Optimizing SuperConductor Transport Properties Through Large-Scale Simulation

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OSCon

http://www.oscon-scidac.org/

Outline

Critical Current by Design *see Poster A1 (18)*

- Experimental validation
- Non-additivity of defects
- Prediction of critical currents

Intelligent optimization of Superconductors

- Approach
- Examples

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Extracting, Tracking, and Visualizing of Vortices

- Tracking methods
- Tools
- Next steps

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Model and Pinning

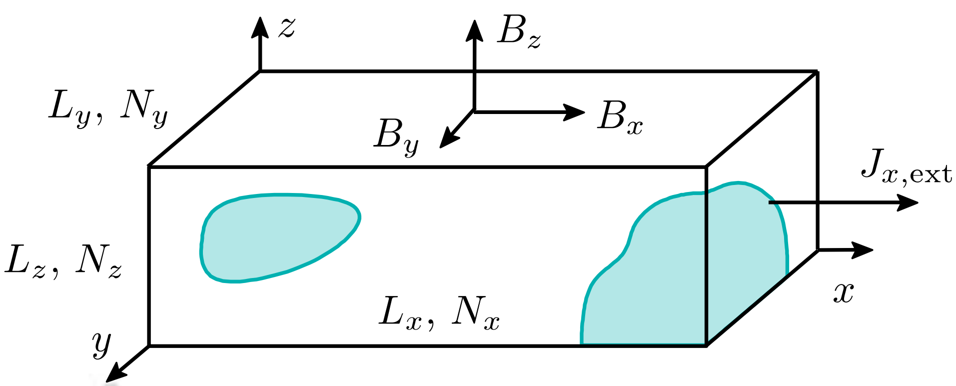
Time dependent GL equations:

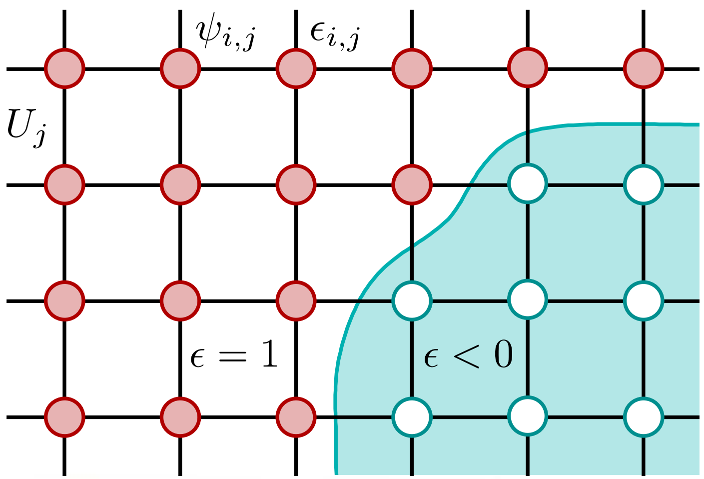
$$\frac{\partial\Psi}{\partial t} = -\frac{\delta\mathcal{F}_{\mathrm{GL}}}{\delta\Psi^*}, \quad \frac{\delta\mathcal{F}_{\mathrm{GL}}}{\delta\mathbf{A}} = 0$$

In dimensionless units:

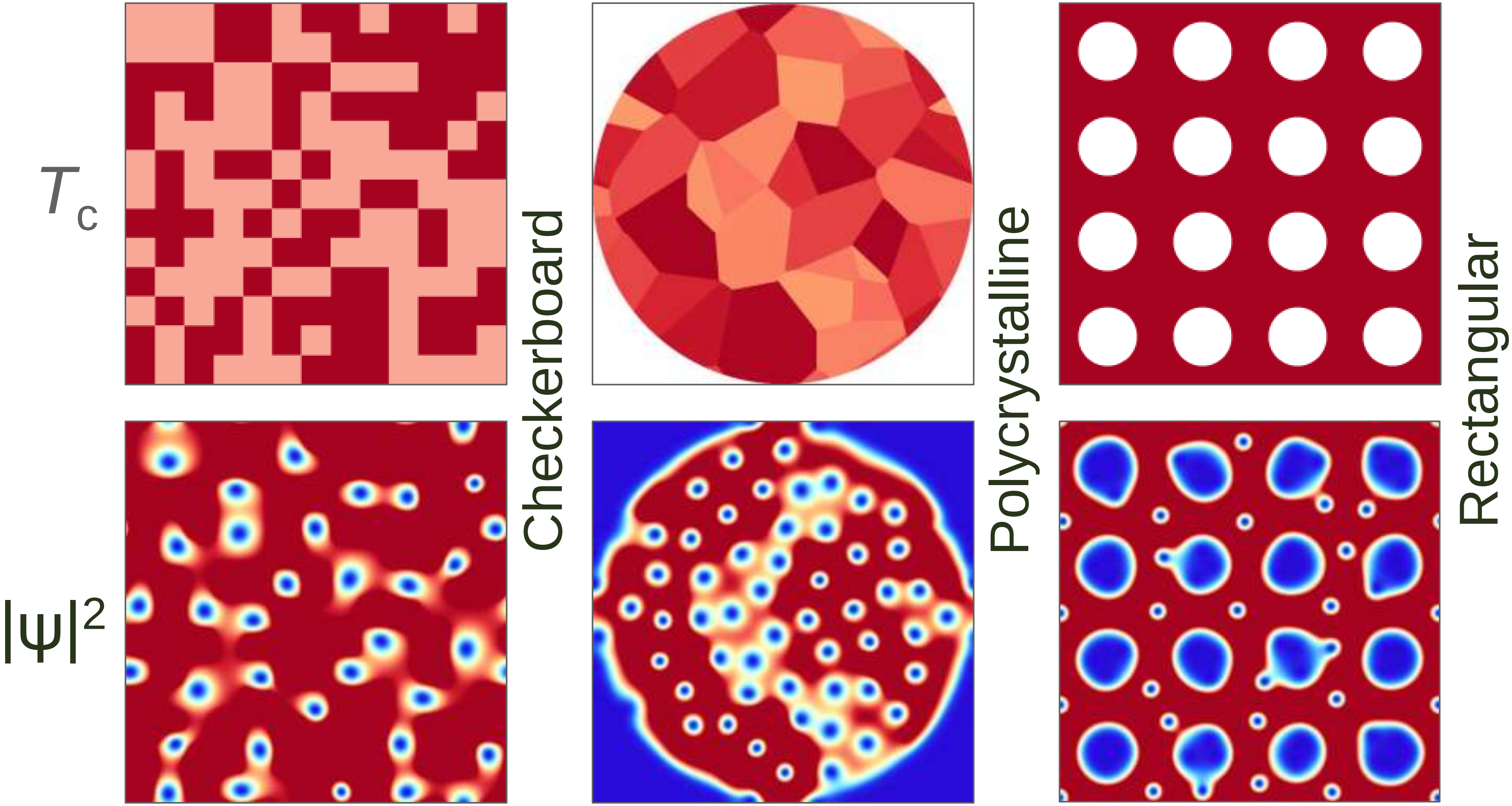
$$u(\partial_t + i\mu)\psi = \epsilon(\mathbf{r})\psi - |\psi|^2\psi + (\nabla - i\mathbf{A})^2\psi + \zeta(\mathbf{r},t)$$
$$\kappa^2\nabla\times(\nabla\times\mathbf{A}) = \mathbf{J}_n + \mathbf{J}_s + \mathcal{I},$$

Inclusions and defects are modeled by critical temperature $T_c(\mathbf{r})$ [$\varepsilon(\mathbf{r})=T_c(\mathbf{r})/T-1$] modulation





Examples: Order parameter ψ(r) follows T_c-pattern

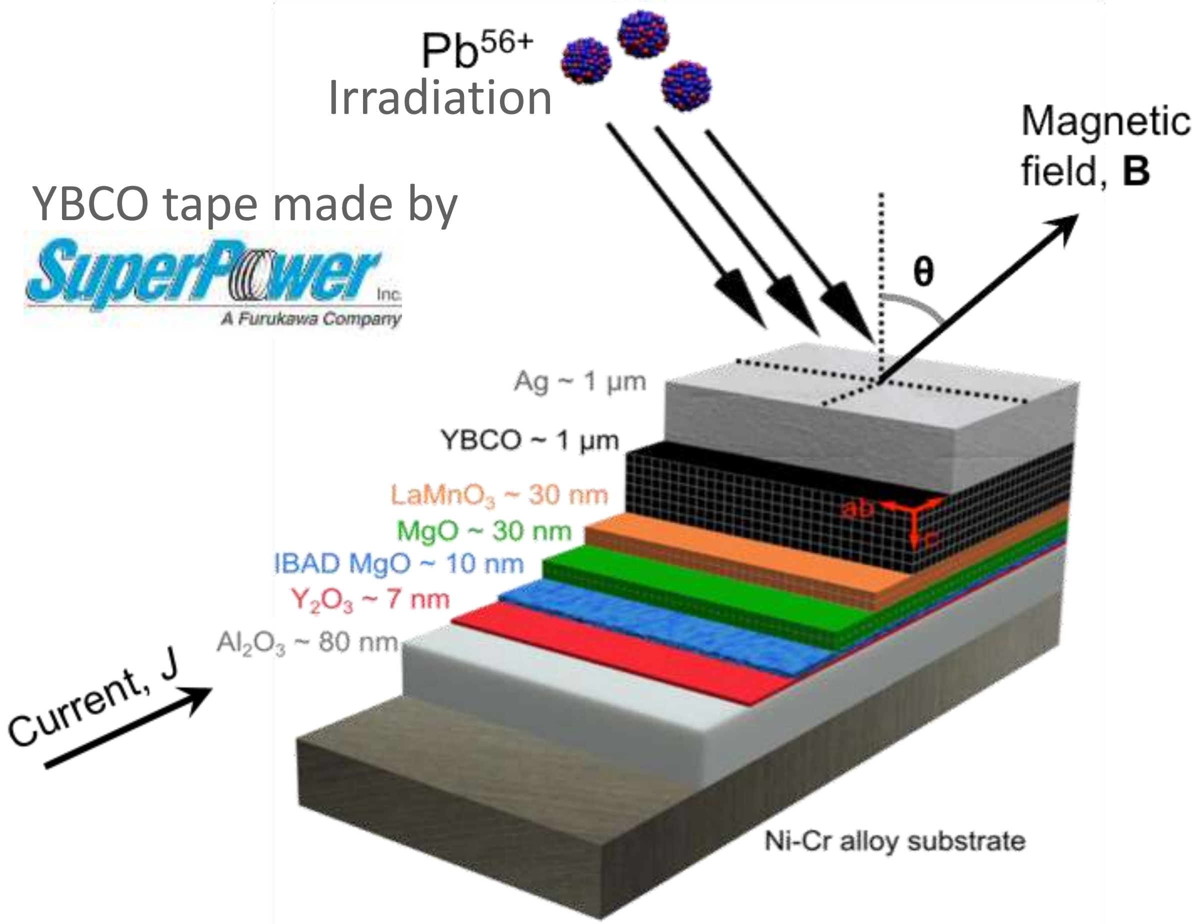


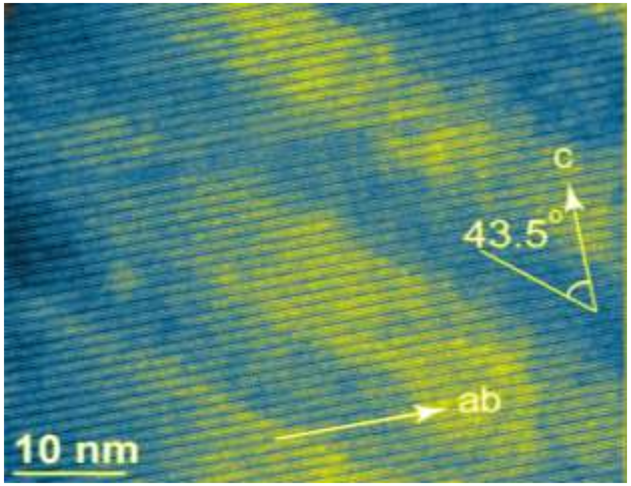
Experimental motivation

Angular dependence of the critical current in commercial REBCO coated conductors

YBCO tape made by

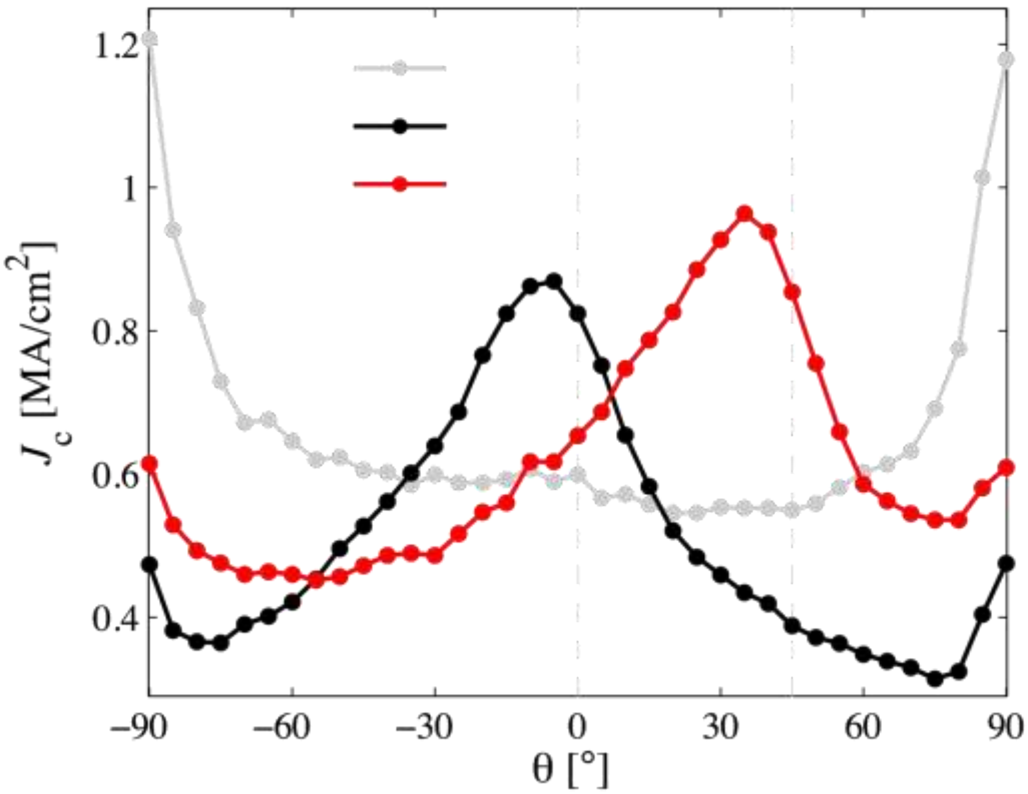
SuperPower Inc.
A Furukawa Company





TEM image of heavy-ion damage tracks

Observation and scientific questions



- Disappearance of central peak after irradiation → Pinning effects are non-additive. Explanation?
- Overall increase of the critical current. Can we increase it more?
- Can we get a more homogeneous critical current?
- **What is the optimal irradiation track concentration?**

Here we use large-scale Ginzburg-Landau simulations to address these questions

→ **Simulation-assisted design of mixed-pinning landscapes with predictable "critical-current-by-design"**

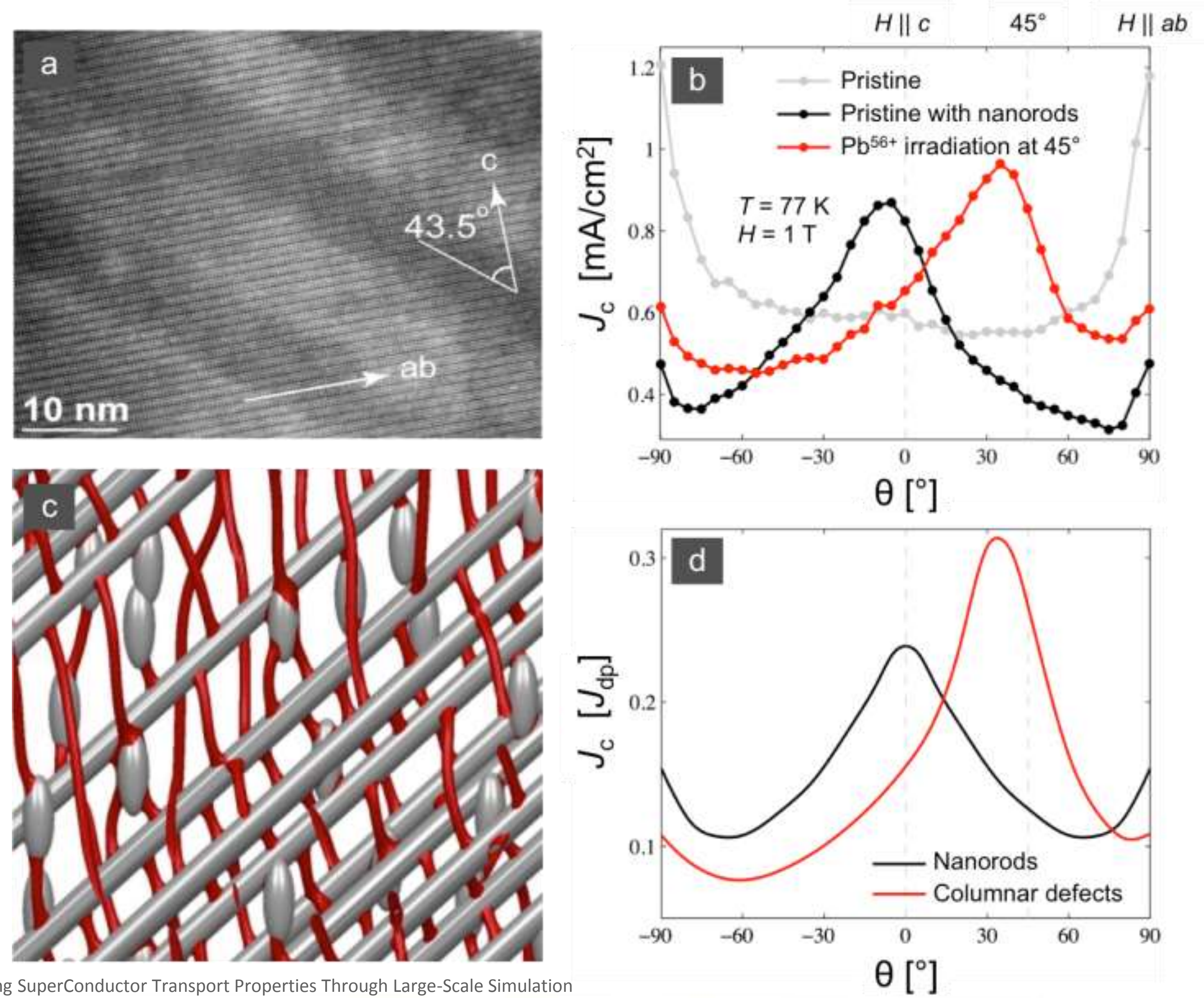
Sample realization

- Sample is realized as a cuboid, discretized using a regular mesh of 10^8 grid points with mesh size of $\xi_0/2$
- (quasi-)periodic boundary conditions
- Inclusions and irradiation tracks are modeled by a different low-T_c component
- Anisotropy in c-direction is implemented by an anisotropy factor $\gamma=5$
- For each field and pinning configuration an IV curve is calculated from which the critical current is obtained

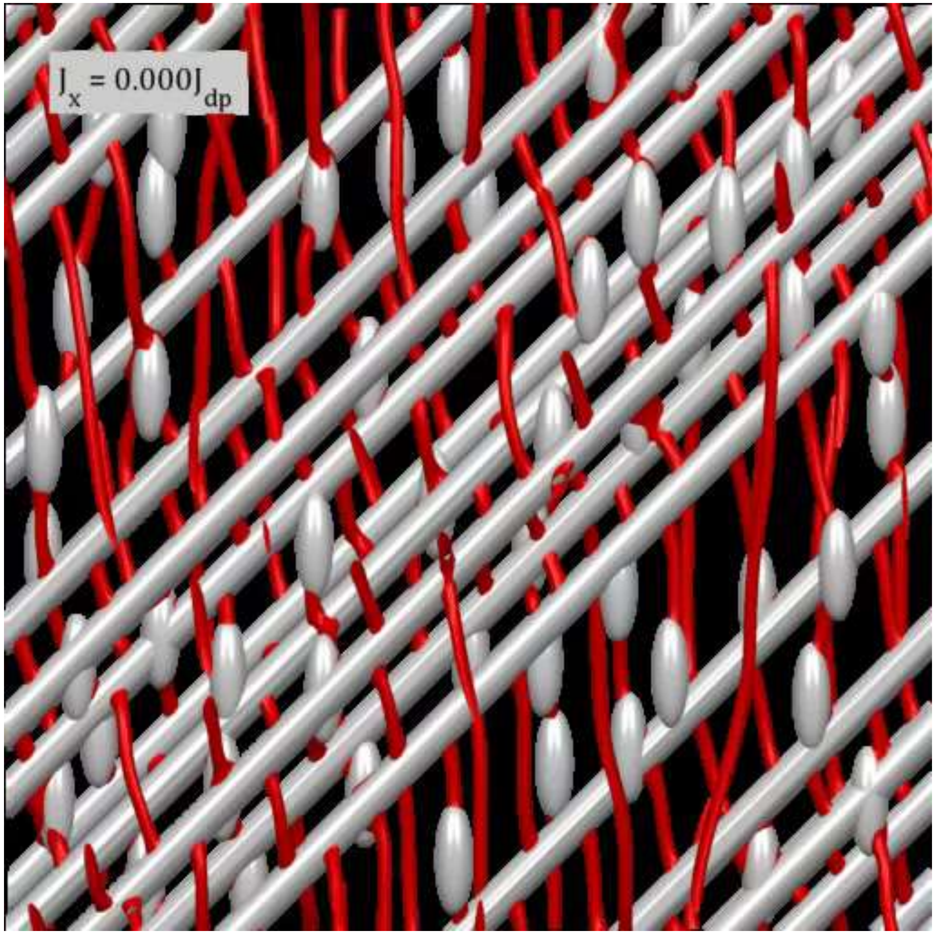
Comparison Experiment & Simulation

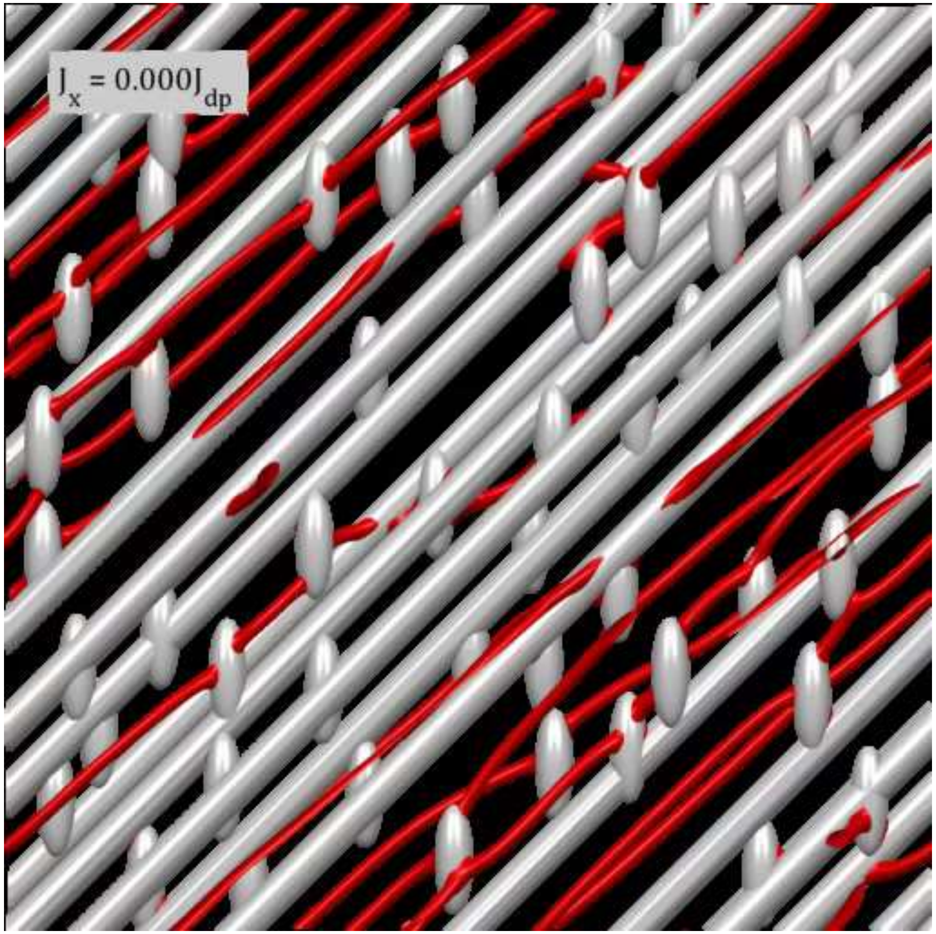
	Experiment	Simulations
Anisotropy / Layers		
Anisotropy	Anisotropy factor ~ 5–7 (more like **7**)	**Anisotropy factor = 5**
Layers	Distance between layers **1.2×10^{-7} cm**	No layered structure
Sample size		
Sample size	• Thickness = 1 μm • Width = 80 μm • Length = 4 mm	• 128 × 512 × 768 grid points • **$64\xi_0 \times 256\xi_0 \times 256\xi_0$ = 96 × 384 × 384 nm** • Quasi-periodic boundary conditions
Coherence length		
ab-plane	• $\xi_0 = \xi(0K)$ ~ **1.5 nm** (from H_{c2} ~ 150 T) • $\xi(77K)$ ~ 3.4 nm (from H_{c2} ~ 28.5 T) • GL model: $\xi(77K) = 1.5/(1–77/92)^{½} = 3.7$ nm	**Unity (ξ_0)**
c-axis	ξ_0/(Anisotropy factor) = 0.21 nm	**ξ_0/(Anisotropy factor)**
Nanorods		
Dimensions	• Diameter ~ 5-10 **nm = 3-6 ξ_0** • Length ~ **100-1000 nm = 60-600 ξ_0**	• Diameter = **$4\xi_0$** • Length = **$128\xi_0$**
Average in-plane spacing between nanorods	~ 20 to 50 nm = 13 to 33 ξ_0	For N nanorods in the simulated volume, $\boldsymbol{L} = \sqrt{\frac{64\times256\times256}{128\times N}}$, e.g for N=100, L=$18\xi_0$ • $18\xi_0$
Irradiation induced columnar defects		
Dimensions	~5-10 nm	**$4\xi_0$**
Concentration	• ~ 1e11 cm^{-2} • Average spacing ~ 30 nm • Matching field, B_Φ = 2 T	• Average spacing = $20\xi_0$ = 30 nm • For N columnar defects, $L = \sqrt{\frac{64\times256}{N}}$, e.g. N~40 for L=20, Varied from 5 to 100

Validation of the simulation

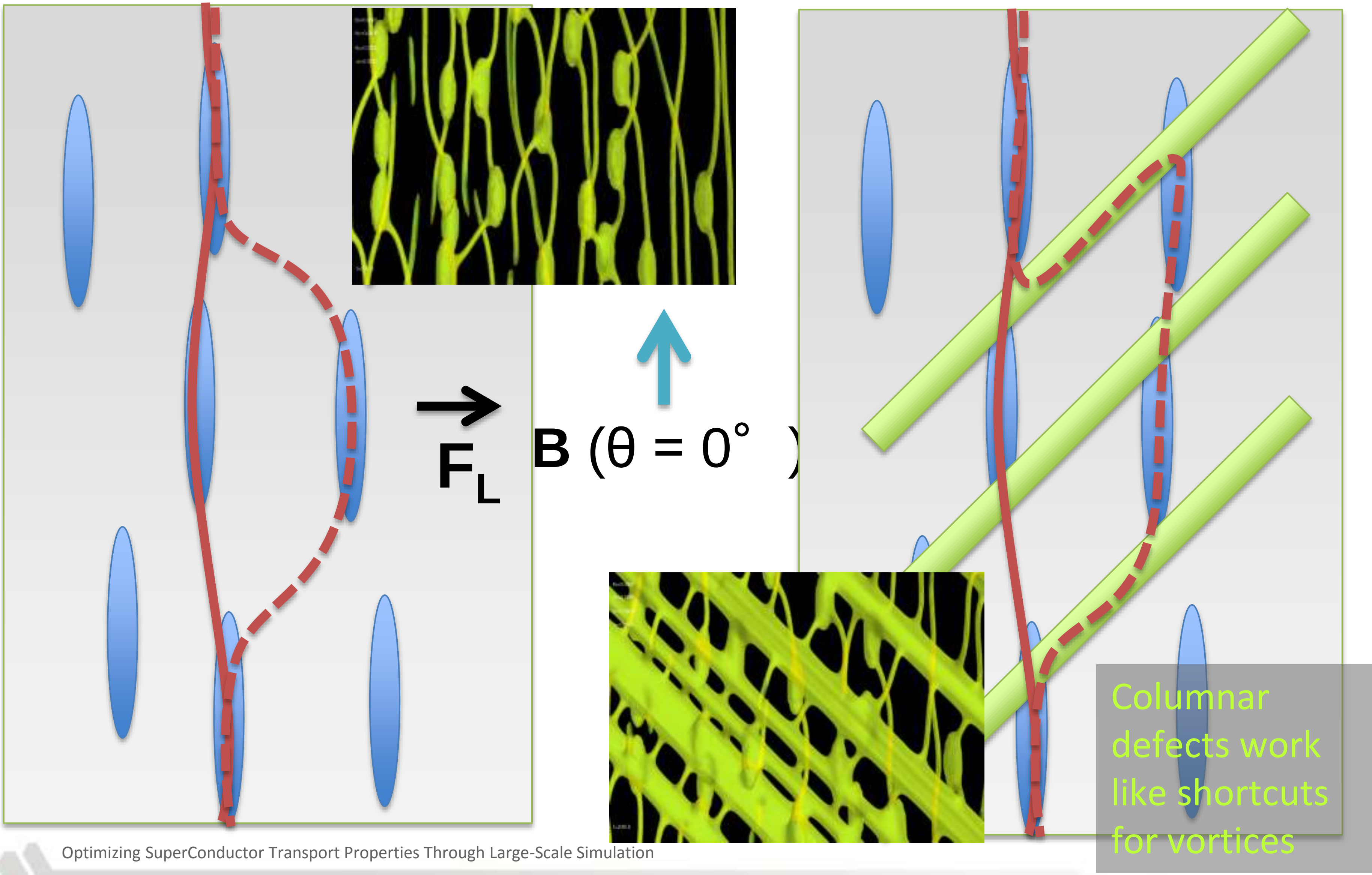


Depinning in fixed field **B** (θ = 0°　/45°　)=0.08

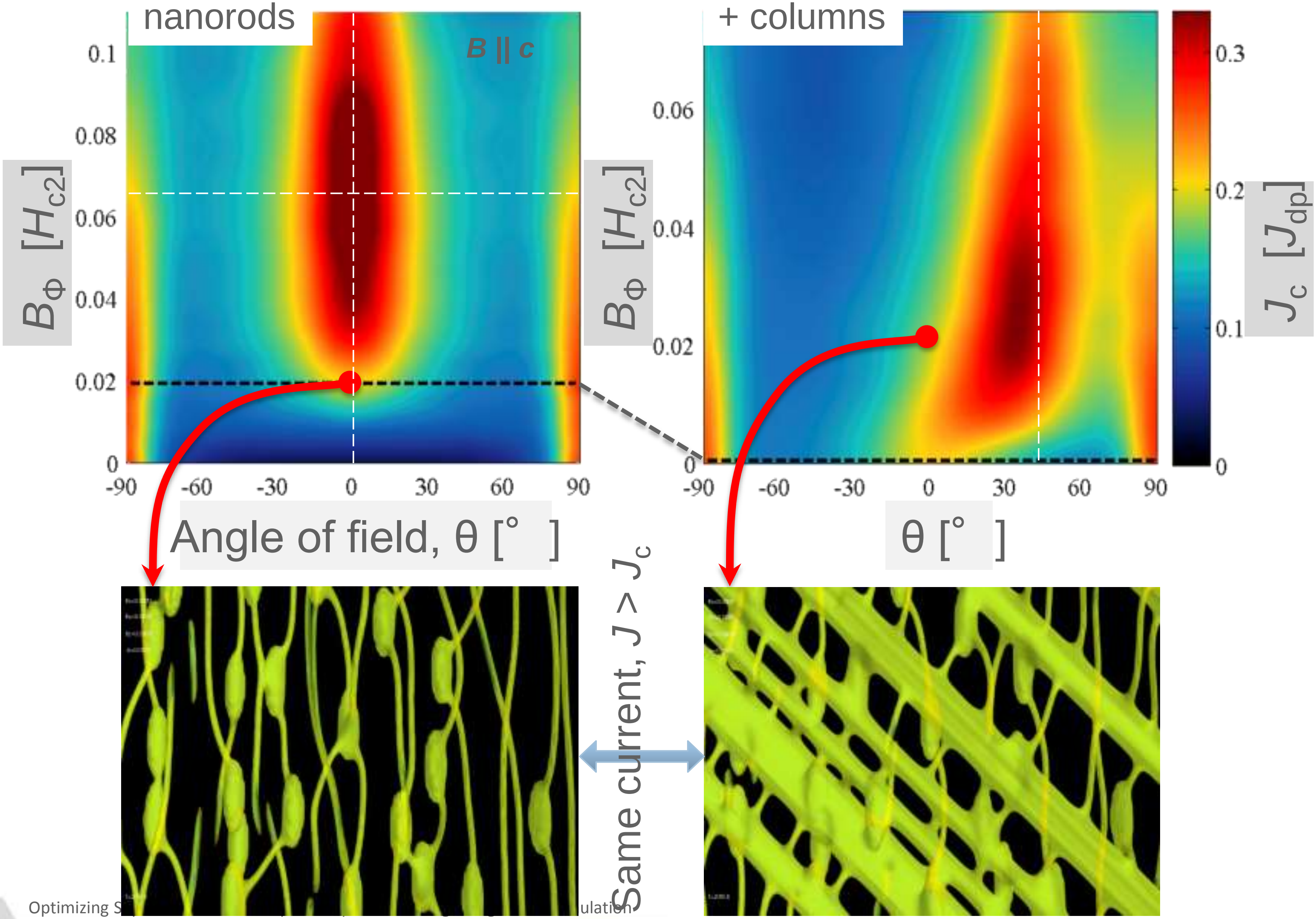




Discovery of novel mechanism: Non-additivity of defects



Predication of the critical current in irradiated samples



Sadovskyy et. al., submitted to Nature Materials (2015)

Critical Current by Design

- Experimental validation
- Non-additivity of defects
- Prediction of critical currents

Intelligent Optimization of Superconductors

- Approach
- Example

see Poster A2 (19)

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Optimization Challenge & Approach

Desired output

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

Challenge

- We need to calculate the critical current for many configurations with small fluctuations (requires disorder averaging)
- A typical pinning landscape has about 10 free parameters

Approach

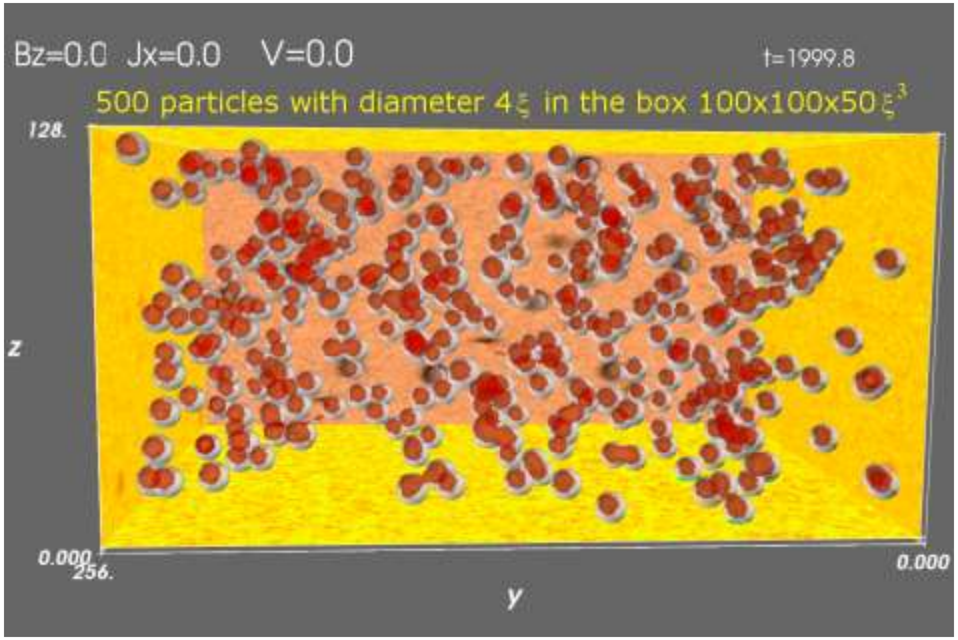
- Fully automated derivative-free optimizer:
  Define possible parameter ranges and the optimizer samples promising pinning configurations
- Can handle arbitrary combination of different defect types

Example: 2 parameter optimization of random spherical inclusions

with diameter a and density n_p

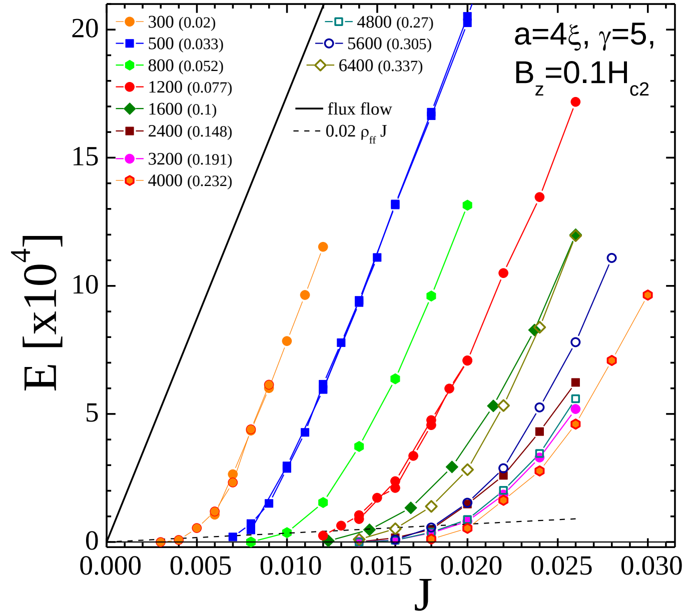
Occupied volume fraction $f \approx n_p V_p$

Overlap: $f \to f - f^2/2$

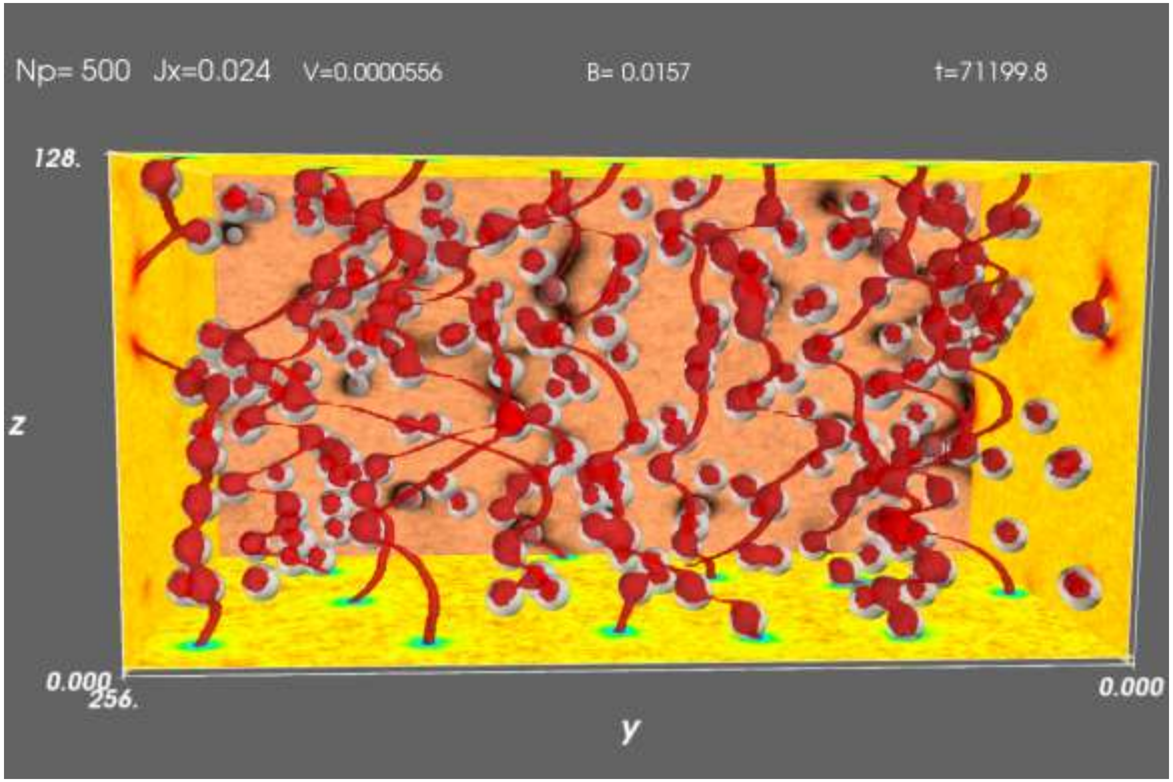


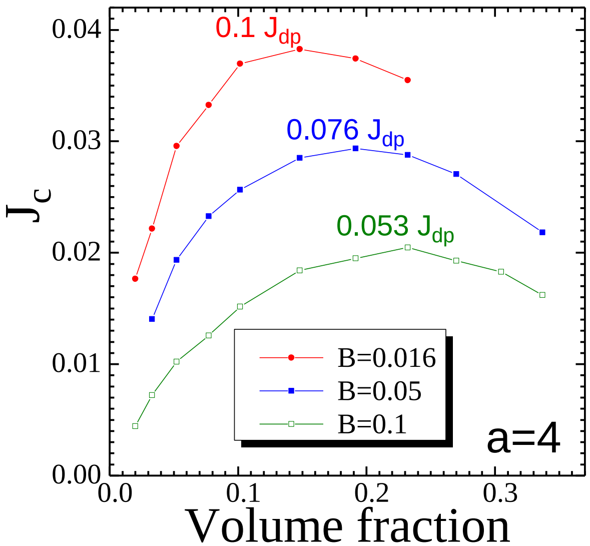
System size: 100x100x50 ξ^3
[256x256x128 mesh points]
Simulation time=10^5 per current

Optimal particle density at fixed magnetic field



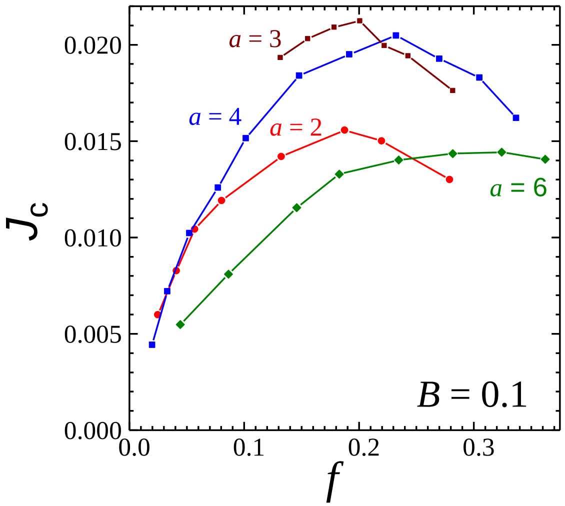
IVs for different numbers of particles (occupied volume fractions)



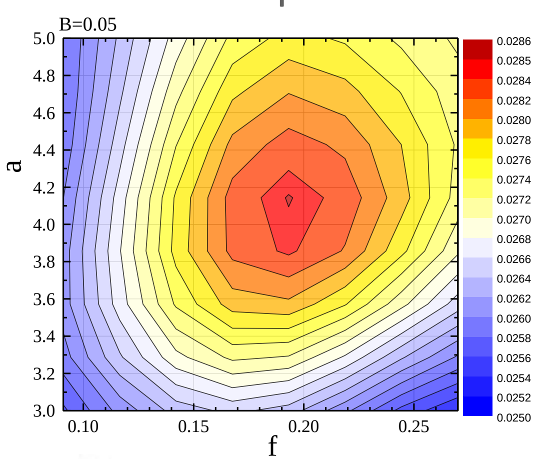


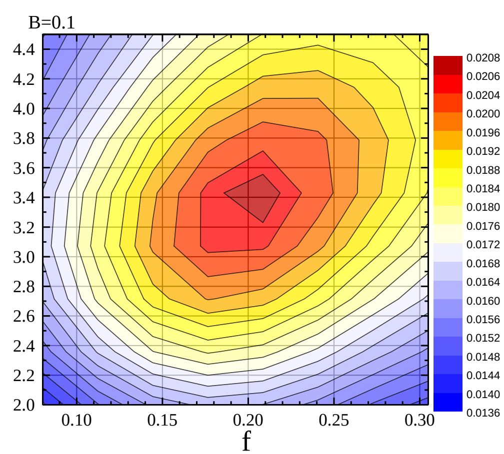
Optimal parameters

Critical current vs particle density for different particle sizes

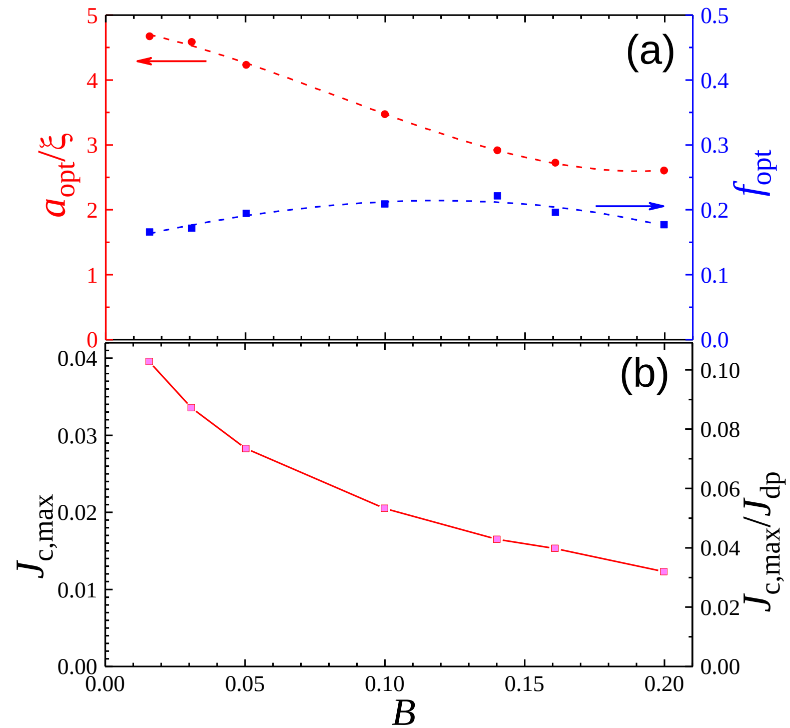


Contour plots of critical current



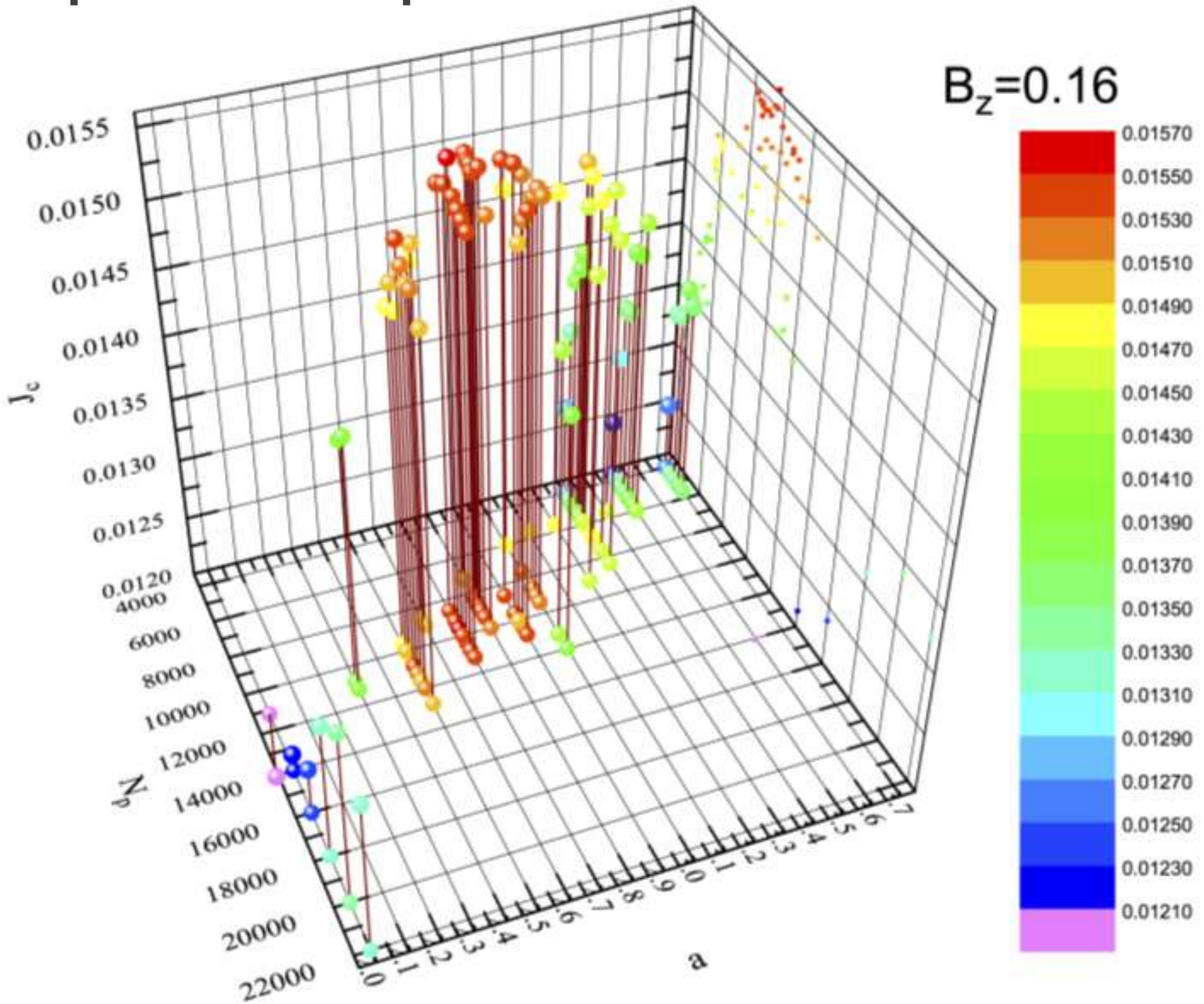


Dependences of optimal parameters on magnetic field



- Optimal particle diameter decreases with field
- Optimal volume fraction = 18-20%

Sampling in parameter space



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Extracting, Tracking, and Visualizing of Vortices

- Extraction & tracking methods
- Tools
- Next steps

see Poster B1 (19)

SDAV

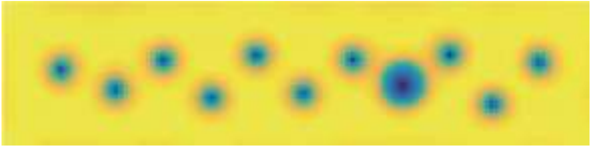
Vortices in superconductors

- Vortices are defined as topological defects of the order parameter field ψ, which are a locus of points satisfy

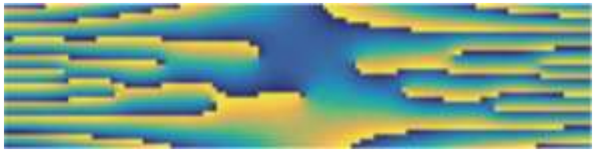
$$|\psi| = 0 \text{ and } -\oint_C \nabla\theta \cdot d\mathbf{l} = 2n\pi,$$

  n is usually +/-1, indicating the chirality
- Vortices are 1D curves in 3D space
- The vortices are fundamentally different from vortices in fluid flow

Amplitude |ψ|

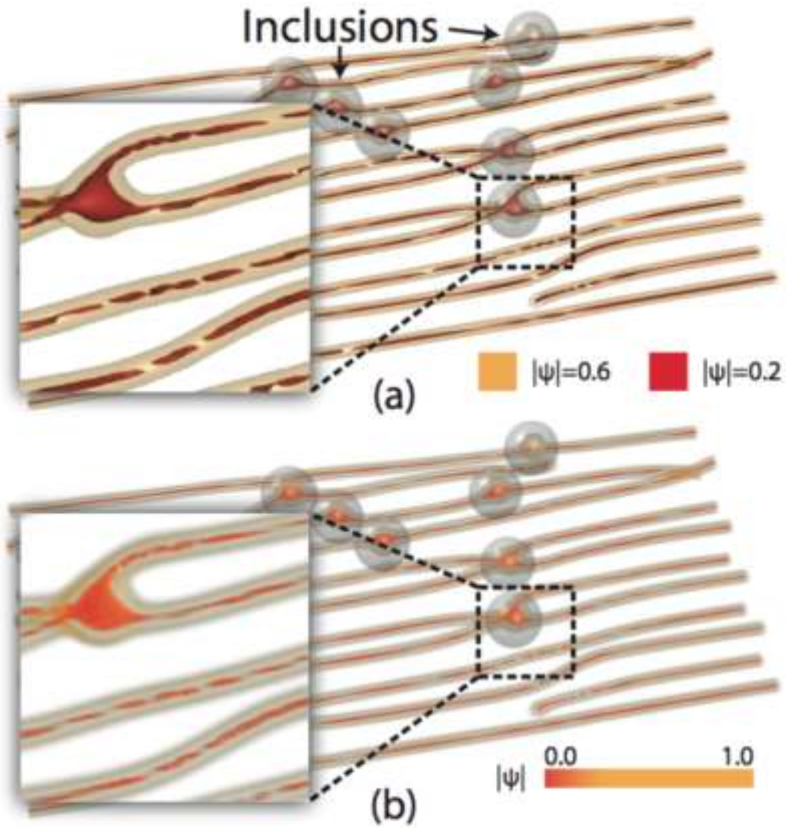


Phase θ



TDGL Data Visualization

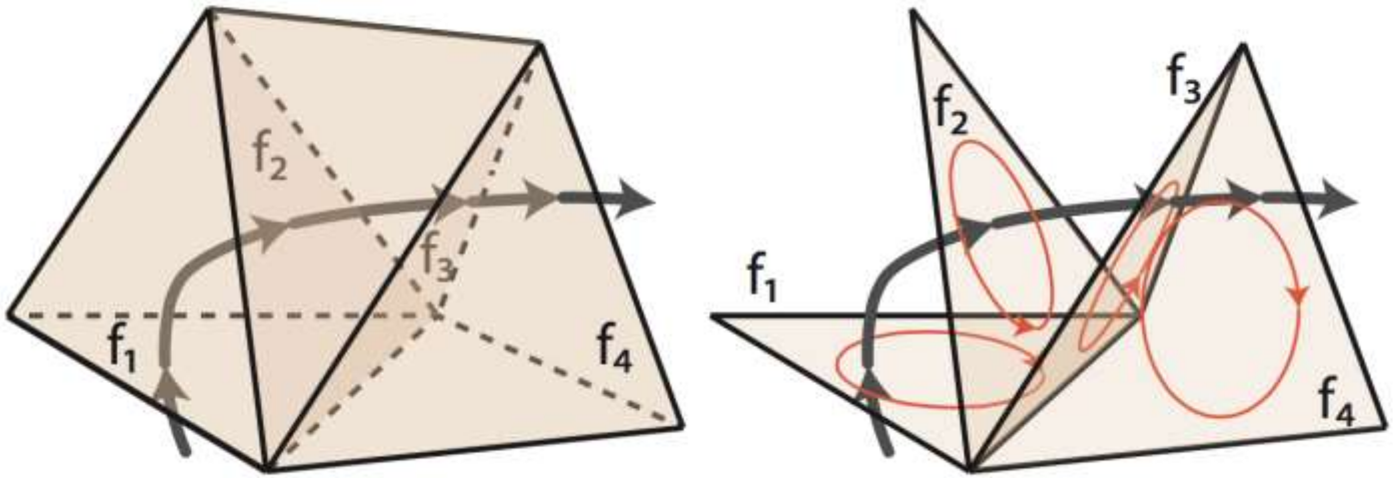
- Little research has been done in visualizing complex-field data
  - Volume rendering/isosurface blur fine features
  - Vortex extraction for single frames in regular grid data is proposed by Phillips *et al.* recently
- Extracting, tracking, and visualizing vortices are the keys to understand the dissipative material behaviors and the impact of adding material inclusions.



Deliverables of a detection algorithm

- A vortex extraction algorithm for both structured and unstructured mesh TDGL data
- A vortex tracking algorithm, which is as accurate as the data discretization
- Application of various visualization techniques

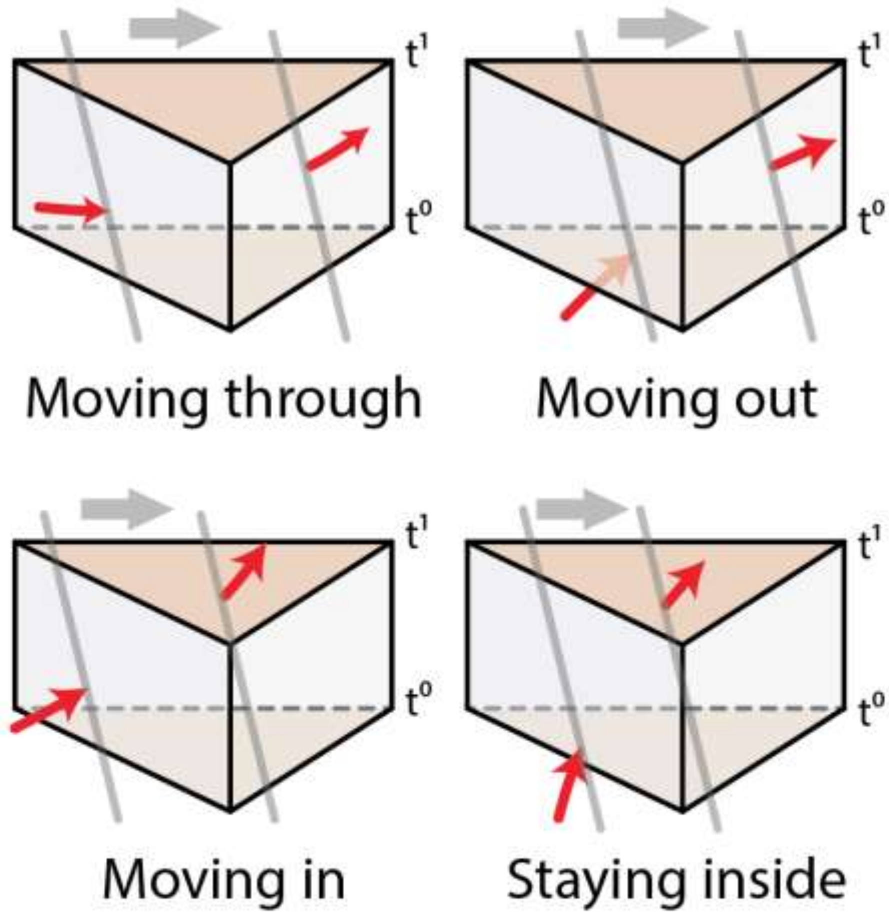
Overview of the Vortex Extraction Algorithm



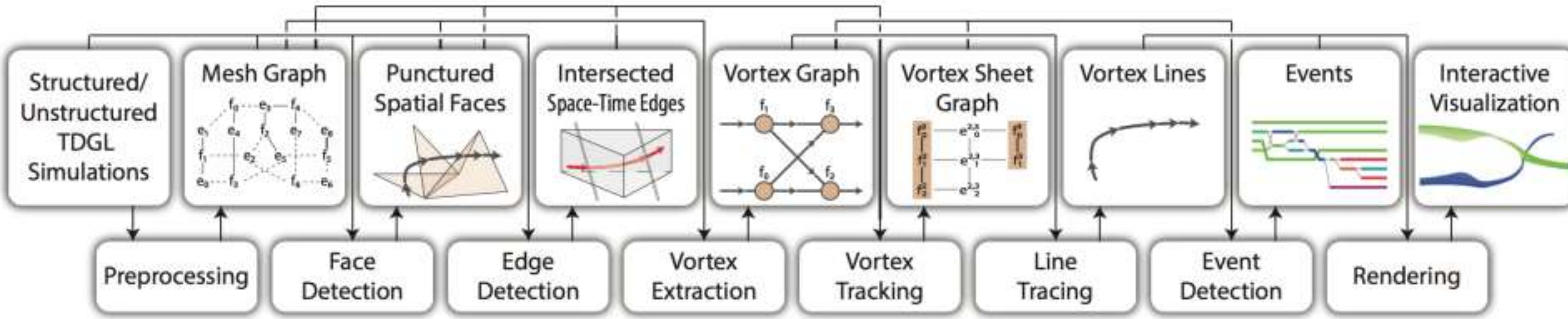
- Vortex extraction locates vortex line at single time frames
  - By definition, singularities can be localized by checking phase jumps over mesh faces.
  - As there are always equal numbers of “ins” and “outs” for each cell, the punctured faces are further connected into vortex lines based on the mesh connectivity.

Overview of the Vortex Tracking Algorithm

- Vortex tracking algorithm relates vortex lines over adjacent frames, unless there are topological changes.
- The movement of a vortex line is detected by checking each space-time edge to see whether it is intersected at an intermediate time between two adjacent frames.



Algorithm Pipeline

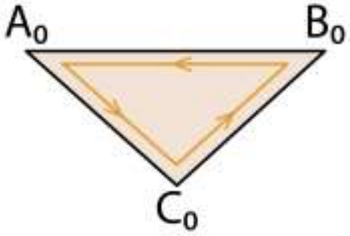


- Load data
- Extract punctured spatial faces
- Extract intersected space-time edges
- Graph-based vortex extraction and tracking

Algorithm Details - Punctured Face/Intersected Edge Detection

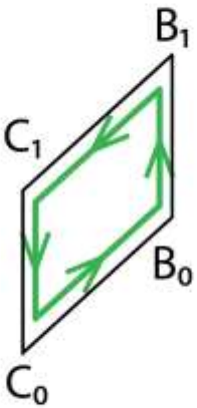
- Phase jump over faces

$$n = -\frac{1}{2\pi}\oint_C \nabla\theta \cdot d\mathbf{l}$$

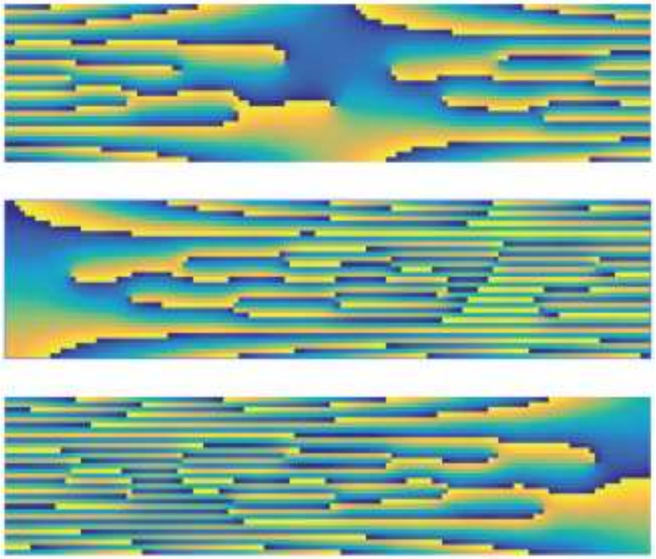


- Phase jump over space-time edges

$$n = -\frac{1}{2\pi}\oint_C \hat{\nabla}\theta \cdot d\hat{\mathbf{l}}$$



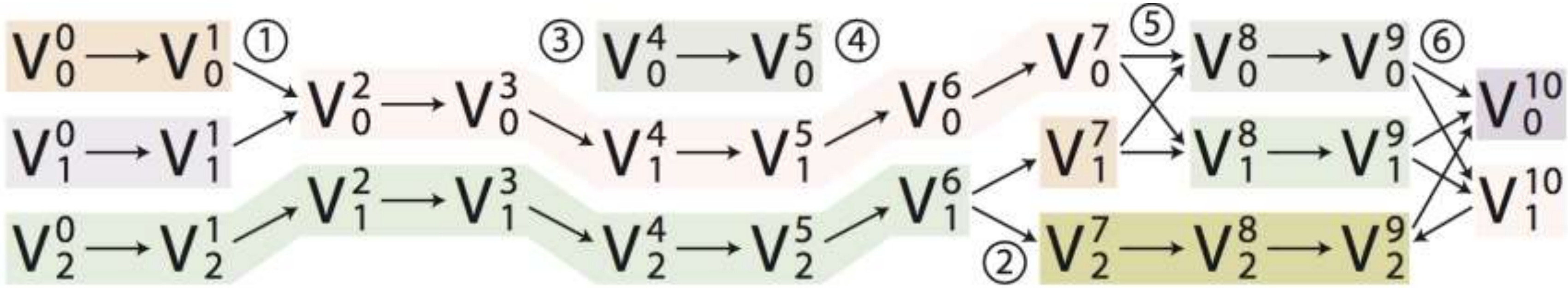
- Gauge transformation



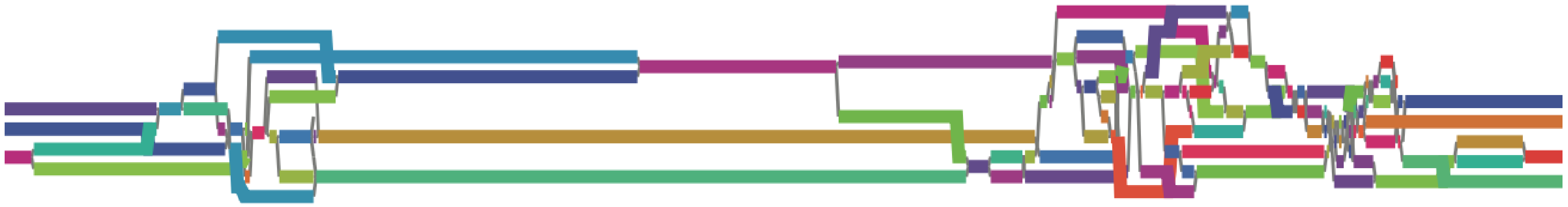
*) Always use local transformations to compute phase jumps

Event Detection and Visualization

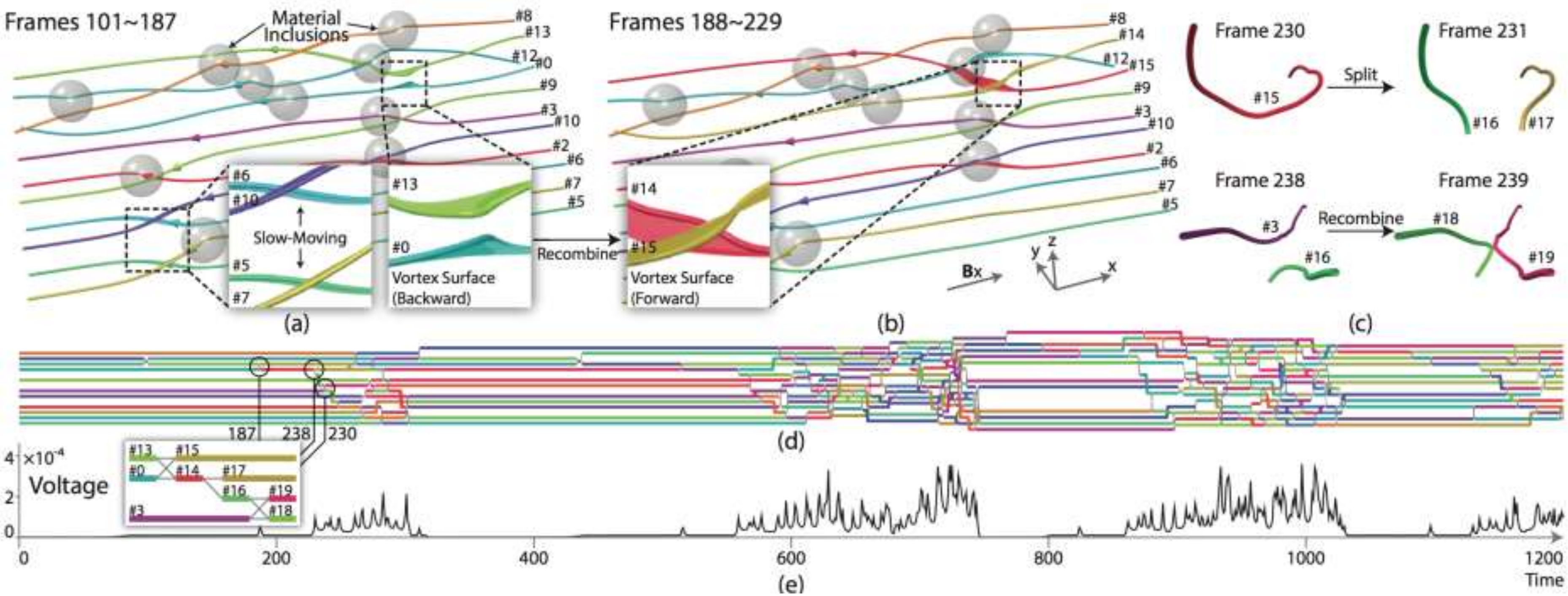
- Events are defined as topological changes of vortex graphs: merging, splitting, birth, death, recombination/crossing, etc.



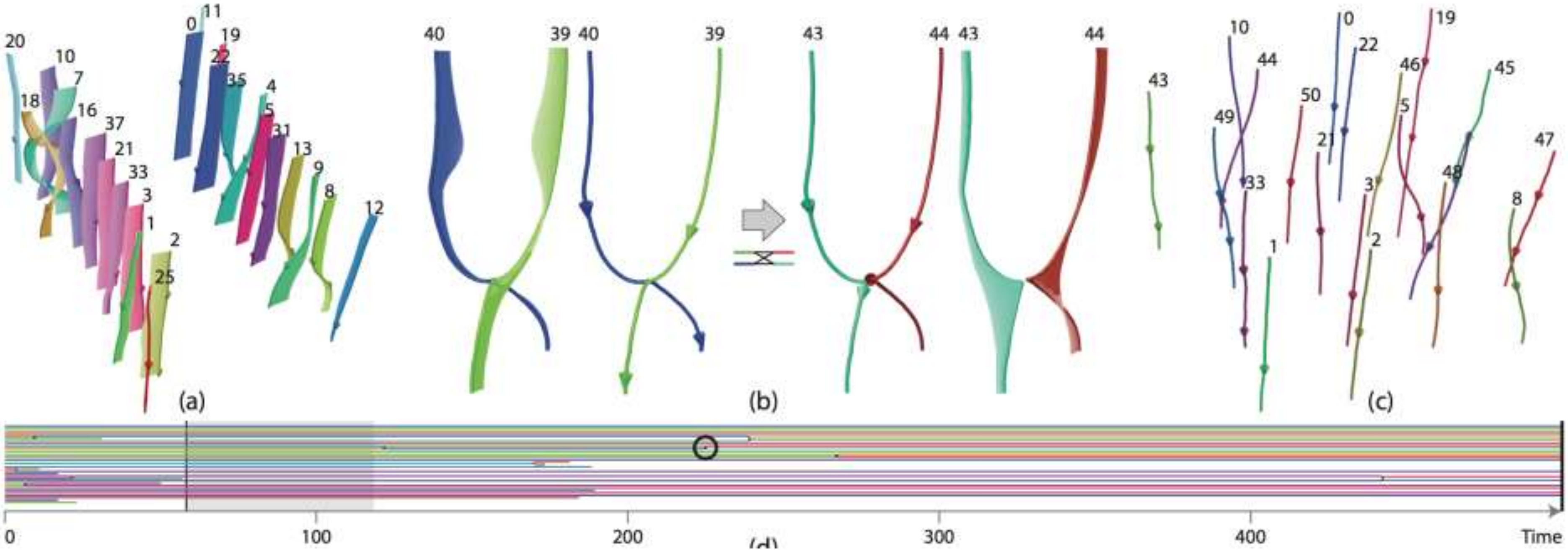
- Event visualization is based on storyline-like visual representations [Tanahashi and Ma 2012]



Results – 3D Structured Grid Data



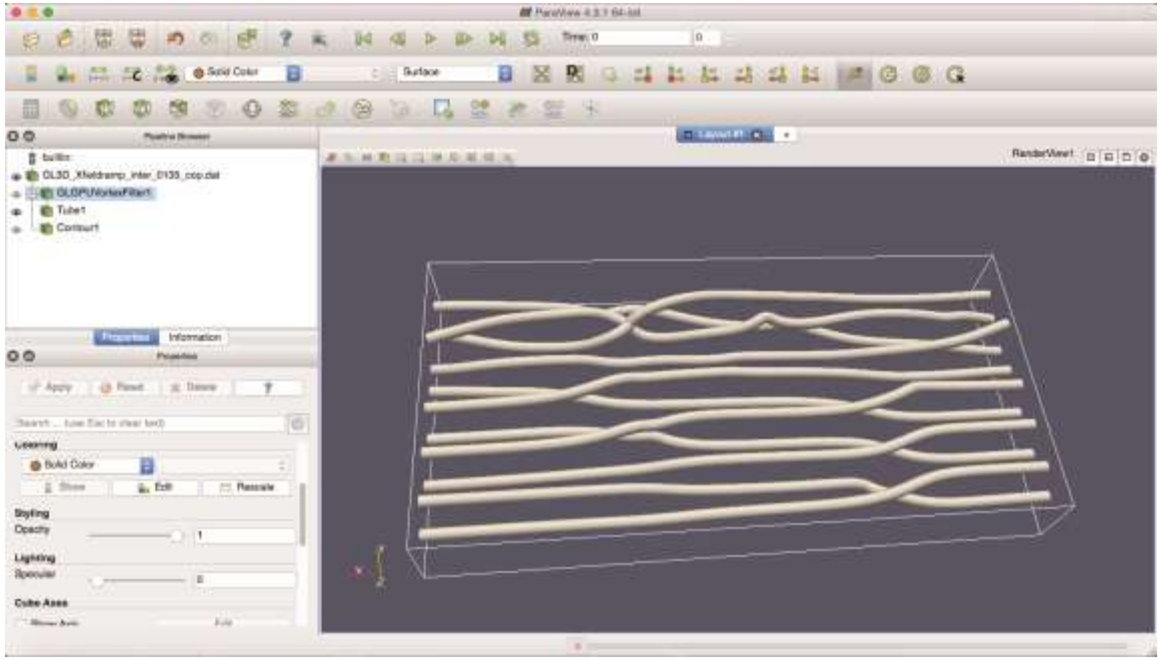
Results – 3D Unstructured Data



Guo et. al., Proc. IEEE SciVis (2015)

Software Development and ParaView Plugins

- A standalone visualization tool, as well as a ParaView plugin are developed for loading, analyzing, and visualizing TDGL simulation data.
- The unstructured mesh data structures are based on libMesh, which is the finite element library used by the simulation. The framework can be integrated with the simulation for in-situ analysis in the future.

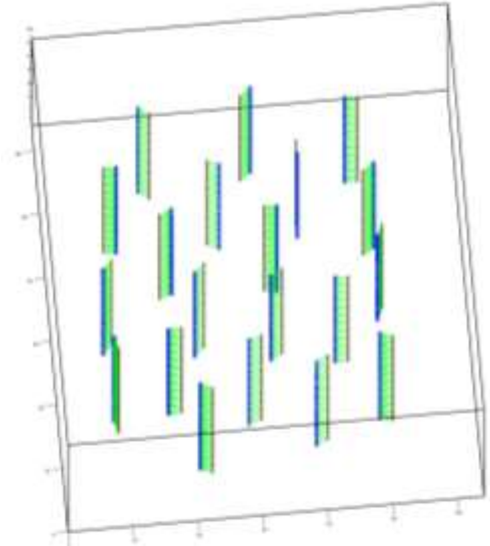


ParaView

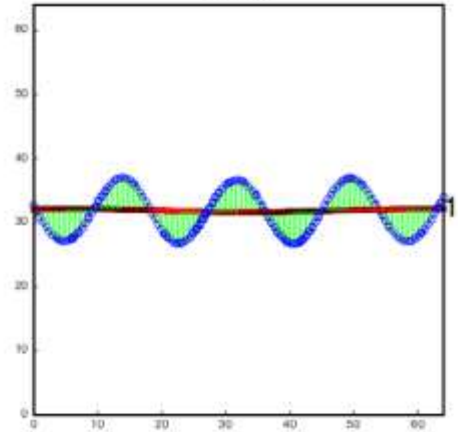
Next steps: Twist, Writhe, and Stabilizing Helical Vortices

- 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.

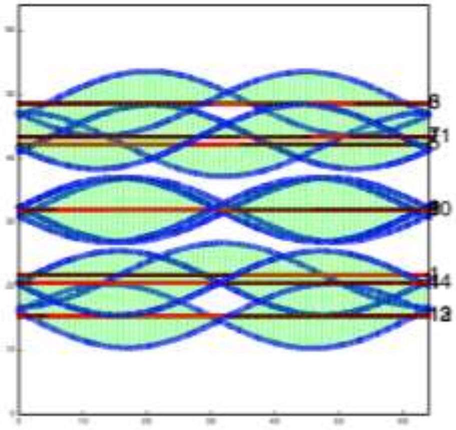
No Twist



Twisting phase field



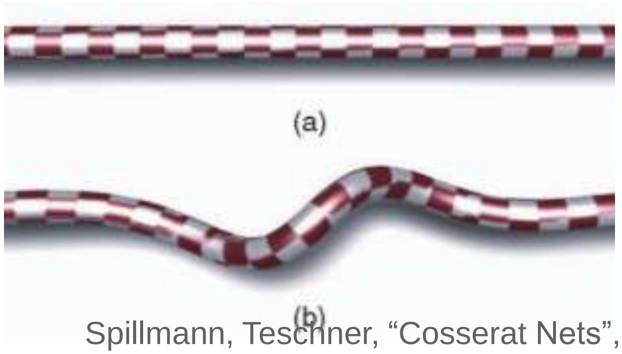
Twisting phase field



Excess Twist leads to Writhe

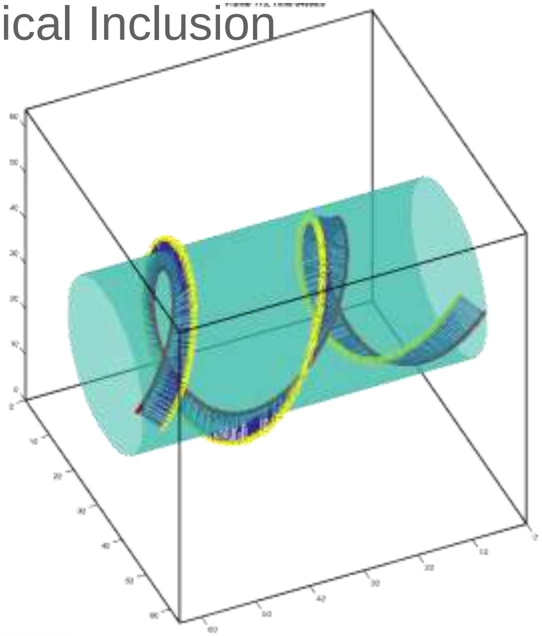
- Twist → Buckling Instability → Writhe of Filament/Rod/Vortex
- Perpendicular Lorentz Forces on writhing vortex → helical coils unstable. "Blows up" (Superconducting state lost): New criterion for upper limit of the critical current
- However, if vortex inside a cylindrical inclusion, cylinder can "traps" helical vortex state. (Superconducting state retained)

Twisted Rod Buckles and Writhes



Spillmann, Teschner, "Cosserat Nets", 2009

Stable Helical Twisted Vortex in Cylindrical Inclusion



Acknowledgements

The OSCon Team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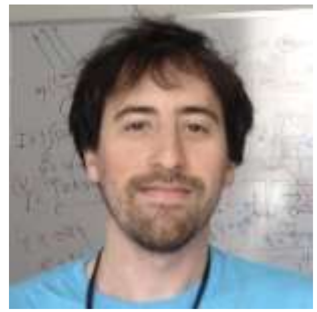
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