Iterative unstructured-mesh Ginzburg-Landau solver on MPI clusters

Dmitry Karpeev[1], Igor Aronson[2], George Crabtree[2], Andreas Glatz[2], Alexei Koshelev[2], Todd Munson[1], Stefan Wild[1]
[1]Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439, USA
[2]Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, USA

GL model

Time-dependent Ginzburg-Landau

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

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

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

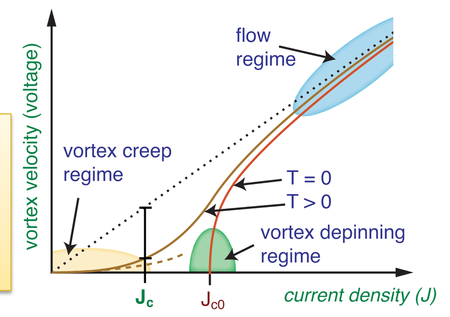
ψ	complex order parameter characterizing density of Cooper pairs
$\mathbf{A}$	vector potential for magnetic field
ζ and $\mathcal{I}$	fluctuations
Γ, a, b	phenomenological parameters from microscopic theory
$\epsilon(\mathbf{r}) = \frac{T_c(\mathbf{r}) - T}{T} \to 0$	for $T \to T_c$ (critical temperature)

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

Total current: $\mathbf{J} = \mathbf{J}_s + \mathbf{J}_n$

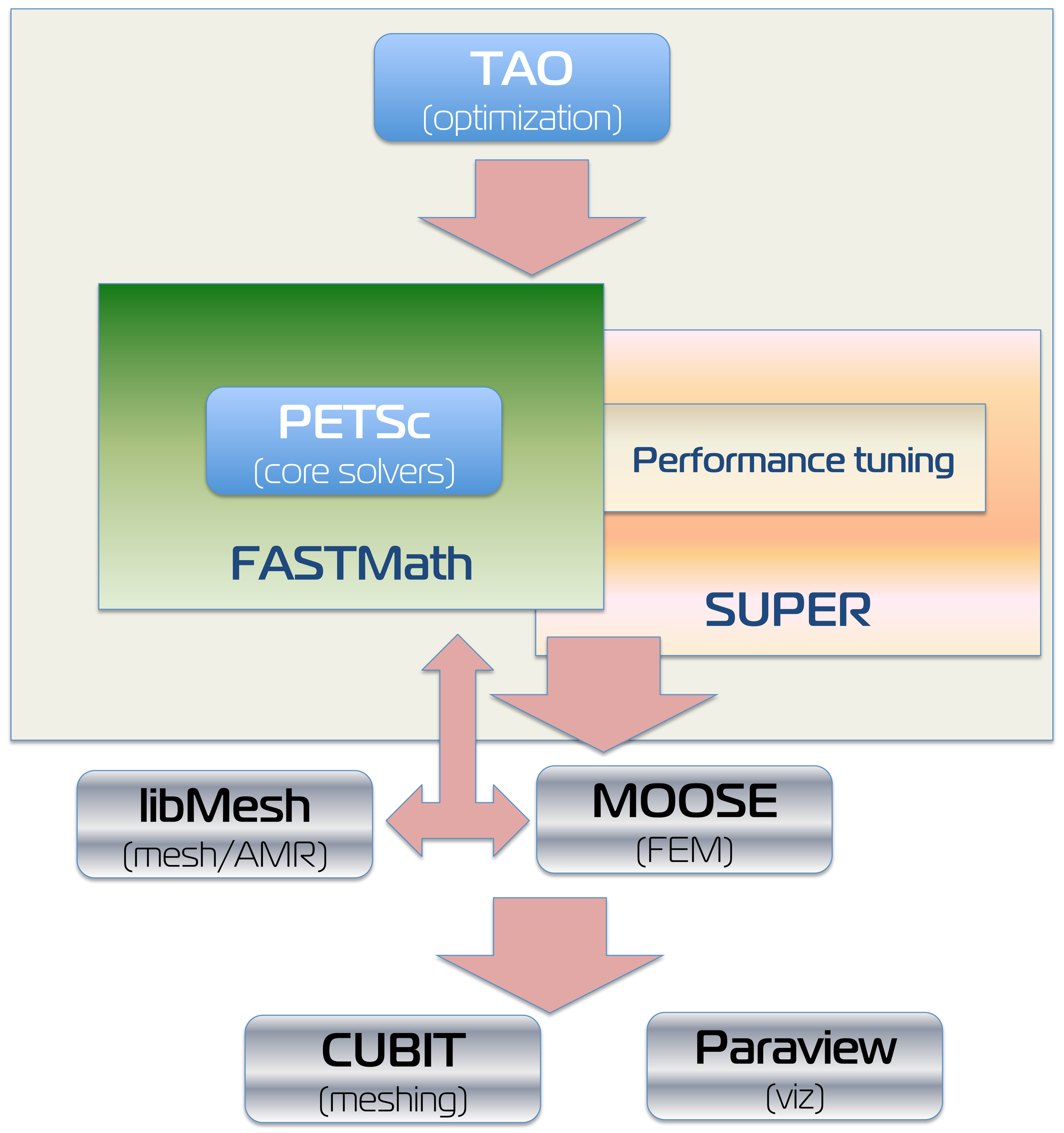
$$\mathbf{J} = \mathrm{Im}\left[\psi^*(\nabla - i\mathbf{A})\psi\right] - (\nabla\mu + \partial_t \mathbf{A})$$

critical current J_c:
- no unique definition
- usually defined when voltage V is a small percentage δ (here 1%) of the free flow value V_{ff}
- ***J_c calculated e.g. by a bisection method***

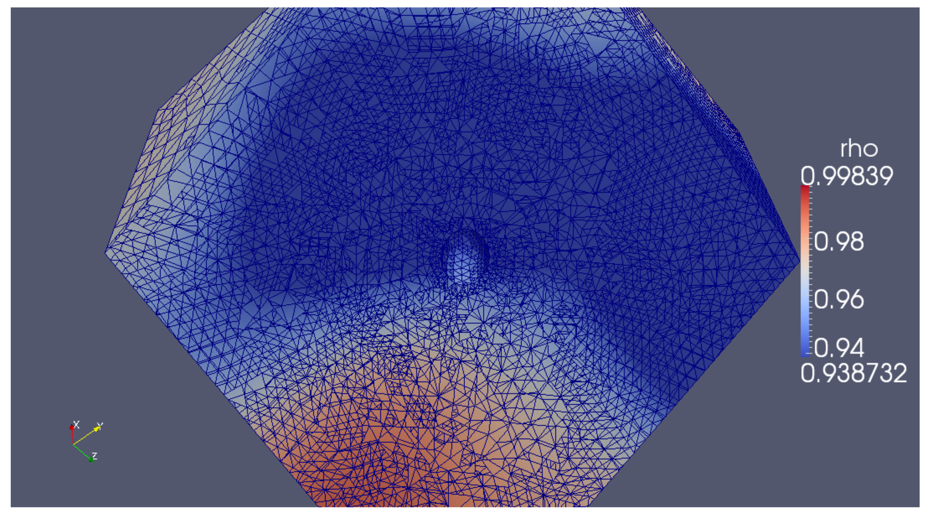


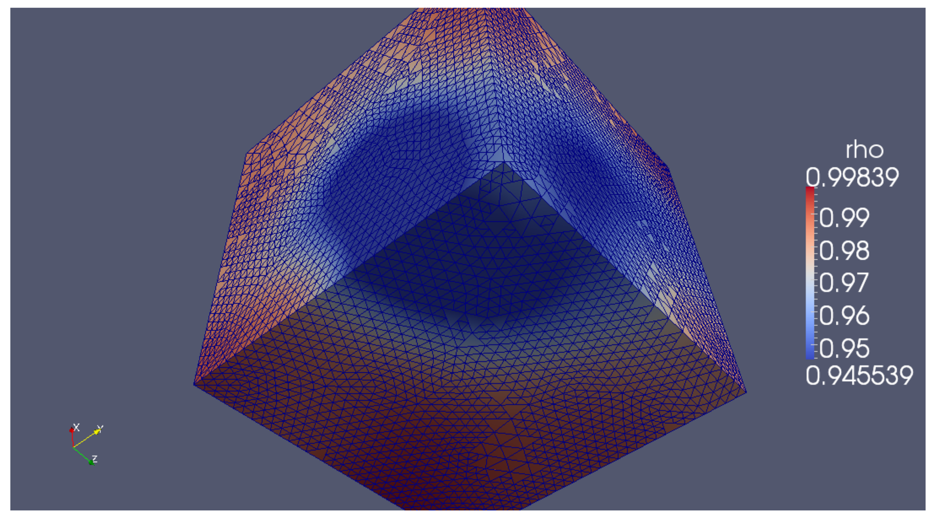
Software/algorithm stack

Leveraging power of SciDAC Institutes



Discretization/Meshing





- **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**

Simulation

Long-time integration

- Need to obtain reliable statistics on J_s independent of transient, fluctuations
- Requires long-time integration ($\sim \Gamma/a_0$ millions of timesteps)
- Alleviated using implicit time-integration

$$\begin{aligned} \frac{\psi^{n+1} - \psi^n}{\Delta t} &= \left(\frac{\epsilon}{u} - i\mu^{n+1}\right)\psi^{n+1} + \frac{1}{u}\Delta_{\mathbf{A}^{n+1}}\psi^{n+1} + F_i^{n+1} + F_e^n, \\ \frac{\mathbf{A}^{n+1} - \mathbf{A}^n}{\Delta t} &= -\frac{c\kappa^2}{\sigma}\nabla \times \left(\nabla \times \mathbf{A}^{n+1}\right) + G_i^{n+1} + G_e^n, \end{aligned}$$

Parameters u and κ are related to Γ, a_0, b, ϵ as well as the fundamental coherence length ξ_0 and magnetic penetration length λ_0.

- $\psi^{n+1}, \mathbf{A}^{n+1}$ are the approximations at time t_{n+1} being determined from the approximations at t_n
- $\Delta_{\mathbf{A}} = (\nabla + i\mathbf{A})^2$ is the modified Laplace operator
- F_i^{n+1} and F_e^n are a splitting of the remaining nonlinear terms into implicit and explicit parts

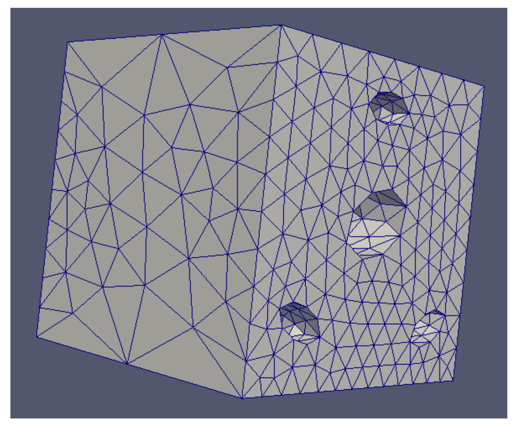
- Fully implicit methods correspond to $F_i = F,\ G_i = G,\ F_e = G_e = 0$ and generally enjoy the best stability properties.
- Linearly implicit methods (with $F_i = G_i = 0, \Delta_{\mathbf{A}^n} = \Delta$) have certain advantages
- Can be obtained as special cases of the general implicit method.

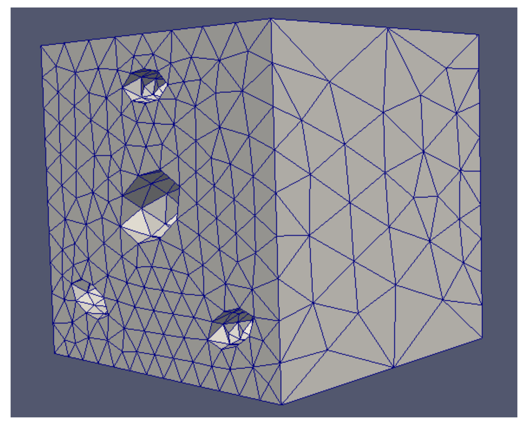
Boundary conditions

Quasiperiodic conditions define the current

- **Can be dealt with using an appropriate gauge transformation on a structured mesh**

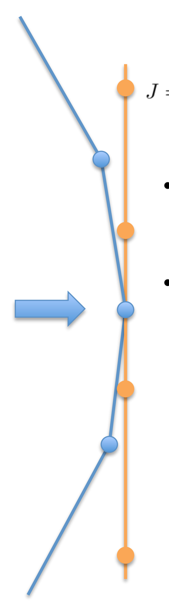
- **Quasiperiodicity on an unstructured mesh:**
- **Master-slave paradigm similar to mortar elements**
- **Requires point location**
- **Introduces implicit coupling not captured by the mesh topology**
- **Residual/Jacobian assembly requires slave-to-master transfer**
- **Slaves are linear combinations of master variables**
- **Linear constraints complicate linear solve**





Preconditioners

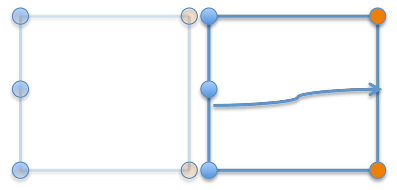
Master-Slave contact
Mortar Elements



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

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

$$\hat{J} = \begin{pmatrix} K_{LL} & K_{LS} & 0 \\ K_{SL} & K_{MM} & K_{MR} \\ 0 & K_{RM} & K_{RR} \end{pmatrix}$$

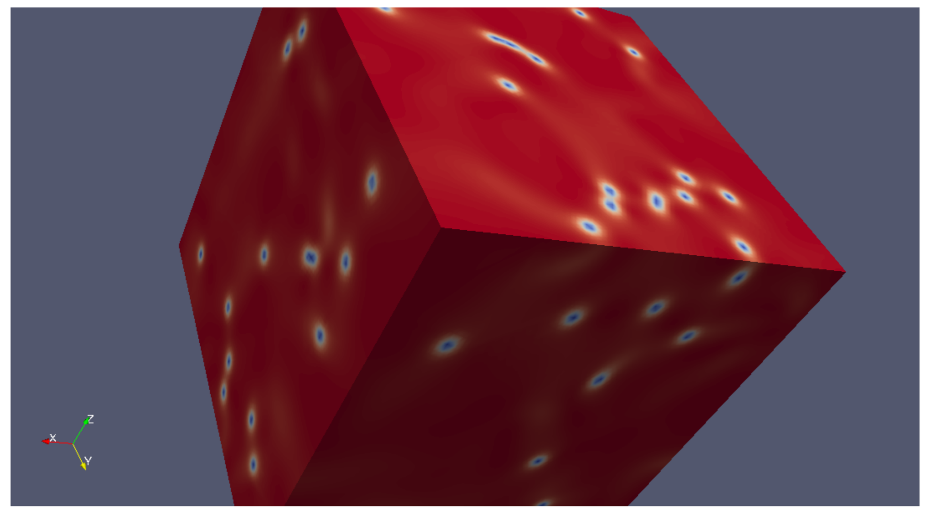


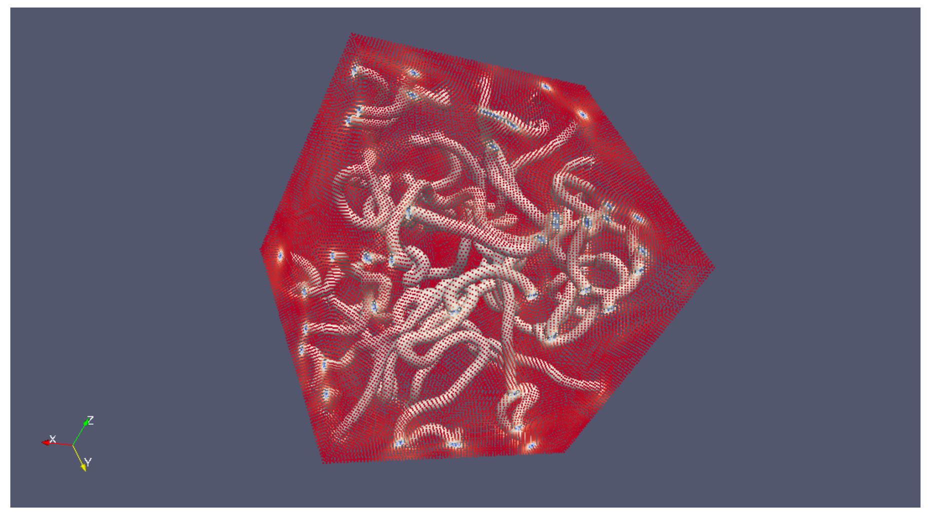
- For GL coupling S to M is an appropriate gauge transformation

- **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**

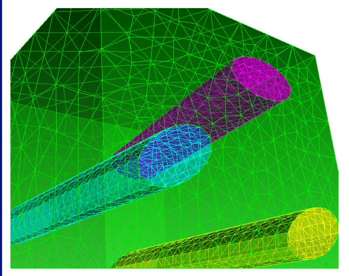
Performance & Outlook

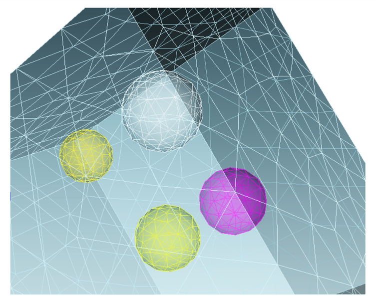
- **Assembly of constraints nontrivial in current software framework**
  - **Requires parallel point location**
  - **Preallocation of Jacobian entries of ordinarily disconnected nodes**
  - **Underallocation harmful: insertion of elements into sparse matrix**
  - **Overallocation harmful: transfer/insertion of many zero entries from Slave to Master**
- **Zero-current boundary conditions simulations highly scalable**

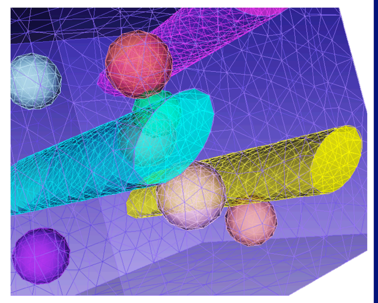




Shape optimization







- Requires solution of adjoint operator
- How does noise enter into the adjoint?
- How to compute derivatives with respect to shape?
- Preliminary work on the temperature modulation model of inclusions

- Adjoint must be solved back in time – final condition for GL generates an initial for adjoint
- Forward problem state must be stored and reused later

$$u(\partial_t + i\mu)\psi' = \epsilon'\psi + \epsilon(\mathbf{r})\psi' - 2|\psi|^2\psi' - \psi^2\psi'^* + (\nabla - i\mathbf{A})^2\psi' + \zeta(\mathbf{r},t)$$

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