

Iterative unstructured-mesh Ginzburg-Landau solver on MPI clusters

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GL model

Time-dependent Ginzburg-Landau

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

$$u(\partial_t + i\mu)\psi = \epsilon(\mathbf{r})\psi - |\psi|^2\psi + (\nabla - i\mathbf{A})^2\psi + \zeta(\mathbf{r}, t)$$

$$\kappa^2 \nabla \times (\nabla \times \mathbf{A}) = \mathbf{J}_n + \mathbf{J}_s + \mathcal{I},$$

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
- $\epsilon(\mathbf{r}) = \frac{T_c(\mathbf{r}) - T}{T_c} \rightarrow 0$ for $T \rightarrow T_c$ (critical temperature)

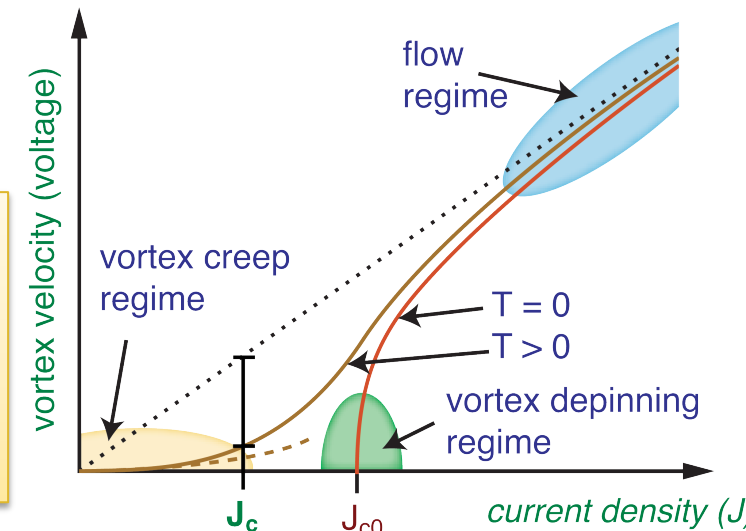
$$\mathbf{B} = \nabla \times \mathbf{A}, \quad \mathbf{E} = -\frac{1}{c}\partial_t \mathbf{A} - \nabla \mu$$

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

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

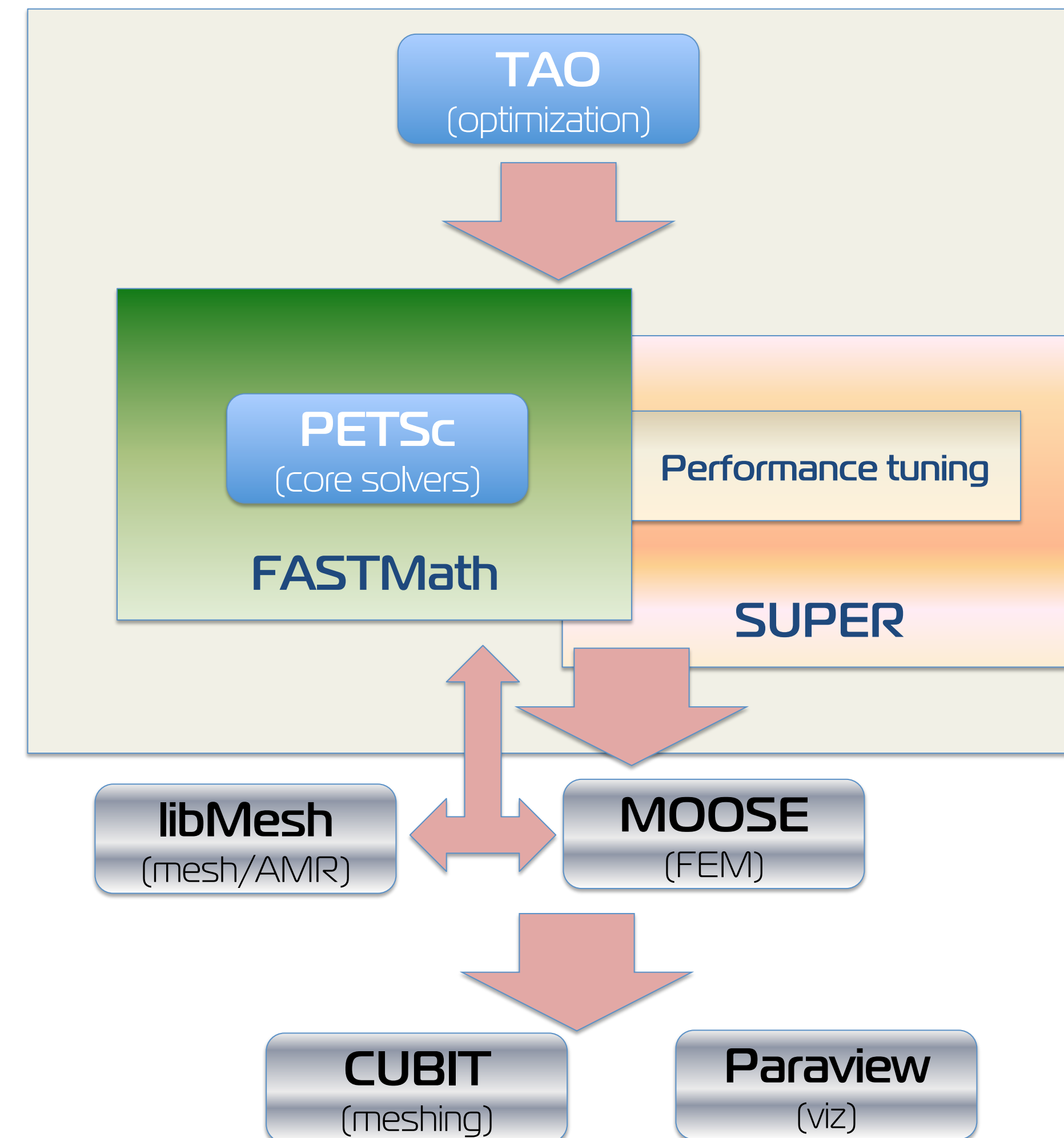
critical current J_c :

- 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

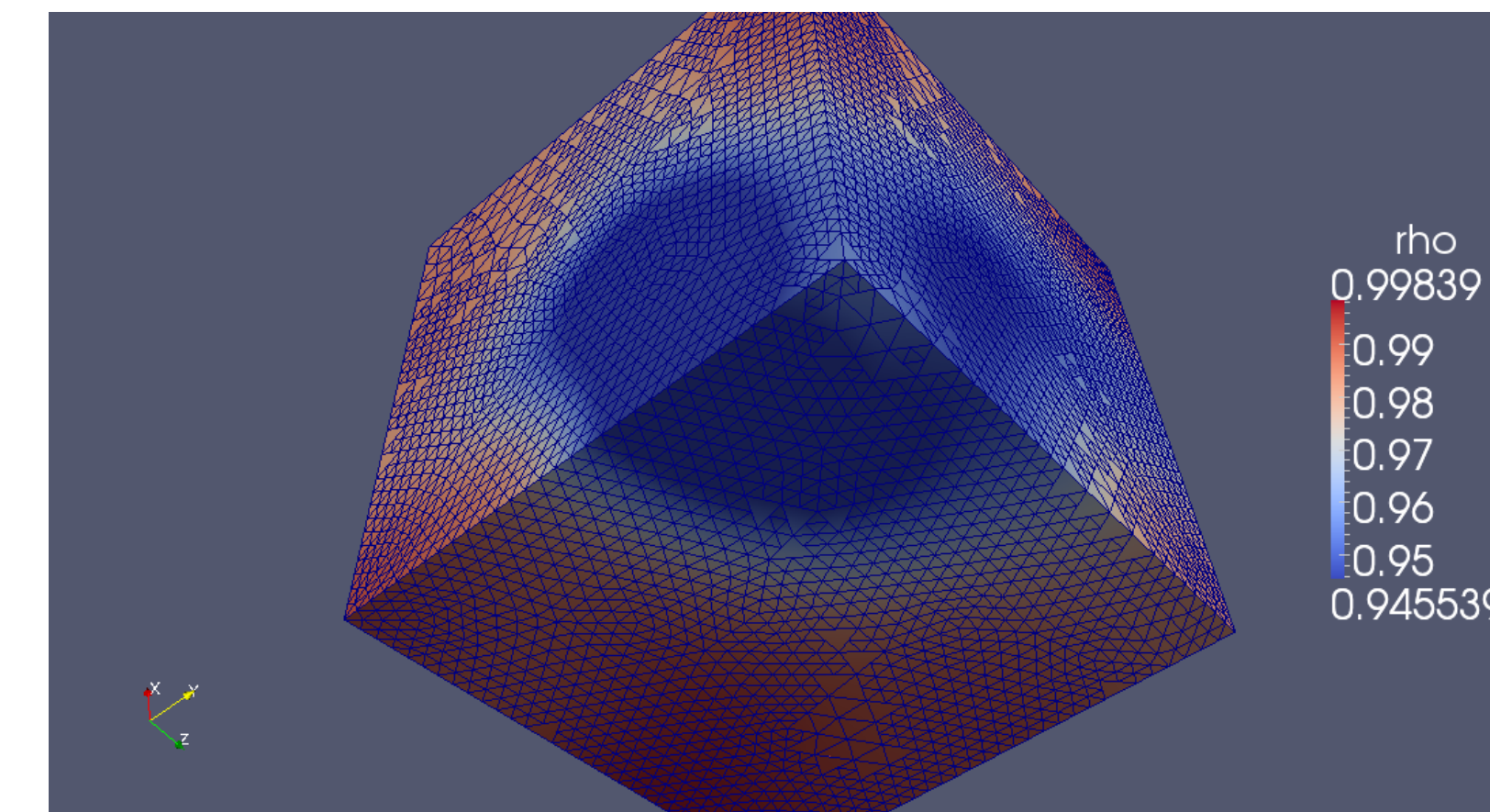
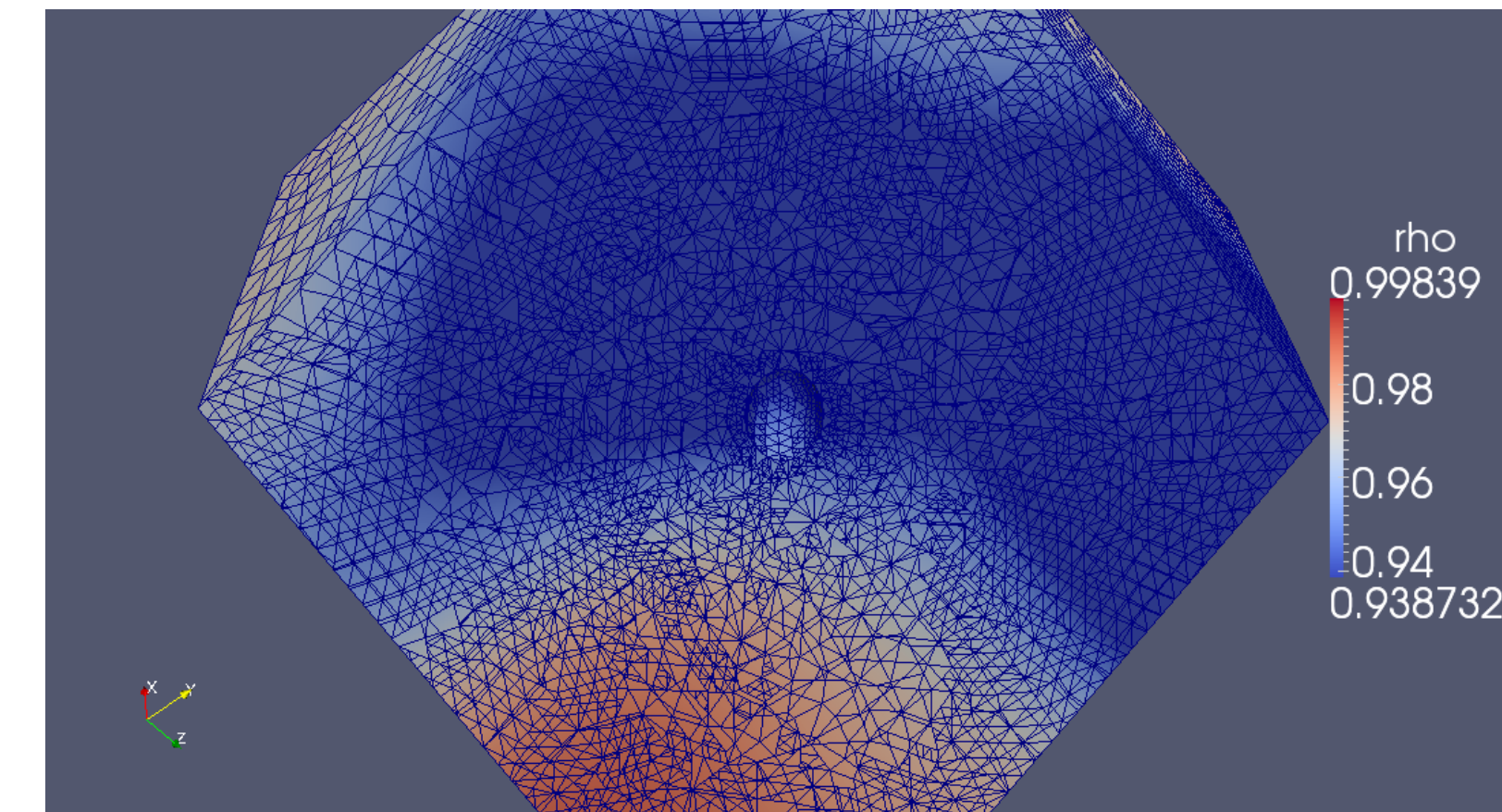


Software/algorithm stack

Leveraging power of SciDAC Institutes



Discretization/Meshing



- AMR: memory/cycles savings once solution features have stabilized
- Mapping to/from refined/derefining 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

$$\frac{\psi^{n+1} - \psi^n}{\Delta t} = \left(\frac{\epsilon}{u} - i\mu^{n+1} \right) \psi^{n+1} + \frac{1}{u} \Delta_{\mathbf{A}^{n+1}} \psi^{n+1} + F_i^{n+1} + F_e^n,$$

$$\frac{\mathbf{A}^{n+1} - \mathbf{A}^n}{\Delta t} = -\frac{c\kappa^2}{\sigma} \nabla \times (\nabla \times \mathbf{A}^{n+1}) + G_i^{n+1} + G_e^n,$$

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.

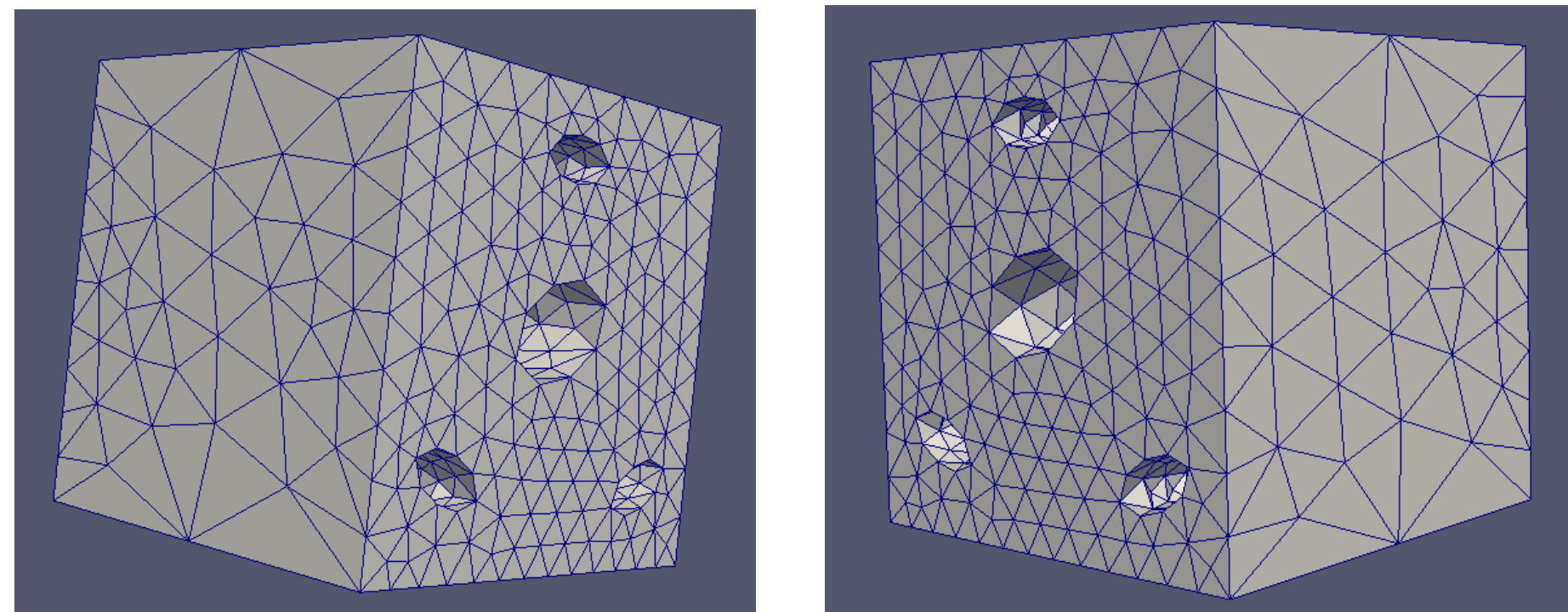
- Linearly implicit methods (with $F_i = G_i = 0, \Delta_{\mathbf{A}^n} = \Delta$) have certain advantages

- Can be obtained as special cases of the general implicit method.

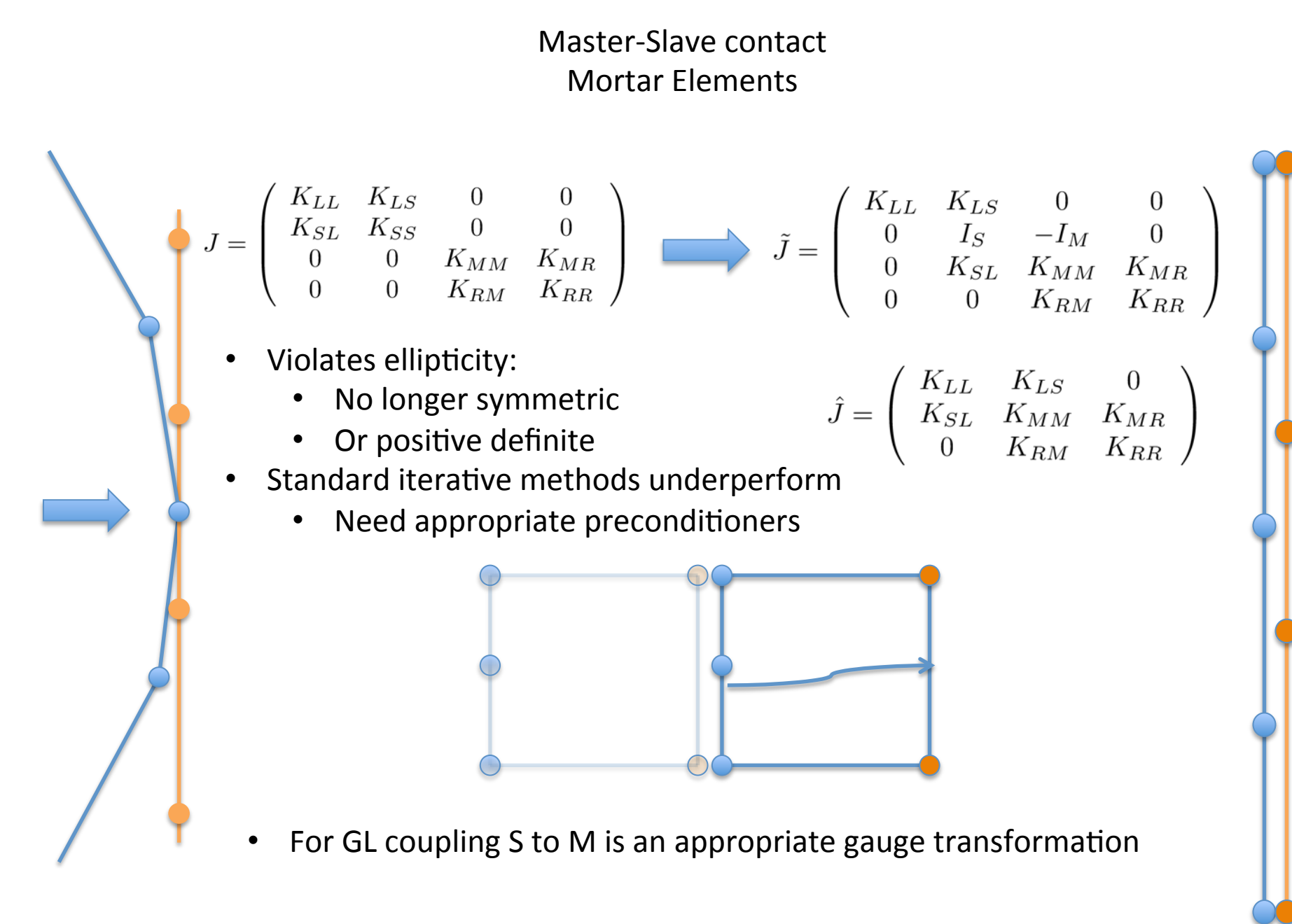
Boundary conditions

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



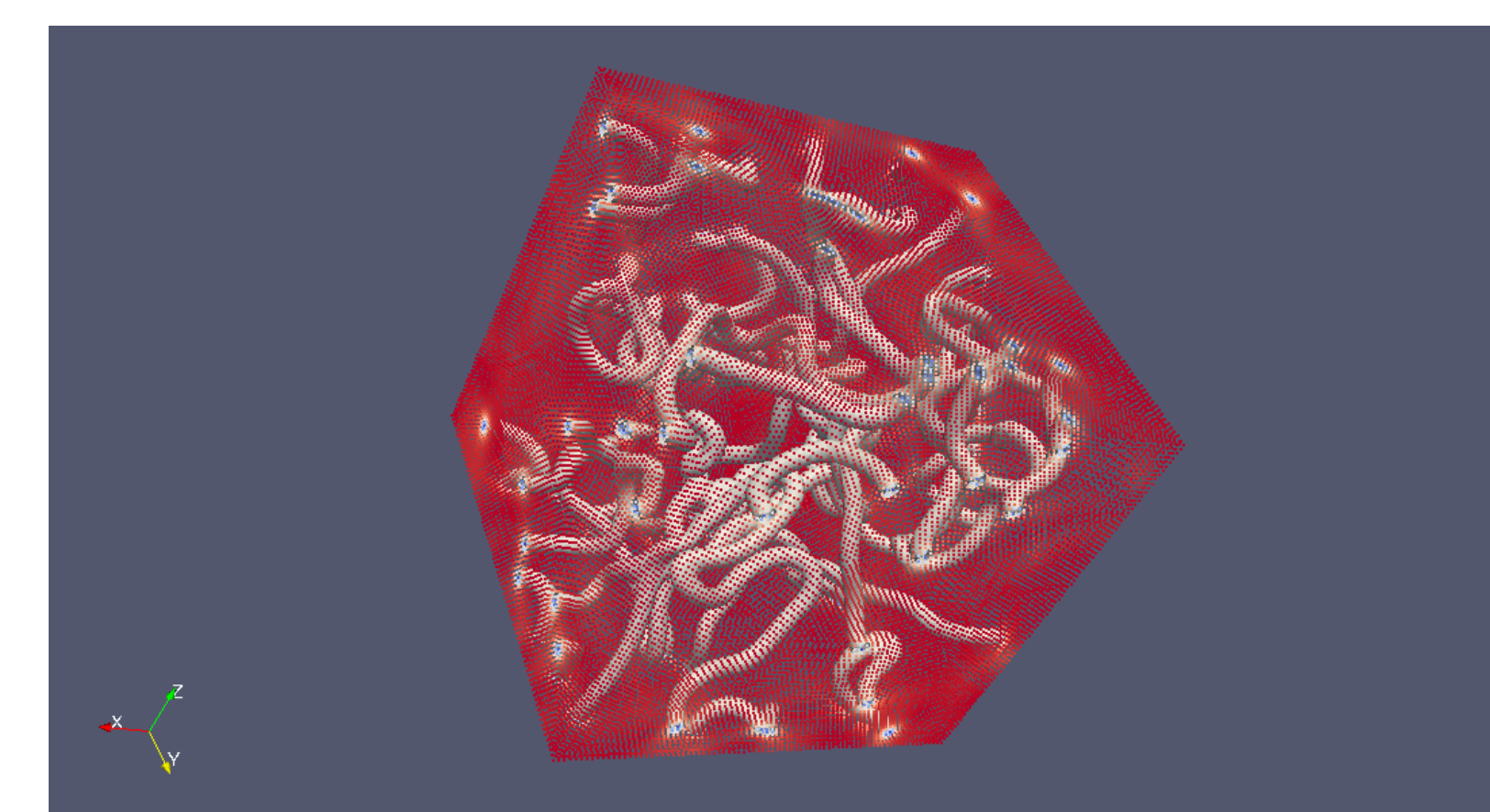
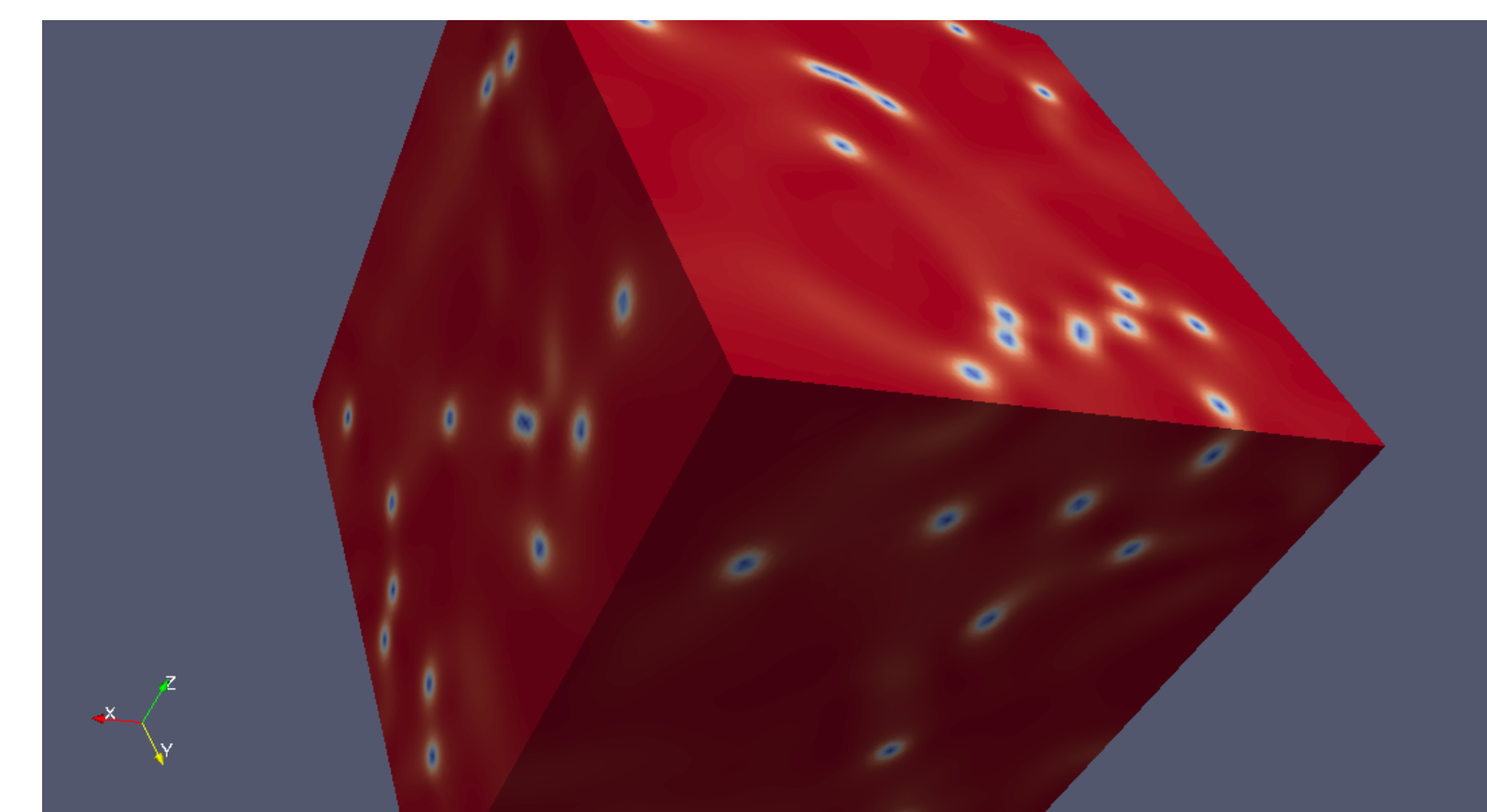
Preconditioners



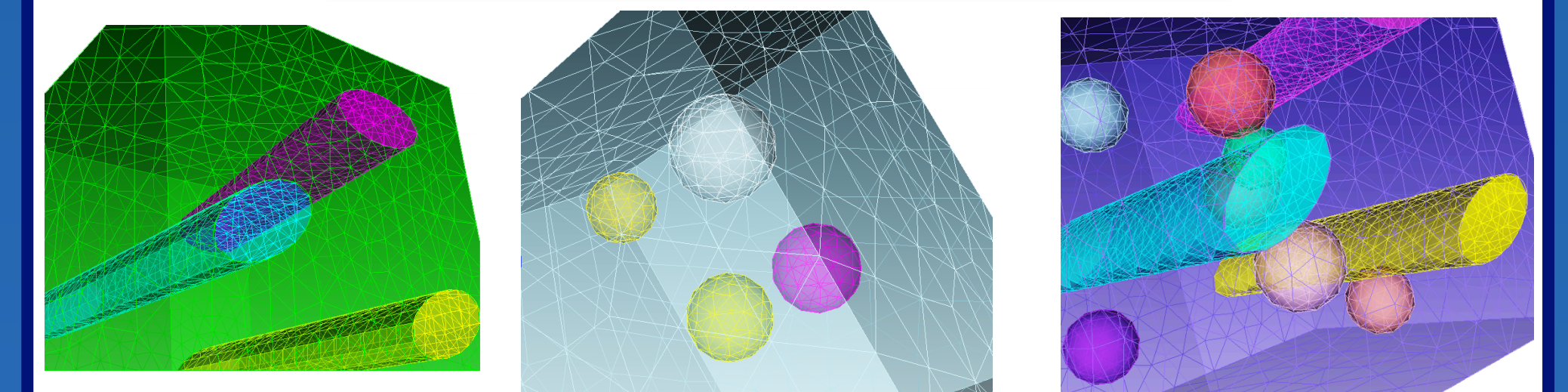
- Use splitting to isolate the constraints
- Constraint elimination results in an SPD Schur complement S
- Precondition S
 - Matrix-free using block P
 - Assemble S
 - Use multigrid or domain-decomposition
- PETSc provides flexible splitting/recombination preconditioner machinery
 - PCFieldSplit

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

