Iterative unstructured-mesh Ginzburg-Landau solver on MPI clusters

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Model

• Time-dependent Ginzburg-Landau

TDGL equations:

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

In dimensionless units:

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

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

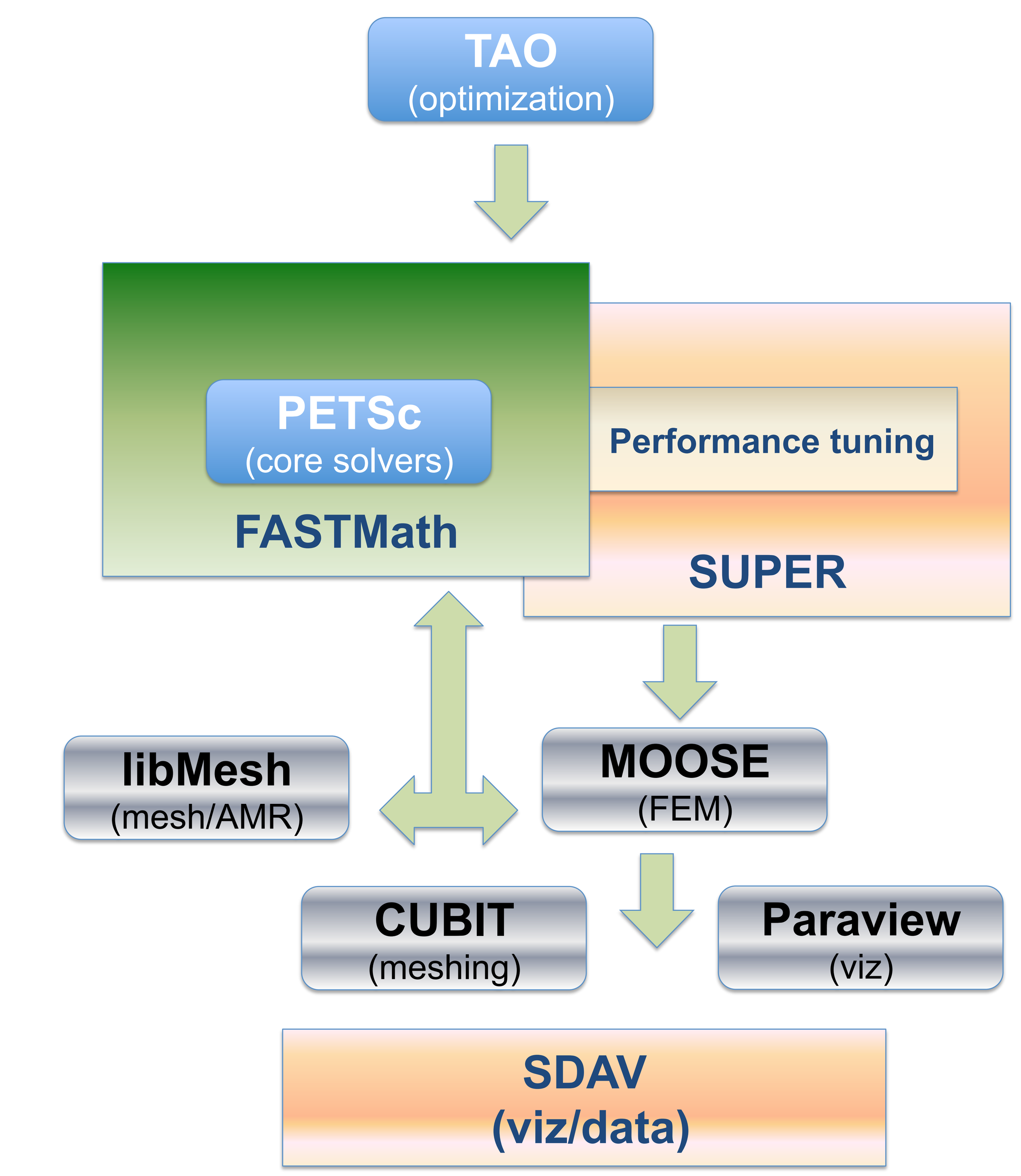
Coupled system for ψ and $\mathbf{A}$:

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)

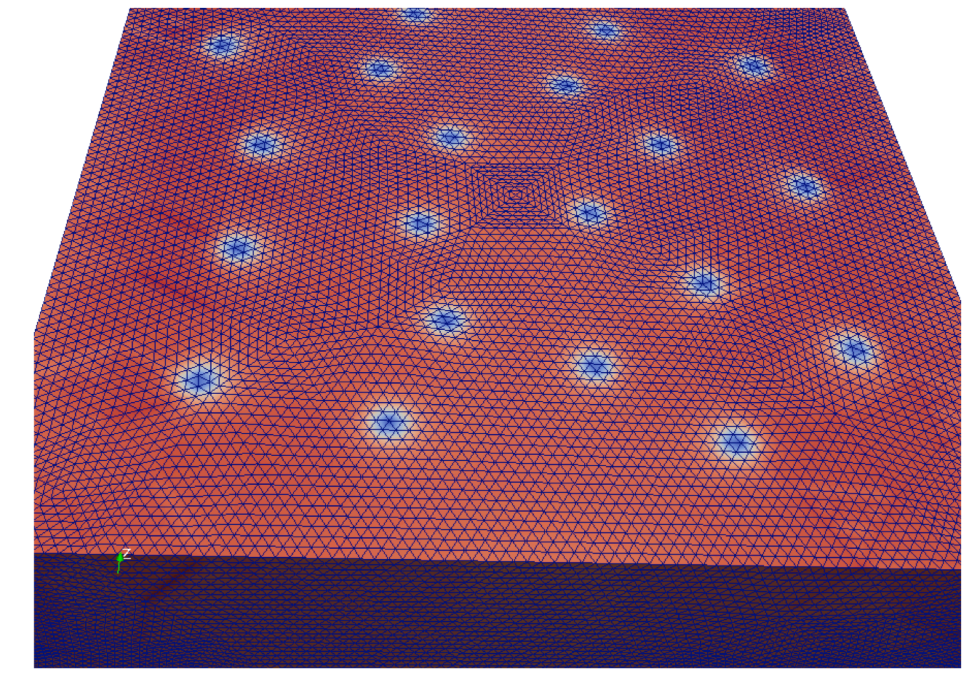
Total current: $\mathbf{J}=\mathbf{J}_s+\mathbf{J}_n$ $\quad \mathbf{J} = \mathrm{Im}\left[\psi^*(\nabla - i\mathbf{A})\psi\right] - (\nabla\mu + \partial_t \mathbf{A})$

Software/Algorithm stack

Leveraging power of SciDAC Institutes



Discretization/Meshing

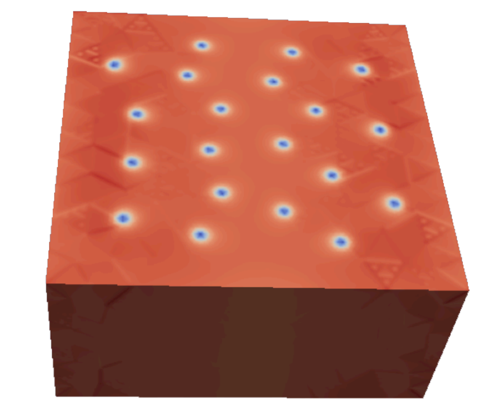


Mapping to refined geometry carries substantial overhead during relaxation from random state

Automatic refined: memory/cycles savings *once* solution features have stabilized

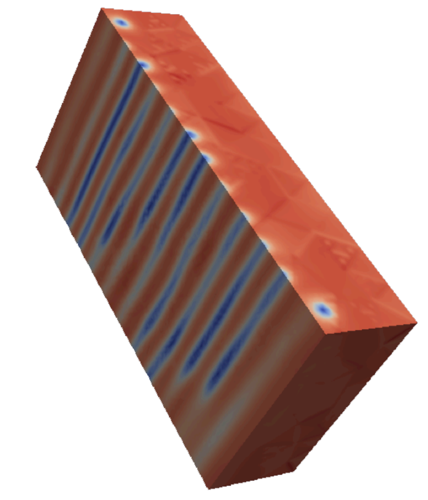
Needs to be used sparingly and intelligently
- ✓ Mesh coarse geometry
- ✓ Refined uniformly
- ✓ Relax solution on uniformly refined mesh
- ✓ Derefinement on relaxed solution

Validation/Visualization



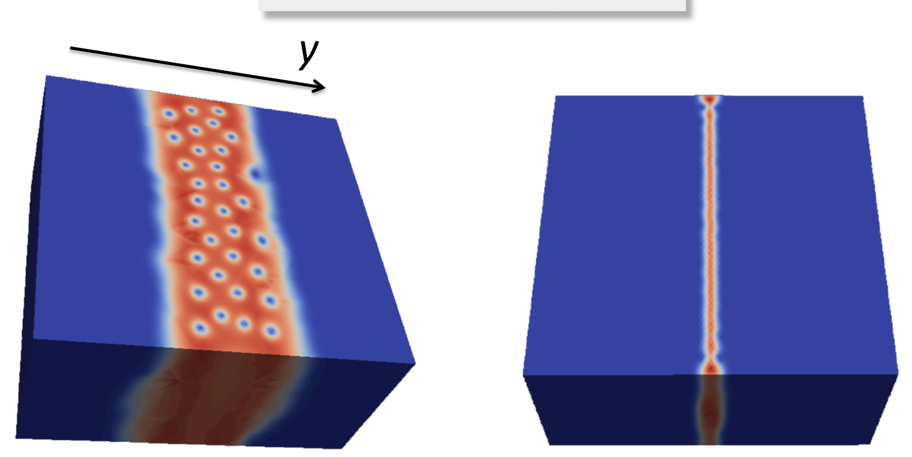
Uniform system relaxes to Abrikosov lattice

Straightforward visualization requires a lot of data: 30 sec movie requires 200 GB of "raster" data



Vortex detection allows to save data in "vector" format

Challenges



The value of gradient term with strong magnetic field becomes enormously large

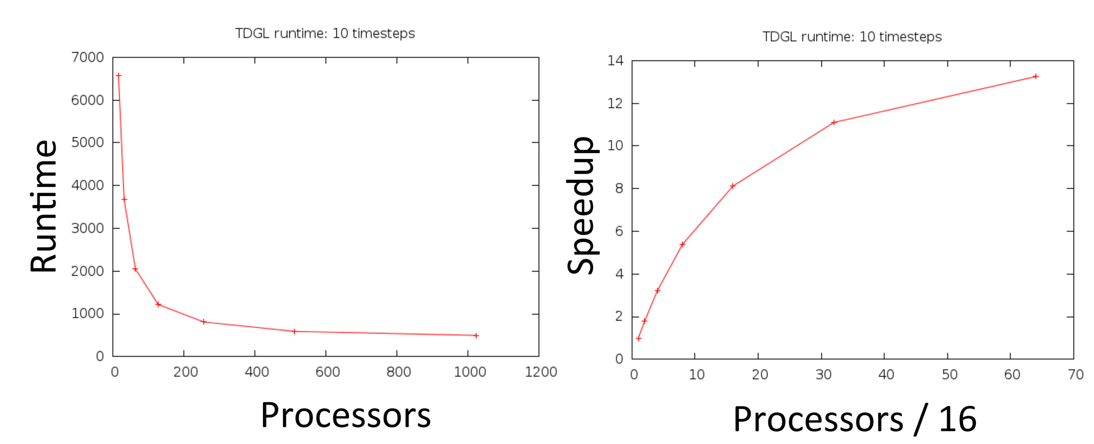
Vortex detection allows to save data in "vector" format

$$A_x = -yB_z: \quad (\nabla_x + iyB_z)^2 = \nabla_x^2 + 2iB_z y\nabla_x - \boxed{B_z^2 y^2}$$

Solution: $(\nabla_x - iA_x)^2 \to e^{-ixyB_z}\nabla_x^2 e^{ixyB_z}$

- Reformulate finite-element discretization using "link-variables"
- Works for time-invariant/spatially-uniform magnetic fields (implementation in progress)
- Suggests an approach to the time-varying case: "Maxwell's equation" for link variables

Parallel performance

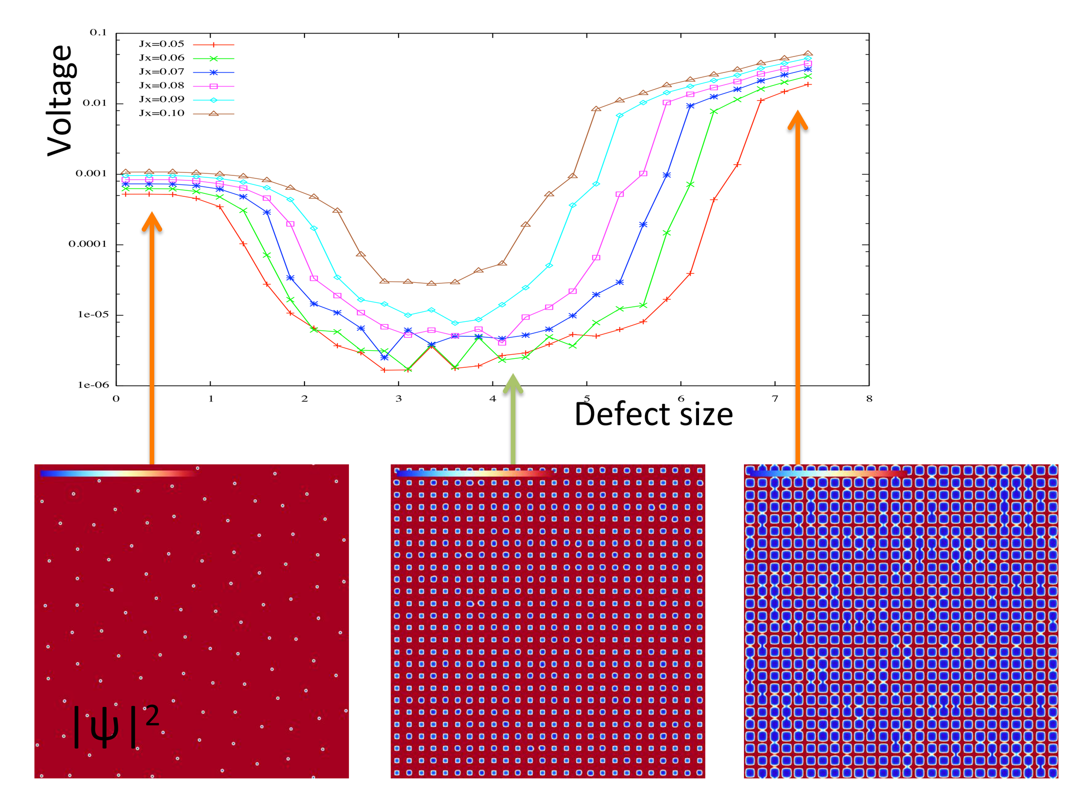


- Good strong scaling: Saturates at 512 cores

- Communication-limited
- Run overhead: amortized with longer runs

- Overcome the communication "wall"
- Better on-the-node performance
- Relatively simple geometry – higher order methods
- Spectral elements – dense linear algebra, more flops per packet and load/store
- Prompted conversation with FASTMath

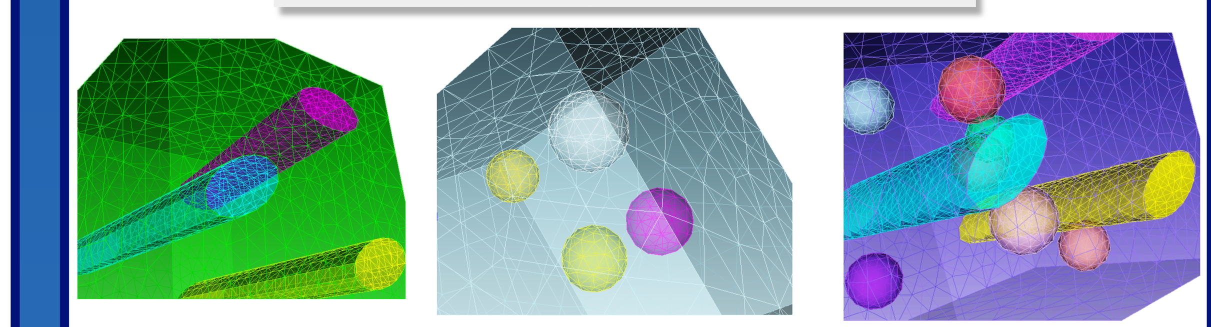
T_c modulation



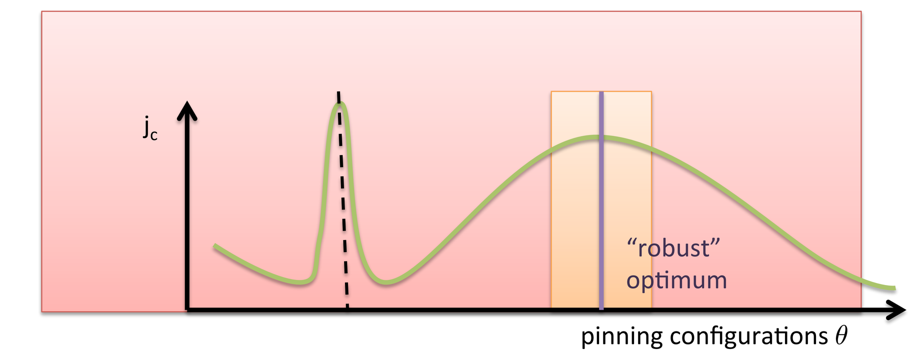
- Determine optimal inclusion configuration for maximizing critical current
- Use derivative-based/derivative-free optimization

- Engaged PhD student
- Initial input to optimization partners (FASTMath)

Shape optimization



Determining optimal robust pinning landscape:
- Optimize critical current
- Minimize deviations from best case
- Min-max or min rms



Requires solution of adjoint operator

- Langevin noise vs backward evolution?
- Temperature modulation model of inclusions?

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