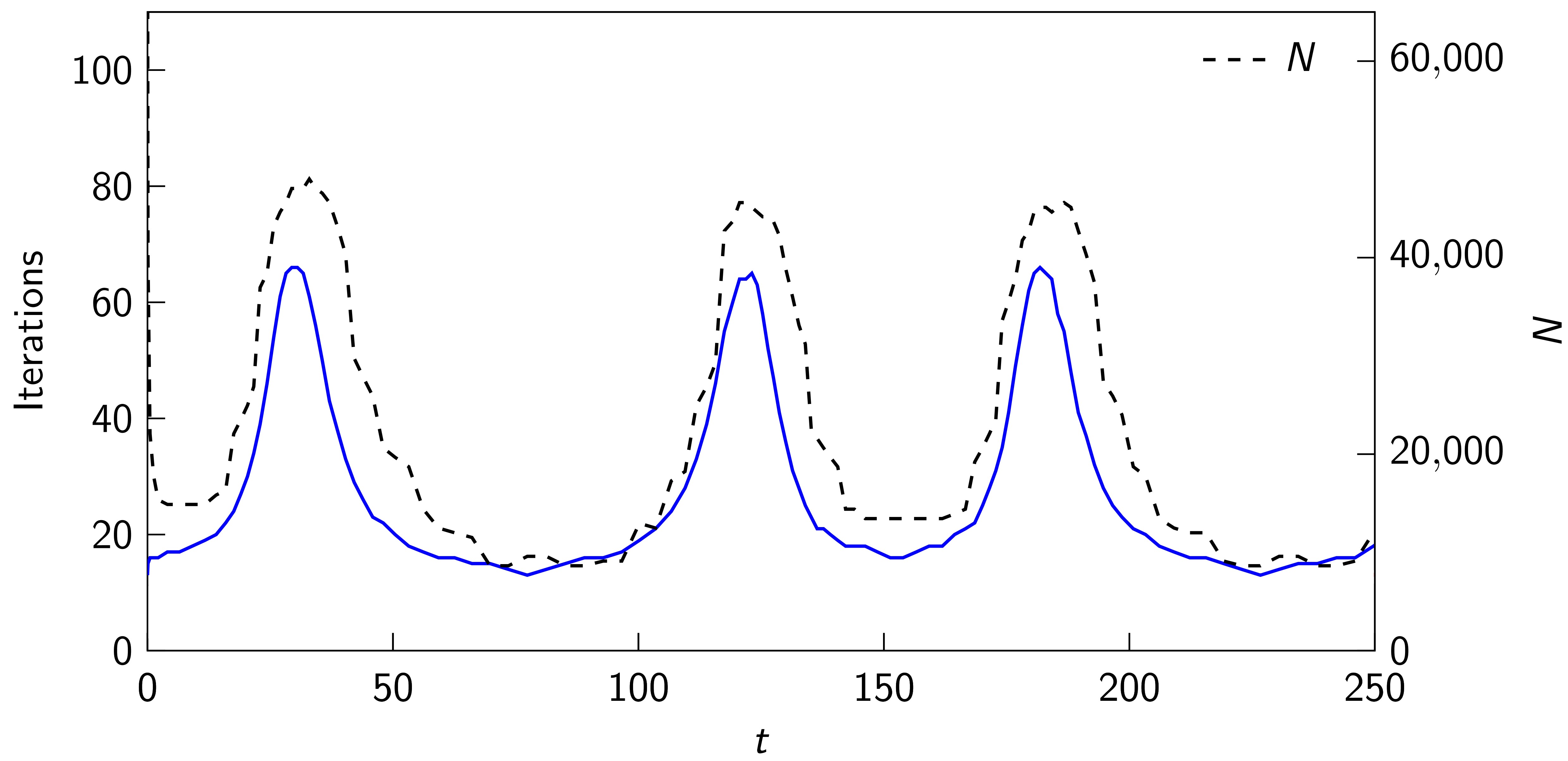

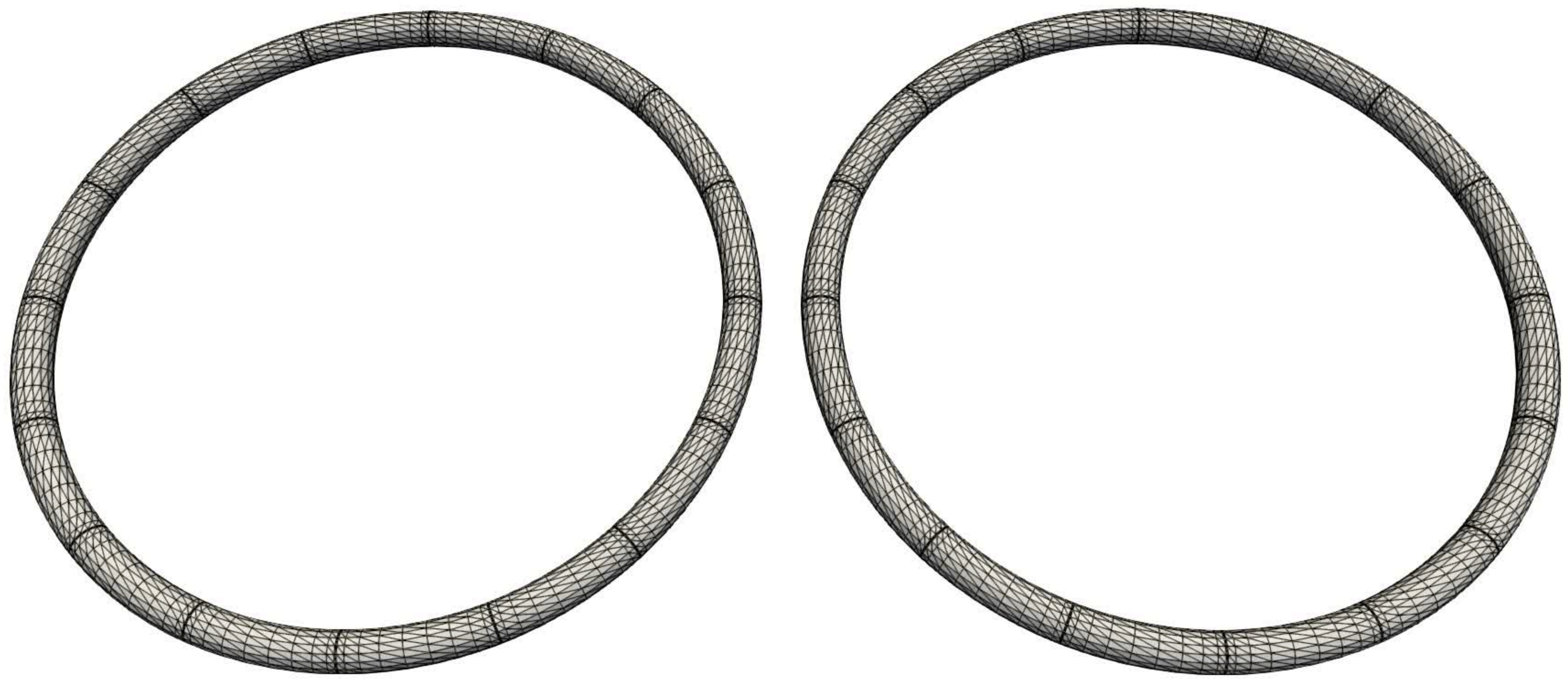

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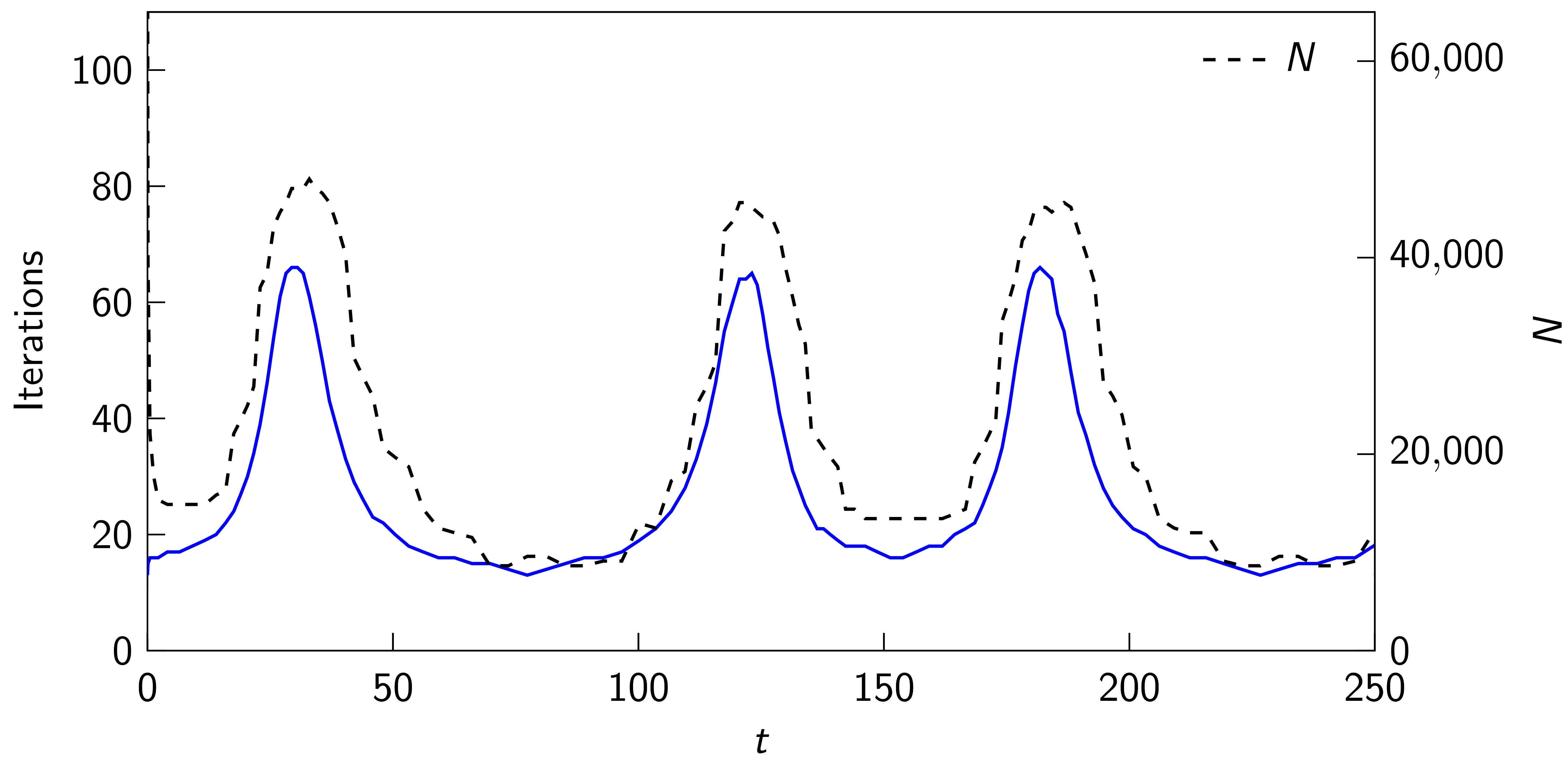

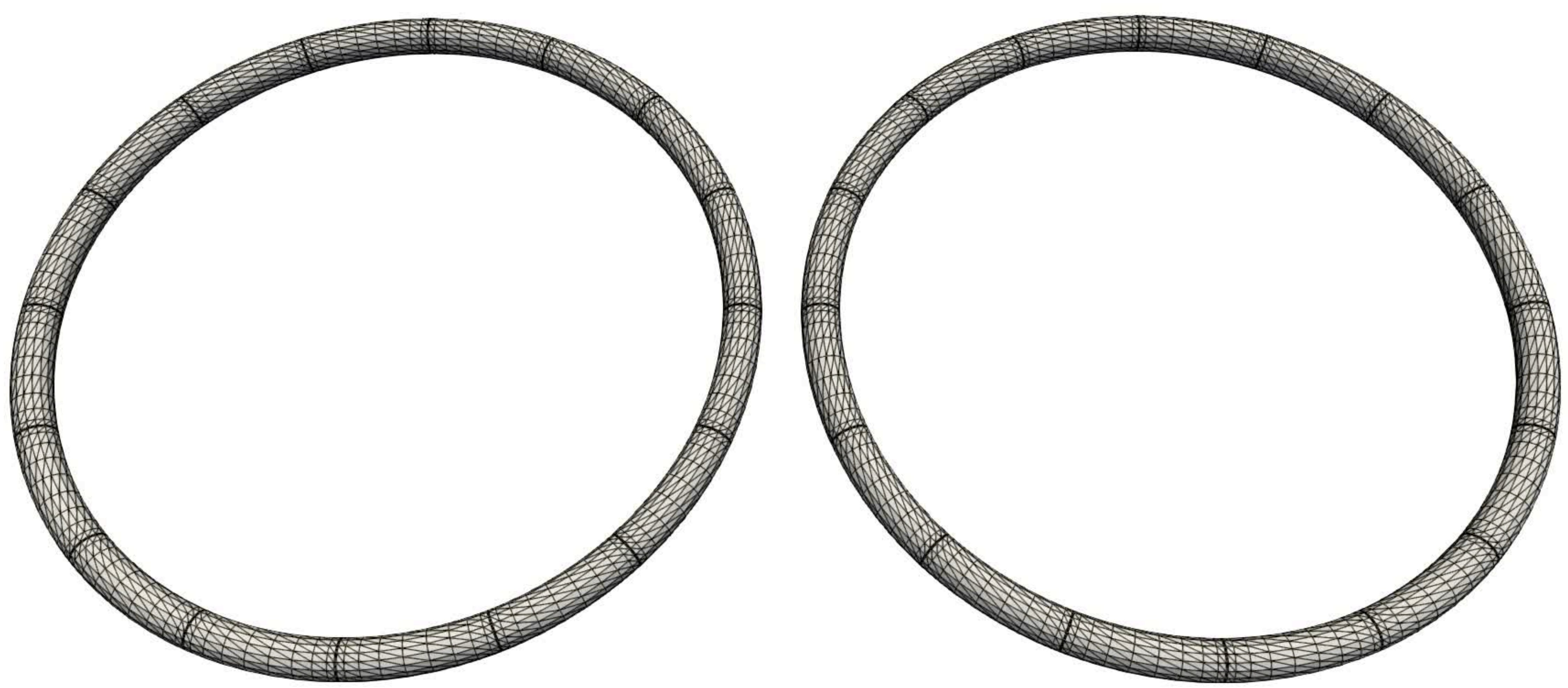

Close interactions:

~5× more GMRES iterations
~5× more unknowns
× ~5× smaller Δt

>125× **slower**!

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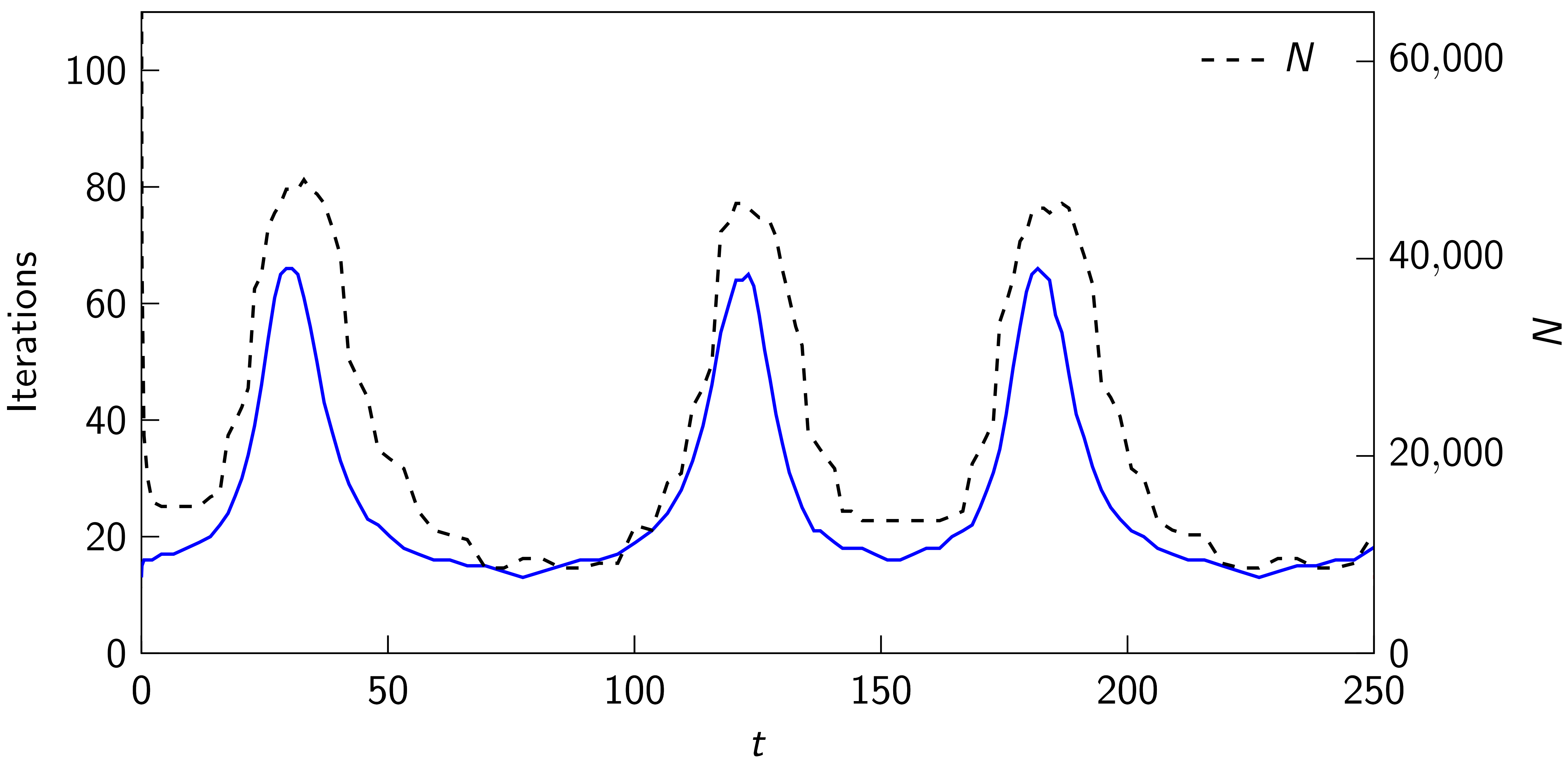

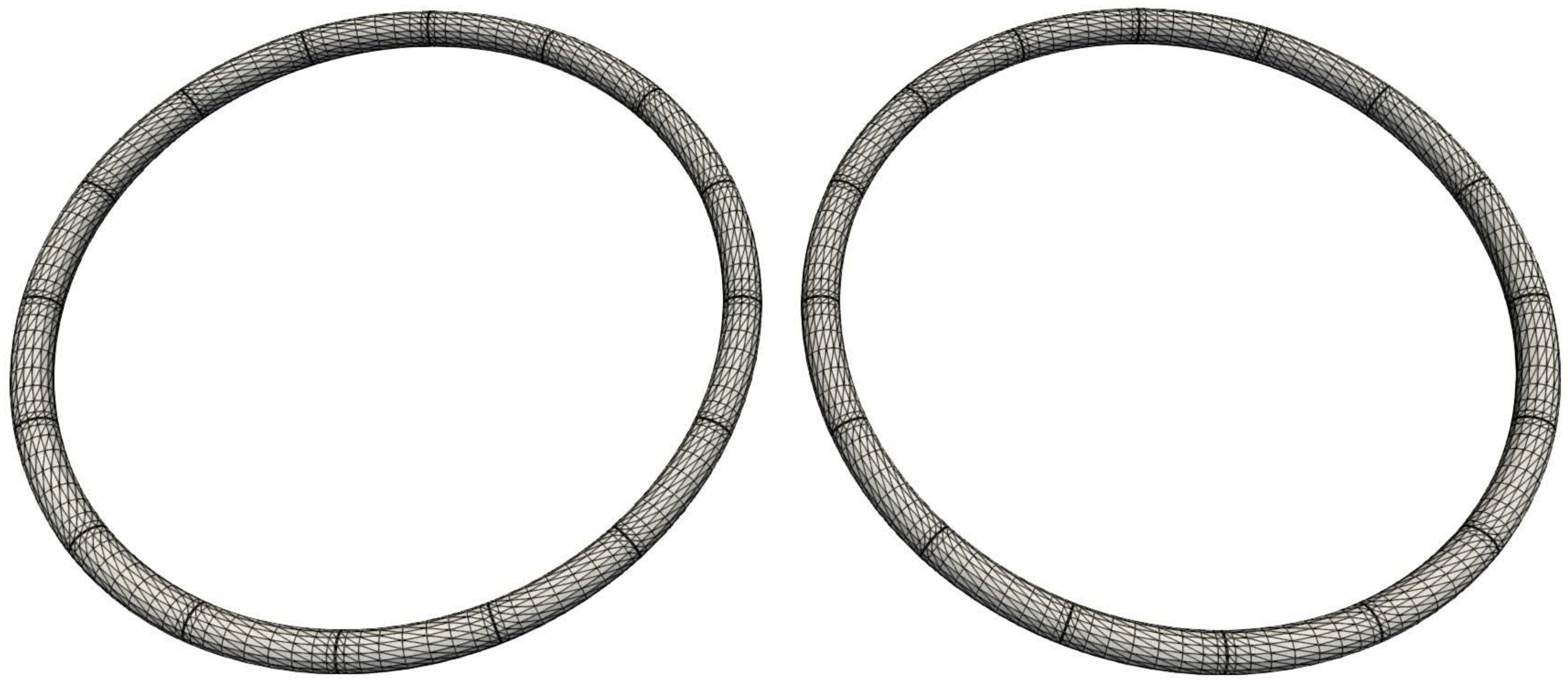

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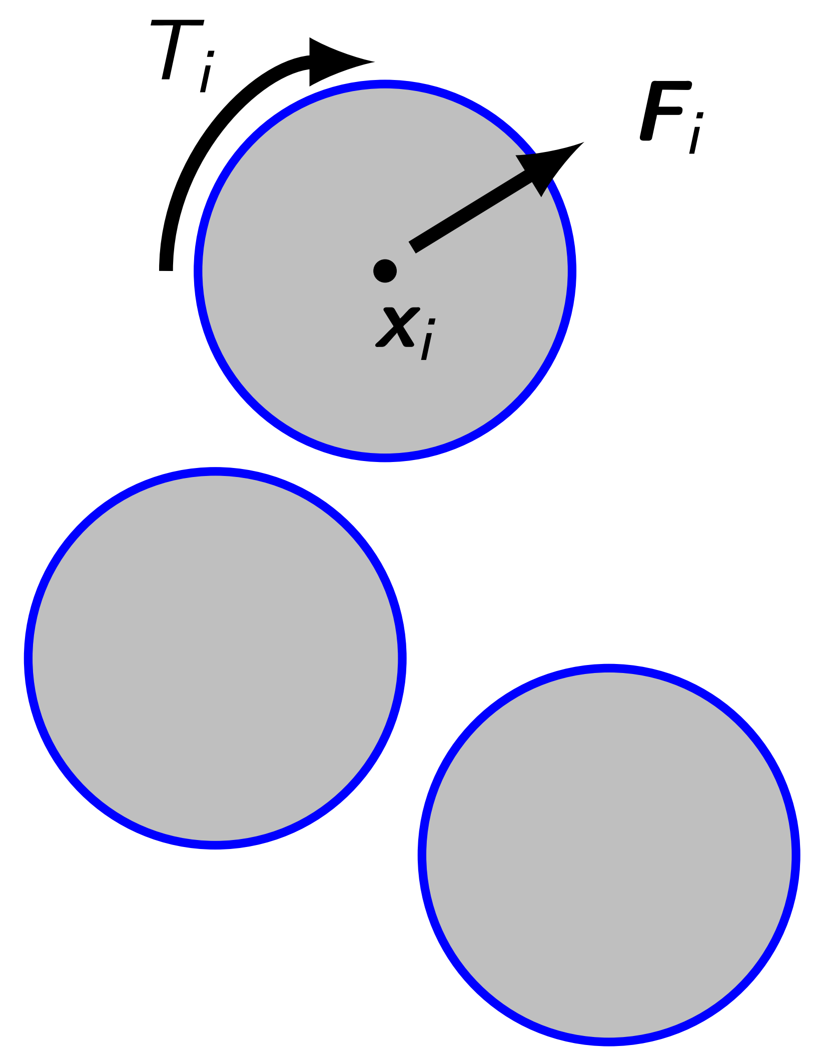
Consider a collection of identical rigid discs $\Omega = \bigcup_{i=1}^{N_\Omega} \Omega_i$ immersed in a Stokesian fluid:

$$\begin{aligned} \Delta \boldsymbol{u} - \nabla p &= 0 \quad \text{in } \mathbb{R}^2 \setminus \Omega \\ \nabla \cdot \boldsymbol{u} &= 0 \quad \text{in } \mathbb{R}^2 \setminus \Omega \\ \boldsymbol{u} &\to 0 \quad \text{as } \boldsymbol{x} \to \infty \end{aligned}$$

$$\int_{\partial\Omega_i} \boldsymbol{f}_i = -\boldsymbol{F}_i$$

$$\int_{\partial\Omega_i} \boldsymbol{f}_i \cdot (\boldsymbol{x} - \boldsymbol{x}_i)^\perp = -T_i$$

fluid traction



along with velocity boundary conditions

$$\boldsymbol{u} = \boldsymbol{V} + \boldsymbol{u}_s \quad \text{on } \partial\Omega$$

where $\boldsymbol{V}(\boldsymbol{x}) = \boldsymbol{v}_i + \boldsymbol{\omega}_i \times (\boldsymbol{x} - \boldsymbol{x}_i)$ is the rigid body velocity of disc i and $\boldsymbol{u}_s$ is a given slip velocity.

Stokes mobility problem
Setup

Consider a collection of identical rigid discs $\Omega = \bigcup_{i=1}^{N_\Omega} \Omega_i$ immersed in a Stokesian fluid:

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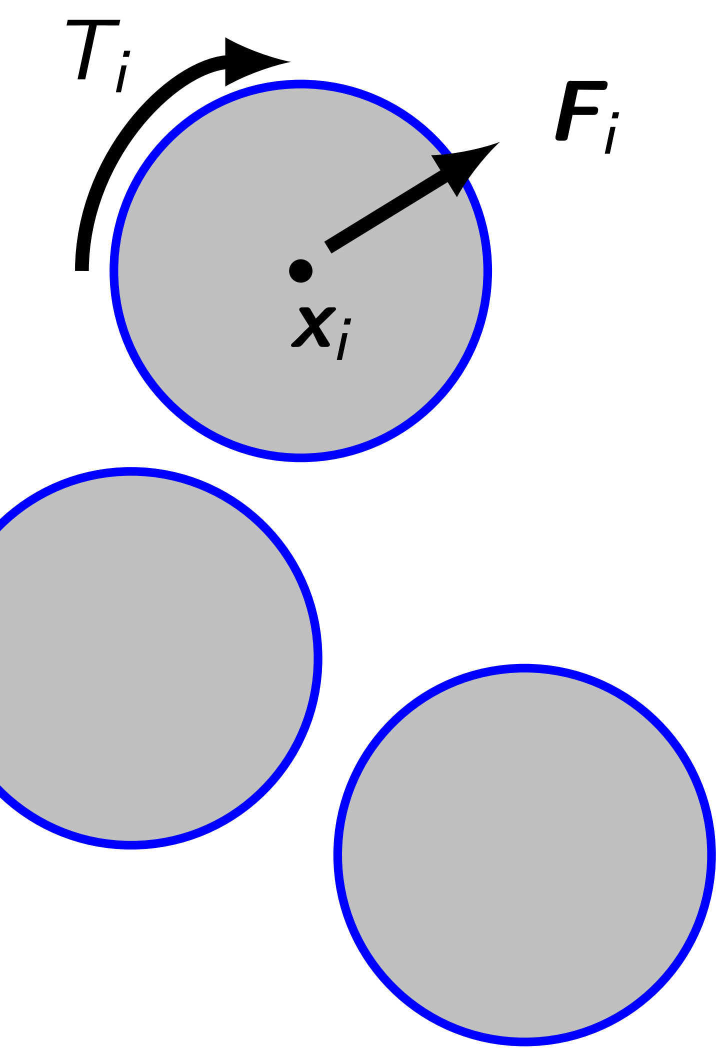

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Stokes mobility problem: Given prescribed forces $\boldsymbol{F}_i$ and torques T_i on each disc, find the unknown rigid body velocities $(\boldsymbol{v}_i, \omega_i)$.

Stokes mobility problem
Boundary integral formulation

Represent fluid velocity using Stokes single- and double-layer potentials:

$$S(\boldsymbol{r}) = \frac{1}{4\pi}\left(\log\frac{1}{|\boldsymbol{r}|}\boldsymbol{I} + \frac{\boldsymbol{r}\otimes\boldsymbol{r}}{|\boldsymbol{r}|^2}\right)$$

$$D(\boldsymbol{r}) = \frac{1}{\pi}\frac{\boldsymbol{r}\otimes\boldsymbol{r}}{|\boldsymbol{r}|^4}(\boldsymbol{r}\cdot\boldsymbol{n})$$

$$\boldsymbol{u}(\boldsymbol{x}) = \int_{\partial\Omega} S(\boldsymbol{x}-\boldsymbol{y})\underbrace{\boldsymbol{\nu}}_{\text{known (“completion flow”)}}(\boldsymbol{y})d\boldsymbol{y} + \int_{\partial\Omega} D(\boldsymbol{x}-\boldsymbol{y}){\color{red}\boldsymbol{\sigma}}(\boldsymbol{y})d\boldsymbol{y}$$

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[Pozrikidis, 1992]

[Rachh & Greengard, 2016]

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$$\boldsymbol{V} = -\sum_{i=1}^{3N_\Omega}\mathfrak{v}_i\mathfrak{v}_i^T\boldsymbol{\sigma}$$

orthonormal basis for rigid body motion on disc i

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orthonormal basis for rigid body motion on disc i

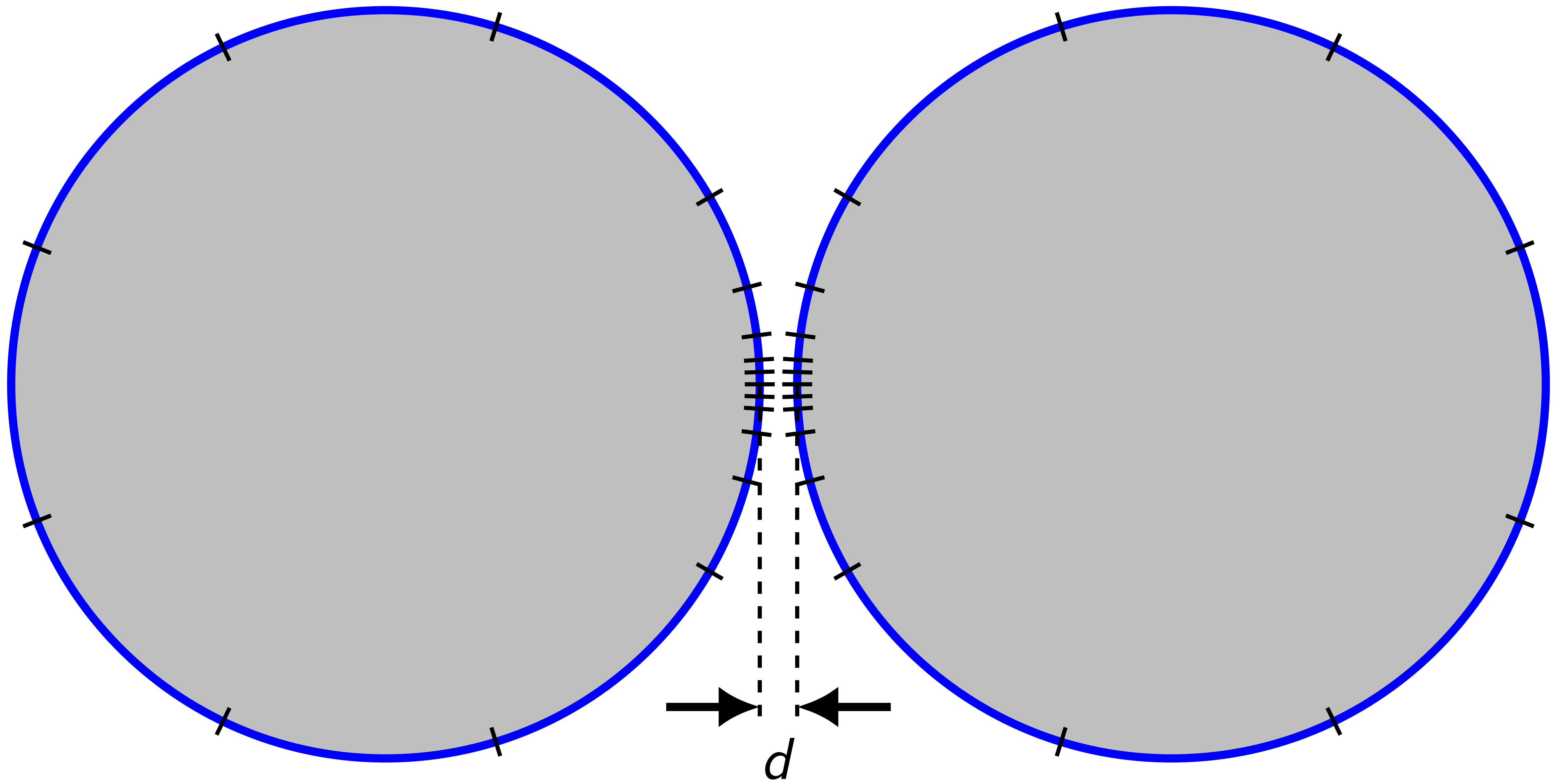
Apply boundary conditions:

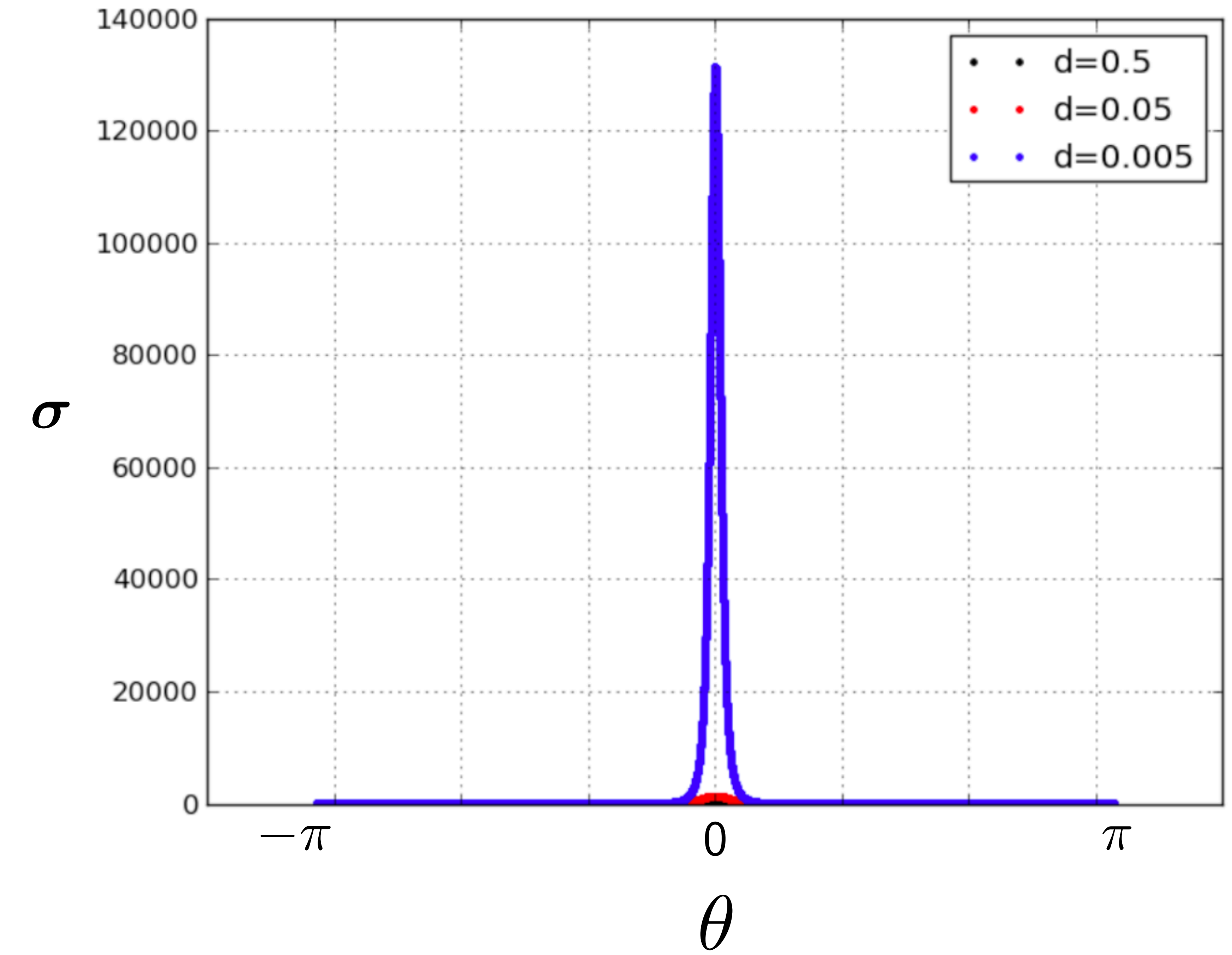
$$\left(I/2 + D + \sum_{i=1}^{3N_\Omega} \mathfrak{v}_i \mathfrak{v}_i^T\right)\boldsymbol{\sigma} = \boldsymbol{u}_s - S\boldsymbol{\nu}$$

(second kind BIE)

[Pozrikidis, 1992]
[Rachh & Greengard, 2016]

Nyström discretization
Close interactions





- Discretize $\partial\Omega$ into high-order panels
- Construct layer potential operators
  - Adaptive quadrature for near integrals
  - Special quadrature for singular integrals
- Solve BIE: $K\boldsymbol{\sigma} = g$

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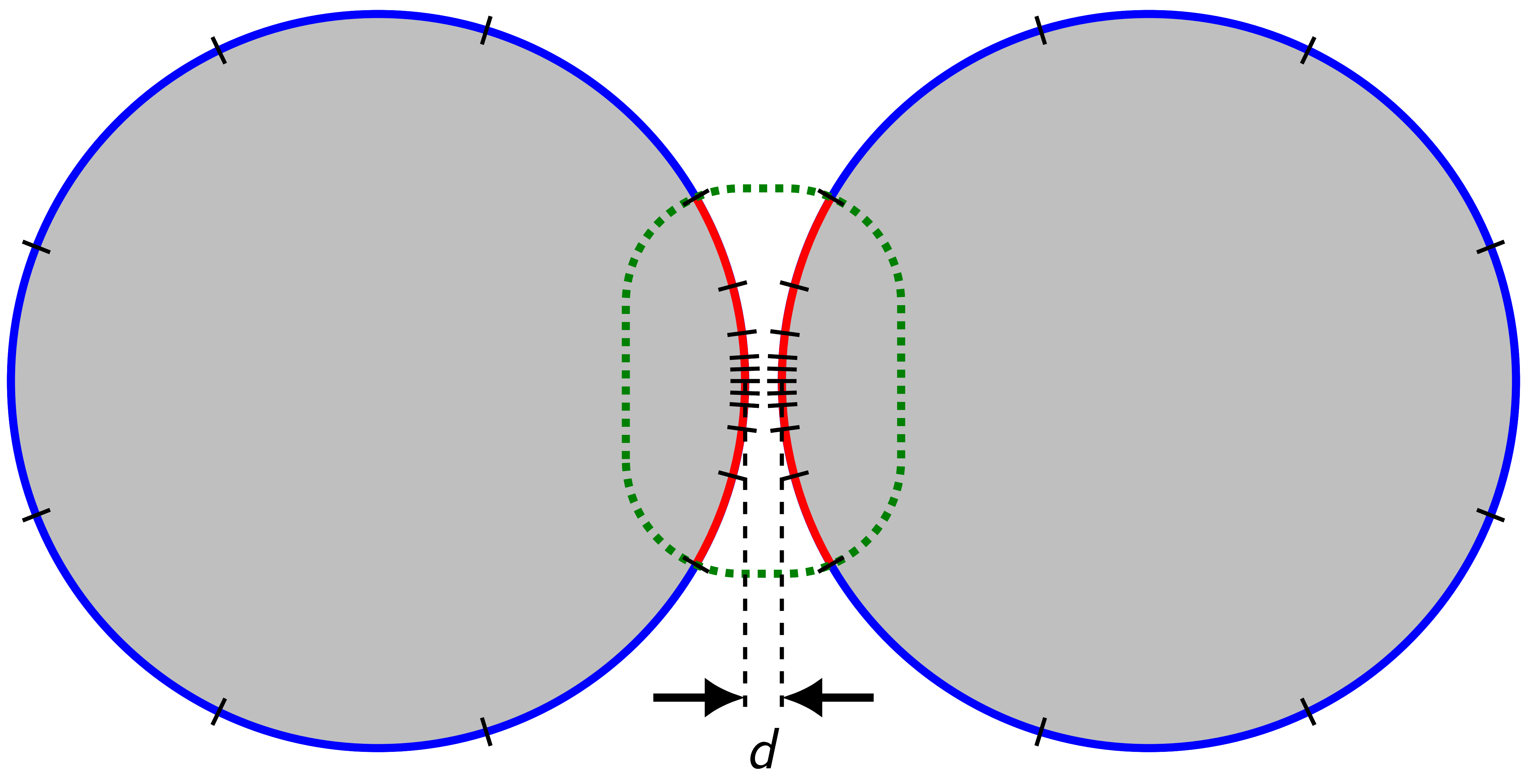
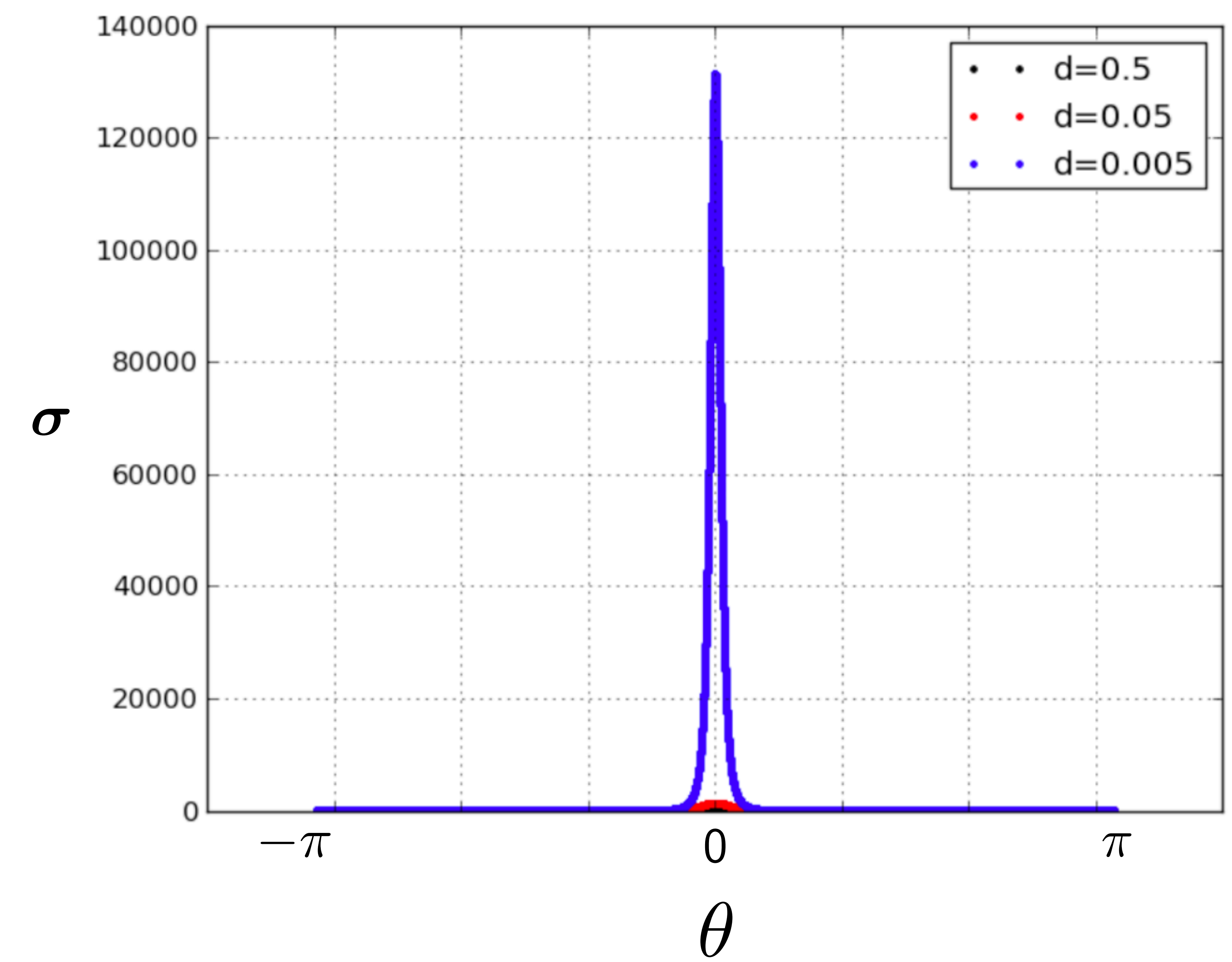
Close interactions





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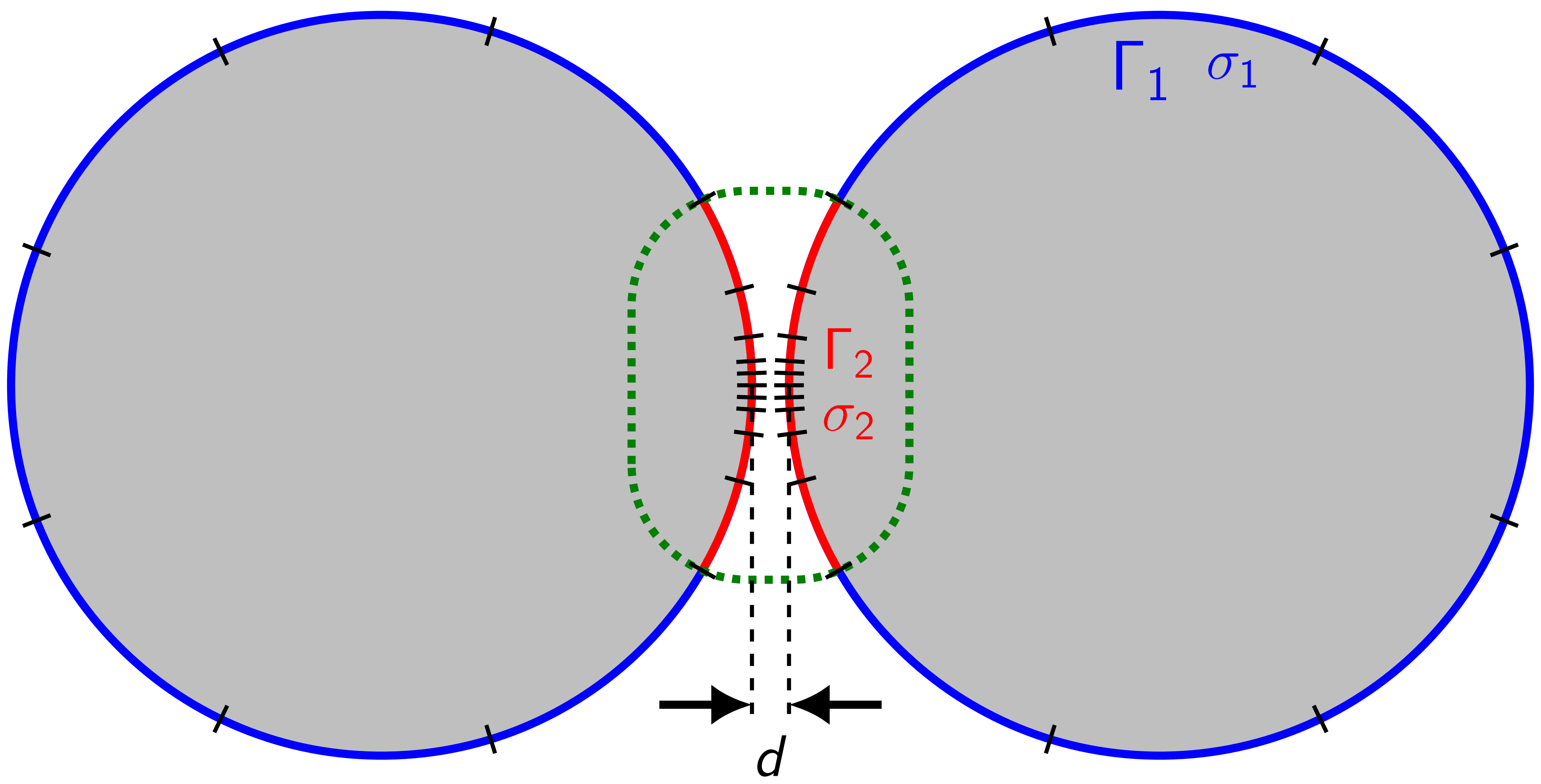
Compress close interactions

Compressing close interactions
Recursively compressed inverse preconditioning (RCIP)



$$\begin{pmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{pmatrix} \begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}$$

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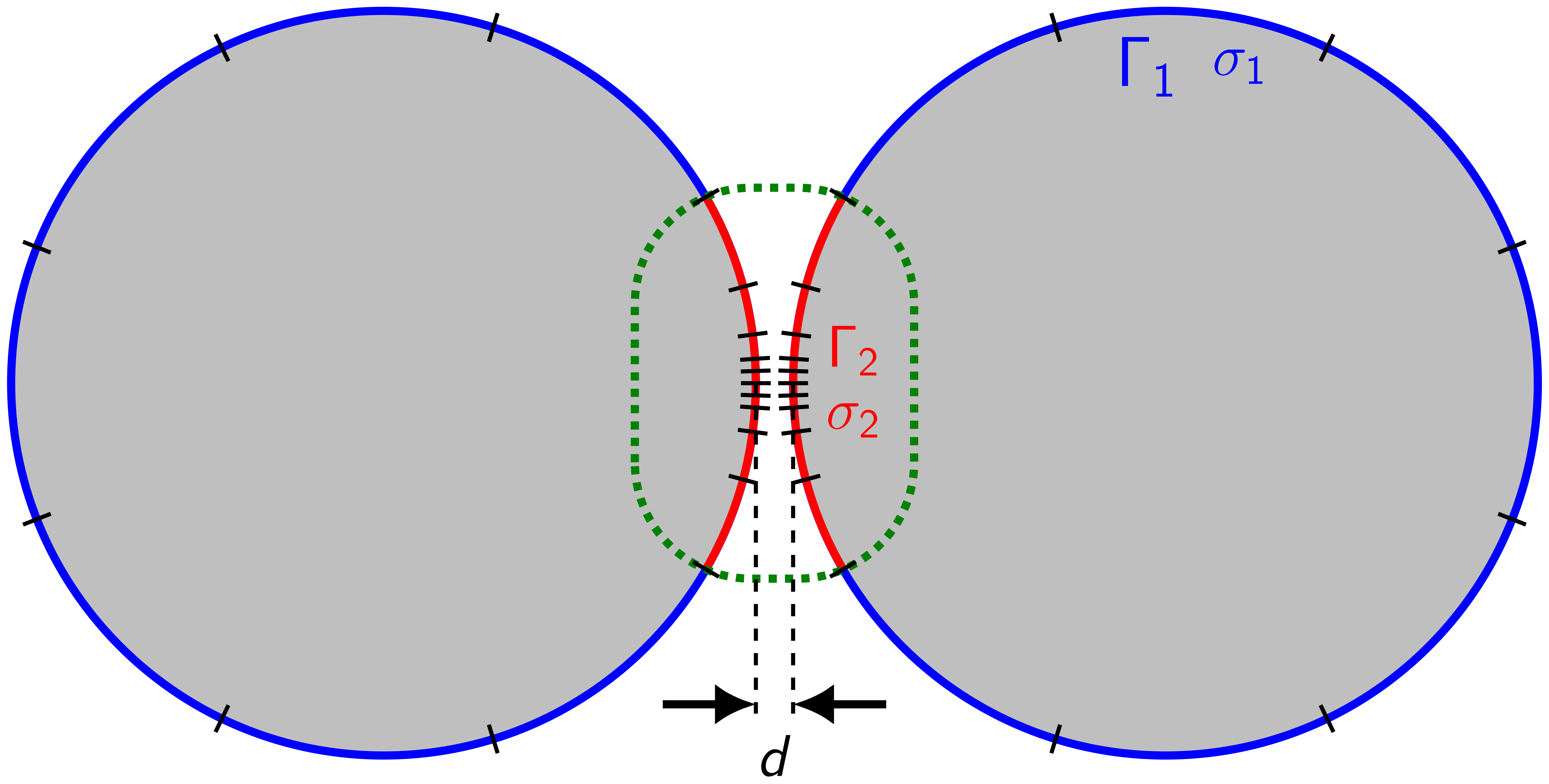

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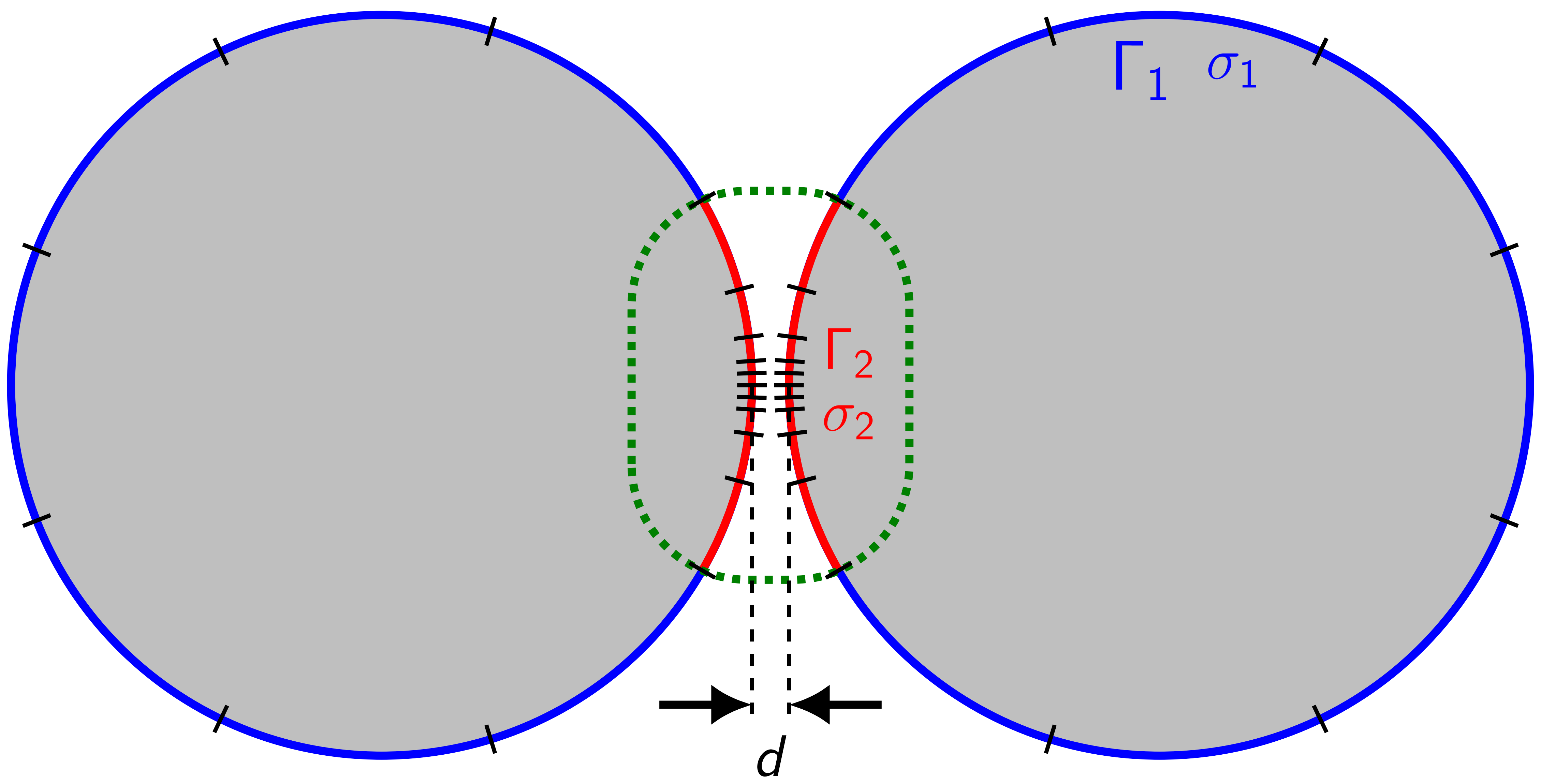

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Build compressed operator using RCIP [Helsing, 2012]

Right precondition with $\begin{pmatrix} I & 0 \\ 0 & K_{22}^{-1} \end{pmatrix}$:

$$\begin{pmatrix} K_{11} & K_{12}K_{22}^{-1} \\ K_{21} & I \end{pmatrix} \begin{pmatrix} \sigma_1 \\ \overline{\sigma}_2 \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}$$

Then $\overline{\sigma}_2 = K_{22}\sigma_2$ is smooth and $K_{12}K_{22}^{-1}$ is low rank.

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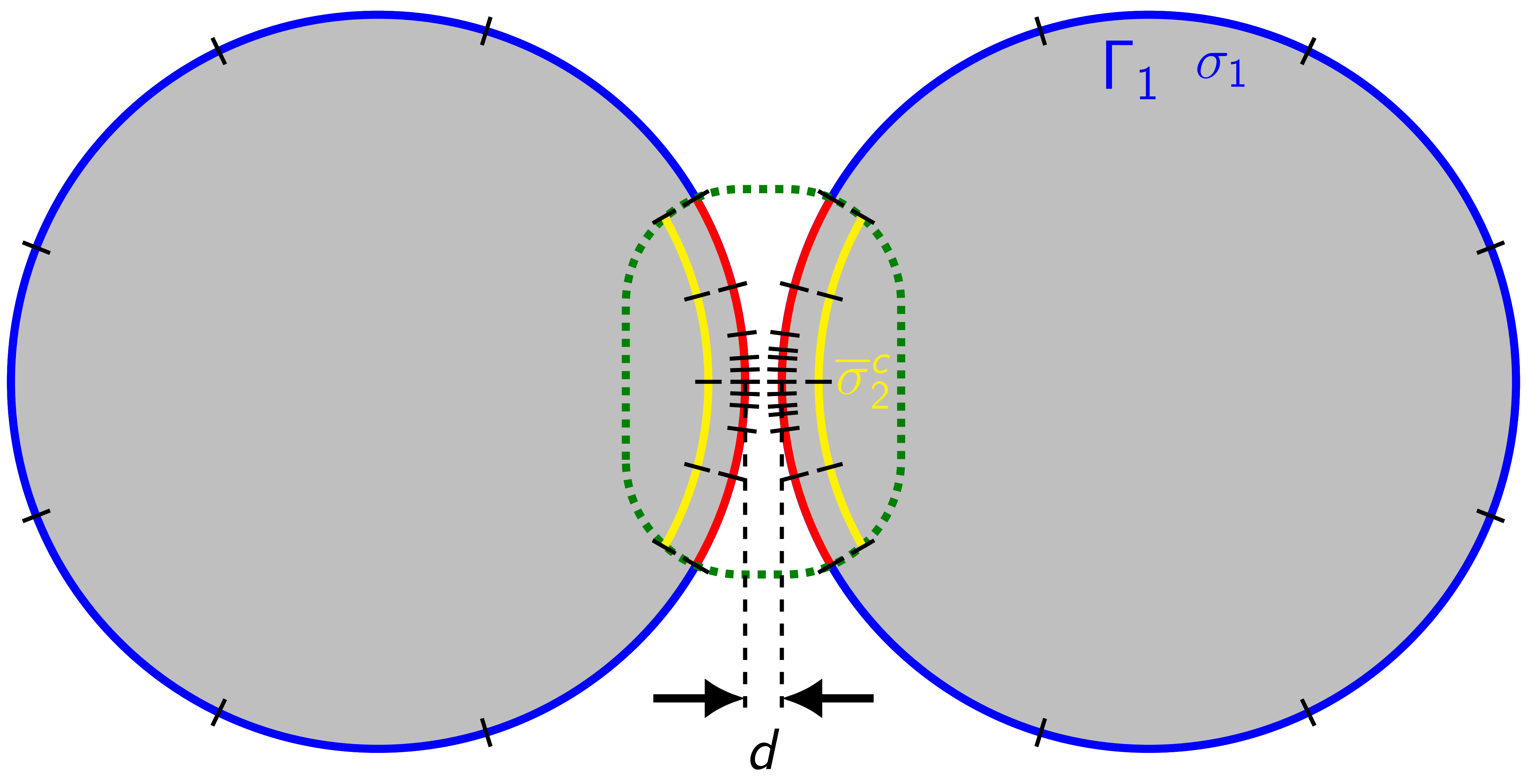

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Then $\overline{\sigma}_2 = K_{22}\sigma_2$ is smooth and $K_{12}K_{22}^{-1}$ is low rank.

Project onto a coarse mesh:

$$\begin{pmatrix} K_{11} & K_{12}^c R \\ K_{21}^c & I \end{pmatrix} \begin{pmatrix} \sigma_1 \\ \overline{\sigma}_2^c \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2^c \end{pmatrix}$$

where $R = \underbrace{\left(W_c^{-1} P^T W_f\right)}_{\substack{L^2 \text{ projection} \\ \text{(fine to coarse)}}} K_{22}^{-1} \underbrace{P}_{\substack{\text{interpolation} \\ \text{(coarse to fine)}}}.$

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Interpolated compressed inverse preconditioning (ICIP)

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(for $\log d$ panels of order p)

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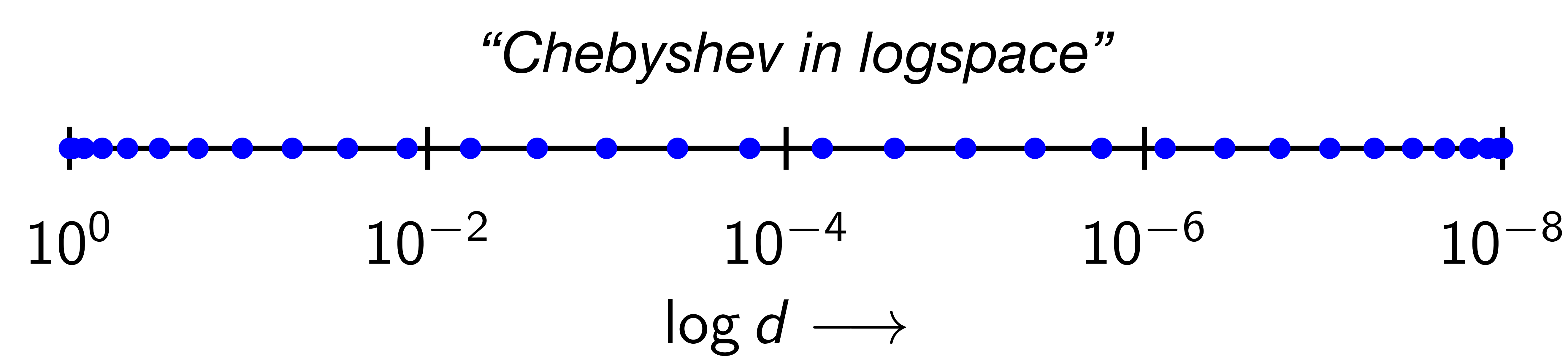
$$[R(d)]_{ij} \approx \sum_{k=0}^{q} [R_k]_{ij} T_k(\log d)$$



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Direct	$p^3(\log d)^3$	$p^6(\log d)^6$
RCIP	$p^3 \log d$	$p^6 \log d$
ICIP	$p^2 q$	$p^4 q$

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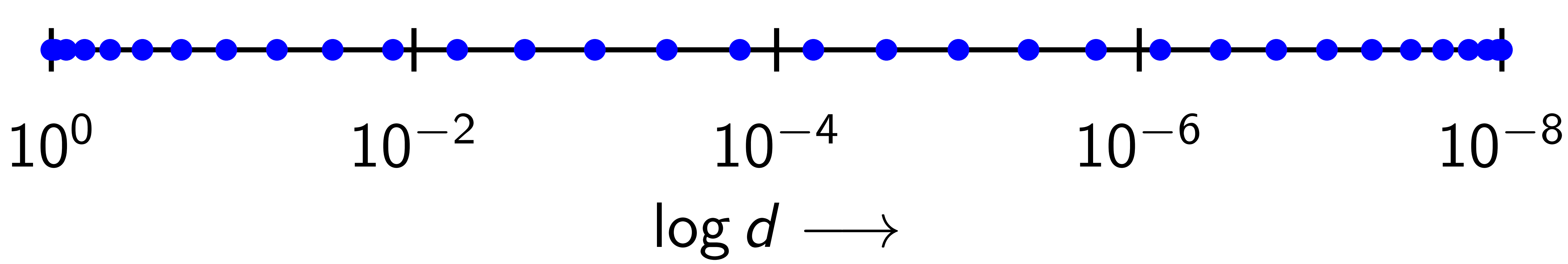
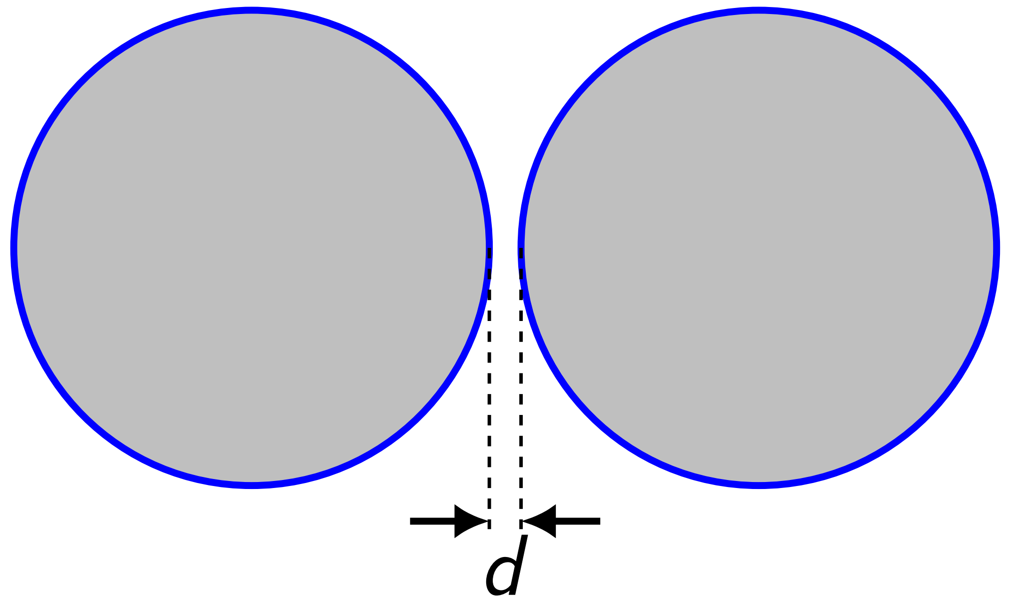
"Chebyshev in logspace"



Results
Convergence of ICIP

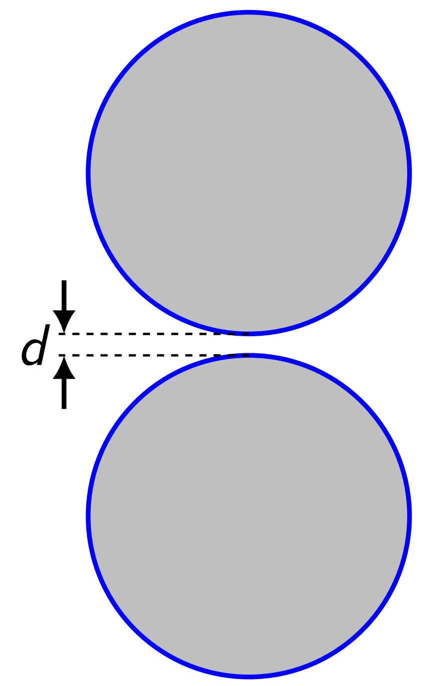
Errors for Stokes mobility with two discs

d	Adaptive discretization	Interpolating $R(d)$				
		$q=8$	$q=16$	$q=24$	$q=32$	$q=40$
10^{-1}	7.6×10^{-15}	1.0×10^{-4}	2.9×10^{-7}	2.1×10^{-9}	9.1×10^{-12}	9.0×10^{-15}
10^{-2}	1.8×10^{-13}	2.8×10^{-3}	3.6×10^{-6}	3.6×10^{-8}	6.5×10^{-10}	1.6×10^{-14}
10^{-3}	4.4×10^{-13}	3.4×10^{-5}	5.6×10^{-10}	4.8×10^{-14}		
10^{-4}	3.8×10^{-11}	1.5×10^{-3}	1.4×10^{-9}	1.4×10^{-13}		
10^{-5}	9.0×10^{-9}	1.5×10^{-5}	2.1×10^{-12}			
10^{-6}	2.0×10^{-7}	6.0×10^{-4}	1.4×10^{-11}			
10^{-7}	4.3×10^{-7}	1.7×10^{-5}	4.1×10^{-11}			
10^{-8}	5.3×10^{-8}	6.3×10^{-4}	3.9×10^{-9}			



Results
GMRES iterations for ICIP

GMRES iteration counts to solve Stokes mobility with $\epsilon = 10^{-8}$



Adaptive discretization

N_{disc}	$d = 10^{-1}$	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
2	15	37	104	337	1283	1848	2344

Interpolated compressed inverse preconditioning (ICIP)

N_{disc}	$d = 10^{-1}$	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
2	18	20	21	21	21	21	21

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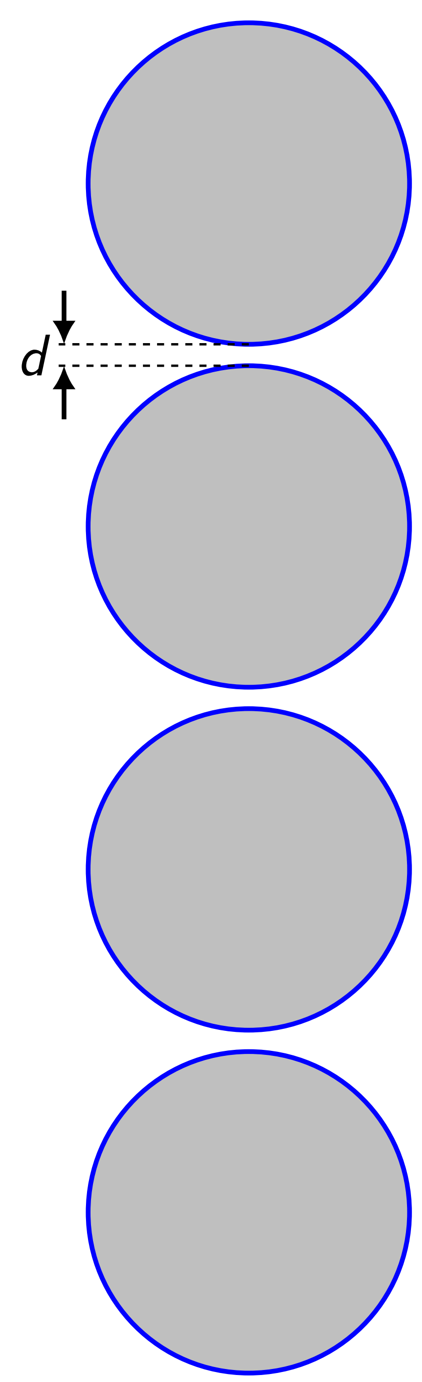
GMRES iteration counts to solve Stokes mobility with $\epsilon = 10^{-8}$



Adaptive discretization

N_{disc}	$d = 10^{-1}$	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
2	15	37	104	337	1283	1848	2344
4	25	75	271	1134	3770	5301	6620

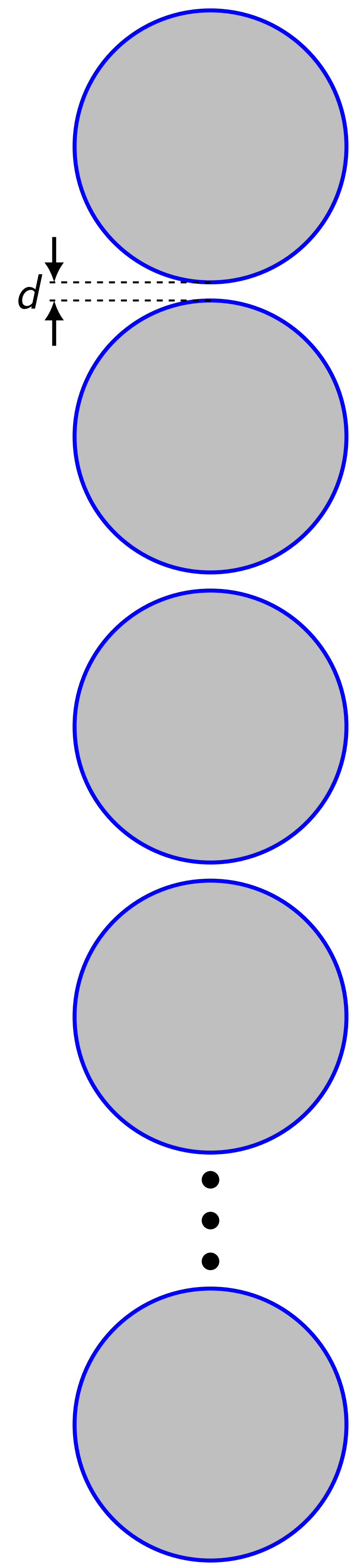
Interpolated compressed inverse preconditioning (ICIP)

N_{disc}	$d = 10^{-1}$	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
2	18	20	21	21	21	21	21
4	28	34	36	37	37	37	37

Results

GMRES iterations for ICIP

GMRES iteration counts to solve Stokes mobility with $\epsilon = 10^{-8}$



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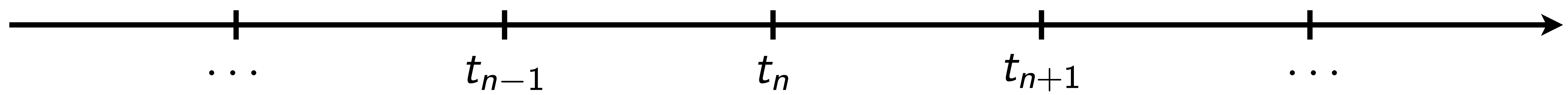
2	15	37	104	337	1283	1848	2344
4	25	75	271	1134	3770	5301	6620
16	35	147	629	2754	8000+	–	–
64	36	148	683	3094	–	–	–
256	37	149	683	3094	–	–	–

Interpolated compressed inverse preconditioning (ICIP)

N_{disc}	$d = 10^{-1}$	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}
2	18	20	21	21	21	21	21
4	28	34	36	37	37	37	37
16	46	71	74	80	86	87	88
64	49	96	108	131	186	237	251
256	49	98	110	134	220	371	608

Accelerating GMRES

Krylov subspace recycling



Forward Euler at timestep n:

- Solve mobility problem using GMRES: $K_n \sigma_n = g_n$
- Advance to t_{n+1}: $\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \Delta t \boldsymbol{V}(\sigma_n)$

Accelerating GMRES

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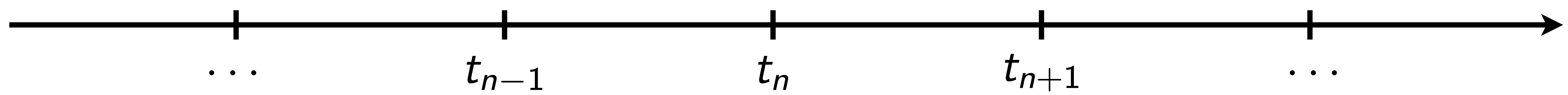

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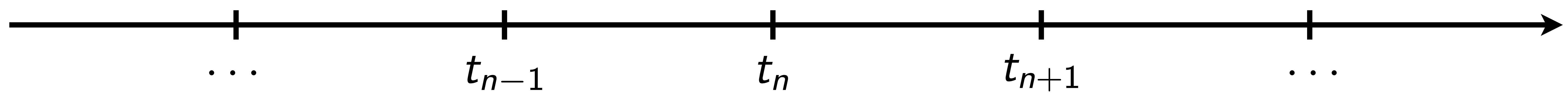
Question: Can we use information from t_{n-1} to accelerate GMRES at t_n?

Accelerating GMRES
Krylov subspace recycling



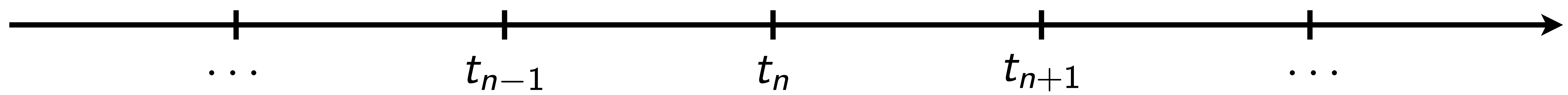
Forward Euler at timestep n:

- Solve mobility problem using GMRES: $K_n \sigma_n = g_n$
- Advance to t_{n+1}: $\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \Delta t\, \boldsymbol{V}(\sigma_n)$

Idea: Use σ_{n-1} as an initial guess to GMRES… doesn't help at all.

Accelerating GMRES

Krylov subspace recycling



Forward Euler at timestep *n*:

- Solve mobility problem using GMRES: $K_n \sigma_n = g_n$
- Advance to t_{n+1}: $\boldsymbol{x}_{n+1} = \boldsymbol{x}_n + \Delta t \, \boldsymbol{V}(\sigma_n)$

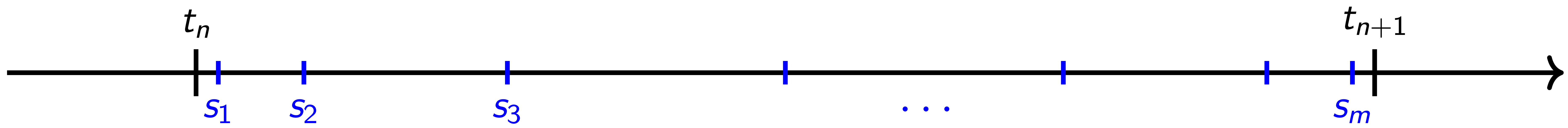
Idea: Reuse Krylov subspace from previous time step… very effective!

- Krylov subspace after *k* iterations: $X = [b \quad Ab \quad \cdots \quad A^{k-1} b]$
- Compute QR decomposition: $QR = AX$
- Define preconditioner: $P = I - QQ^T + XR^{-1}Q^T$

$$\boxed{\begin{aligned} PAx &= x \ \text{ for all } \ x \in \operatorname{span}(X) \\ Py &= y \ \text{ for all } \ y \perp \operatorname{span}(X) \end{aligned}}$$

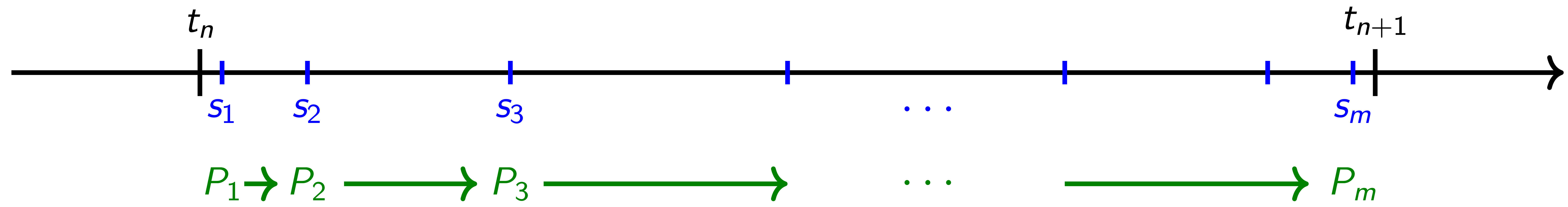
Accelerating GMRES

Krylov recycling with spectral deferred corrections



Accelerating GMRES

Krylov recycling with spectral deferred corrections



Accelerating GMRES

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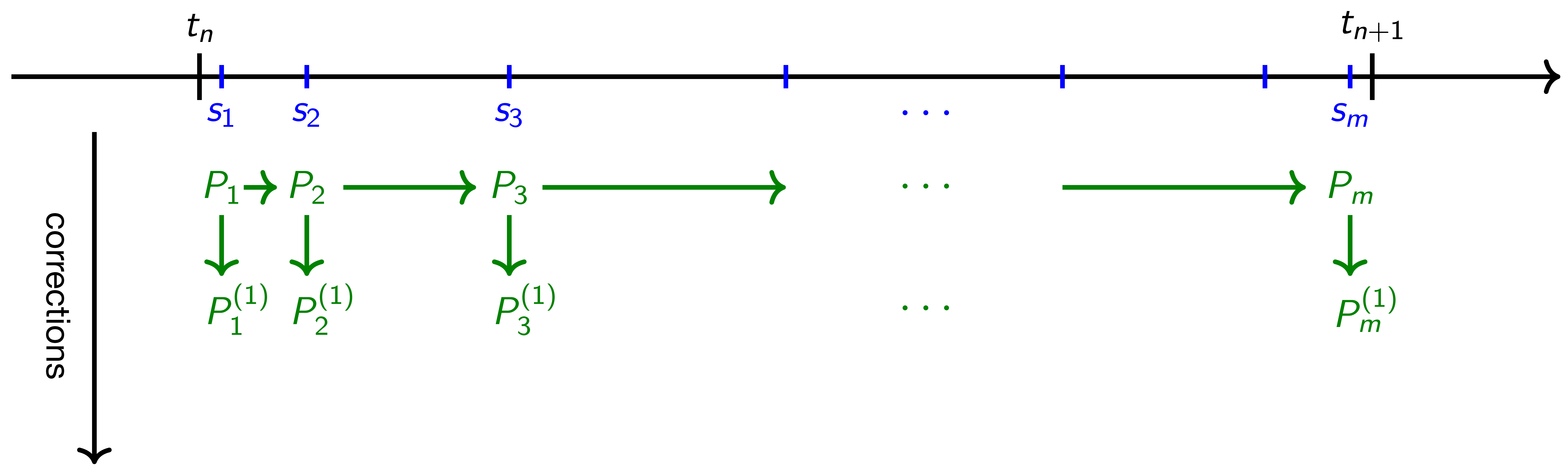
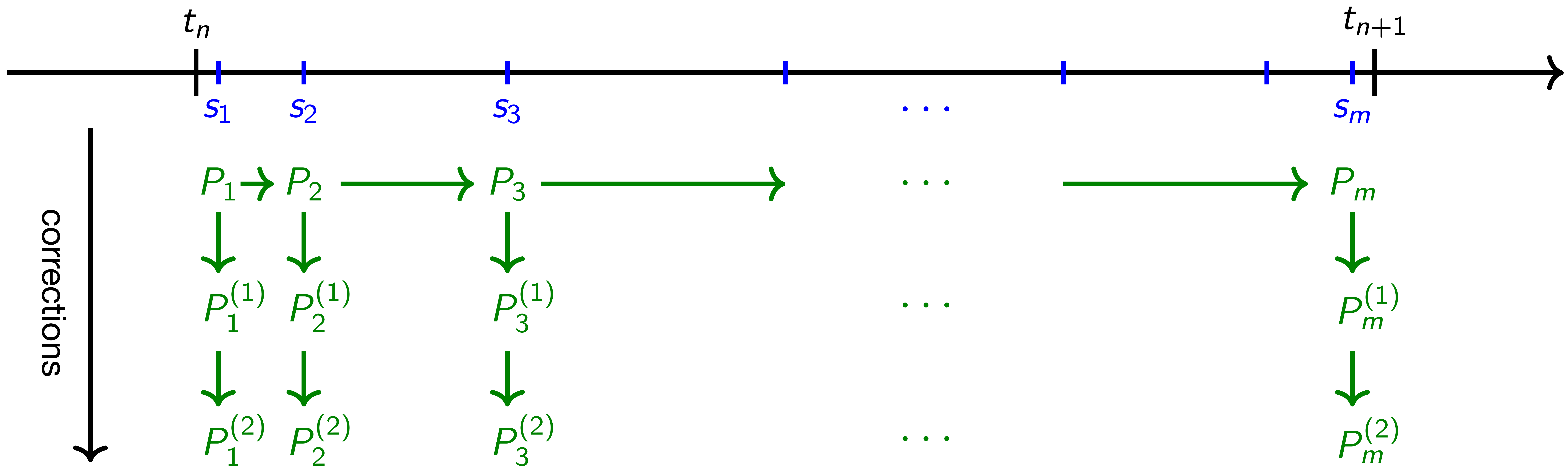


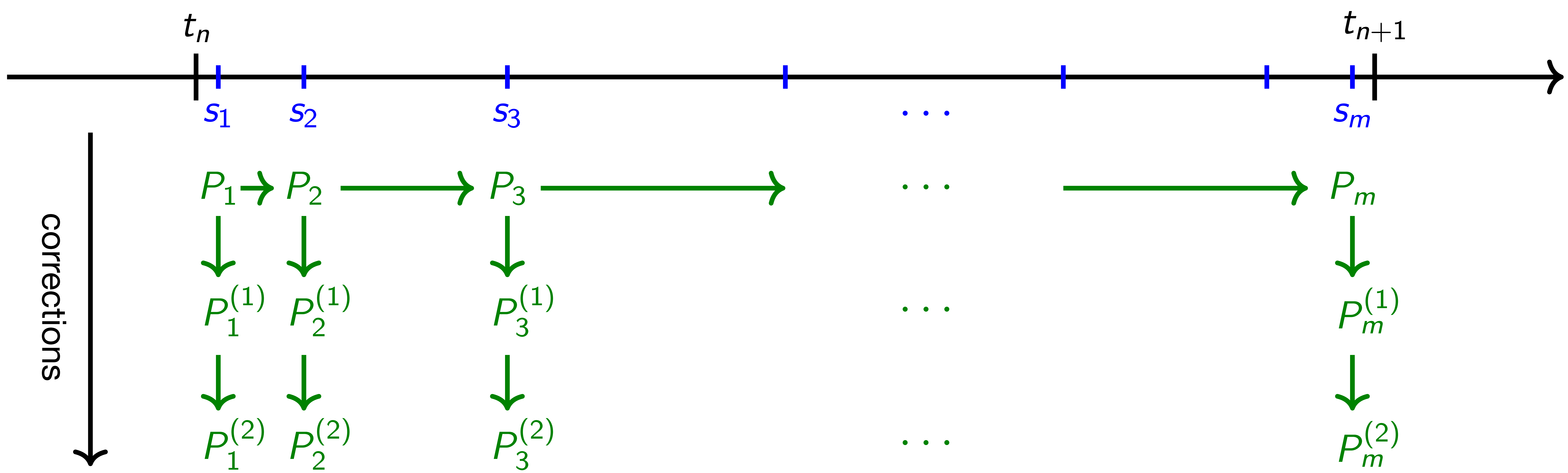
Accelerating GMRES

Krylov recycling with spectral deferred corrections



Accelerating GMRES

Krylov recycling with spectral deferred corrections

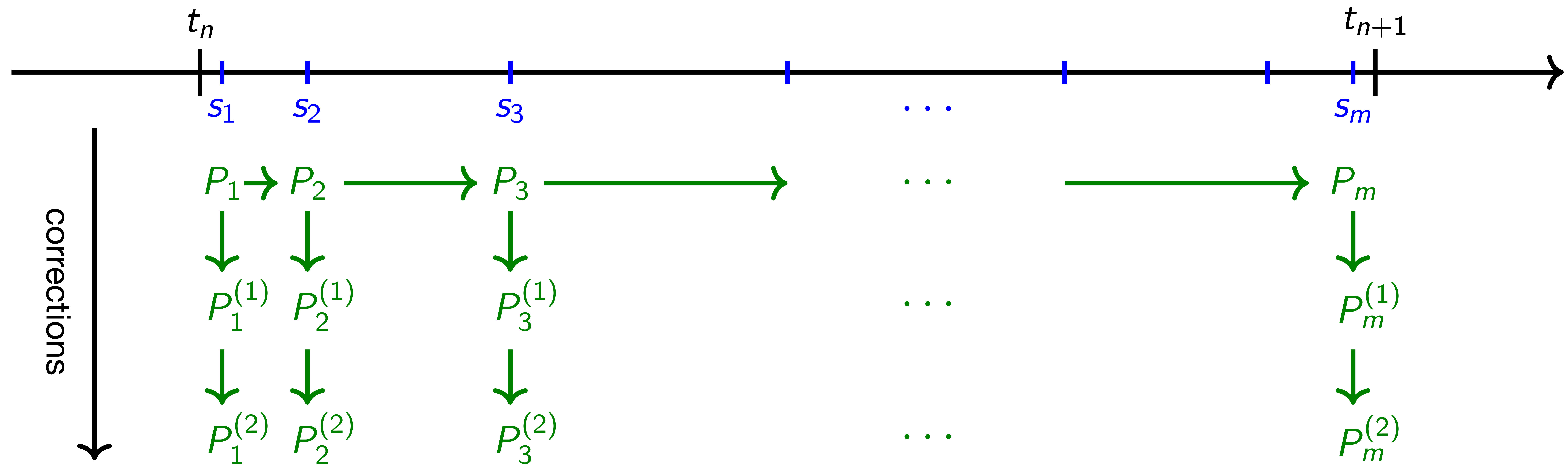


GMRES iterations **without** preconditioner

correction ↓ \ substep →				
66	66	66	66	66
66	66	66	66	66
66	66	66	66	66
66	66	66	66	66

Accelerating GMRES

Krylov recycling with spectral deferred corrections



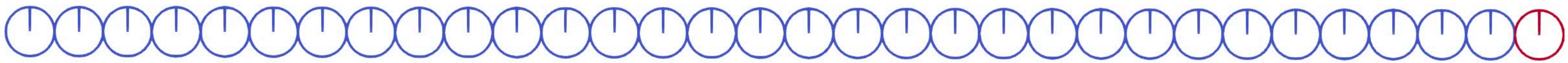
GMRES iterations **without** preconditioner

correction ↓ \ substep ⟶					
	66	66	66	66	66
	66	66	66	66	66
	66	66	66	66	66
	66	66	66	66	66

GMRES iterations **with** preconditioner

correction ↓ \ substep ⟶					
	66	30	22	45	30
	35	17	33	28	24
	8	4	14	5	12
	1	1	2	2	4

Results
A chain of discs



Average GMRES iterations per timestep **without** Krylov preconditioning = 130
with Krylov preconditioning = 30

32 discs (36k unknowns)
10^{-4} minimum distance
10th-order adaptive SDC
7-digit accuracy
~2000 timesteps
64 cores, 48 hours
84 seconds/timestep
1.6 seconds/mobility solve
100k mobility solves
3.2 million iterations

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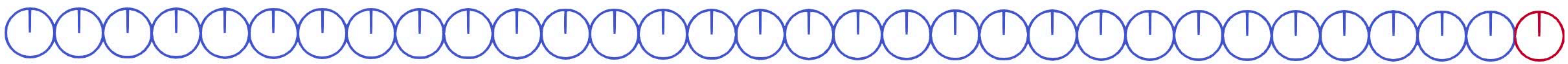

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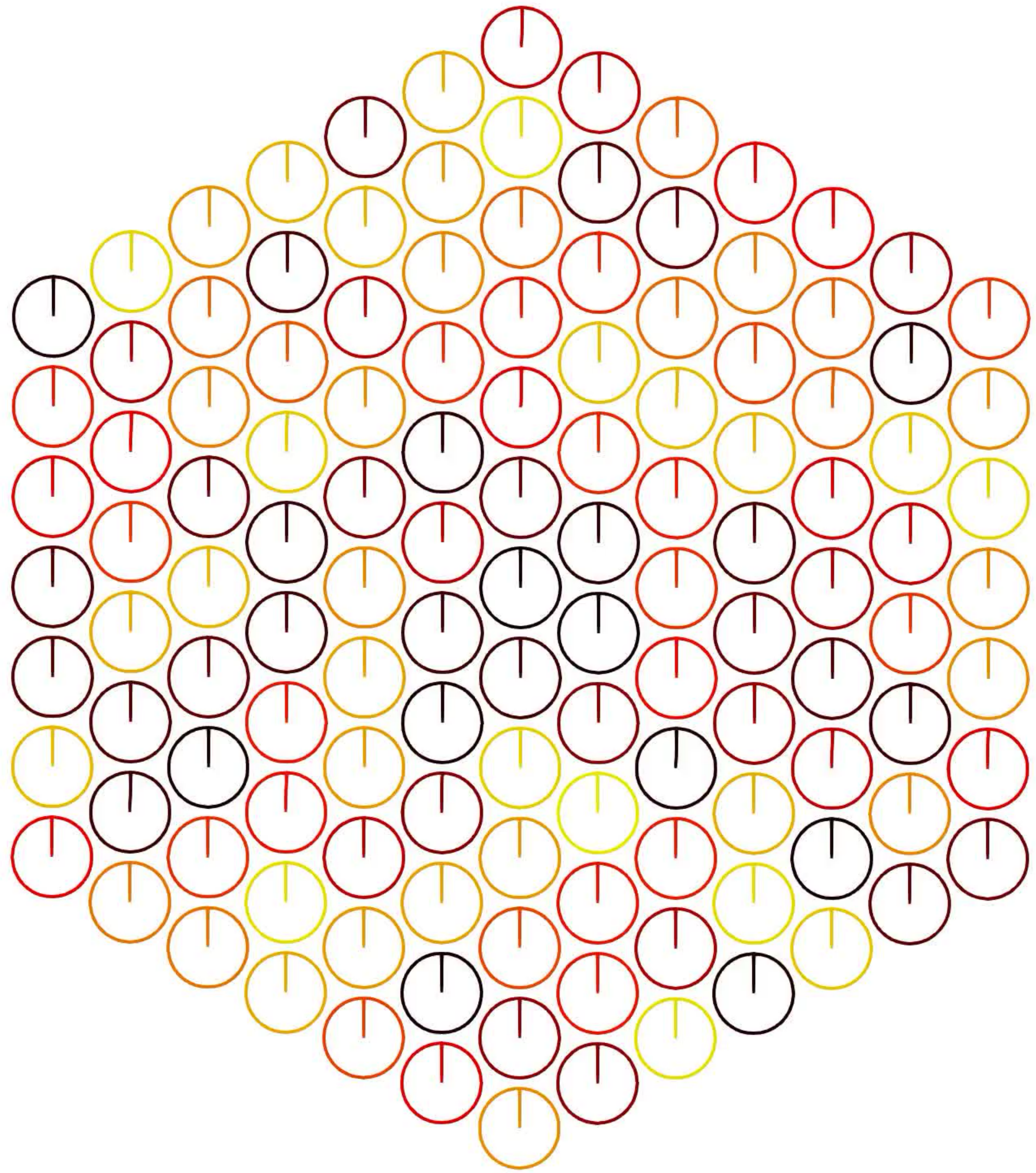
Sedimentation flow



127 discs (200k unknowns)
10^{-4} minimum distance
10th-order adaptive SDC
5-digit accuracy
~200 timesteps
64 cores, 1 week
6,480 mobility solves
1.3m iterations

Results

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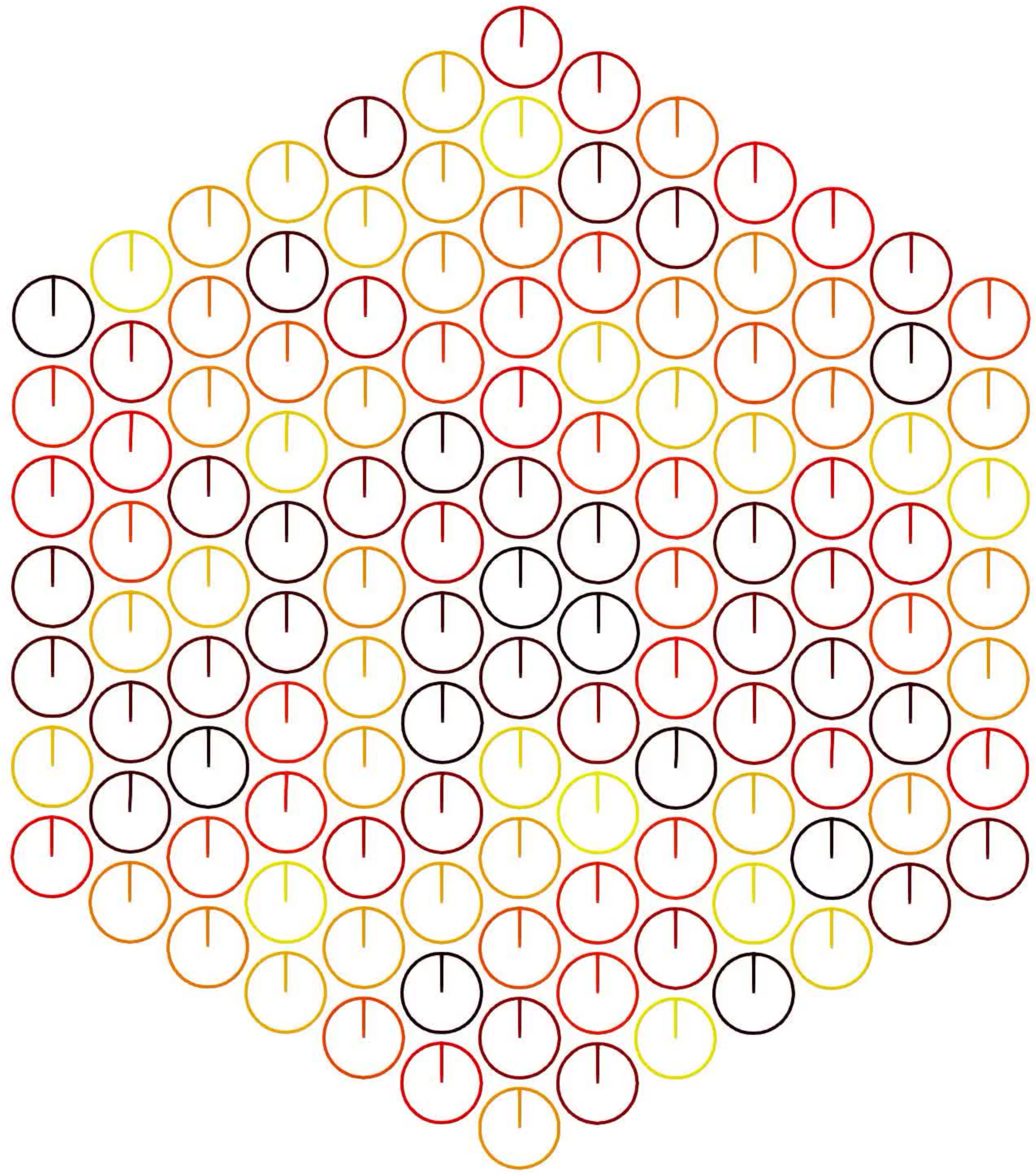

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Conclusions

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- **Krylov subspace recycling** can drastically accelerate high-order timestepping.
- Ongoing work: flows in confined geometries, extension to spheres in 3D.
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Thanks!

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