Many-Particle Simulations using the Fast Boundary Method

NSF EAR 0911094 and EAR 1215800

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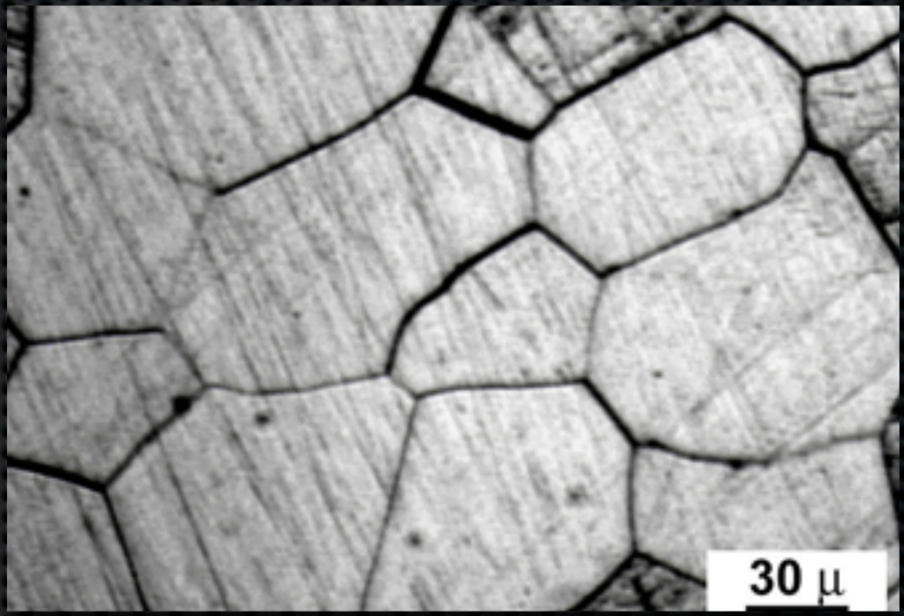
Overview

- Introduction to Stokes Flow and Boundary Methods.
- Computational Difficulties and Acceleration Techniques.
- Analysis and Implementation Details.
- Overview of Application Areas.

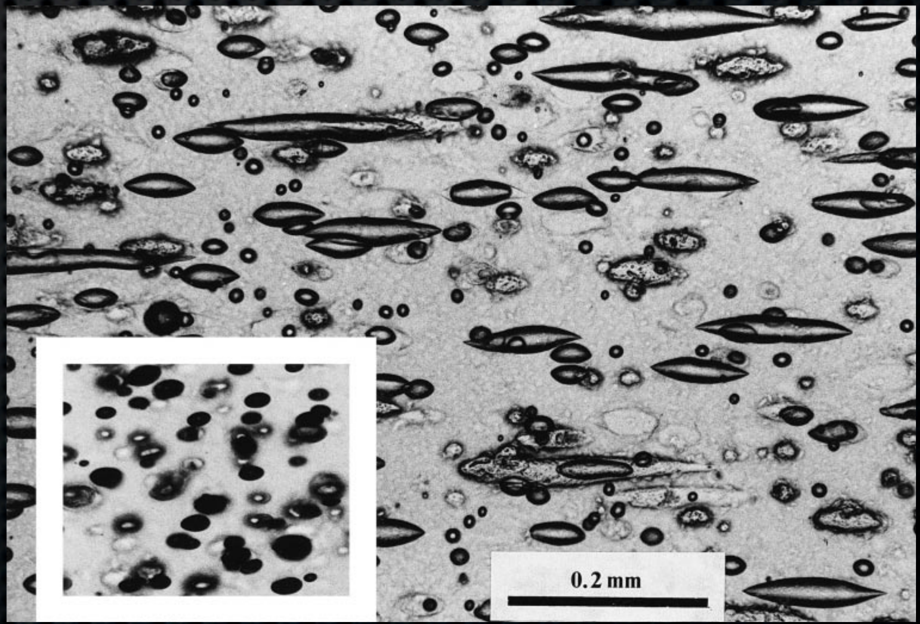
Geophysical Applications

Geophysical Applications

- Micro-scale simulation:
  - Heterogenous flows.
  - Exploring the evolution at the Core-Mantle Boundary.
  - Anisotropic grain-grain stresses.
  - Large viscous flows (volcanic flows).
  - Binary fluid separation.



Crystal Grain Structure [Edward Pleshakov, Wikimedia 2008]

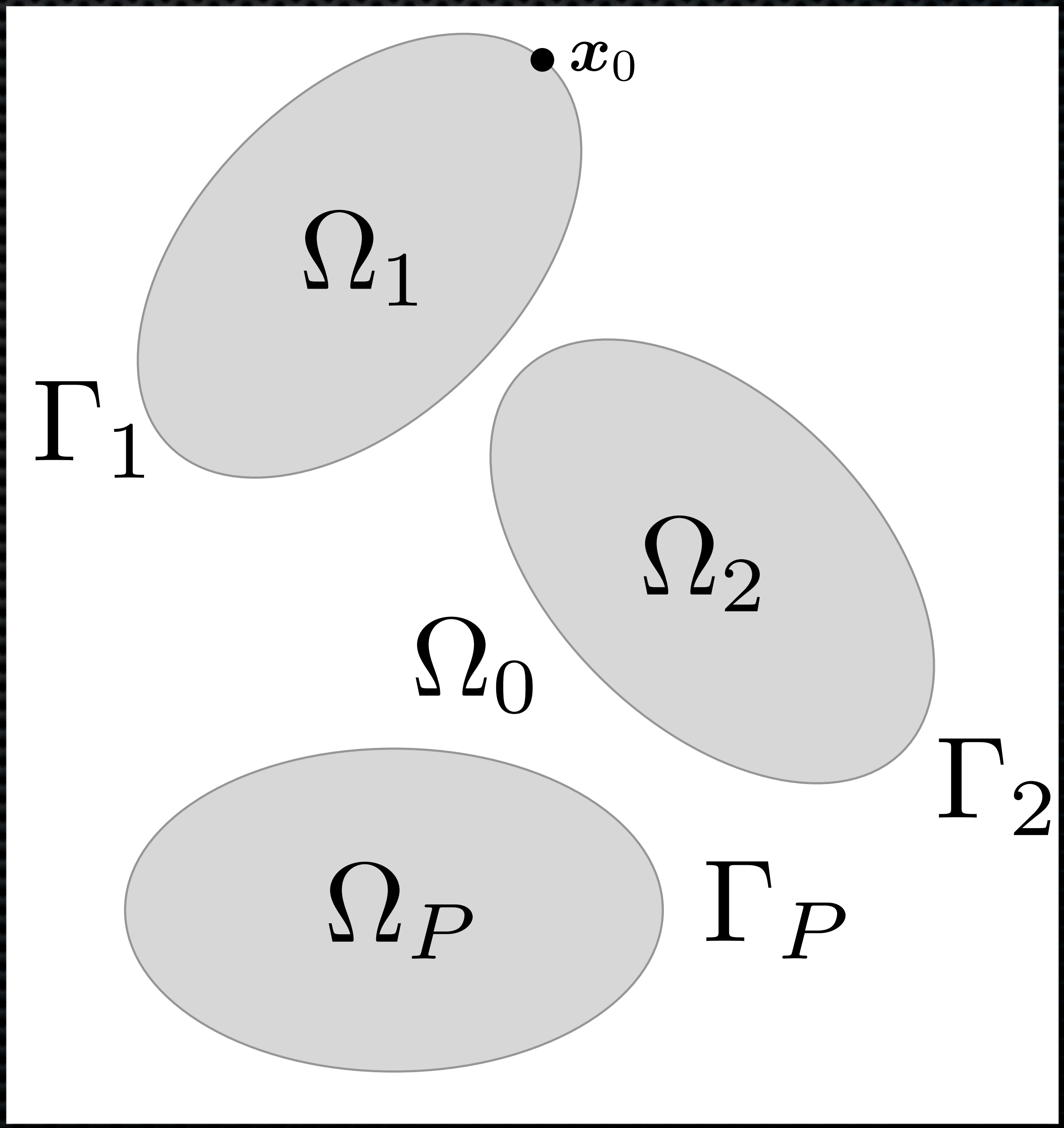


Micro bubbles Map of ULVZs [Manga et al. 1998]

The Physical Problem

$$-\nabla P + \mu \nabla^2 \boldsymbol{u} + \rho \boldsymbol{b} = 0$$

- Each domain may have different physical properties.
- Explicitly track boundary nodes during creeping flows.
- Possibility for unbounded domains.



Governing Equation

- The Stokes Boundary Integral Equation (BIE) for multiple domains [Pozrikidis 2001].

$$\frac{1+\lambda_q}{2} u_j(\boldsymbol{x}) = u_j^{\infty}(\boldsymbol{x}_0) - \sum_{p=1}^{P} \frac{1}{4\pi \mathcal{C}a} \int_{\Gamma_p} \Delta f_i^{(p)}(\boldsymbol{x}) U_{ij}(\boldsymbol{x}, \boldsymbol{x}_0) \, \mathrm{d}\Gamma_m(\boldsymbol{x})$$

$$+ \sum_{p=1}^{P} \frac{1-\lambda_p}{4\pi} \int_{\Gamma_p}^{\mathcal{PV}} u_i(\boldsymbol{x}) T_{ijk}(\boldsymbol{x}, \boldsymbol{x}_0) \hat{n}_k(\boldsymbol{x}) \, \mathrm{d}\Gamma_p(\boldsymbol{x})$$

- The dimensionless parameters:

$$\mathcal{C}a = \frac{\mu_m u_c}{\gamma_c} \qquad \lambda_p = \frac{\mu_p}{\mu_m}$$

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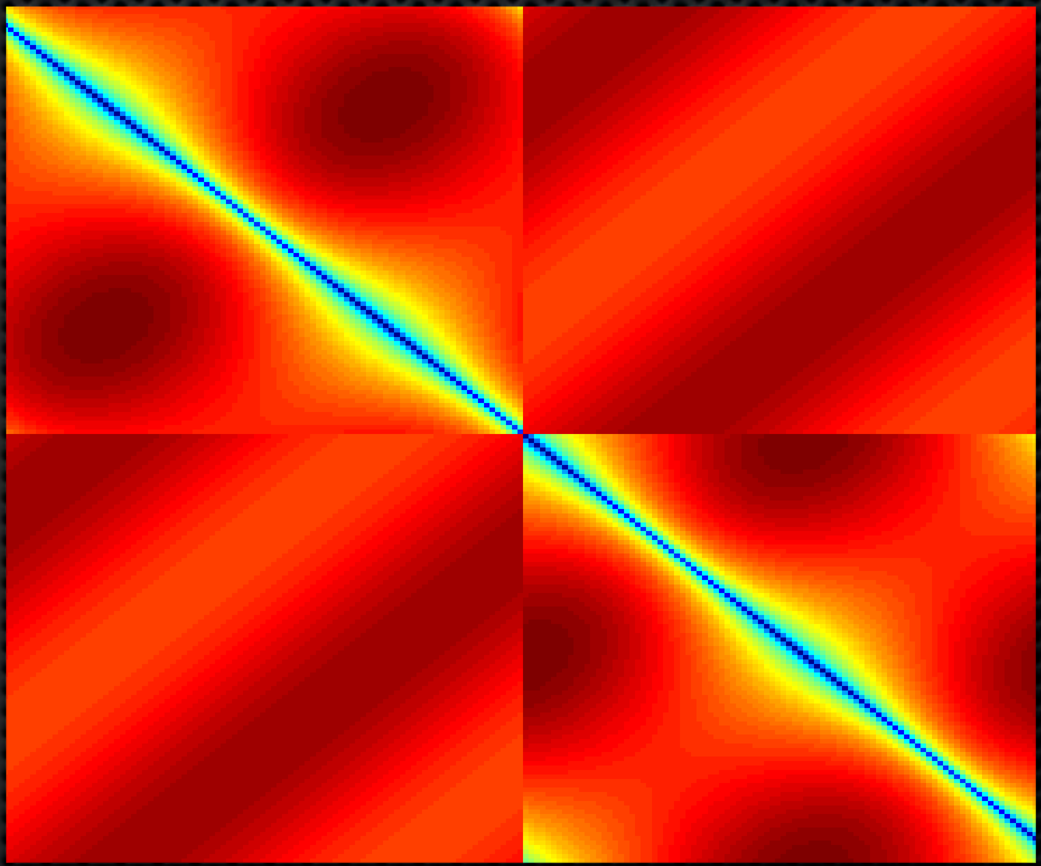
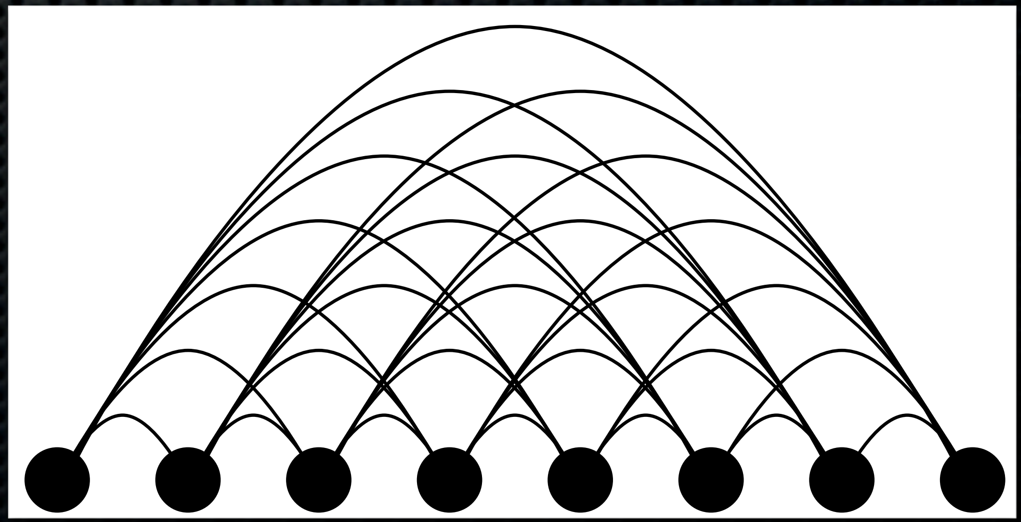
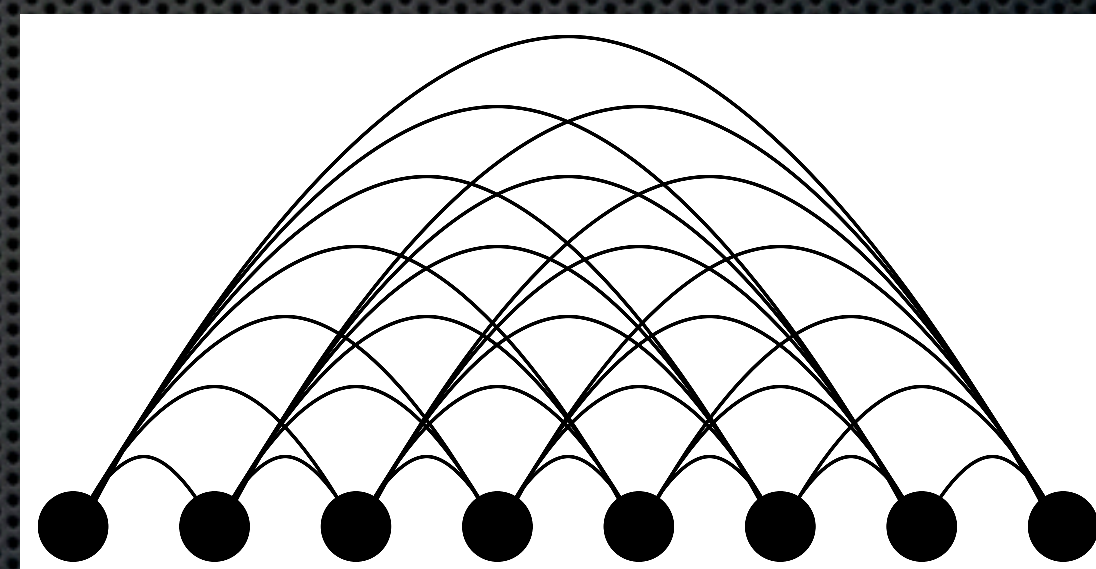
Direct Computation

- Collocation Method.
- Generally **dense** and asymmetric.
- Kernel functions have infinite support.
- Limits size of problem. (32,768 nodes is 1GB matrix).





Fast Multipole Method



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- Move series expansions up and down a tree.
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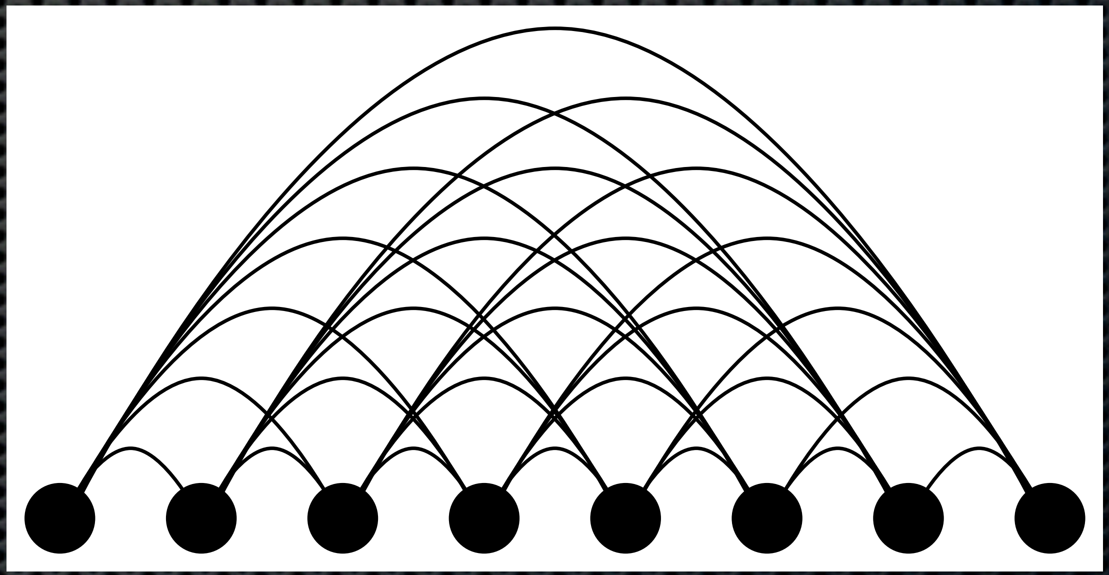

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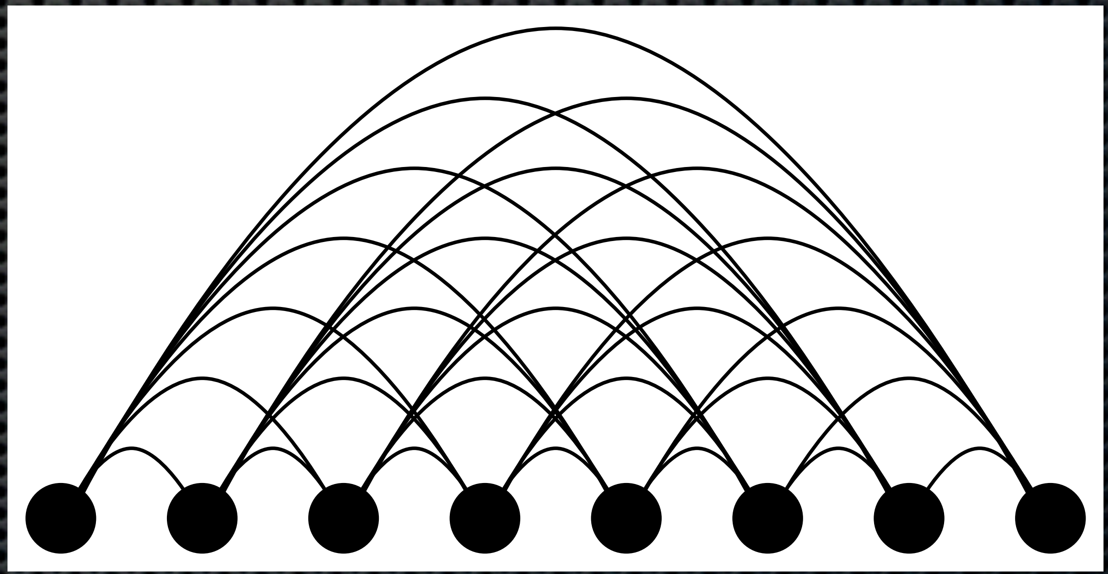

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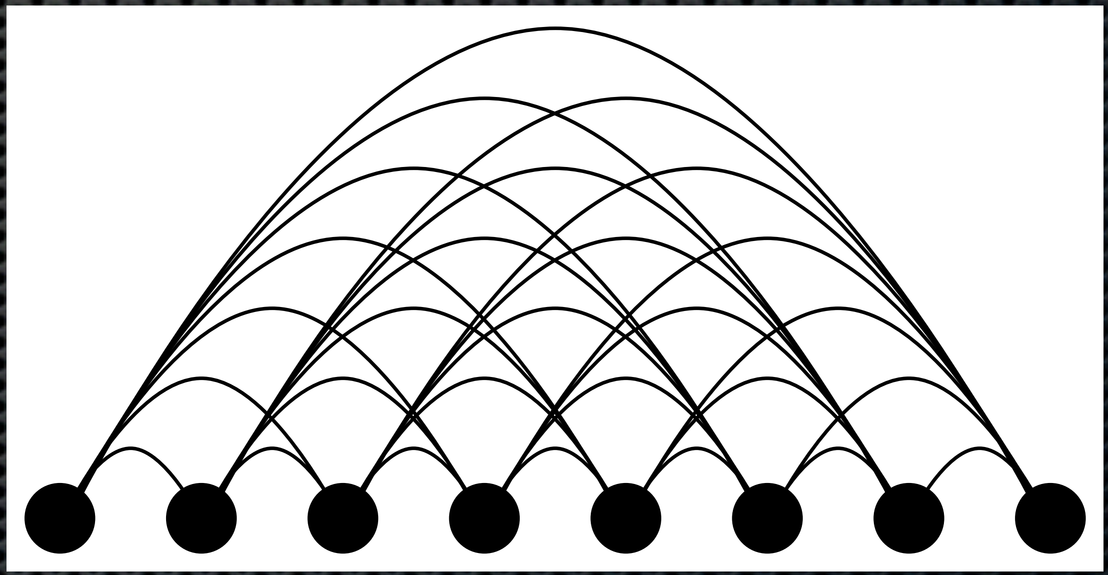

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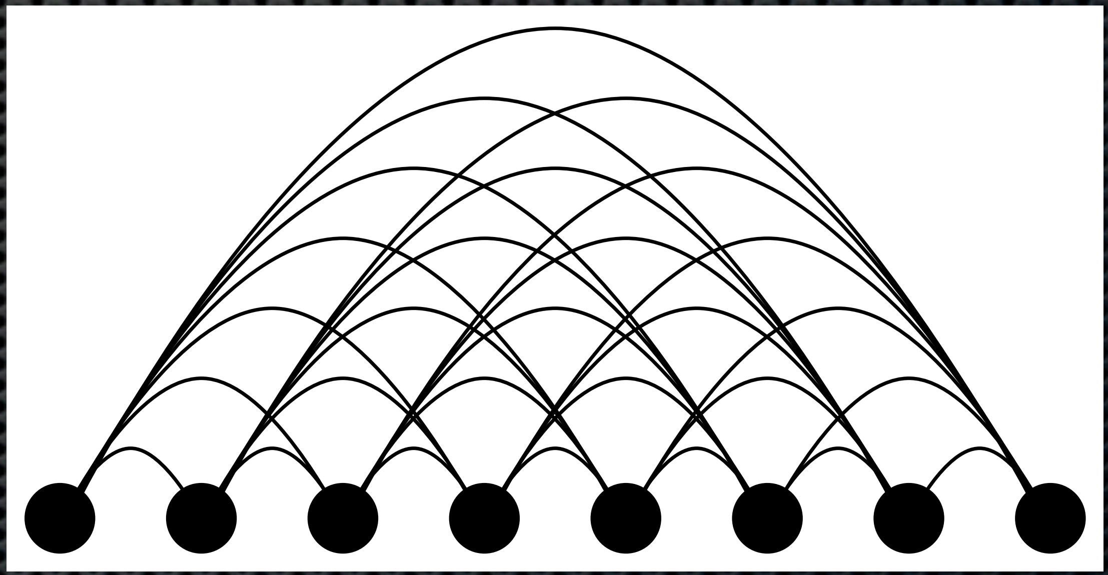

Direct Method

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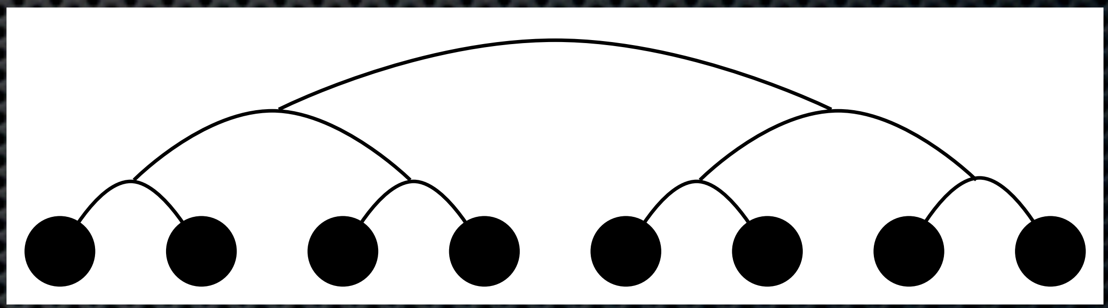

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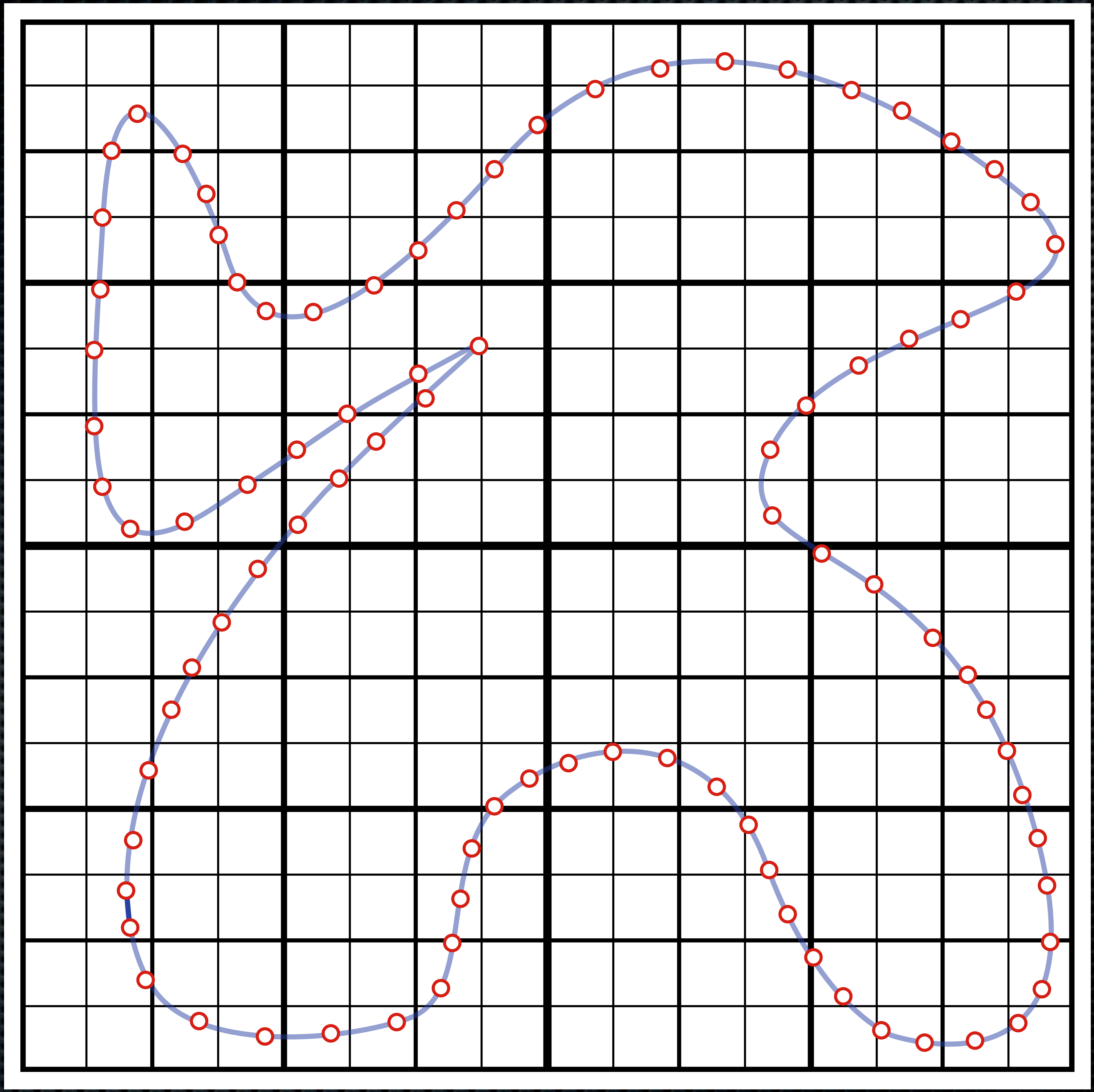

Far Field Expansion

- Example for Potential: $\int_{\Gamma_e} G(z_0, z) t(z) \, d\Gamma_e$

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$$G(z_0, z) = \log(z_0 - z) = \log(z_0 - z_c) + \log\left(1 - \frac{z - z_c}{z_0 - z_c}\right)$$

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- Taylor Expand (requires $|z - z_c| \ll |z_0 - z_c|$)

$$= \sum_{k=0}^{\infty} O_k(z_0 - z_c) I_k(z - z_c) \quad O_k = \begin{cases} \log(z) & k = 0 \\ \frac{(k-1)!}{z^k} & k > 0 \end{cases} \quad I_k = \frac{z^k}{k!}$$

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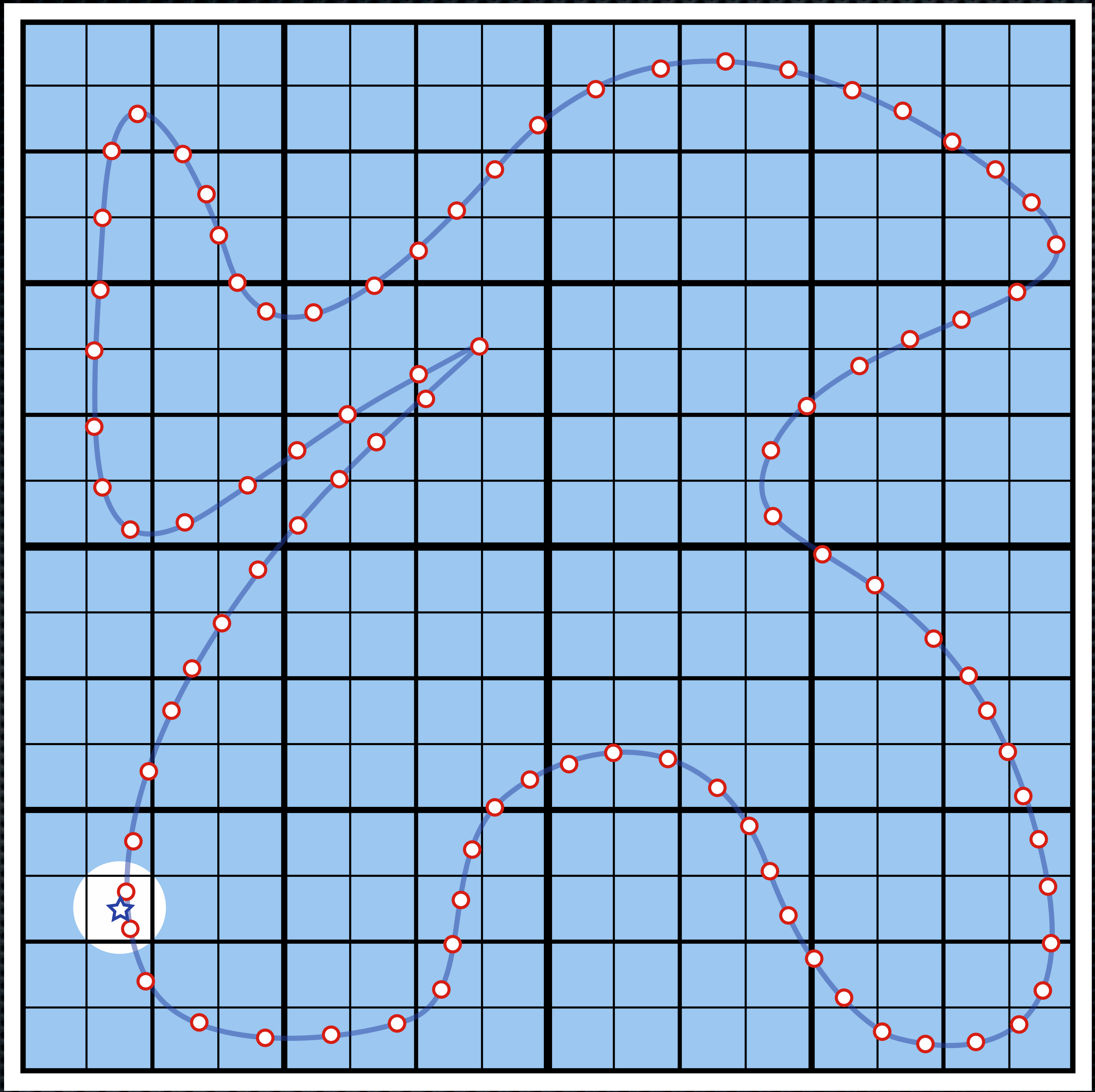

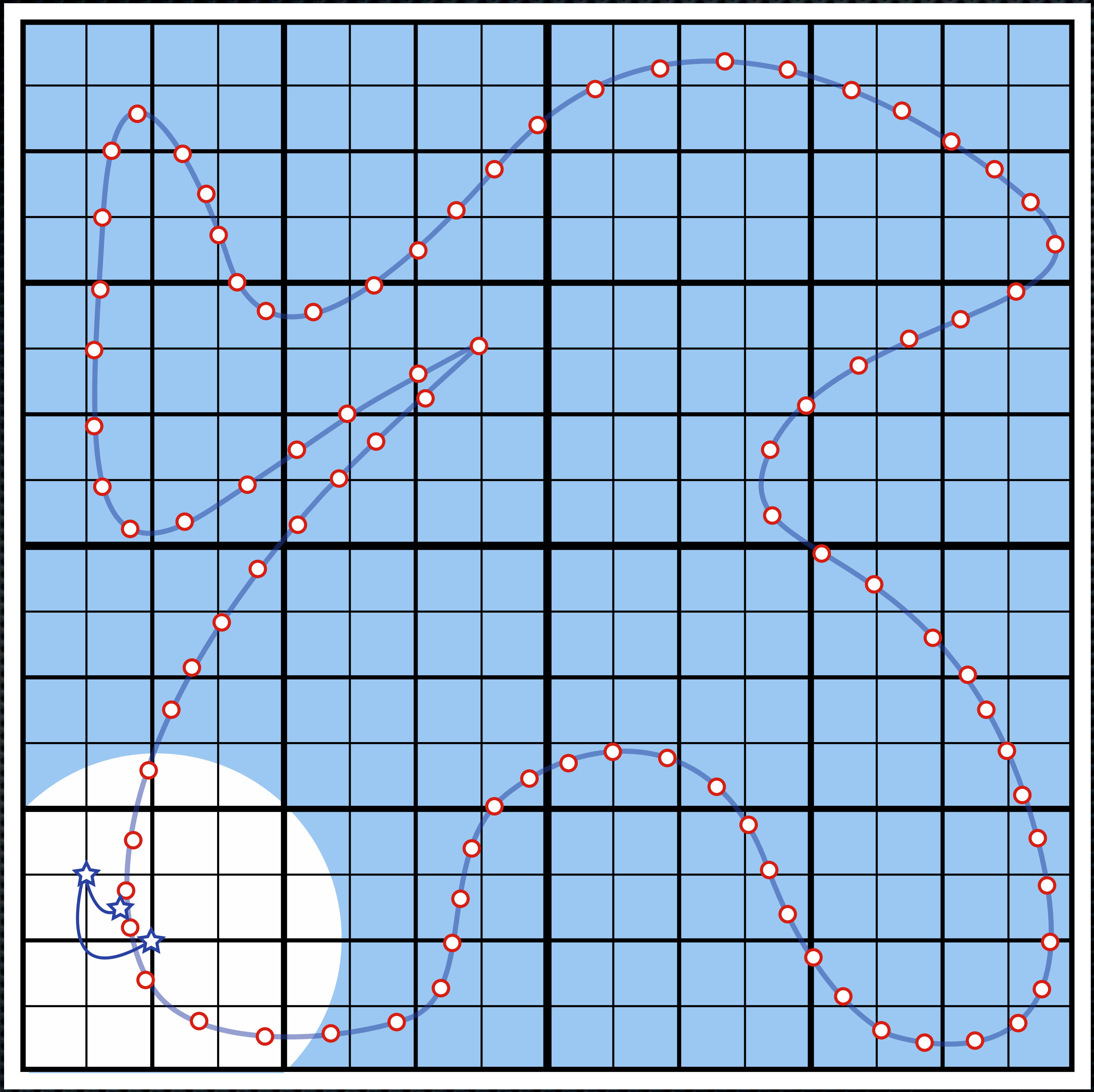

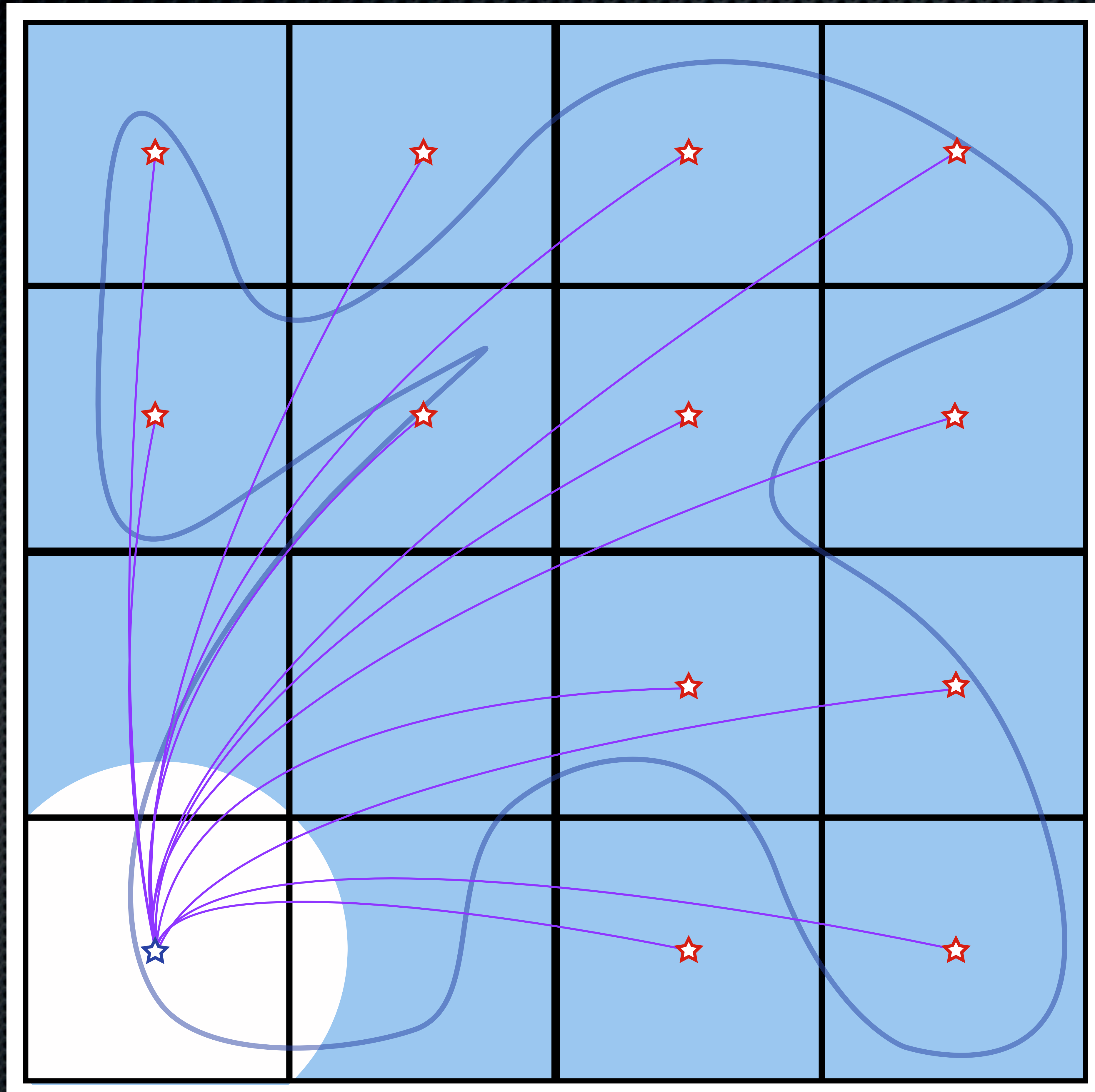

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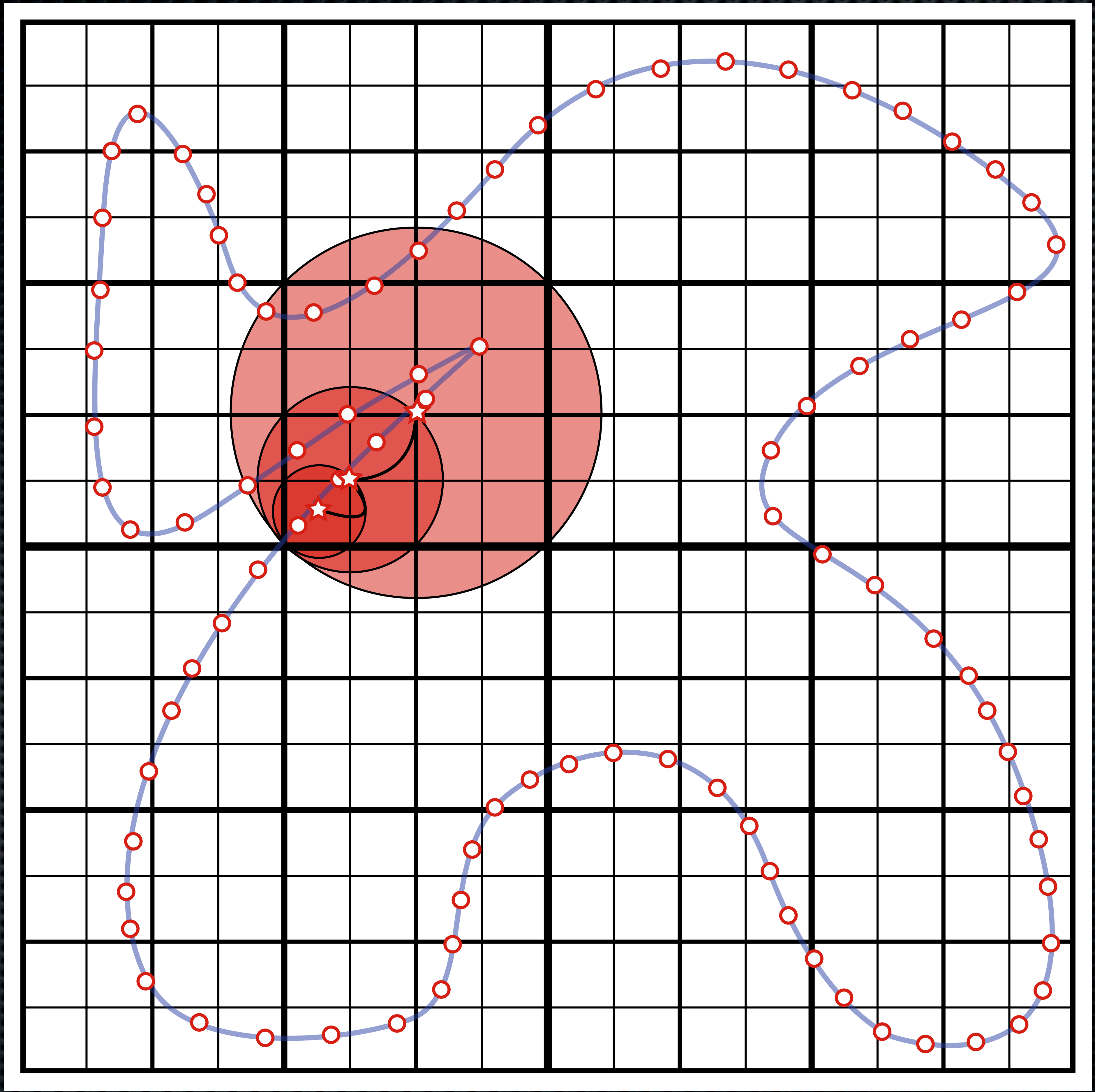

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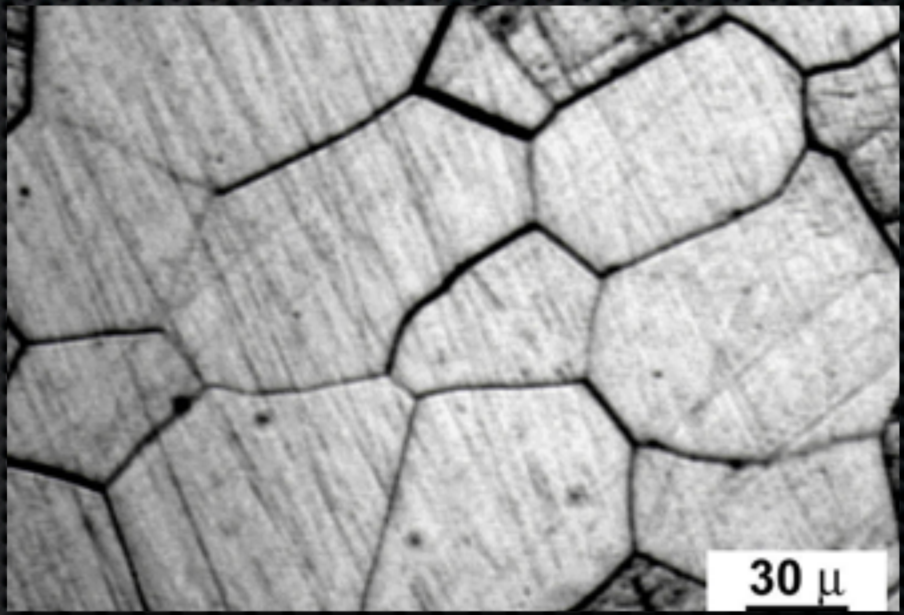

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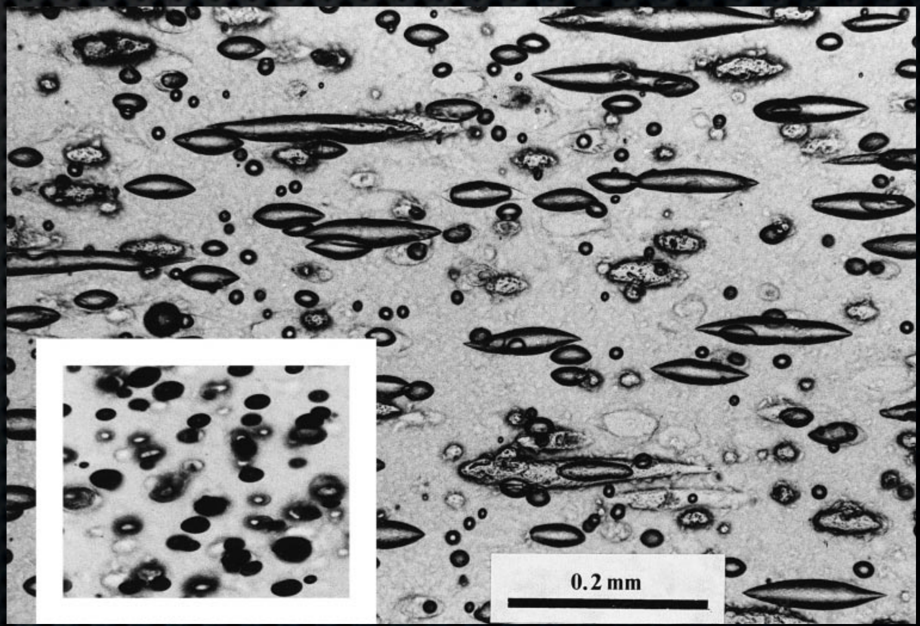

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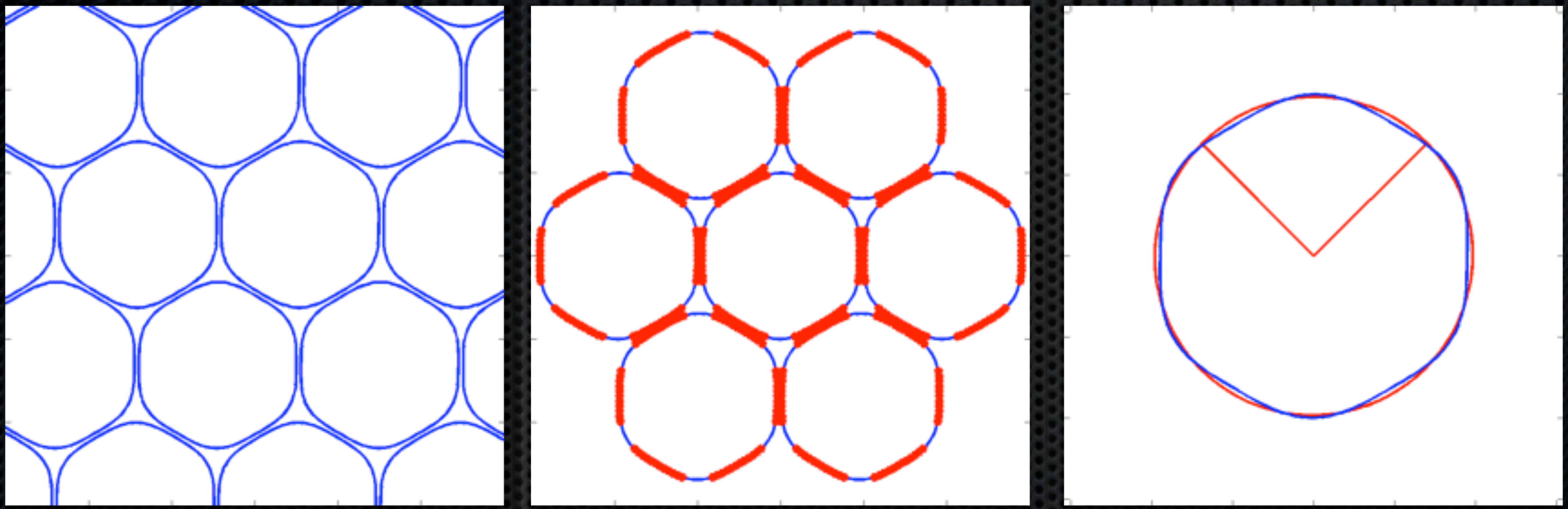
Grain Simulations



- Model a matrix with hundreds of deformable grains.
  - Grain-grain interaction/contact.
  - Deformation and rotation in flow.
  - Derive material properties of flow matrix.

Scaling

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- On Blacklight:
  - Allow for more parameter sweeps of current models.
  - Hundreds of particles.

Blacklight [Pittsburgh Supercomputing Center]

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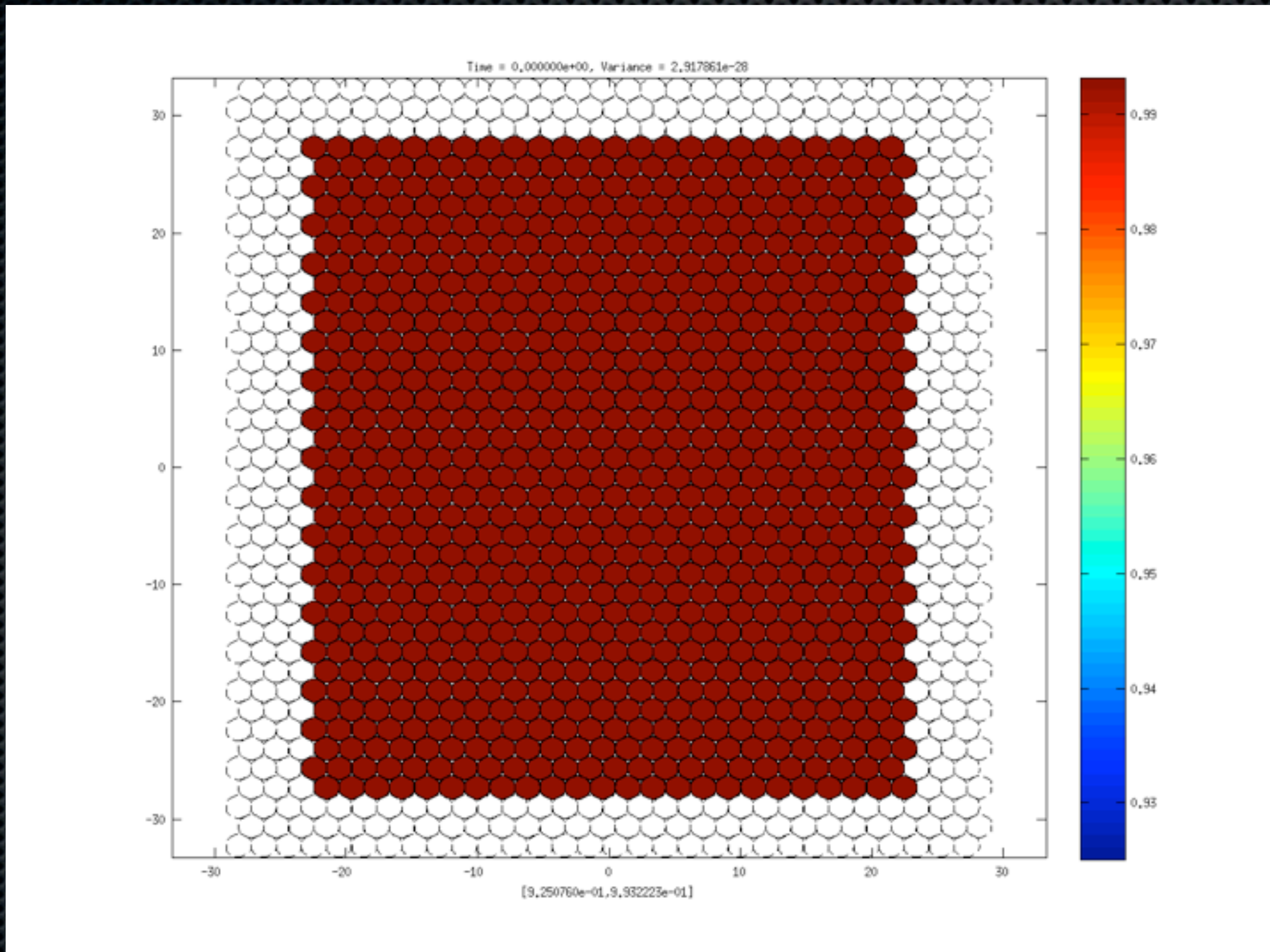
  - Hundreds of particles.
- On Stampeed:
  - 6th Fastest Supercomputer
  - Scale to thousands of particles and beyond...

Blacklight [Pittsburgh Supercomputing Center]

Stampede [Texas Advanced Computing Center]

Geophysical Results



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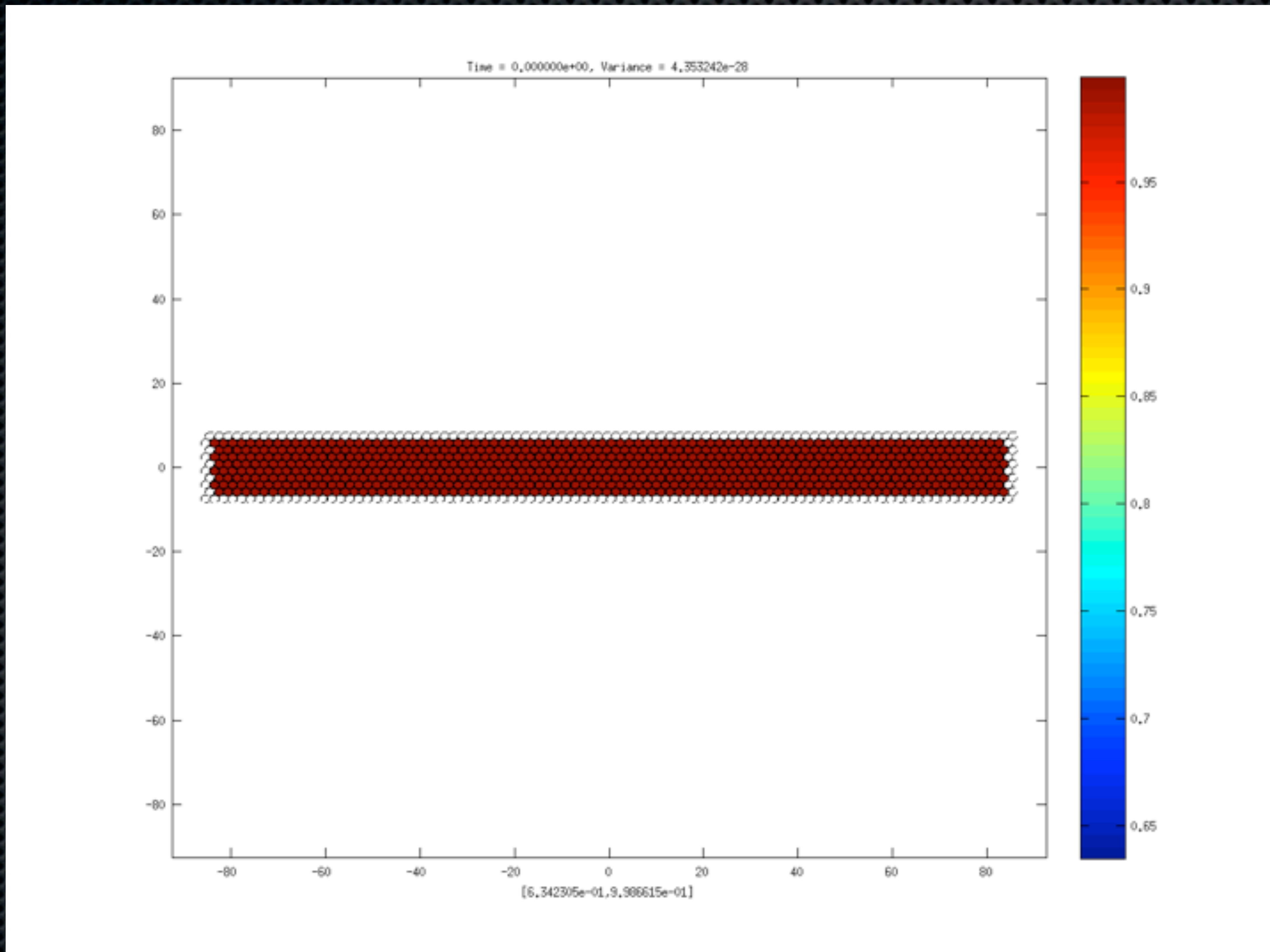

The Big Ideas

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- Fast Multipole Boundary Element Method provides fast method for solving PDEs.
  - Same speed as traditional FDM, FVM, and FEM.
  - Explicitly tracks interfaces.
- Have a multi-domain viscous fluid you need modeled?
  - Material Science, Chemical Engineering, Biology... ... and of course Geophysics!

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References

- X. Gao, “Numerical evaluation of two-dimensional singular boundary integrals--Theory and Fortran code”, Journal of Computational and Applied Mathematics, Volume 118, Pages 44-64, 2006

- E.J. Garnero and A.K. McNamara, “Structure and Dynamics of Earth's Lower Mantle”, Science, Volume 320, Issue 5876, Pages 626-628, 2008

- S. Hier-Majumder and J. Revenaugh, “Relationship between the viscosity and topography of the ultralow-velocity zone near the core–mantle boundary”, Earth and Planetary Science Letters, Volume 299, Pages 382-386, 2010

- D.M. Koch and D.L. Koch, “Numerical and theoretical solutions for a drop spreading below a free fluid surface”, Journal of fluid mechanics, Volume 287, Issue 1, Pages 251-278, 1994

- L.G. Leal, Advanced Transport Phenomena: Fluid Mechanics and Convective Transport Processes, Cambridge Series in Chemical Engineering, 2007

- T.M. Lassak et al., “Core-mantle boundary topography as a possible constraint on lower mantle chemistry and dynamics”, Earth and Planetary Science Letters, Volue 289, Pagrs 232-241, 2010

- Y.J. Liu and N. Nishimura, “The fast multipole boundary element method for potential problems: a tutorial”, Engineering Analysis with Boundary Elements, Volume 30, Issue 2, Pages 371-381, 2006

References

- Y.J. Liu, “A new fast multipole boundary element method for solving 2-D Stokes flow problems based on a dual BIE formulation”, Engineering Analysis with Boundary Elements, Volume 32, Issue 2, Pages 139-151, 2008
- M. Manga and H.A. Stone, “Buoyancy-Driven Interactions Between 2 Deformable Viscous Drops”, Journal of fluid mechanics, Volume 256, Pages 647-683, 1993
- A.K. McNamara, E.J. Garnero, and S. Rost , “Tracking deep mantle reservoirs with ultra-low velocity zones”, Earth and Planetary Science Letters, Volume 299, Pages 1-9, 2010
- C. Pozrikidis, Boundary integral and singularity methods for linearized viscous flow, Cambridge Texts in Applied Mathematics, 1992
- C. Pozrikidis, “Interfacial Dynamics for Stokes Flow”, Journal of Computational Physics, Volume 169, Issue 2, Pages 250-301, 2001
- S. Rost et al., “Seismological constraints on a possible plume root at the core–mantle boundary”, Nature, Volume 435, Issue 7042, Pages 666-669, 2005
- M.S. Warren and J.K. Salmon, “A Parallel Hashed Oct-Tree N-Body Algorithm”, Proceedings of the 1993 ACM/IEEE conference on Supercomputing, AMC, Pages 12-21, 1993