A2

Large-scale Simulation of Vortex Dynamics and Optimization

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Large-scale GL simulation

See Poster A1 for details on the underlying equations.

Why large-scale GL?

Robust optimization of the critical currents for energy applications is challenging:

- ☑ Critical current is determined by long-time evolution of time-dependent Ginzburg-Landau equations
- ☑ Critical current is dominated by rare events of vortex depinning, avalanches, nucleation, splitting, and reconnection
- ☑ Frequency and duration of pinning/depinning depend on configurations of inclusions
- ☑ Suitable pinning configurations can be determined by geometry optimization

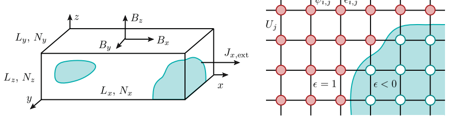
Implementation approaches

1. Regular spatial discretization
   + Fast, easier to implement, less overhead
   – non-rectangular features difficult to handle, the mesh size needs to be adapted to smallest defect
2. FEM with adaptive mesh refinement
   + very flexible geometries possible
   – large overhead, boundary conditions difficult to implement

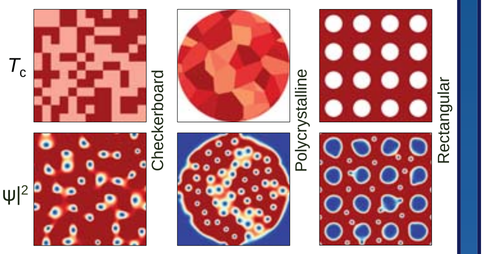
Pattern generator

Pinning landscape

Inclusions and defects are modeled by critical temperature $T_c(\mathbf{r})$ modulation

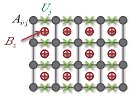


Order parameter ψ(**r**) follows T_c-pattern



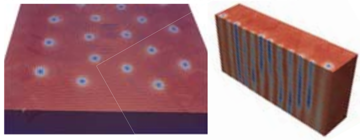
Discretization

Regular simulation grid



- ✓ Direct implementation: CUDA/MPI
- ✓ Stable link variables
- ✓ Better control of boundary conditions
- ✓ T_c-modulated inclusions only

Unstructured simulation grid



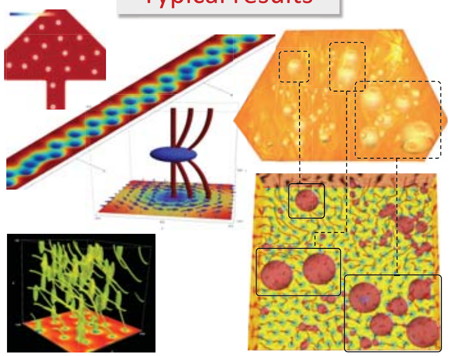
PETSc/ libMesh

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

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

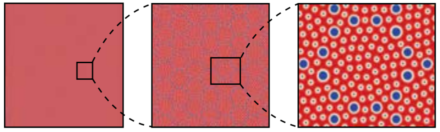
Needs to be used sparingly and intelligently
- ✓ Mesh coarse geometry
- ✓ Refined uniformly
- ✓ Relax solution on uniformly refined mesh
- ✓ Derefinement on relaxed solution

Typical results



Scalability

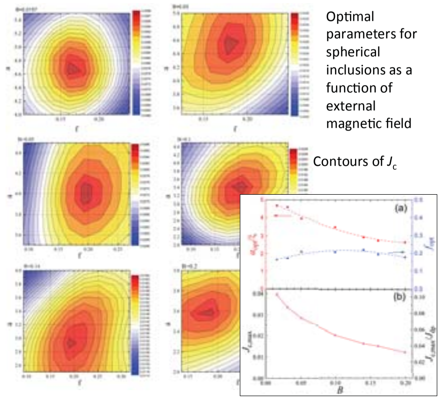
Reaching a steady state in (12 000 ξ)^2 2D or (550 ξ)^3 3D system is a matter of hours



Vortex pinning optimization

Critical current optimization

- ➢ Optimal inclusion configurations for maximal critical current
- ➢ Robustness of these configurations
- ➢ Dependence on magnetic field and temperature

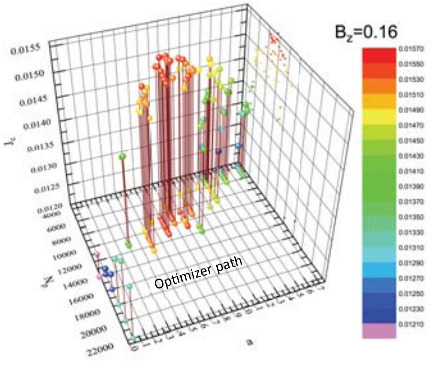


Optimal parameters for spherical inclusions as a function of external magnetic field

Contours of J_c

Systematic approach

- ➢ Fully automatic derivative-free optimizer for GPU/ CPU clusters
- ➢ Arbitrary combination of different defect types



- ➢ Current-by-design concept

SUPER, FASTMath

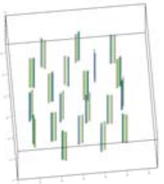
Data analysis

See Poster B1 for details on vortex detection and tracking.

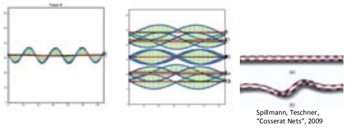
Novel vortex feature analysis: twist & writhe

- ➢ When electrostatic and magnetic fields aligned, phase field twists around the vortex.
- ➢ Shielding supercurrents spirals around vortex rather than form planar loops.
- ➢ Twisting phase field can be numerically extracted from GL simulations. Represented as ribbon.

No twist



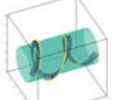
Twisting phase field



Spillmann, Teschner, "Cosserat Nets", 2009

→ Excess twist leads to writhe

- Twist → Buckling Instability → Writhe of Filament/Rod/Vortex
- Perpendicular Lorentz Forces on writhing vortex → helical coils unstable.



SDAV

Next steps & References

Next steps

- ➢ Implement finite-κ PDE (Maxwell equation) on structured grids
- ➢ Continue optimization studies on unstructured grids on ALCF machines
- ➢ Run large-scale multi-parameter optimizations

See also posters A1 & B1

Technical References:

[1] I. A. Sadovskyy, A. E. Koshelev, C. L. Phillips, D. A. Karpeev, and A. Glatz
Stable large-scale solver for Ginzburg-Landau equations for superconductors
J. Comp. Phys. **294**, 639 (2015)

[2] D. A. Karpeev, I. A. Sadovskyy, H. Guo, and A. Glatz
Gauge-invariant unstructured FEM discretization of the Ginzburg-Landau equations
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[3] C. L. Phillips, T. Peterka, D. Karpeyev, and A. Glatz
Detecting vortices in superconductors: Extracting one-dimensional topological singularities from a discretized complex scalar field
Phys. Rev. E **91**, 023311 (2015)

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