Computational studies of vortex dynamics and pinning effects in high-Tc superconductors

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OSCon

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Part I: Ginzburg-Landau solver on regular meshes with GPUs

- Introduction
- Meshing & Implementation
- Examples & Application

see Poster 31.1

Part II: Adaptive mesh solver & Optimization

- Periodic boundary conditions
- Adaptive refinement
- Sensitivity

see Poster 31.2

Basic equations

Time dependent GL equations:

$$\frac{\partial \Psi}{\partial t} = -\frac{\delta \mathcal{F}_{\mathrm{GL}}}{\delta \Psi^*}, \quad \frac{\delta \mathcal{F}_{\mathrm{GL}}}{\delta \mathbf{A}} = 0$$

$$u(\partial_t + i\mu)\psi = \epsilon(\mathbf{r})\psi - |\psi|^2\psi + (\nabla - i\mathbf{A})^2\,\psi + \zeta(\mathbf{r},t)$$
$$\kappa^2 \nabla \times (\nabla \times \mathbf{A}) = \mathbf{J}_n + \mathbf{J}_s + \mathcal{I},$$

$$\mathbf{B} = \nabla \times \mathbf{A}, \quad \mathbf{E} = -\frac{1}{c}\partial_t \mathbf{A} - \nabla\mu$$

Coupled system for ψ and $\mathbf{A}$:

ψ	complex order parameter characterizing density of Cooper pairs
$\mathbf{A}$	vector potential for magnetic field
ζ and $\mathcal{I}$	thermal fluctuations
$\epsilon(\mathbf{r}) = \frac{T_c(\mathbf{r})-T}{T} \to 0$	for $T \to T_c$ (critical temperature)

External current and pinning

Total current: **J=J$_s$+J$_n$**

$$\mathbf{J} = \mathrm{Im}\left[\psi^*(\nabla - i\mathbf{A})\psi\right] - (\nabla\mu + \partial_t\mathbf{A})$$

critical current J$_c$:

- usually defined when voltage V is small percentage ± (here 1%) of free flow value V$_{ff}$
- ***J$_c$ calculated e.g. by a bisection method***

- separate dc electric field

$$\begin{aligned}\mu(\mathbf{r}) &= -E_x x + \tilde{\mu}(\mathbf{r}) \\ \psi(\mathbf{r}) &= \tilde{\psi}(\mathbf{r})\exp(iKx)\end{aligned}$$

- fix the current (ordinary differential equation for K)

$$J_{\mathrm{ext}} = \mathrm{Im}\left[\left\langle\tilde{\psi}^*(\nabla_x - iA_x)\tilde{\psi}\right\rangle\right] + K\left\langle|\tilde{\psi}|^2\right\rangle + \partial_t K$$

this gives the voltage-current characteristics E$_x$(J$_{ext}$) through ∂_tK=E$_x$ which we use to obtain the critical current J$_c$

- solve the Poisson equation for [1] (follows from current conservation)

$$\boxed{\Delta\tilde{\mu} = \nabla\cdot\mathrm{Im}\left[\tilde{\psi}^*(\nabla - i\mathbf{A})\tilde{\psi}\right] + K\nabla_x|\tilde{\psi}|^2}$$

→ solved by super-relaxation with Jacobi iterations

$$\partial_\tau\tilde{\mu} = -\Delta\tilde{\mu} + \nabla\cdot\mathrm{Im}\left[\tilde{\psi}^*(\nabla - i\mathbf{A})\tilde{\psi}\right] + K\nabla_x|\tilde{\psi}|^2$$

Discretization

Here we consider the large-λ (or κ) limit:

- in this case our equation system reduces to the GL equation only, and we can keep the magnetic vector potential constant.
- we choose the gauge for the vector potential as $\mathbf{A} = -B_z y \mathbf{e}_x^{(0)}$ i.e. we have constant magnetic field in z-direction
- the current simplifies to $\mathbf{J} = \mathrm{Im}\left[\psi^* (\nabla - \imath\mathbf{A})\psi\right] - \nabla\mu$

- time discretization

$$\psi_m - \psi_m^- = dt\left[\epsilon_m \psi_m^{\bowtie} - \frac{\beta}{2}|\psi_m|^2\psi_m - \frac{\beta}{2}|\psi_m^-|^2\psi_m^- + \gamma\left(\nabla - \imath\mathbf{A}\right)^2\psi_m^{\bowtie} + \zeta_m(t)\right]$$

implicit Crank-Nicolson, with

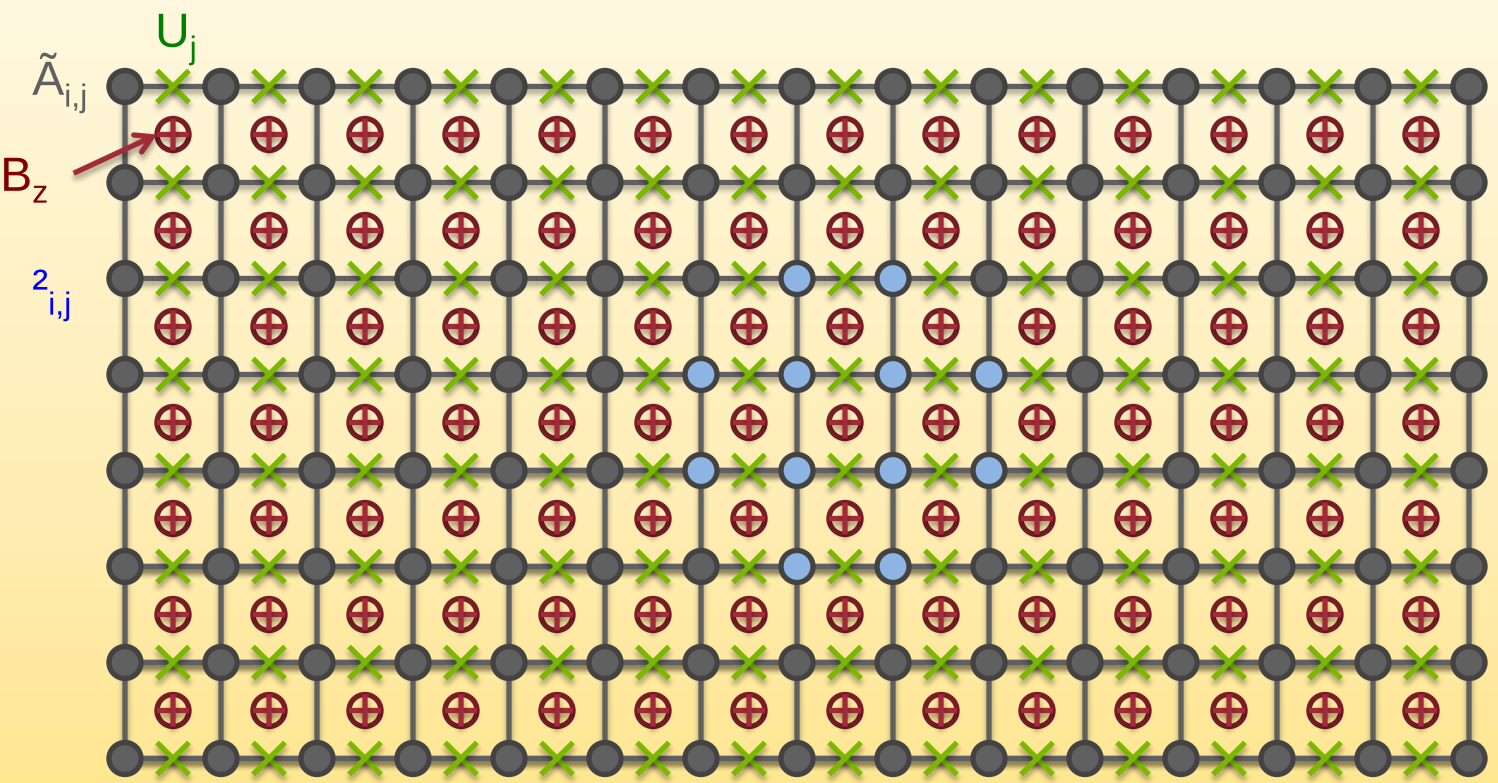
$$\begin{aligned}\psi_m &= \psi_{x,y,z}(t)\\ \psi_m^- &= \psi_{x,y,z}(t-dt)\\ \psi_m^{\bowtie} &= \left(\psi_m + \psi_m^-\right)/2\end{aligned}$$

- Laplacian

$$\left(\nabla - \imath\mathbf{A}\right)^2\psi_m = \frac{U_j\psi_{i+1,j,k} + U_j^*\psi_{i-1,j,k} - 2\psi_m}{dx^2} + \frac{\psi_{i,j+1,k} + \psi_{i,j-1,k} - 2\psi_m}{dy^2} + \frac{\psi_{i,j,k+1} + \psi_{i,j,k-1} - 2\psi_m}{dz^2}$$

with $\mathbf{A} = -B_z y \mathbf{e}_x^{(0)}$, $U_j = e^{\imath j\, dx\, dy\, B_z}$ "link" variables

Simulation grid and pinning



Inclusions and defects are modeled by T_c **modulation → corresponding to normal metallic pinning centers: spatial variation of ²(r), i.e., the linear coefficient of the order parameter in the TDGL** [positive in the superconductor, negative in the defect]

- **arbitrary geometry, but**
- **on a regular grid (see posters)**

Boundary conditions

- at surfaces, we use the no-current condition: $$\partial_{x,y,z}\psi = 0 \text{ and } \partial_{x,y,z}\tilde{\mu} = 0$$
- not applicable in x-direction if external current is applied

→ this defines the Laplacian at the surface layers

- for $\lambda \to \infty$ and finite vector potential (as before) [no current], we can use periodic conditions in x- & z-directions and quasi-periodic in y-direction ($y=0,\ldots,L_y$):

$$\psi_{x,L_y,z} = \psi_{x,0,z} e^{\imath 2\pi B_z x L_y / L_x}$$

(challenge on unstructured/refined meshes)

- for finite λ (finite κ) we also have boundary conditions for the vector potential.

Iterative solver on GPUs

- due to the laplacian, an explicit time integration requires very small dt, i.e., it takes a long time to reach a steady state (easy to parallelize)
- due to the boundary conditions, we cannot use a FFT-based spectral solver for *arbitrary* magnetic field (for certain discrete values it is possible)

➔ **use iterative solver for the implicit time integration**

- the GL equation can be written in the simple form $\boxed{\mathcal{M}\Psi = \mathbf{b}}$

$$\begin{aligned} \Psi &= (\psi_0, \ldots, \psi_{N-1})^T \\ \mathbf{b} &= (b_0, \ldots, b_{N-1})^T \end{aligned}$$

- in order to invert the matrix M on a parallel machine, we use the Jacobi iteration

we write $\mathcal{M} = \mathcal{D} + \mathcal{R}$ where D=diag(M)

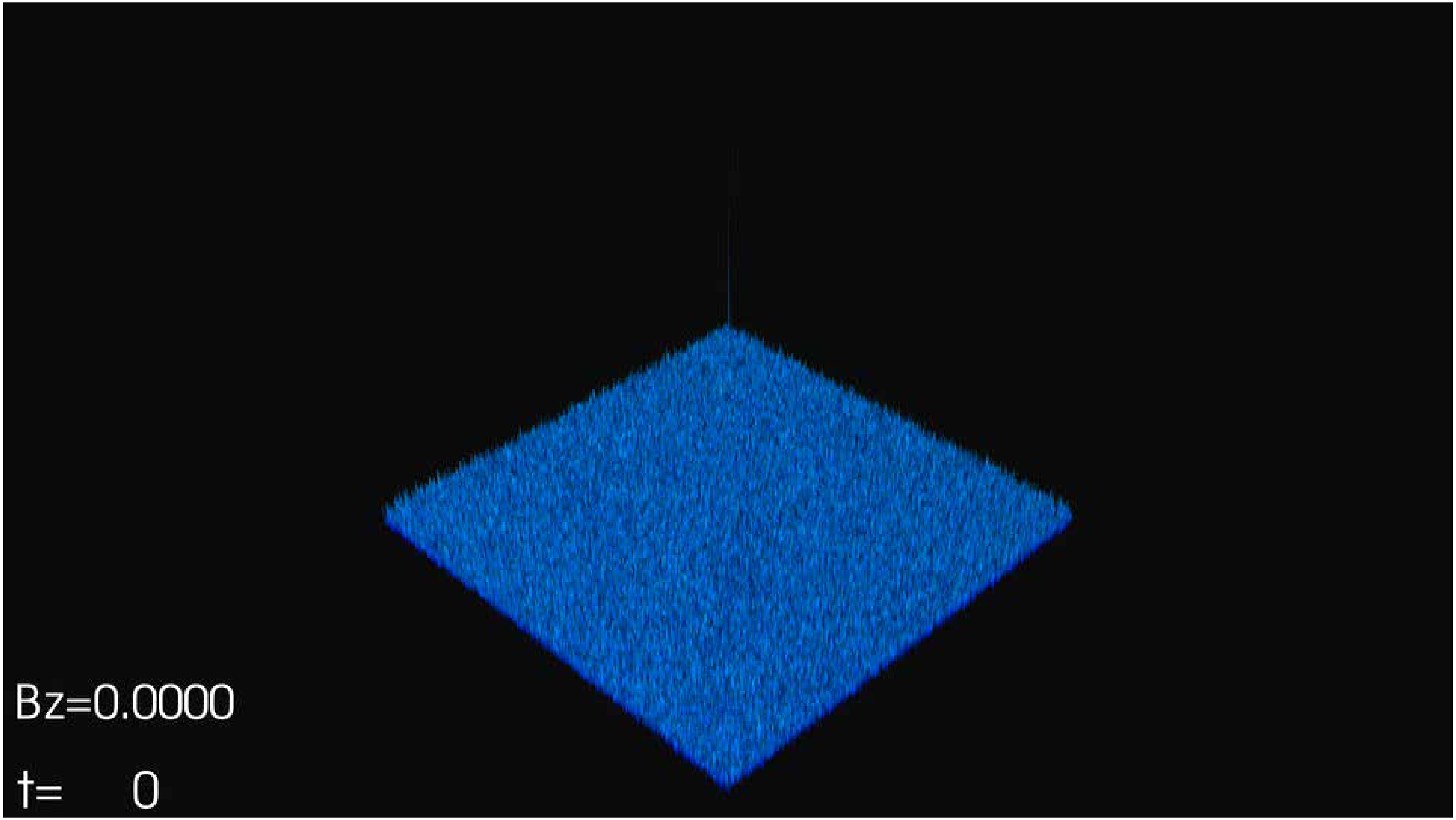
then iterate $\boxed{\Psi^{(k+1)} = \mathcal{D}^{-1}\left(\mathbf{b} - \mathcal{R}\Psi^{(k)}\right)}$

convergence criterion $\|\mathbf{r}_k\|_{\max} \ll 1$

residual $\mathbf{r}_k \equiv \mathbf{b} - \mathcal{M}\Psi^{(k)}$

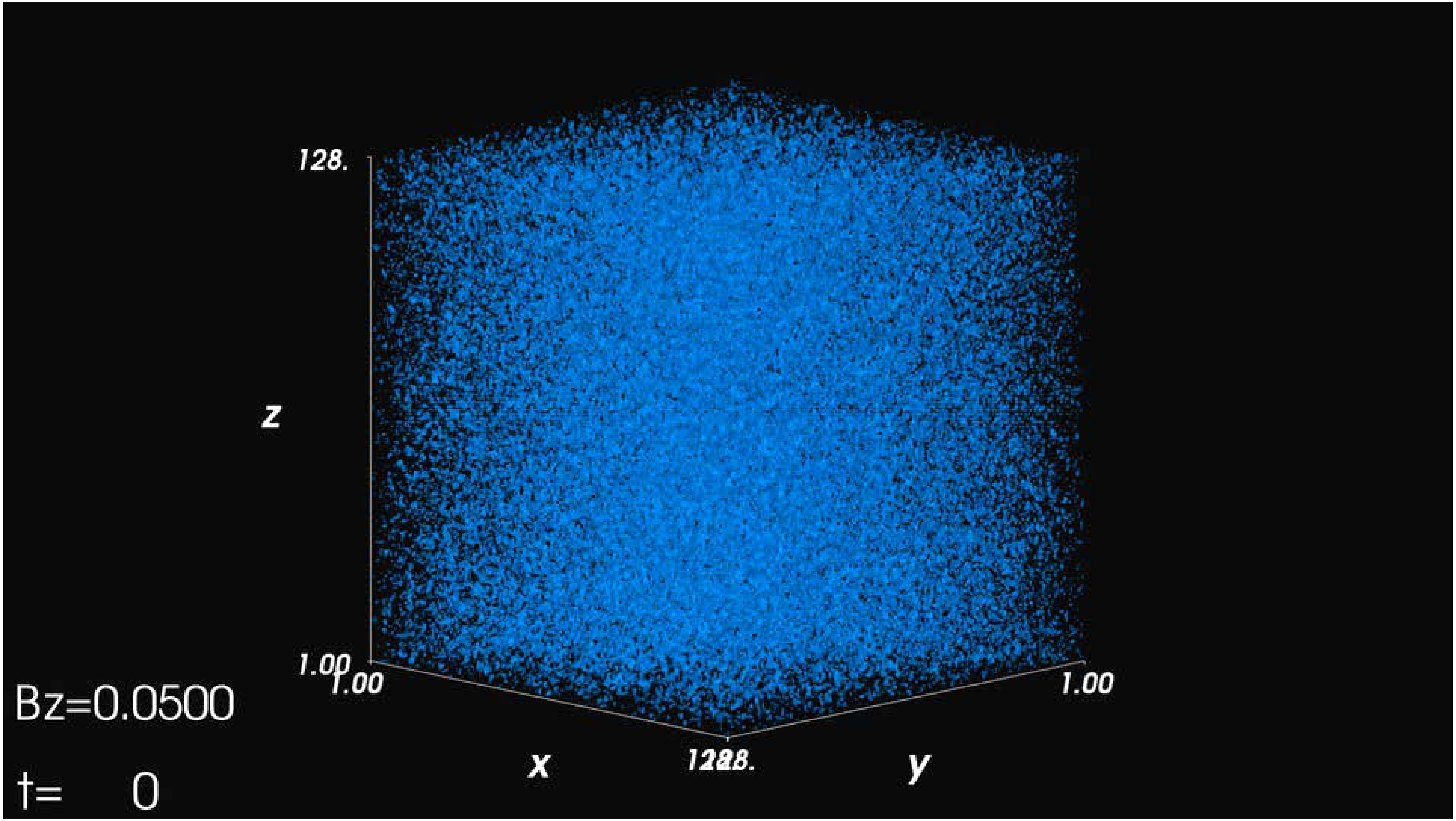
This scheme is implemented for GPUs and requires for a typical dt=0.1 and dx=dy=dz=0.5, **4-5 iterations** only to reach an accuracy of 10^{-6}

Example results for the structured grid solver



2D with surface, increasing field, 512^2 mesh points

...



3D with surface, relaxation in fixed field, 512^3 grid points

Pinning by nanoparticles in YBCO films

best practical way to enhance critical currents

Isolated particles (BZO, BSO,Y211 …)

MacManus-Driscoll *et al.*, APL 2004

Song *et al.,* APL 2006

Gutiérrez *et al.*, Nat. Mat. 2007, APL 2007

Kim *et al.*, APL 2007

Yamasaki *et al.*, SuST 2008

Polat *et al.*, PR B 2011

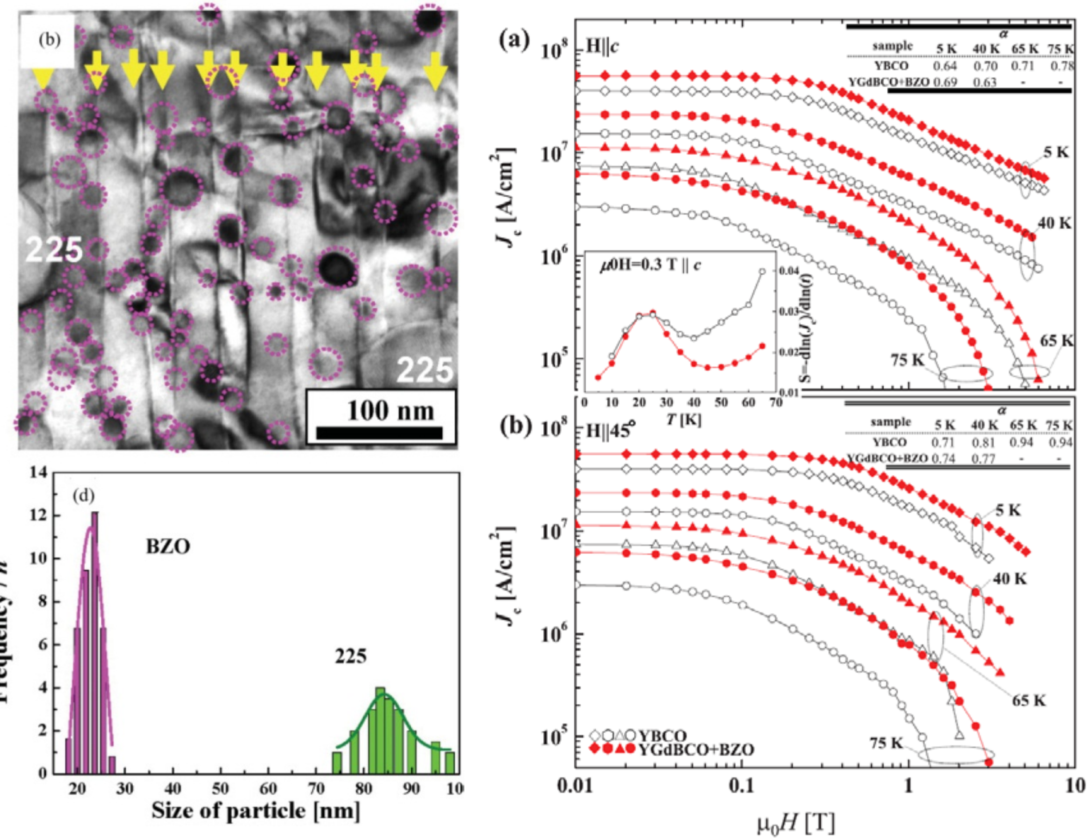
Miura *et al.*, PR B 2011, SUST 2013

Columns; Columns + Particles

Kang *et al.,* Science 2006

Varanasi *et al.,* SuST 2007, JAP 2007, APL 2008

Maiorov *et al.,* Nat. Mat. 2009

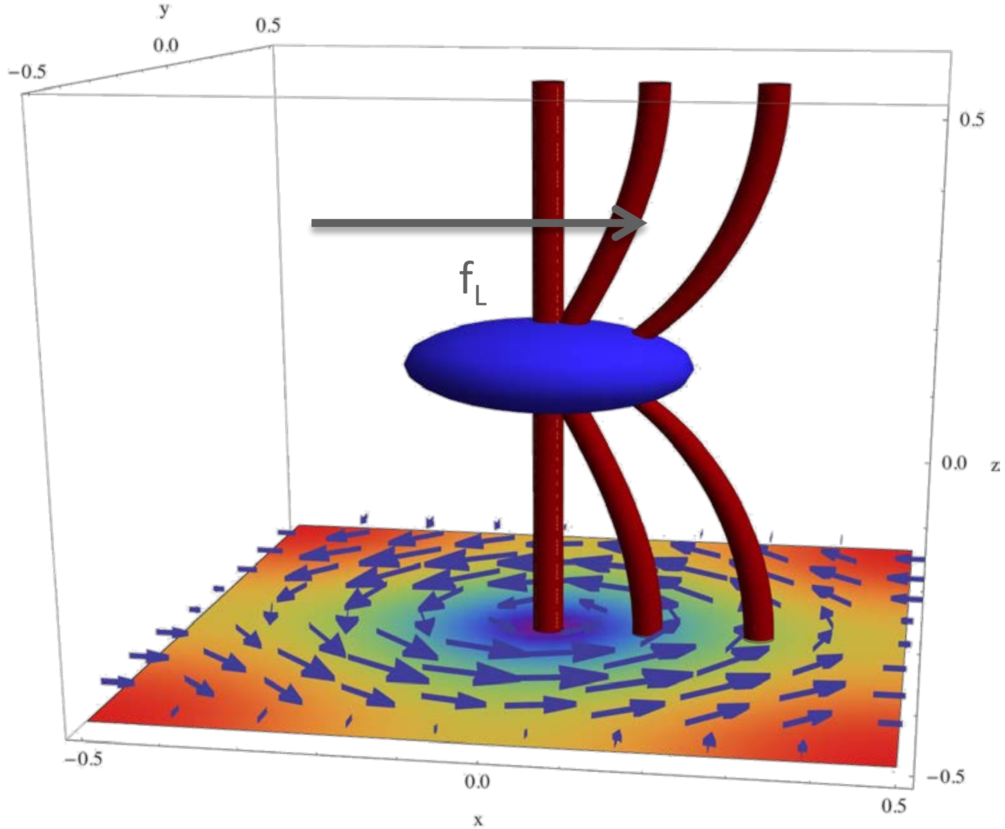


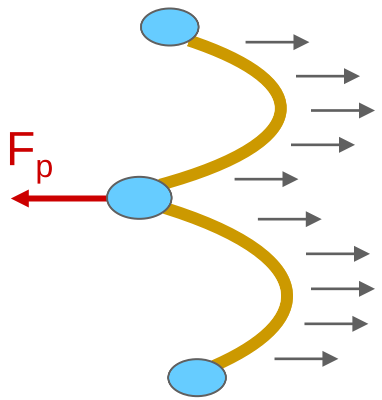
Miura *et al.*, Phys. Rev., B **83**, 184519 (2011)

Find the critical current without applied current

Find the pin-braking force to detach a vortex from a single nanoscale ellipsoidal inclusion

- key parameter in strong-pinning theory
- expect non-trivial dependence on defect size

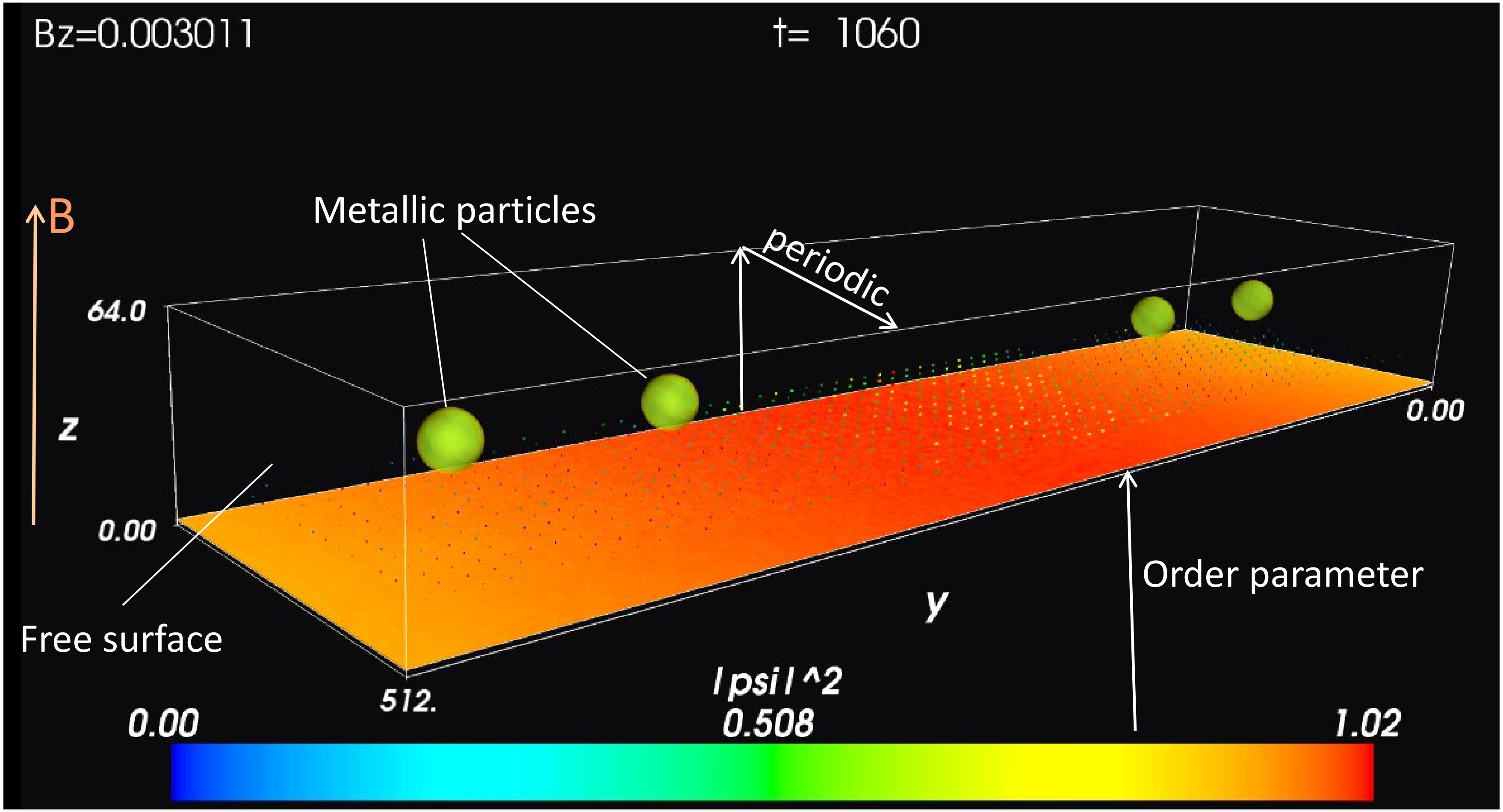




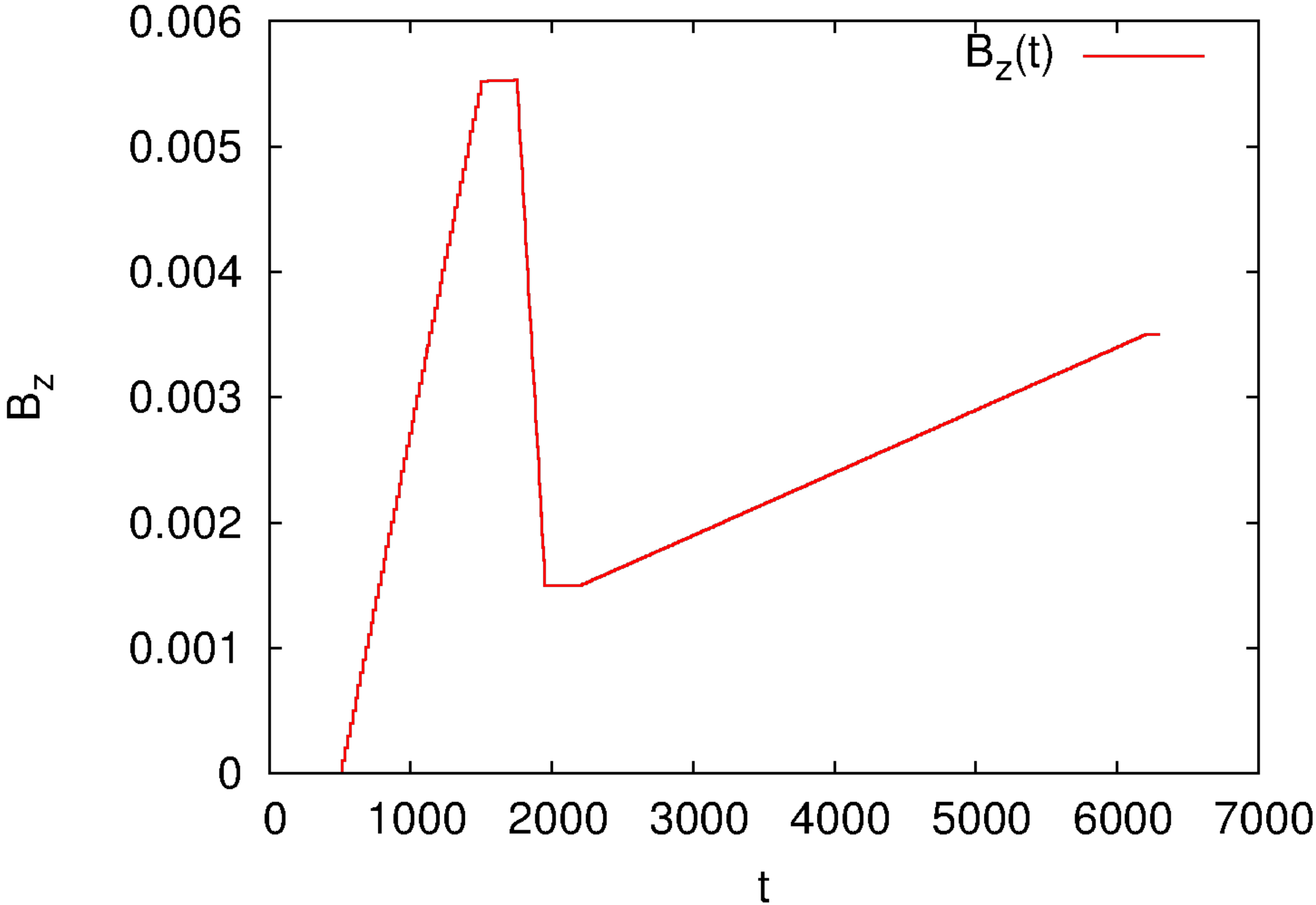
→ prepare the initial state for a single free vortex, relax to a steady state with inclusion, then slowly increase the current.

Simulation of pin-trapping and pin-breaking

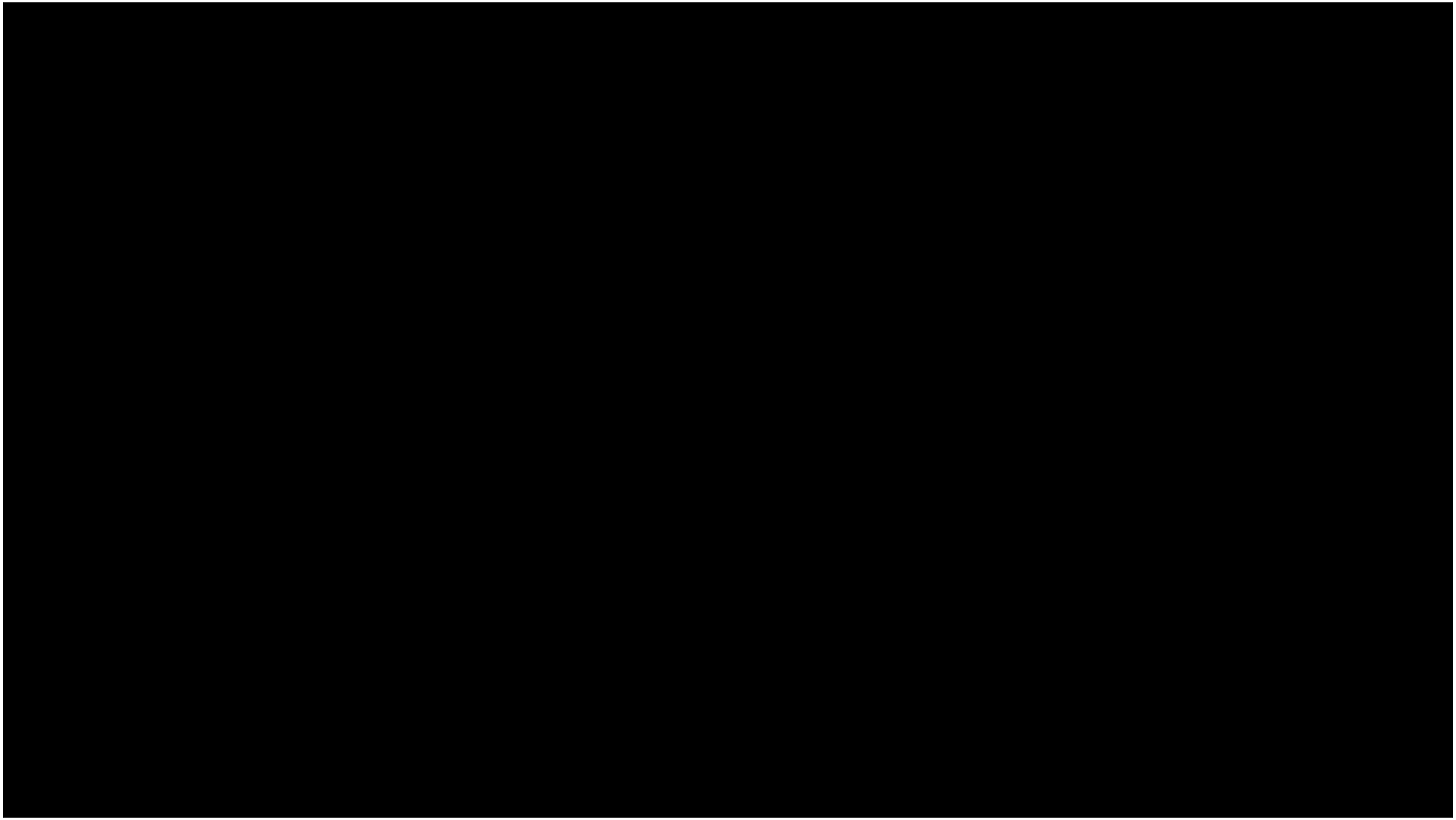
size 50ξx200ξx25ξ, particle diameter 8ξ



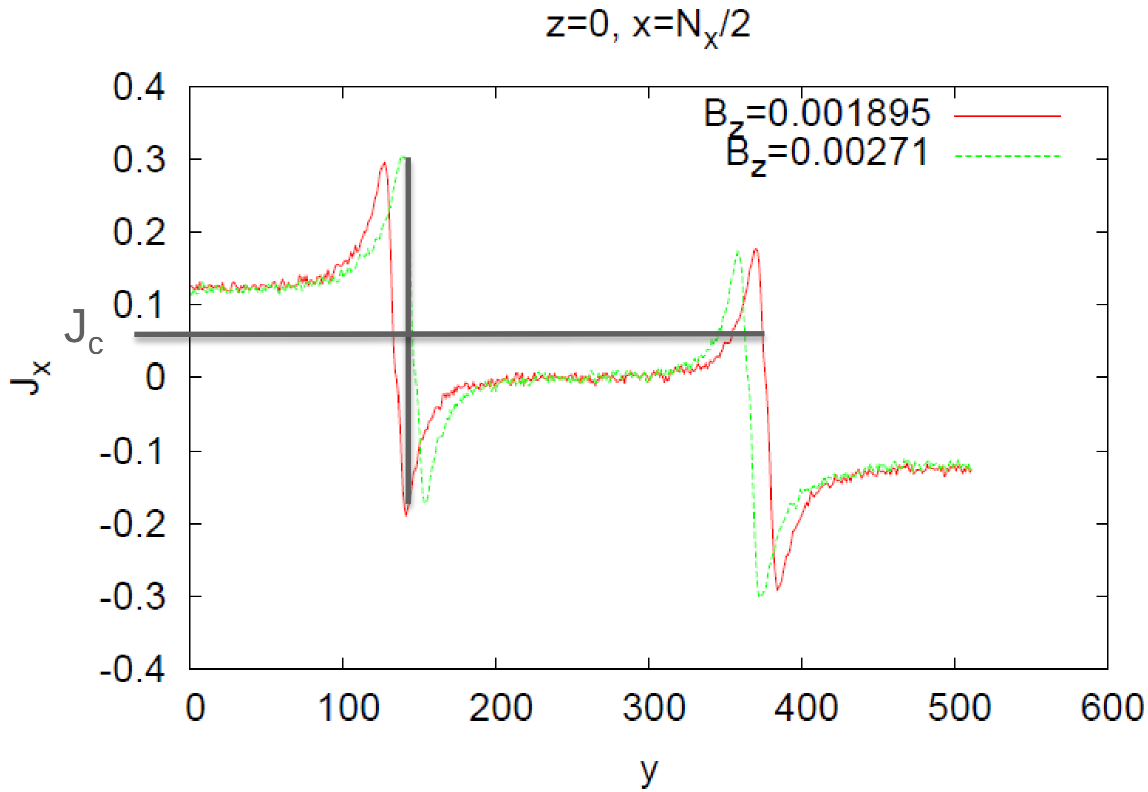
Magnetic field protocol

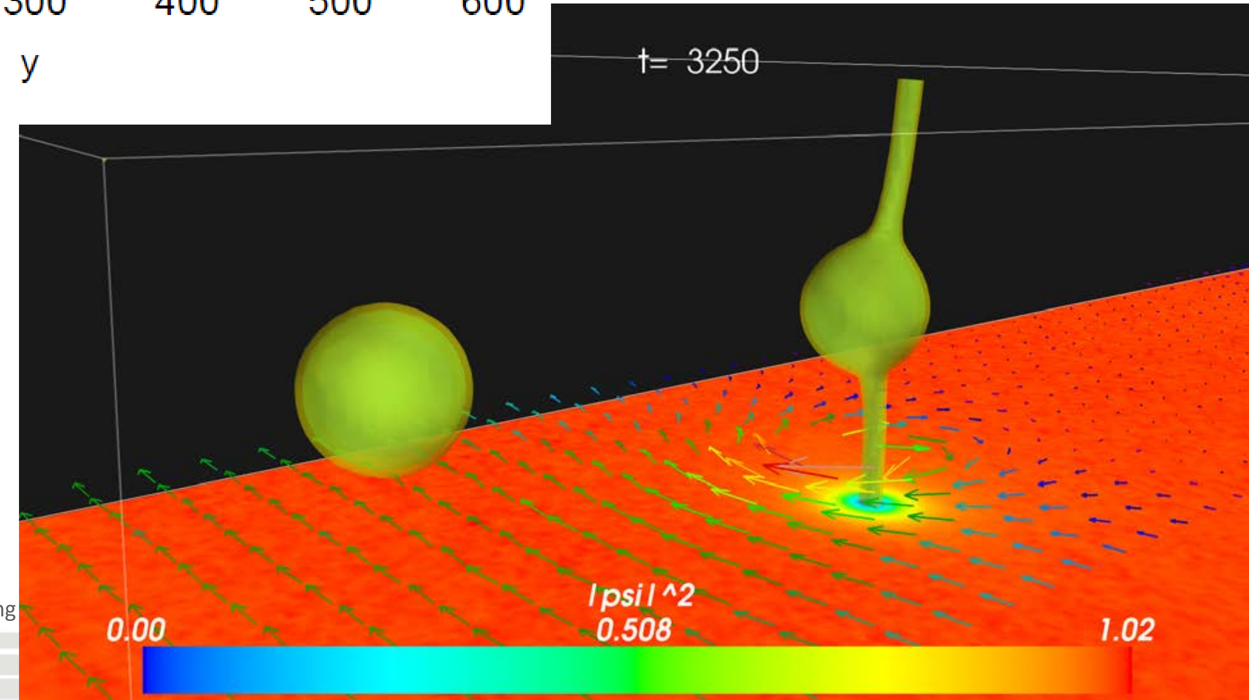


Dynamics



Current Profile





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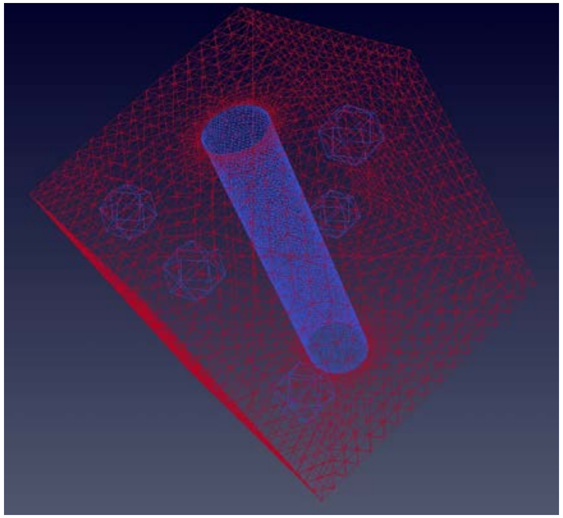
Computational Challenge: Complexity

Typical simulation complexity

- Simulations of $O(10^6)$ timesteps for reliable V values
- Sample volumes $O(10^6)$»^{3} + with cell mesh size $O(10^{-1})$»
  → *$O(10^9)$ degrees of freedom (DoF) per realization of pinning configuration μ.*



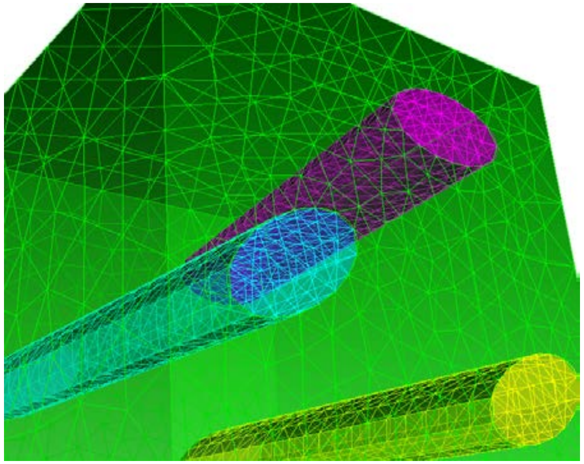
Computational demand for 10^3 flops per DoF per timestep

- 10 - 100h on full 100TFlop/s machine *at peak* for single μ
- Optimization increases demand by O(100)-O(1000) x

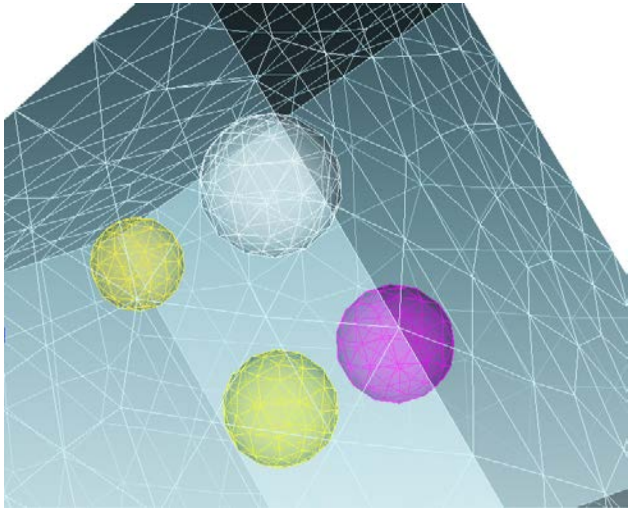
→ **Computational requirements**

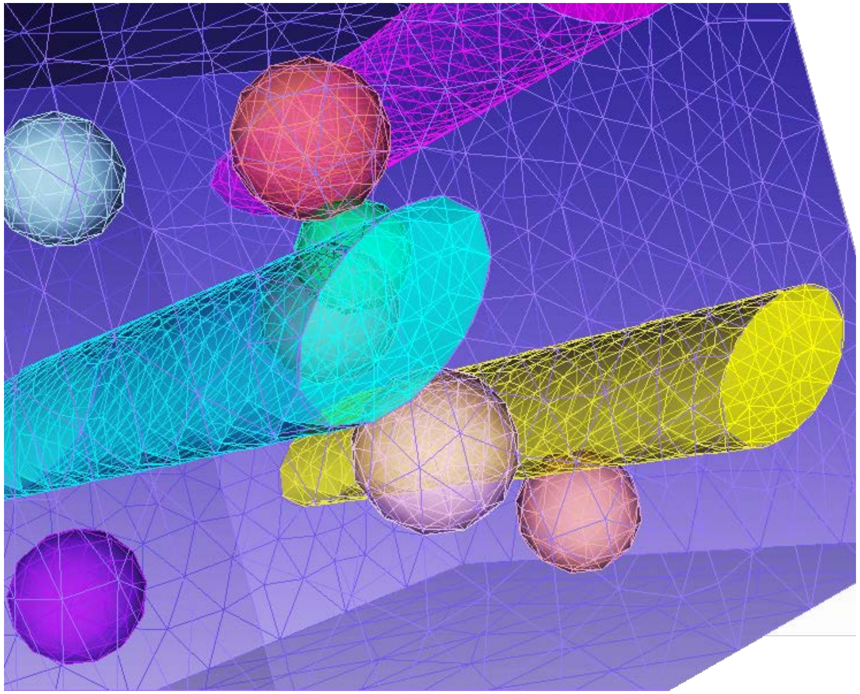
- Leadership-class hardware for computational optimization of pinning structures
- State-of-the-art sampling techniques to minimize the number of probed μ
- Automated meshing of materials with embedded pinning structures
- Fully implicit time-integration to circumvent the timestep size limitation
- Modern iterative methods to solve O(1B) system at each timestep in optimal time.

Computational Challenge: Meshing

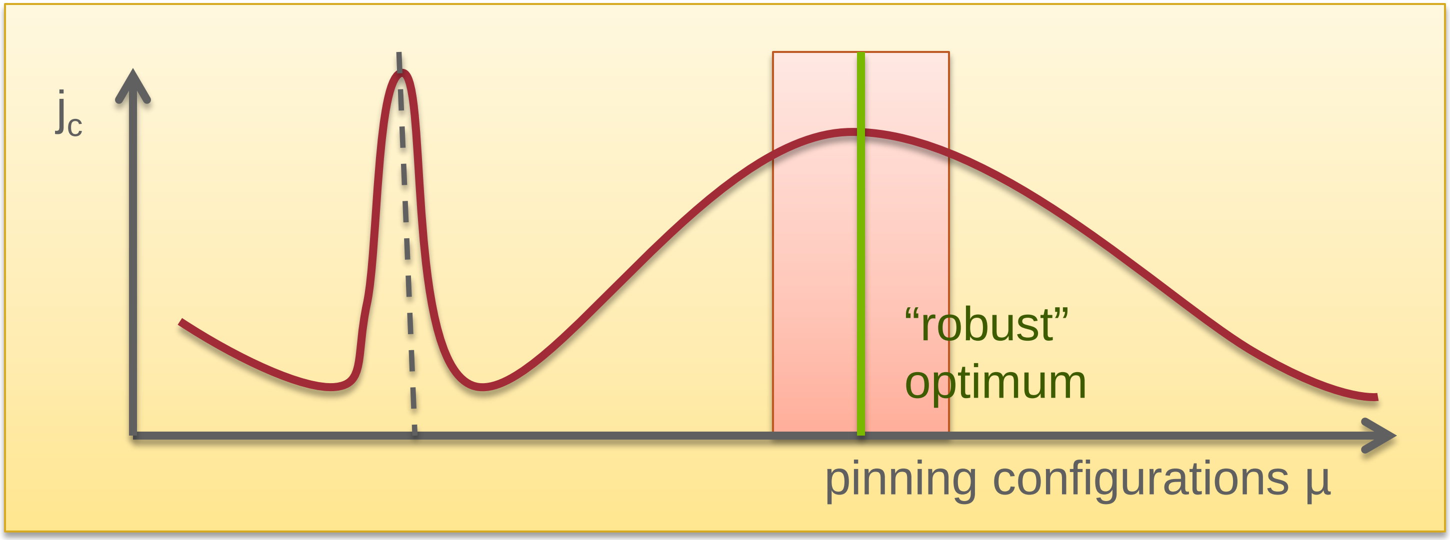


- mesh size needs to be smaller than the coherence length to capture order parameter variations
- near inclusions and defects mesh needs to be finer
  → *Adaptive meshing*
- increased precision by adaptive mesh refinement near vortices





Optimization of pinning for maximal current

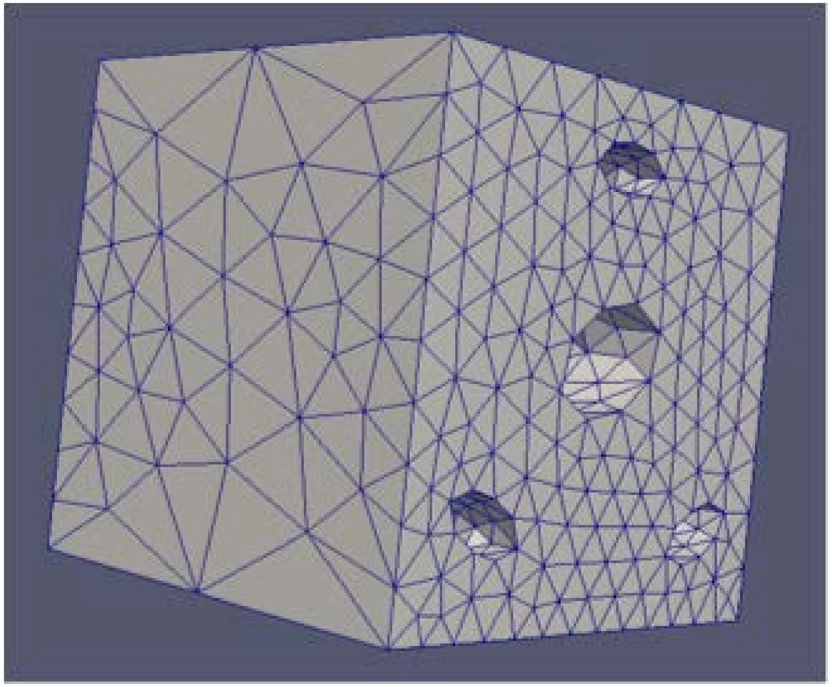


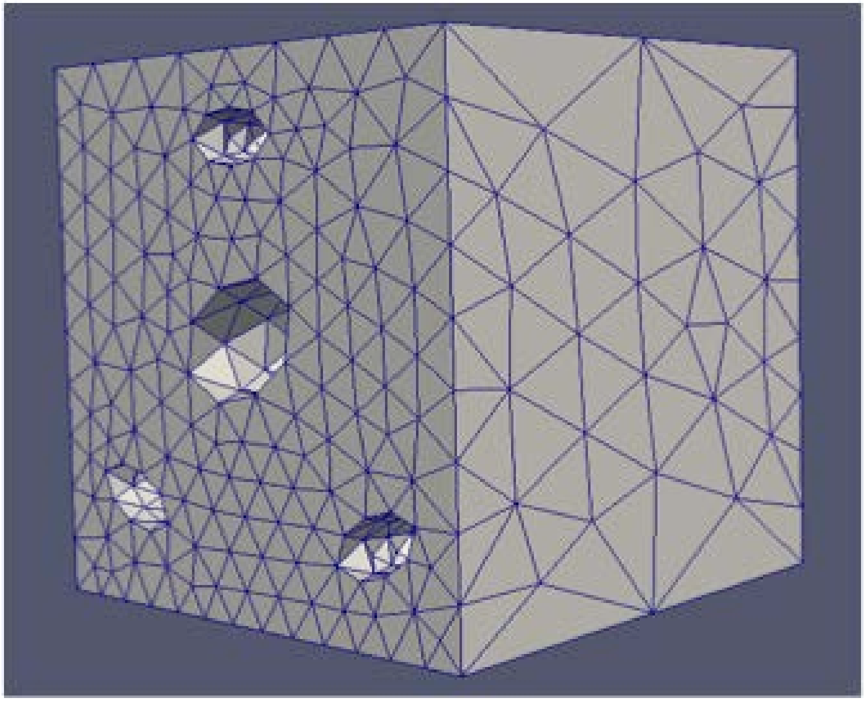
Determining optimal pinning landscape:

- ***Optimize critical current***
- ***Minimize deviations from best case***
- ***Min-max or min rms***

$$
\begin{aligned}
\max_{\theta} \quad & J_c(\theta) \\
\text{such that} \quad & J_c(\theta) = \max_{J} \left\{ J : V_\theta(J) \leq \delta V_{\text{ff}}(J) \right\}, \\
& \theta \in \Theta,
\end{aligned}
$$

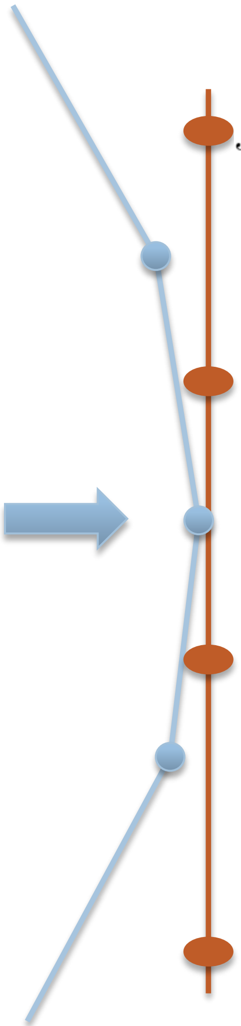
Quasiperiodic BCs on unstructured meshes



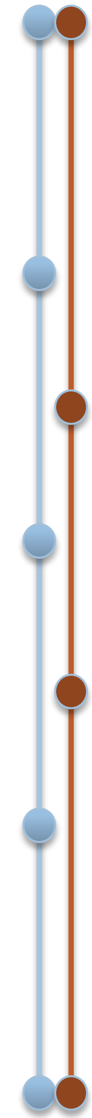


- Implicit coupling not captured by the mesh topology
  - Point location
  - Constraints
  - Solver
  - Preallocation

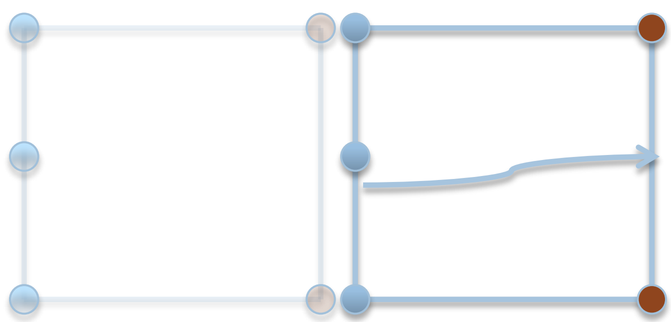
Master-Slave contact
Mortar Elements



$$J = \begin{pmatrix} K_{LL} & K_{LS} & 0 & 0 \\ K_{SL} & K_{SS} & 0 & 0 \\ 0 & 0 & K_{MM} & K_{MR} \\ 0 & 0 & K_{RM} & K_{RR} \end{pmatrix} \quad \Rightarrow \quad \tilde{J} = \begin{pmatrix} K_{LL} & K_{LS} & 0 & 0 \\ 0 & I_S & -I_M & 0 \\ 0 & K_{SL} & K_{MM} & K_{MR} \\ 0 & 0 & K_{RM} & K_{RR} \end{pmatrix}$$



- Violates ellipticity:
  - No longer symmetric
  - Or positive definite
- Standard iterative methods underperform
  - Need appropriate preconditioners



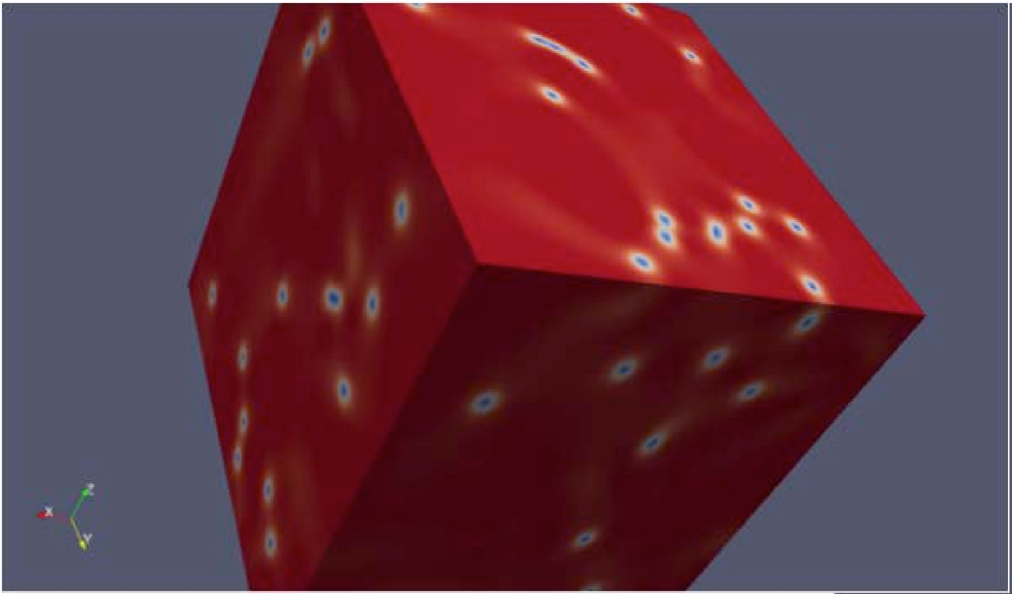
- For GL coupling S to M is an appropriate gauge transformation

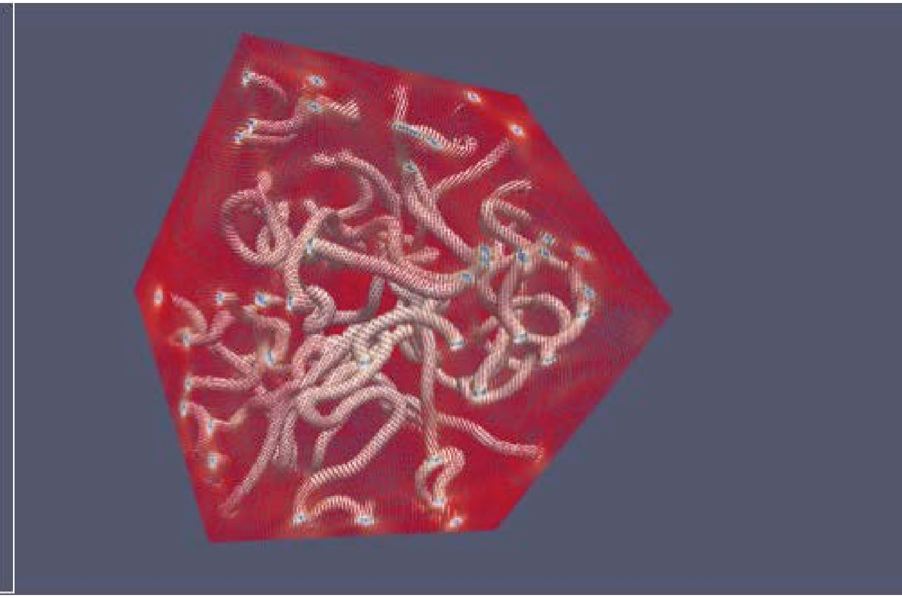
Physics-based Preconditioning (aka PCFieldSplit)

$$\tilde{J} = \begin{pmatrix} K_{LL} & K_{LS} & 0 & 0 \\ 0 & I_S & -I_M & 0 \\ 0 & K_{SL} & K_{MM} & K_{MR} \\ 0 & 0 & K_{RM} & K_{RR} \end{pmatrix} \quad \Rightarrow \quad \hat{J} = \begin{pmatrix} K_{LL} & K_{LS} & 0 \\ K_{SL} & K_{MM} & K_{MR} \\ 0 & K_{RM} & K_{RR} \end{pmatrix}$$

- Use splitting to isolate the constraints
- Constraint elimination results in an SPD Schur complement S
- Precondition S
    - Matrix-free using block P
    - Assemble S
    - Use multigrid or domain-decomposition
- PETSc provides flexible splitting/recombination preconditioner machinery
    - PCFieldSplit

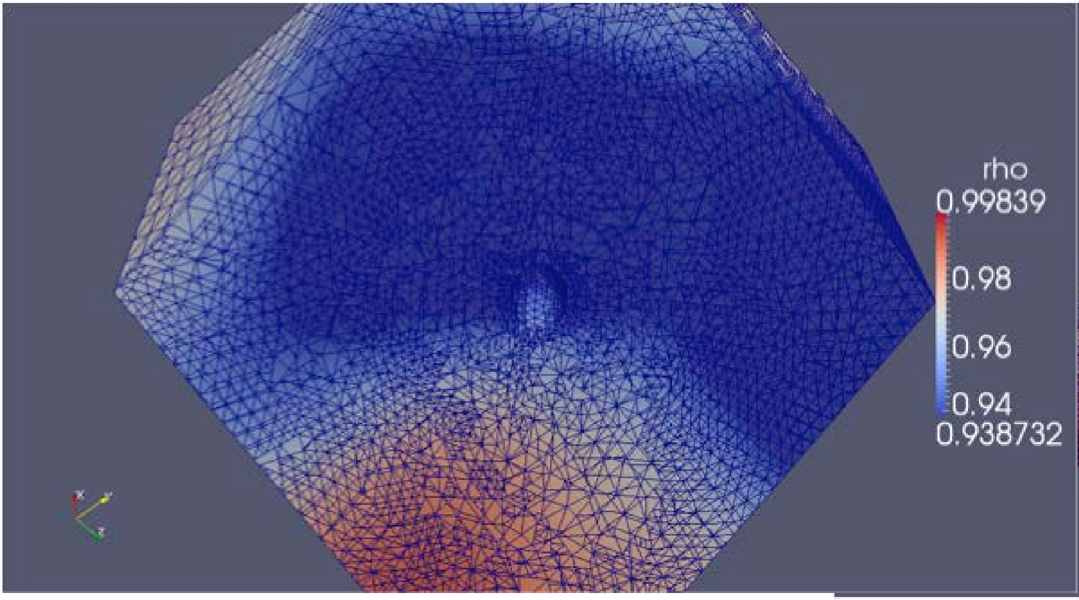
Scalable zero-current BC Simulation

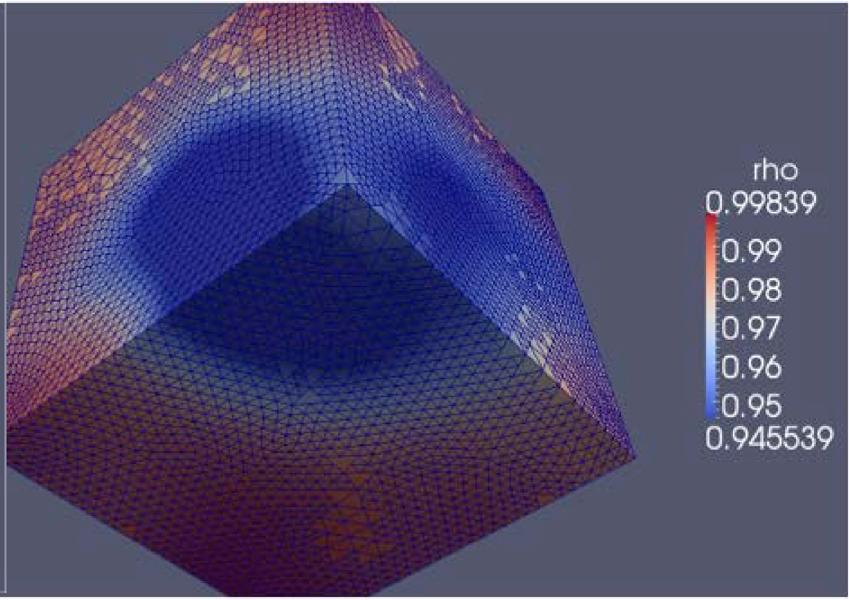




- Highly scalable
- Fully implicit
- Responds to a variety of preconditioners
- Refinement-independent convergence rates

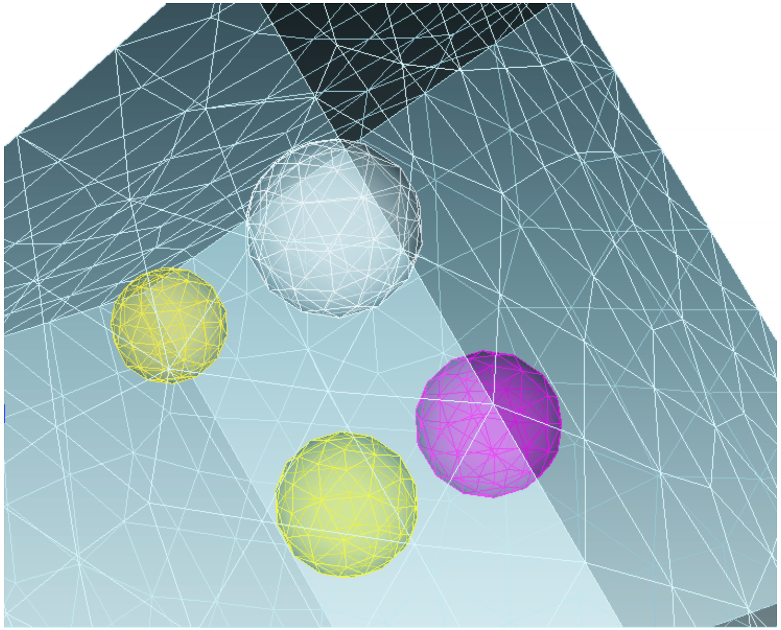
Adaptive Mesh Refinement





- **AMR: memory/cycles savings *once* solution features have stabilized**
- **Mapping to/from refined/derefined geometry carries substantial overhead**
- **Needs to be used sparingly and intelligently**
  - **Mesh coarse geometry**
  - **Refined uniformly**
  - **Relax solution on uniformly refined mesh**
  - **Derefinement to focus on the features of relaxed solution**

Shape Optimization



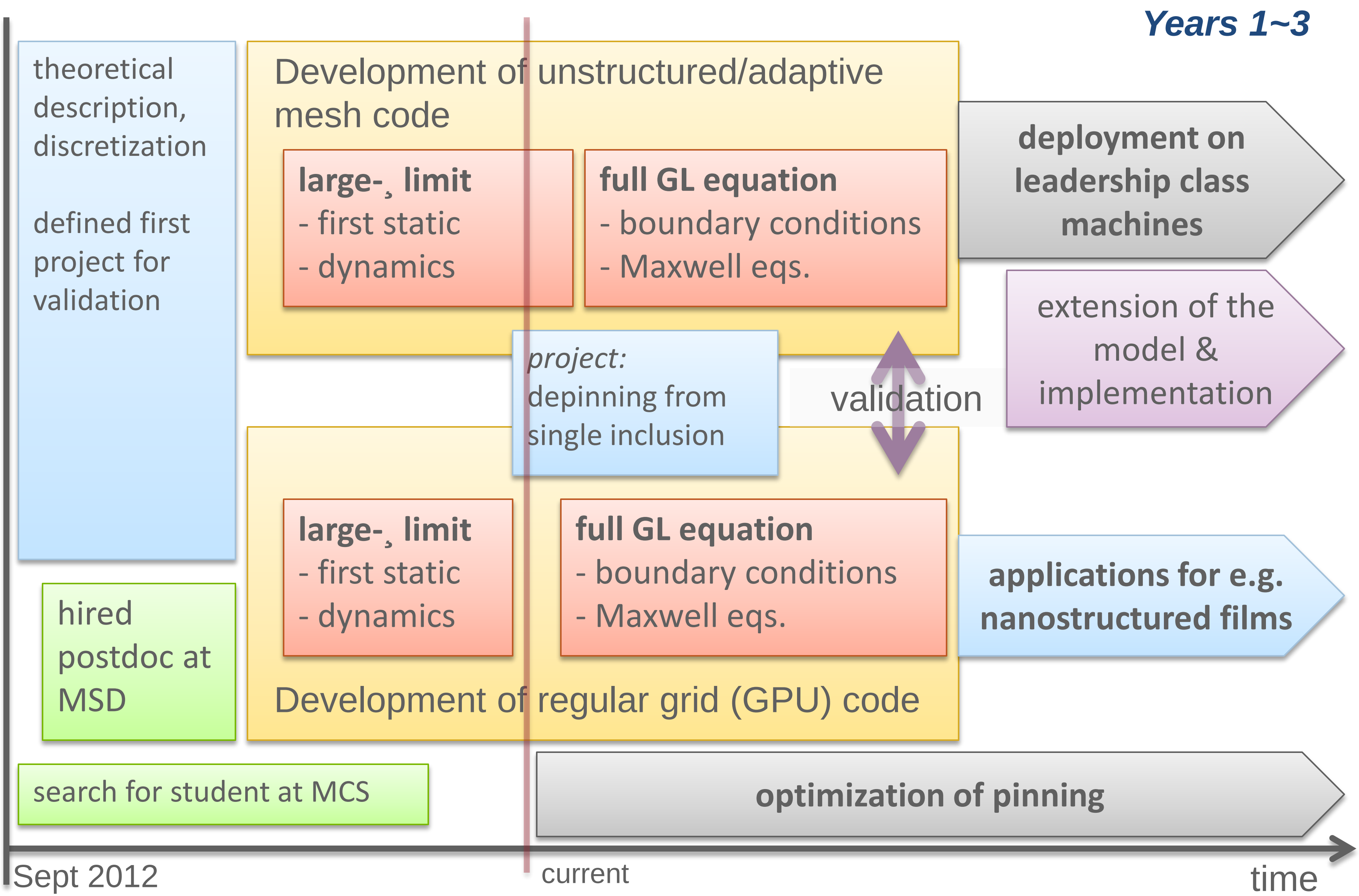
- Naïve sampling of all shape space – slow
- Shape derivatives exist, accelerate convergence
- Require computation of J_c sensitivity p
- Need "reverse mode"

- Preliminary investigation on a structured grid
- Geometry encoded by modulation of T_c
- Investigate simple case:
  - Single sphere of variable radius R

$$u(\partial_t + i\mu)p = \epsilon(\mathbf{r})p - 2|\psi|^2 p - \psi^2 p^* \left(\nabla - i\mathbf{A}\right)^2 p + \tfrac{\delta\epsilon}{\delta R}\psi, \;\; p(T) = 0$$

$$\frac{dJ_c}{dR} = \int_0^T \langle \tfrac{\delta\epsilon}{\delta R}, p \rangle dt$$

OSCon overview



Summary

- *New large-scale parallel TDGL integration method on GPUs*
- *Modeling of inclusion and other pinning centers by T_c-modulation or adaptive meshing with corresponding boundary conditions*

- ***Makes the study of mesoscopic systems including the collective behavior possible***

- ***Close interaction with SciDAC institutes: FASTMath & SUPER and started to work with SDAV on visualization***