Large-Scale Dynamics Simulations of Superconductors: New Fundamental Scientific Insights, Computational Challenge, and Broad Impact

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Outline

- Motivation
- **Vortex Dynamics & Pinning**
- **Ginzburg-Landau Theory**
- **Scientific & Computational Challenges**
- Broader Impact
- SciDAC Team & Collaborations

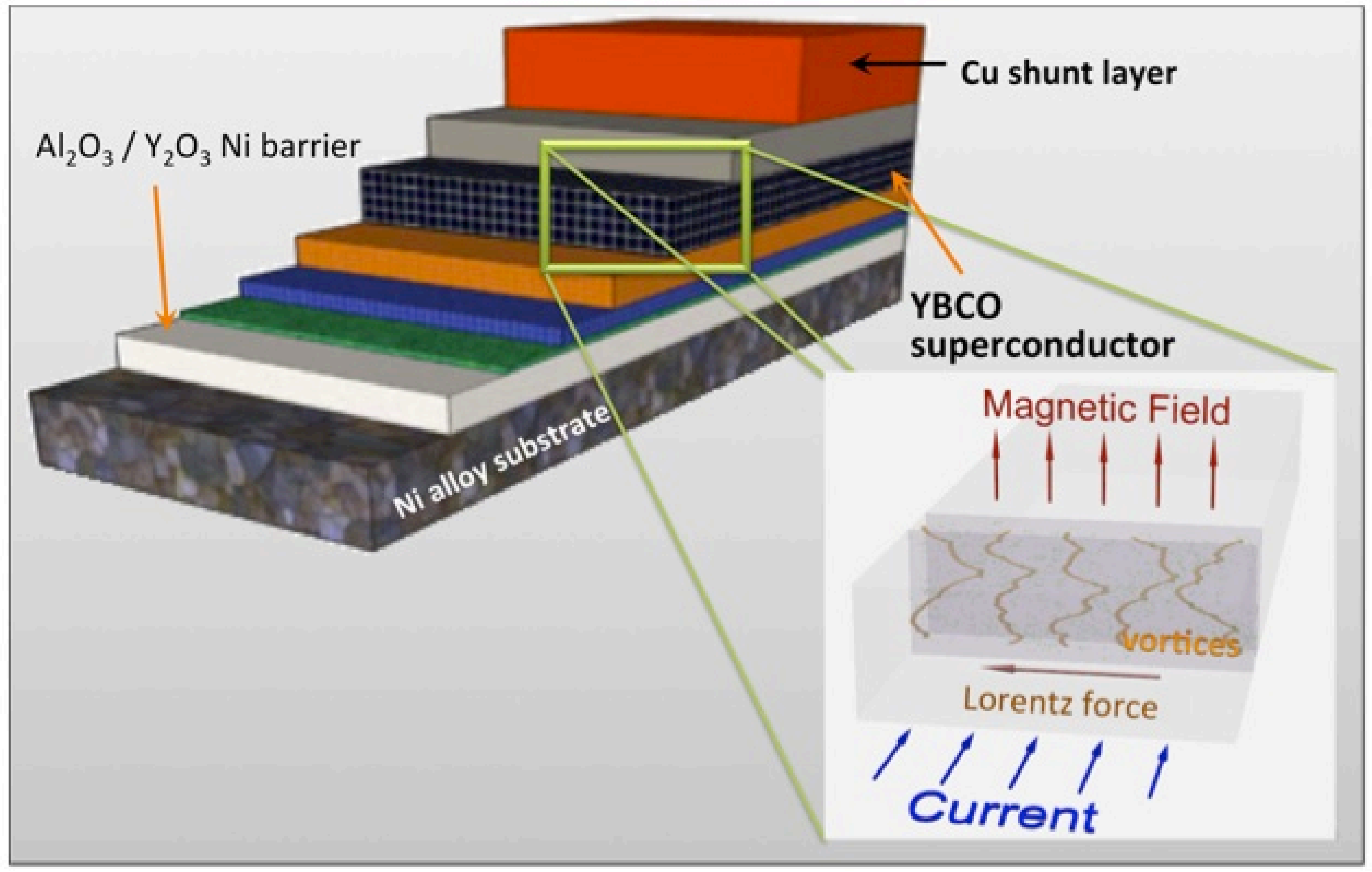
SciDAC OSCon: *"Optimizing SuperConductor Transport Properties through Large-Scale Simulation"*

This SciDAC Partnership will develop and apply novel methods for optimizing superconductors for energy applications using large-scale computational algorithms and tools.

OSCon is a joint effort of Argonne's Materials Science Division (MSD) and the Mathematics and Computer Science Division (MCS)

Motivation: Lossless energy transport in through superconducting cables

1st generation cable including insulation & cooling ↓



← 2nd generation cable with illustration of vortex motion

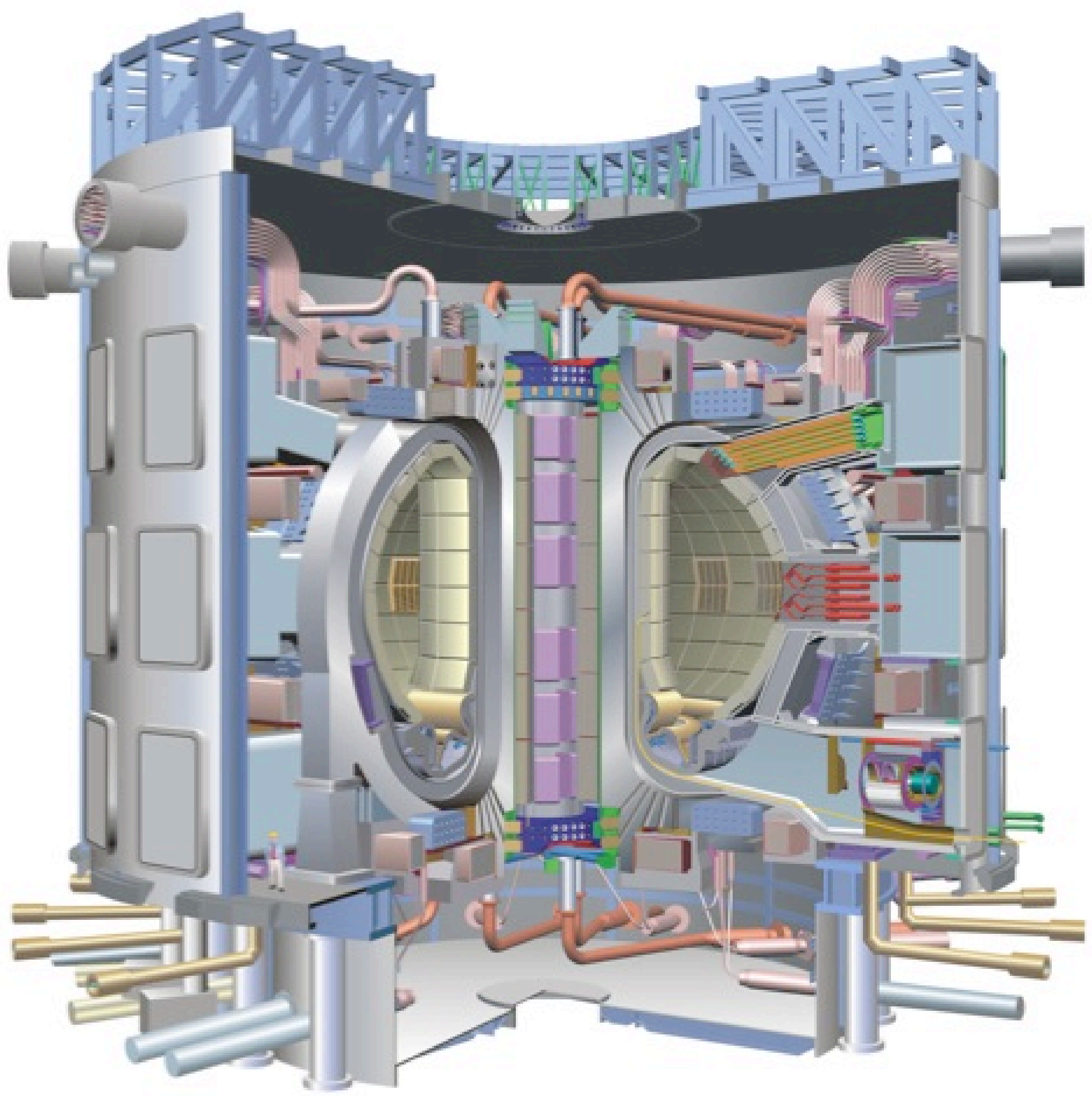
high-current transmission (in urban areas, here NY) ↓

compact generators & motors ↓

Other applications

LHC magnets

Maglev trains



ITER magnets

Diagnostic applications (MNR, MRI, …)

Superconducting cables

- 5x power capacity of copper in same cross-sectional area
  - Relieve urban power bottleneck in cities and suburbs
- Cables operating at 77 K are technically ready
  - in-grid demonstrations at Copenhagen DK, Albany NY, Long Island NY, Columbus OH, New Orleans LA, Amsterdam

Barriers to grid penetration

- Reduce cost by factor 10 - 100 to compete with copper
- Demonstrate reliable multiyear operation

Example: The Power Grid Challenge

capacity

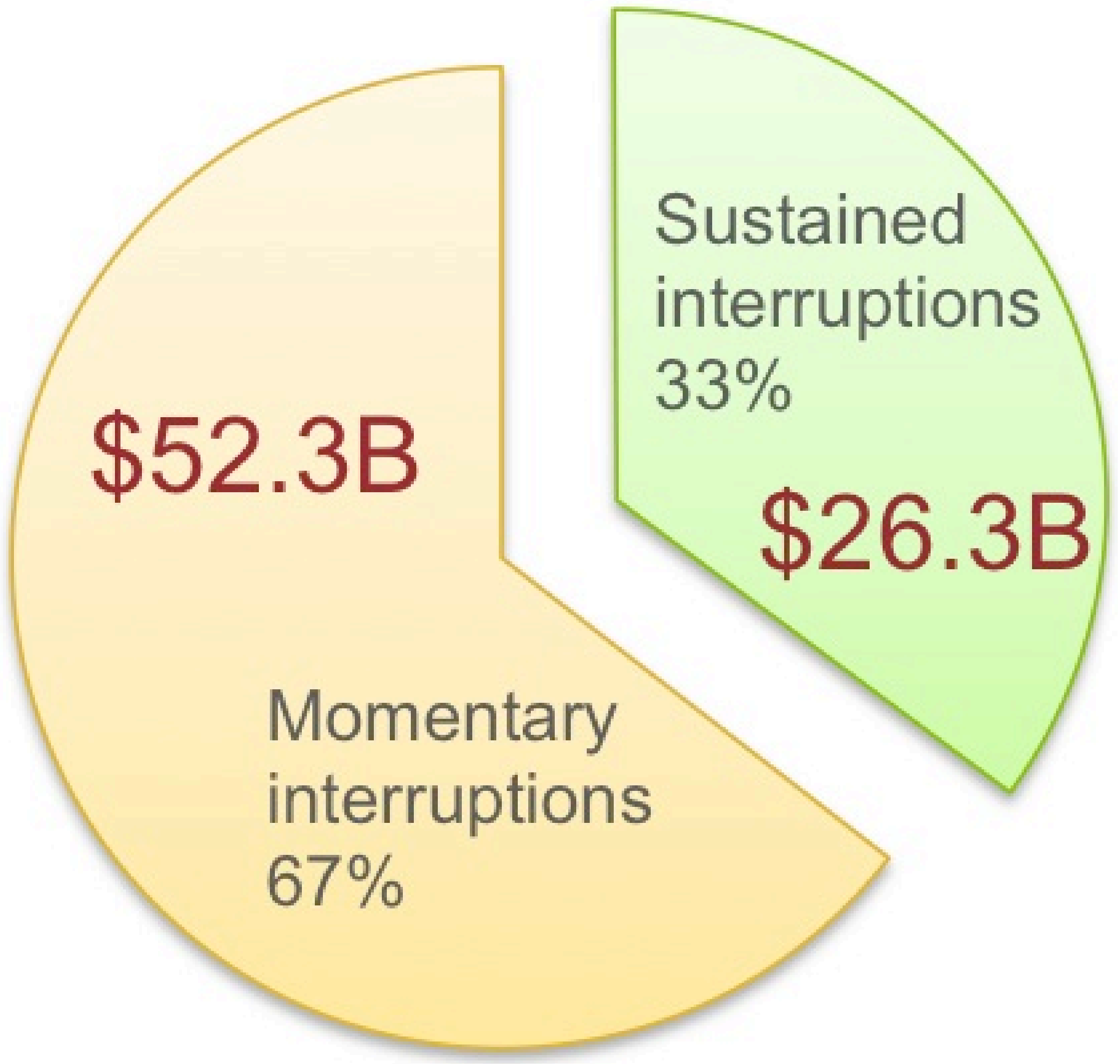
growing demand in cities and suburbs
high people/power density
→ urban power bottleneck

projected:
50% demand growth in the US
100% worldwide by 2030

reliability & power quality

average power loss/customer

	[min/yr]
US	214
France	53
Japan	6 (before 2011)



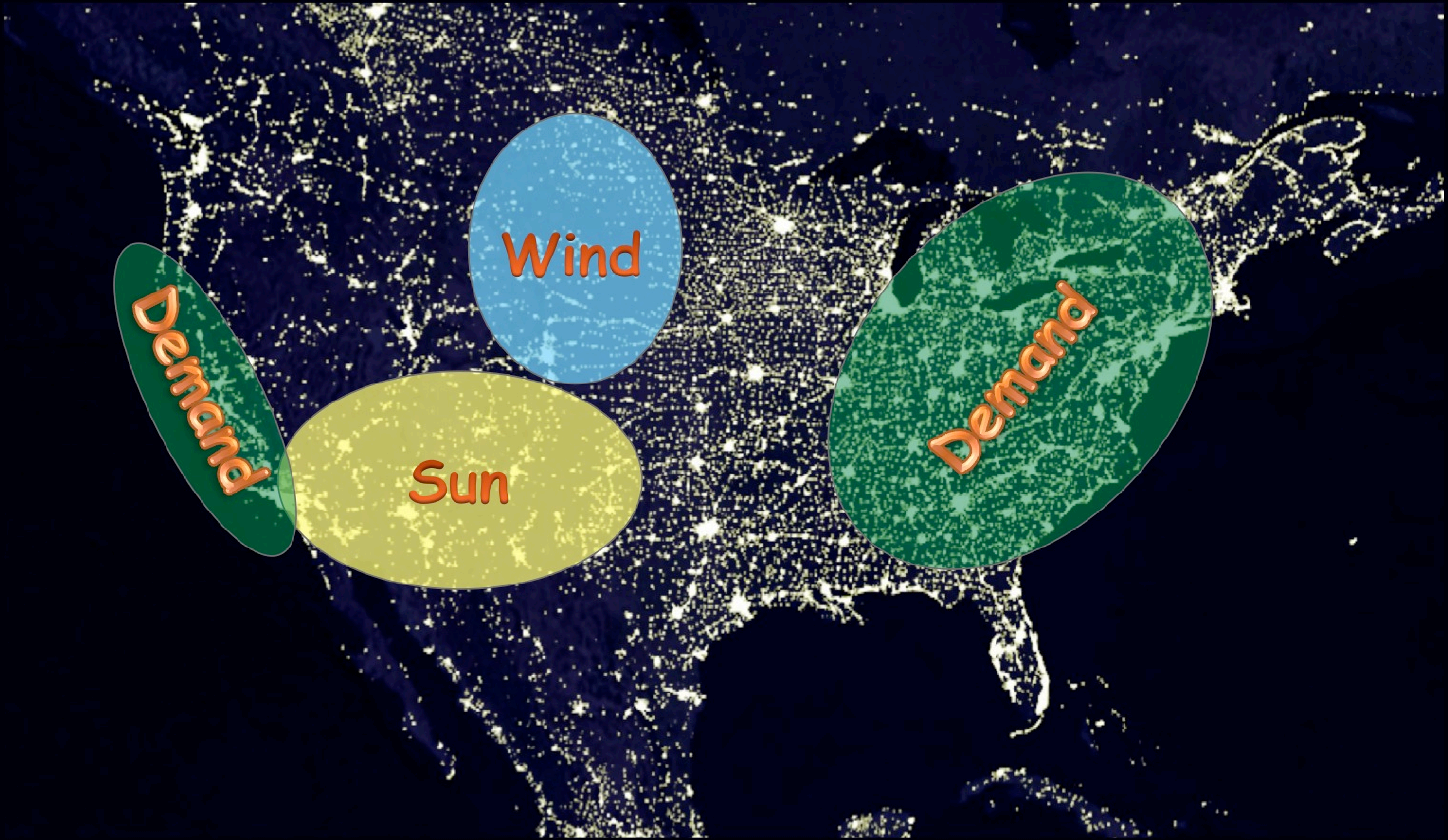
$79B economic loss in US

LaCommare & Eto, Energy 31, 1845 (2006)

accommodation of renewables

17% of total electricity supply by 2020 – sources distant from load centers

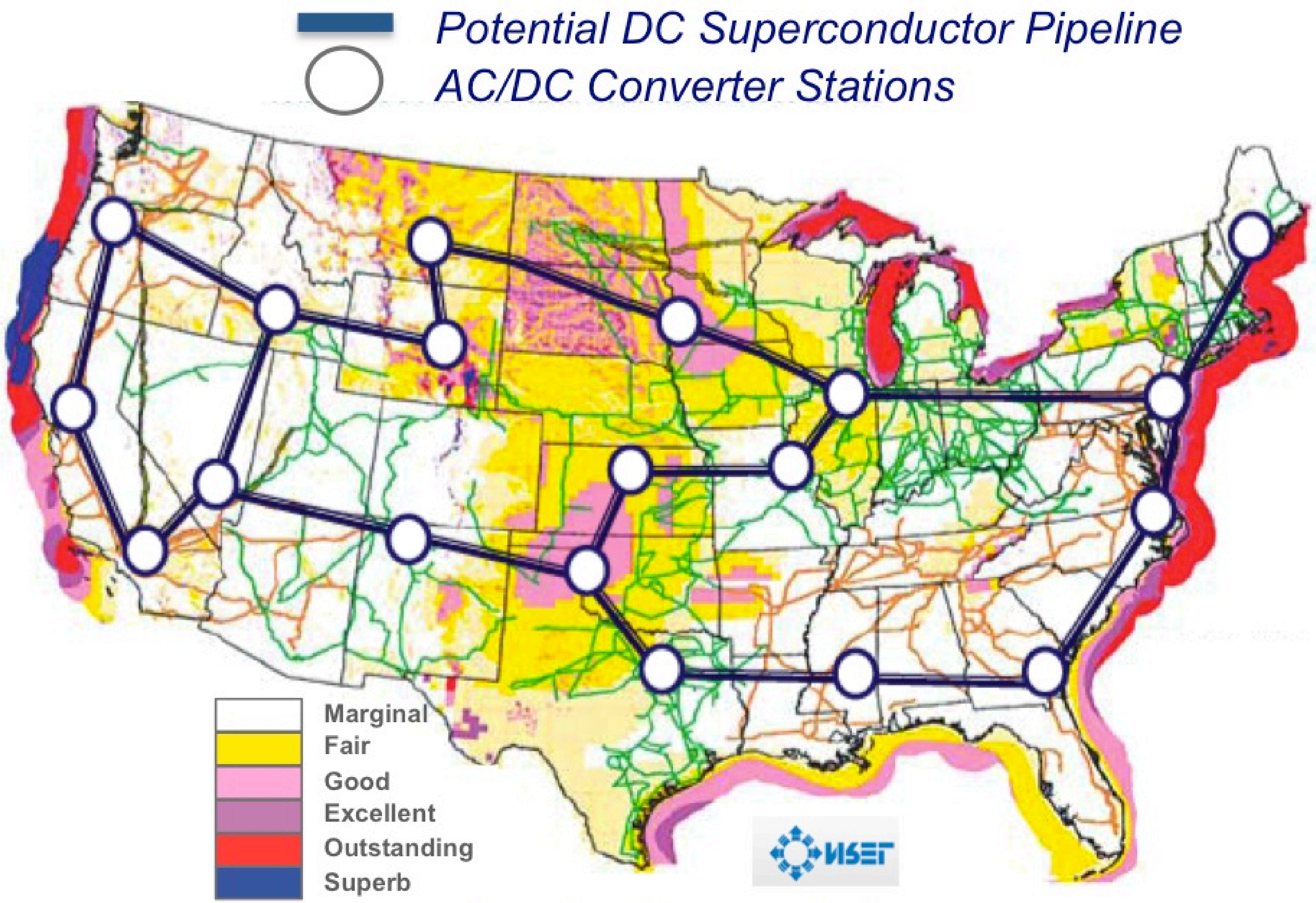
Making the Grid Ready for Renewables



breakthroughs needed for
long distance reliable, efficient delivery of electricity

Long Distance DC Superconducting Transmission

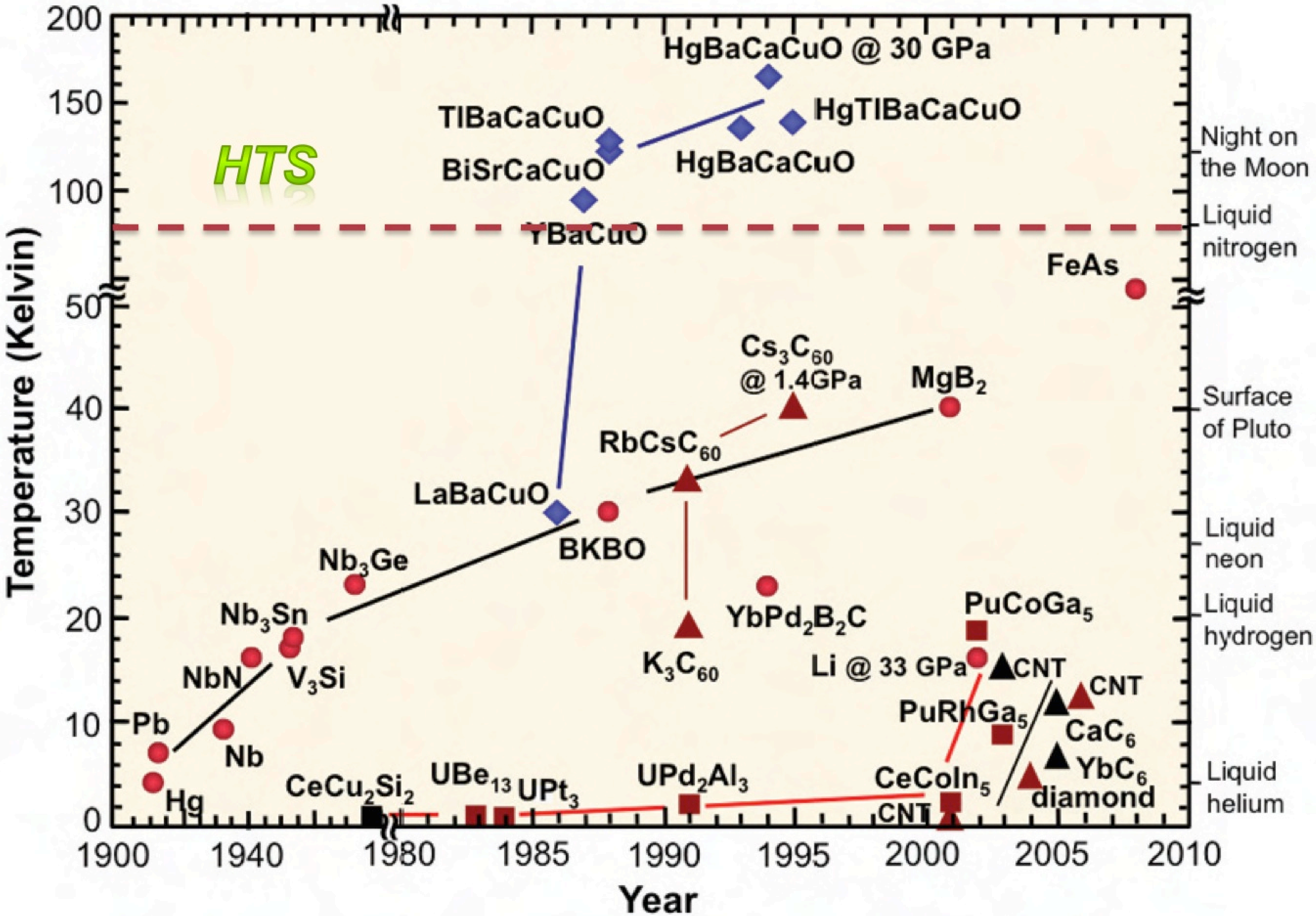
- high capacity: 5 -10 GW
- low voltage: 200 kV vs 765 kV
- reduced right of way:
  25 ft vs 600 ft
- no AC losses: reduced cooling



American Superconductor Corporation

An Interstate Highway System for Electricity

Superconducting Materials

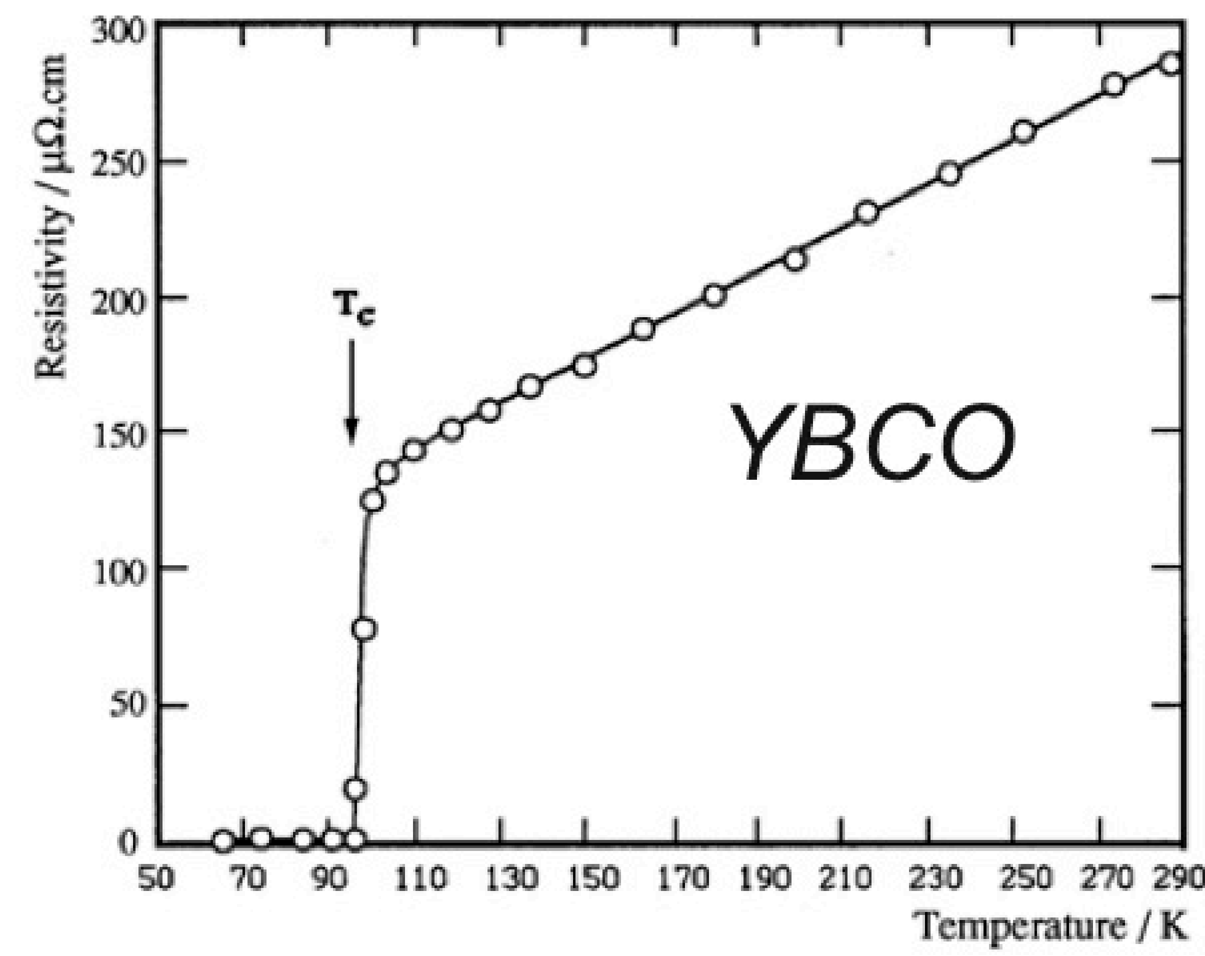


Superconductivity

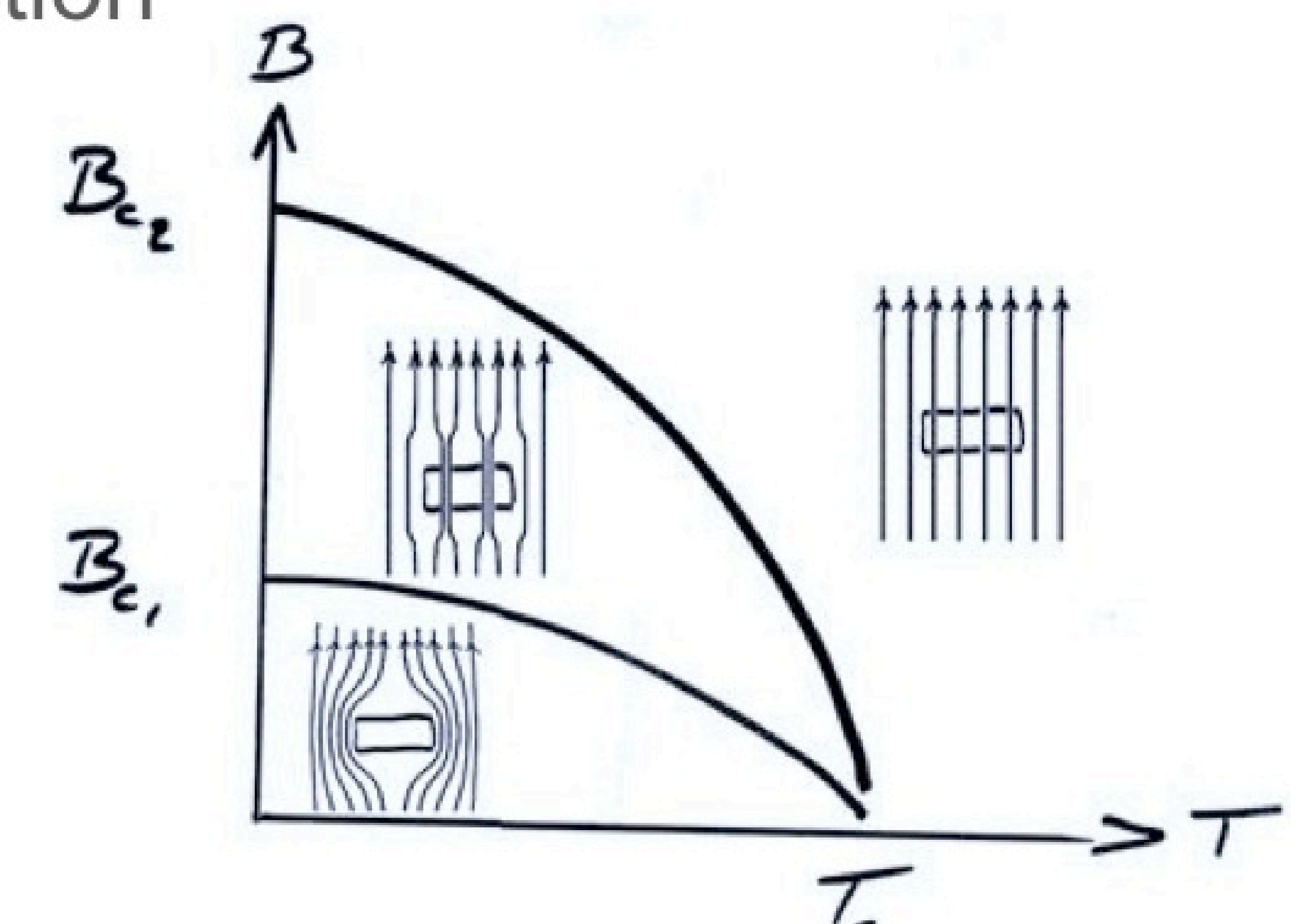
perfect conductor + diamagnet = superconductor

Meissner effect

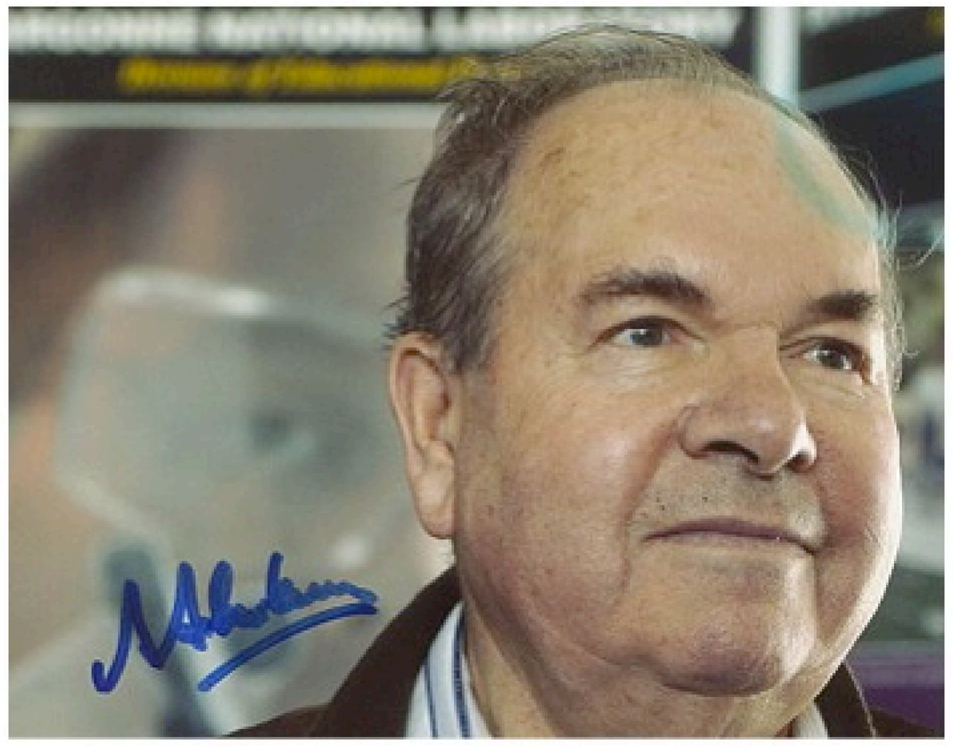
- discovered 1911
- resistance goes to zero at critical temperature T_c
- no dissipation
- type I
  - magnetic field is screened up to B_c, $T_c \rightarrow 0$ above
  - T_c very small
- type II
  - magnet field can penetrate in ***vortices*** without destruction of the SC for $B_{c1}<B<B_{c2}$
  - T_c can be "high"



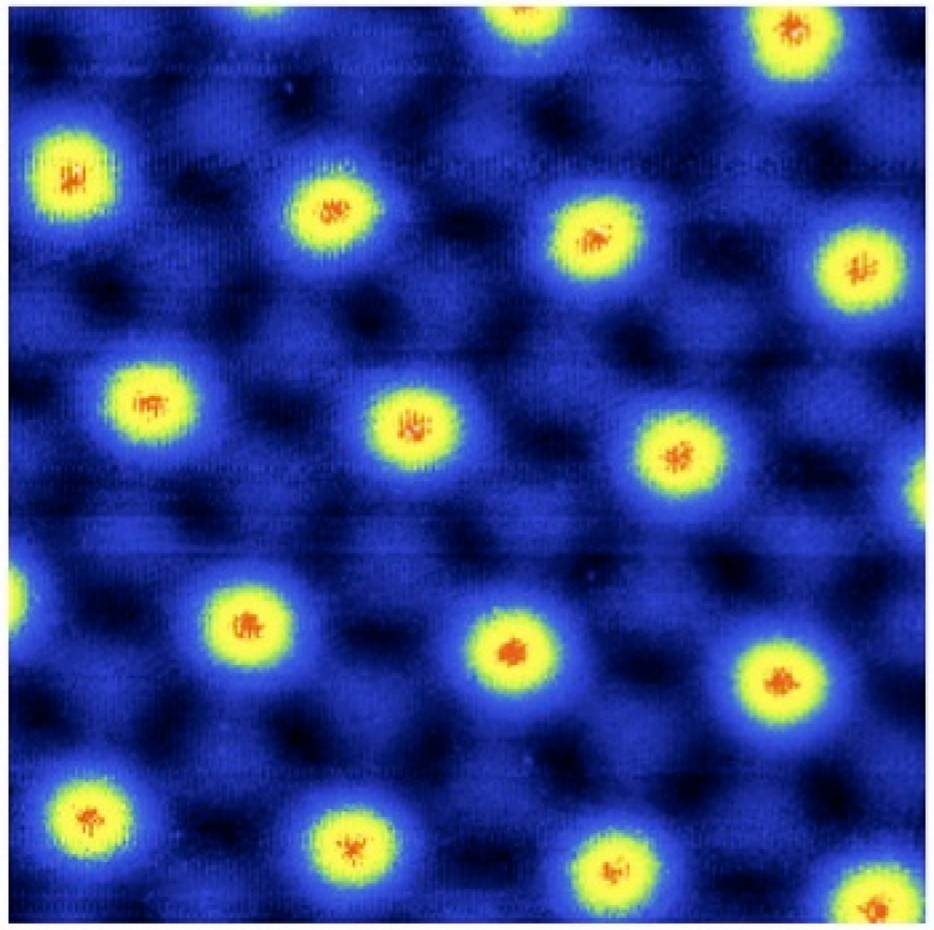
YBCO & BiSCO:
$B_{c1} \approx 0.03T$, $B_{c2} \approx 120T$



Vortices



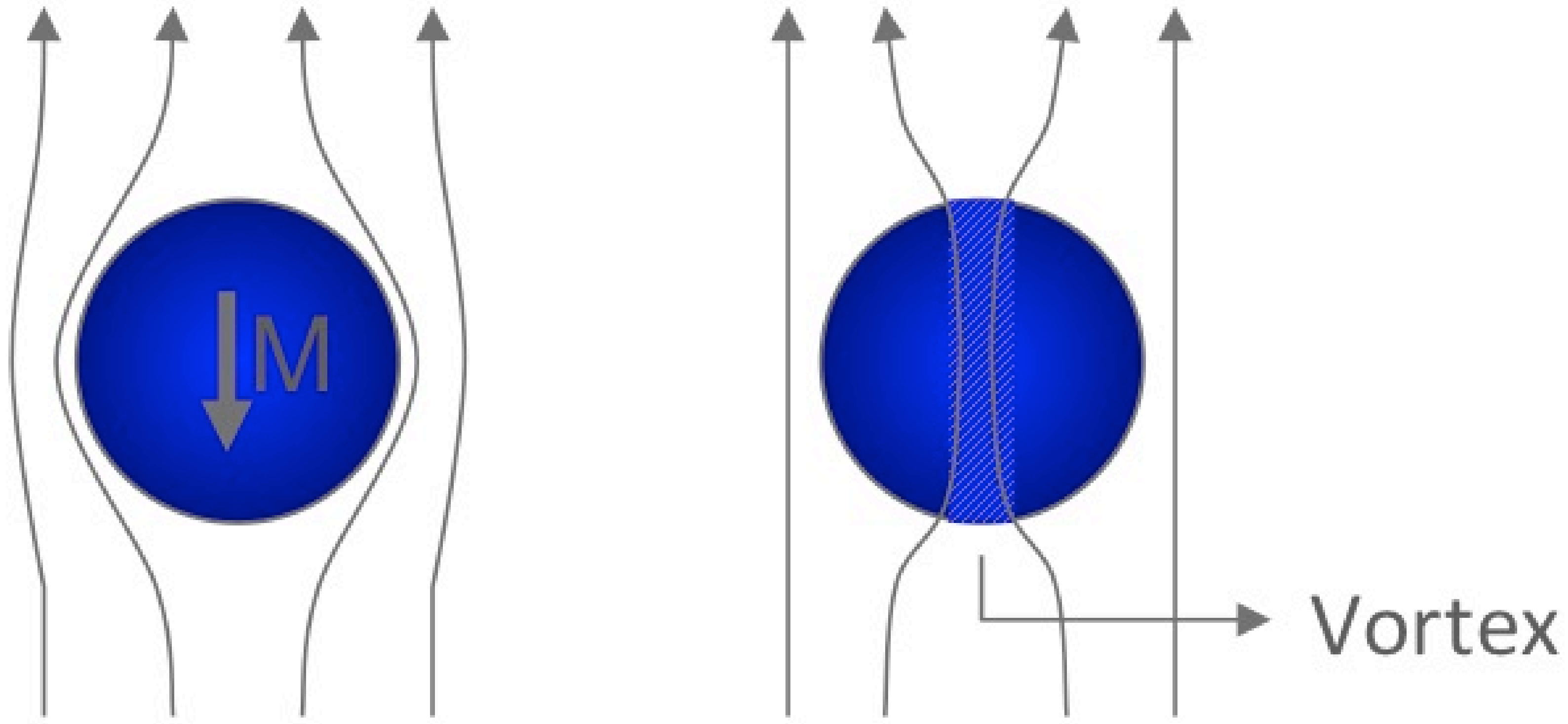
Alexei Alexeyevich Abrikosov *(Nobel Prize 2003)*



vortex lattice (STM image, RIKEN)

Vortices

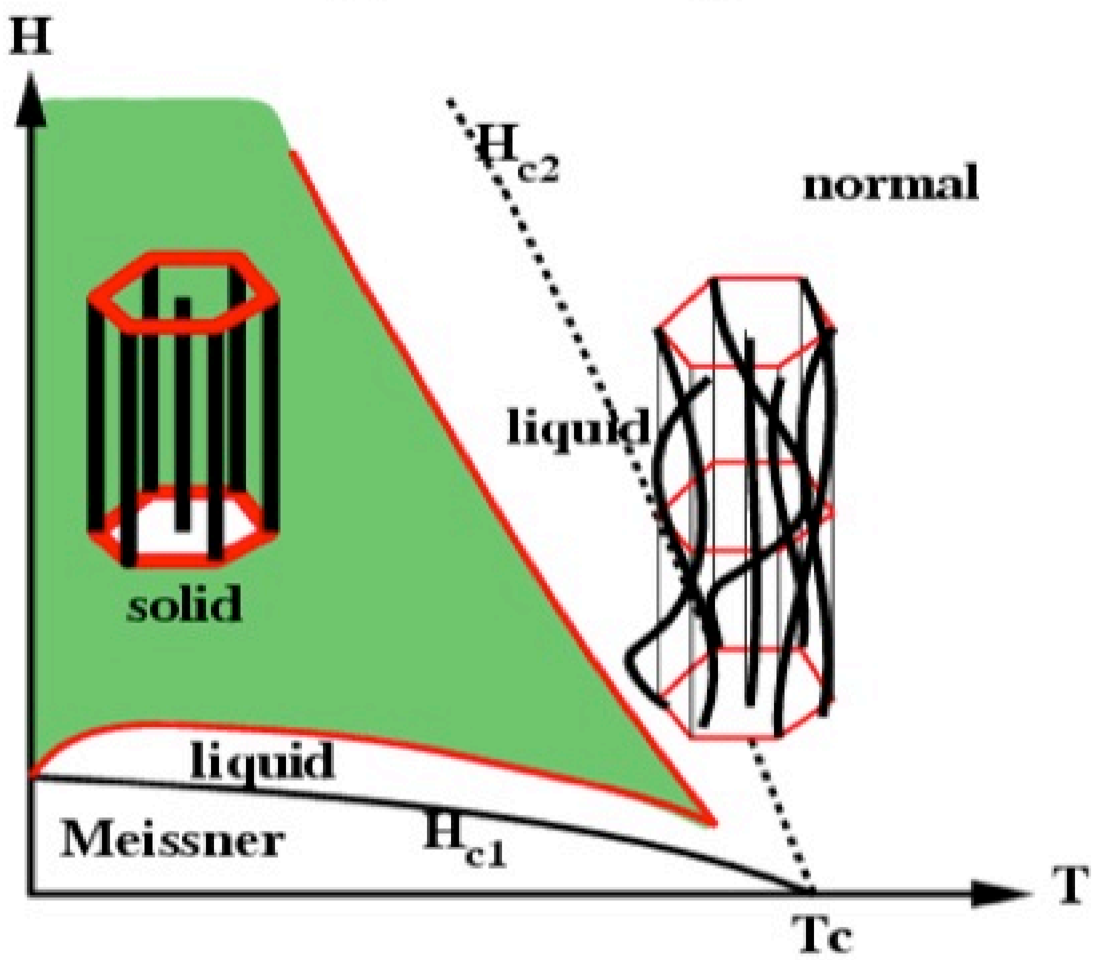
- are (normal) quantized flux tubes
- through which the magnetic field
- penetrates type II superconductors
- they are screened by *supercurrents*

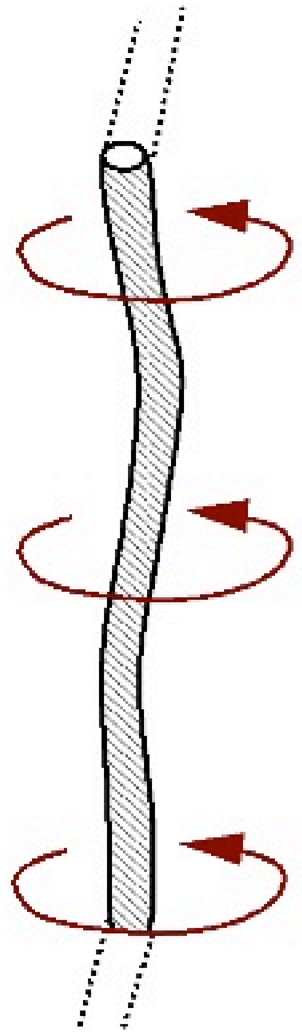


$B < B_c, B_{c1}$

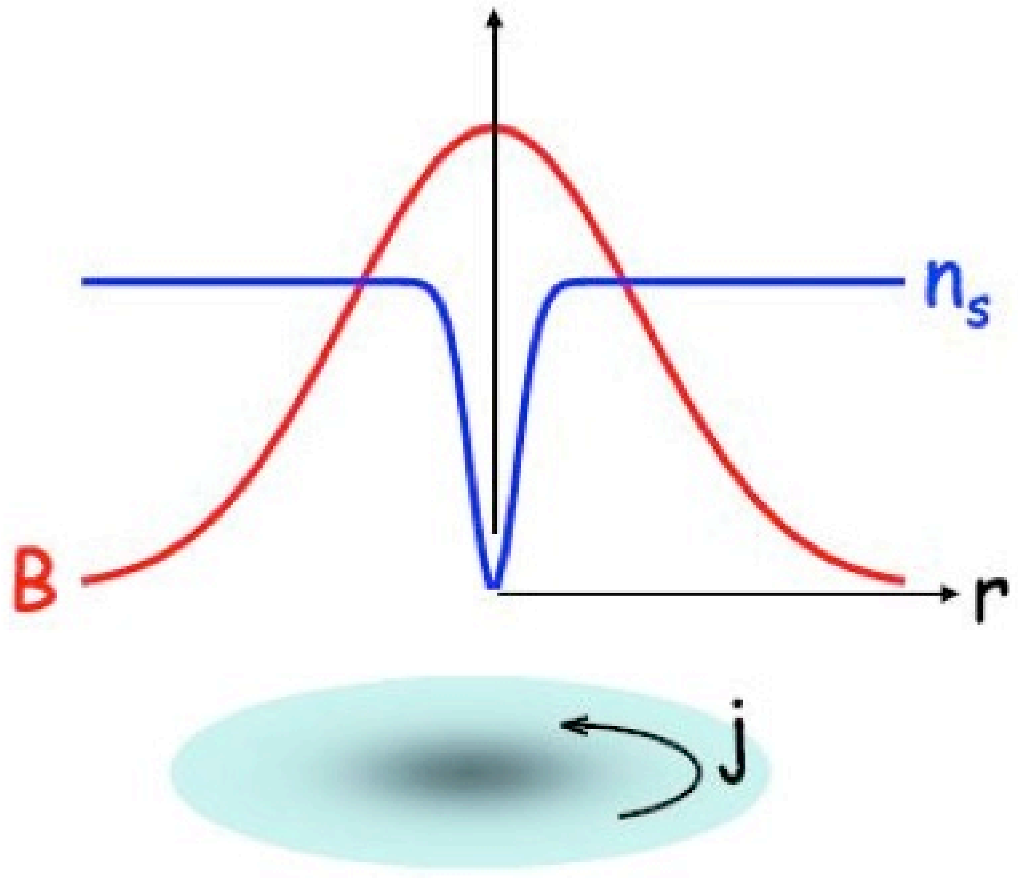
$B_{c1} < B < B_{c2}$

phases of "vortex matter" ➔

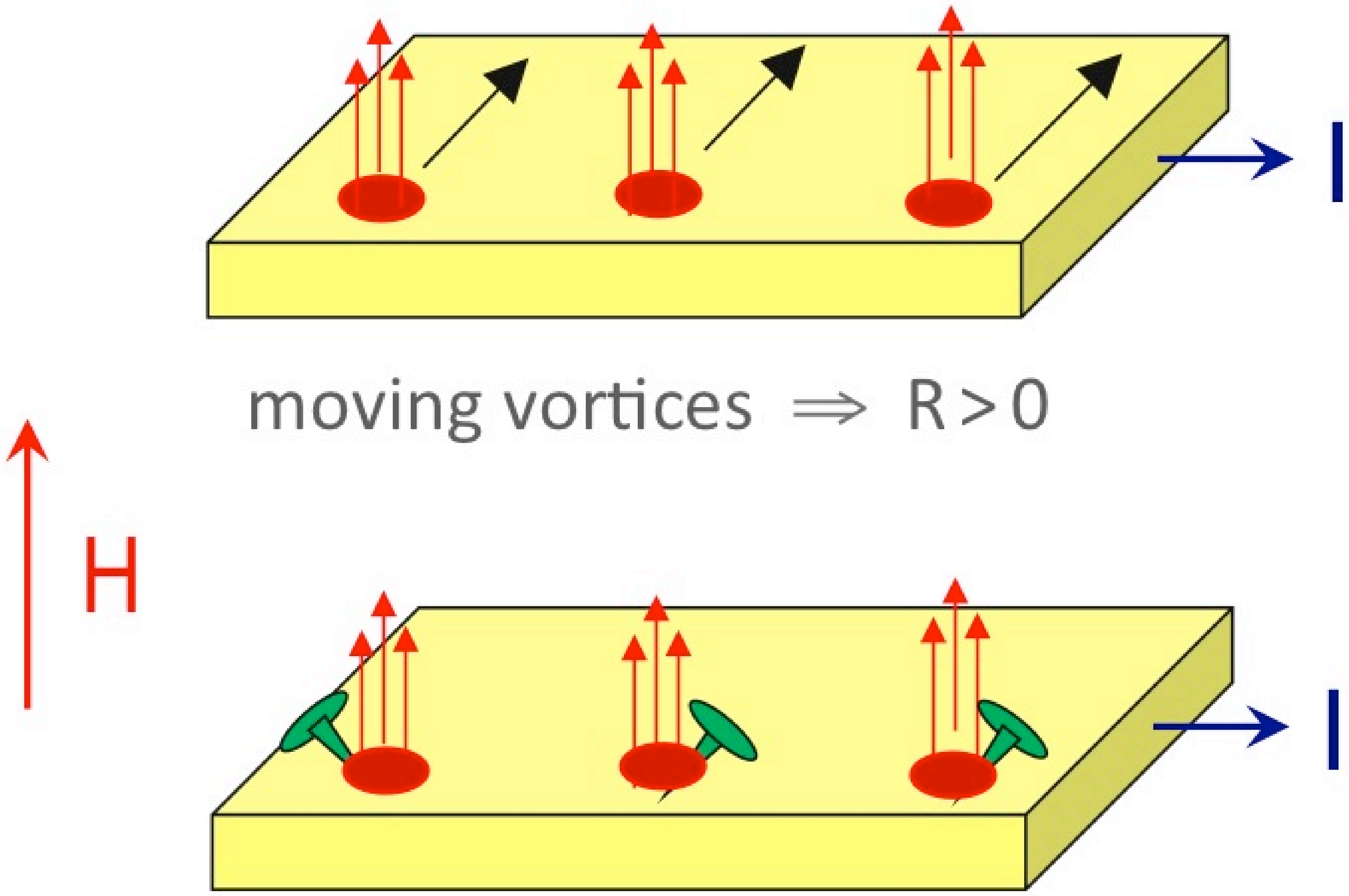




screening currents and field & superconducting density distribution

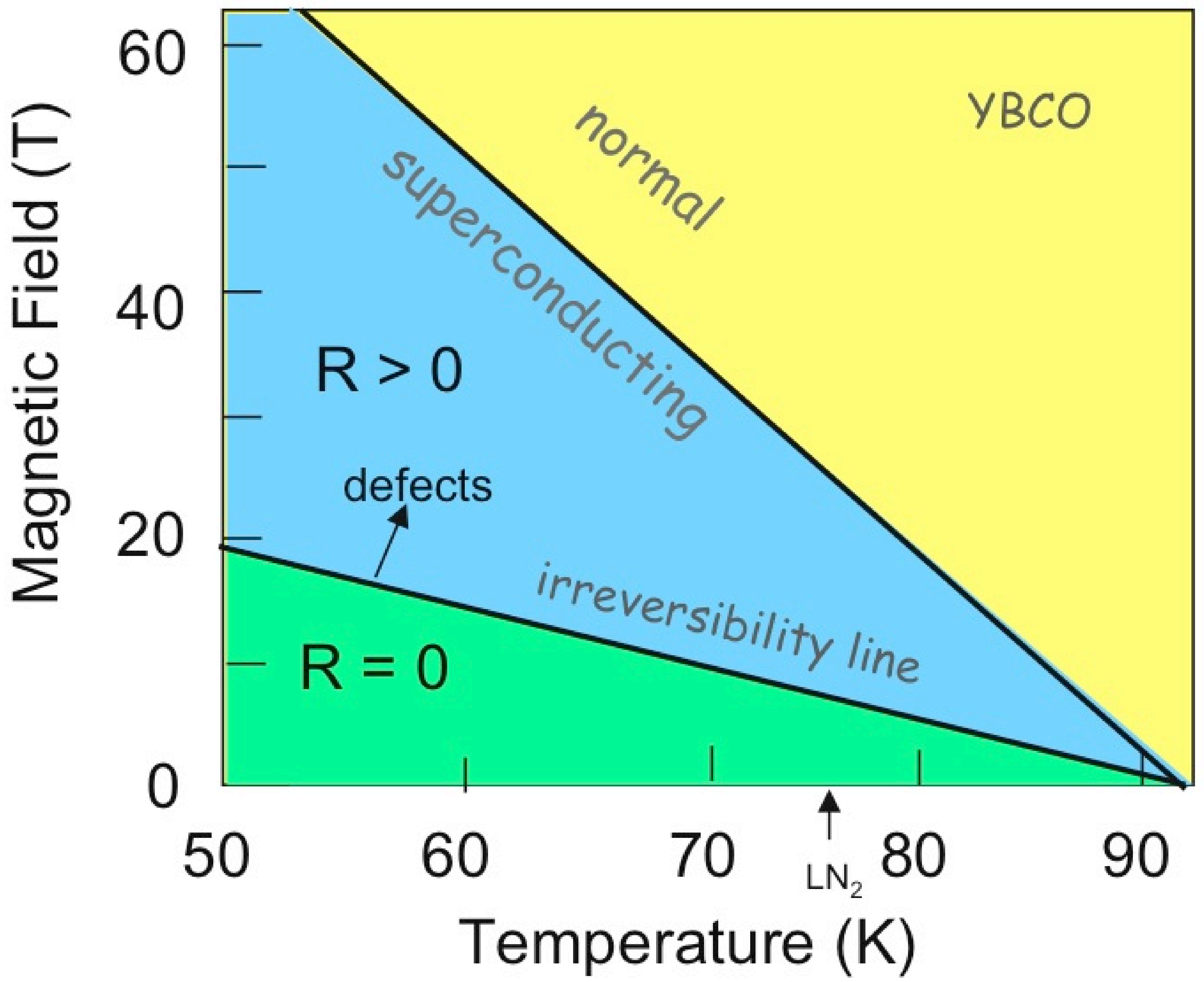


Barriers to superconducting performance: vortex motion & dissipation



moving vortices ⇒ R > 0

pinned vortices ⇒ R = 0



pinning defects:
nanodots, disorder,
2nd phases, dislocations
intergrowths
. . .

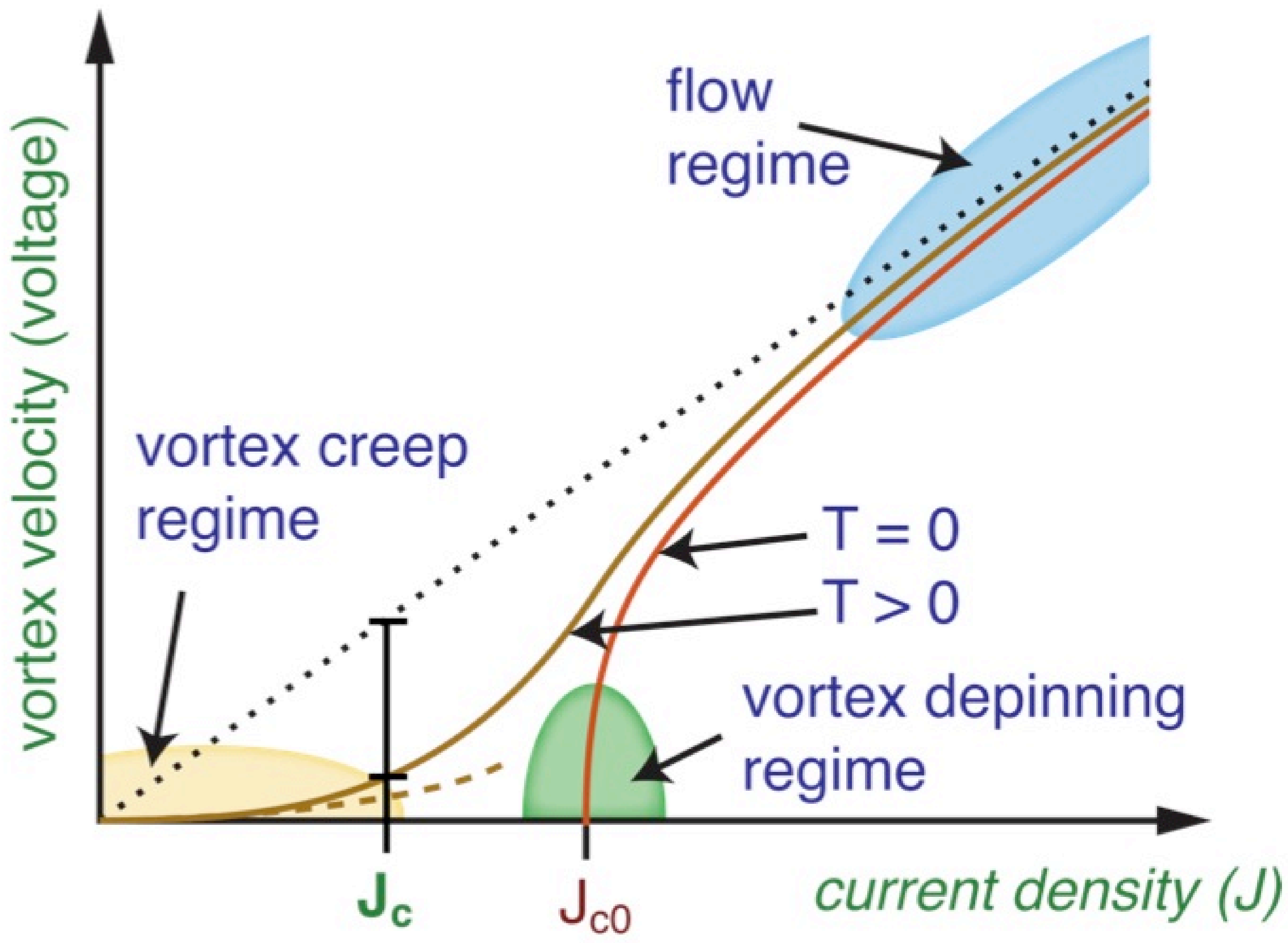
Performance Enhancement

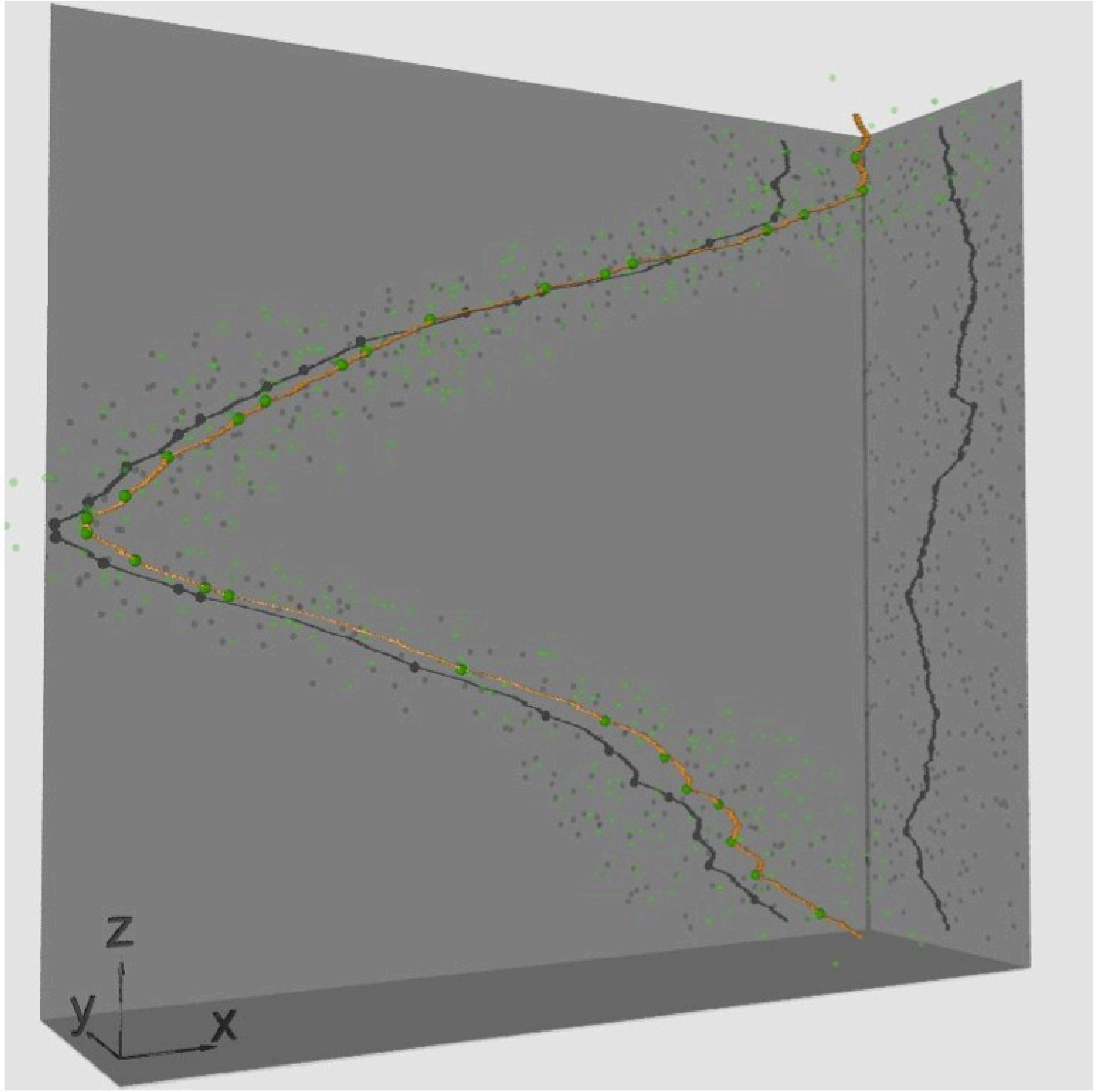
higher transition temperature → new materials

higher currents → control "vortex matter"

Vortex pinning and critical current J_c

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}





Open Question: How to arrange pinning in order to get close to the theoretical limit of the critical current

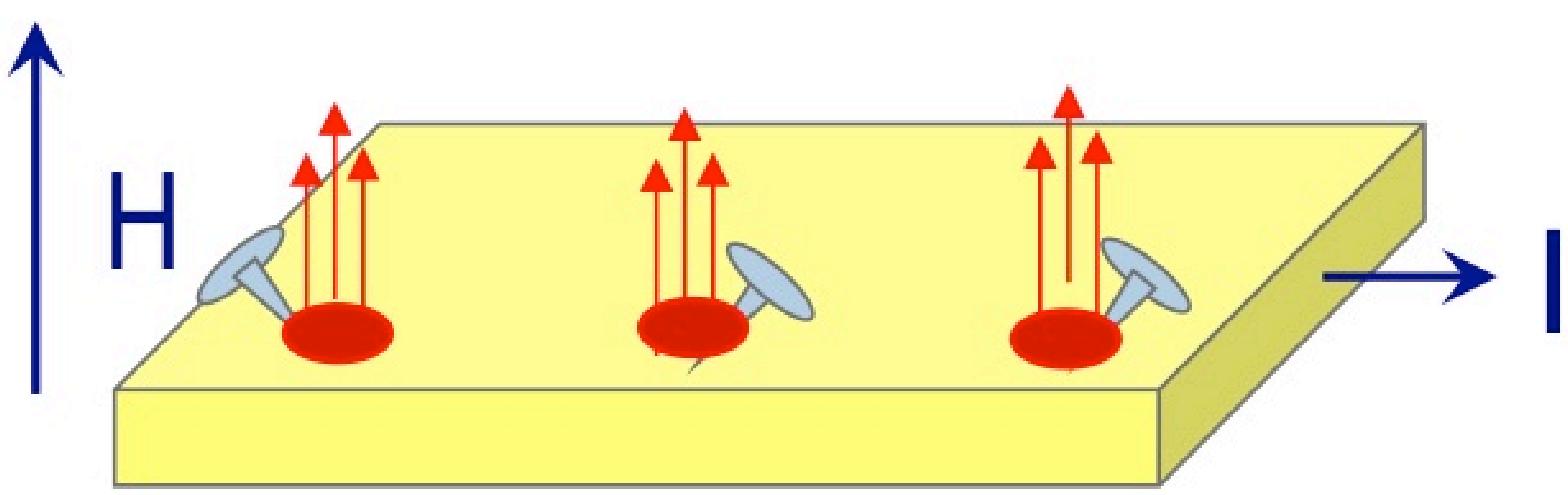
The Grand Challenge for Superconducting Applications

Raise the critical current

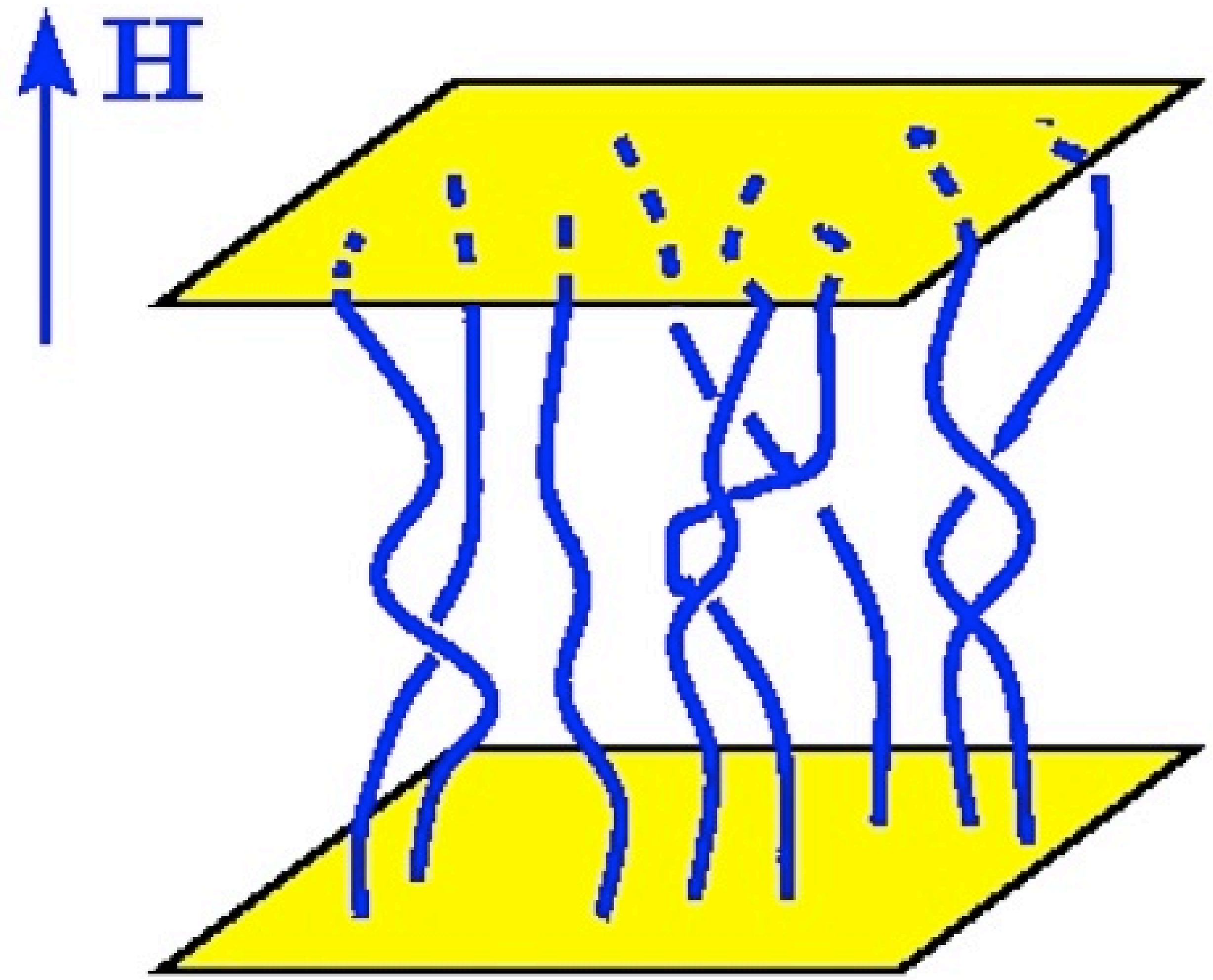
Overcome the "glass ceiling" in critical current: 20% of theoretical limit

Holds for all superconductors – conventional and high temperature

Origin of the glass ceiling is buried in collective dynamics



isolated vortex
one vortex - one pin site



analogy: atomic matter

actual strength $\ll$ theoretical strength

slip at dislocations, grain boundaries

vortex matter

vortex – vortex interaction

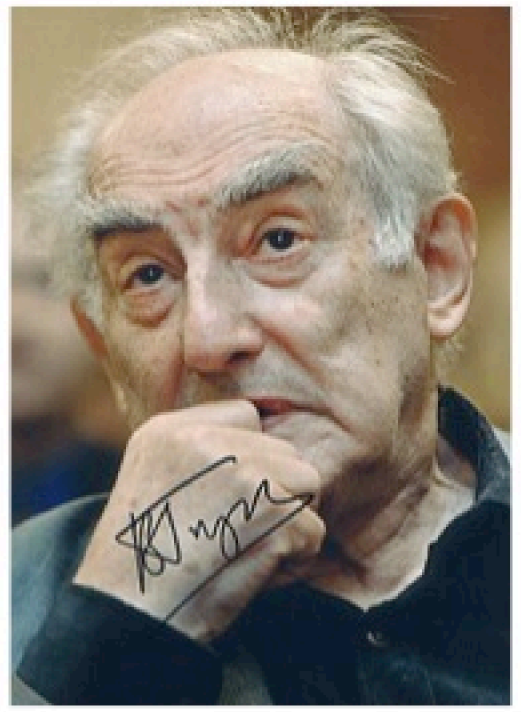
flexible vortices

distribution of point/line/planar pin sites

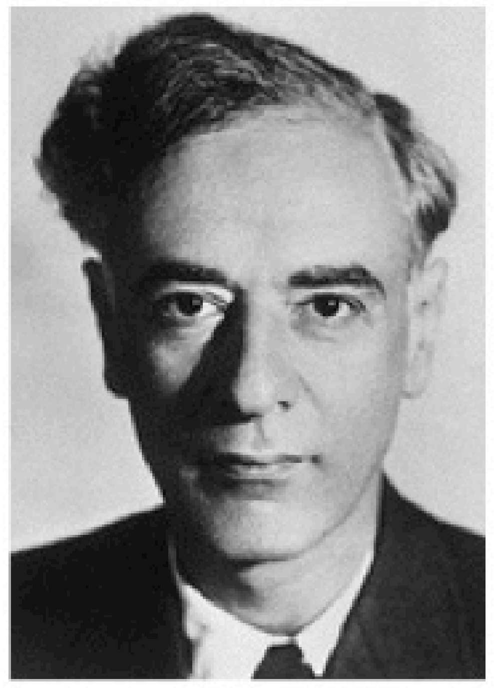
Ginzburg-Landau Theory

- The Ginzburg-Landau model is a phenomenological model to describe phase transitions
- The (complex) Ginzburg-Landau equation is one of the most-studied nonlinear equations in the physics
- Phenomenological, but can be derived from microscopic theory in several cases

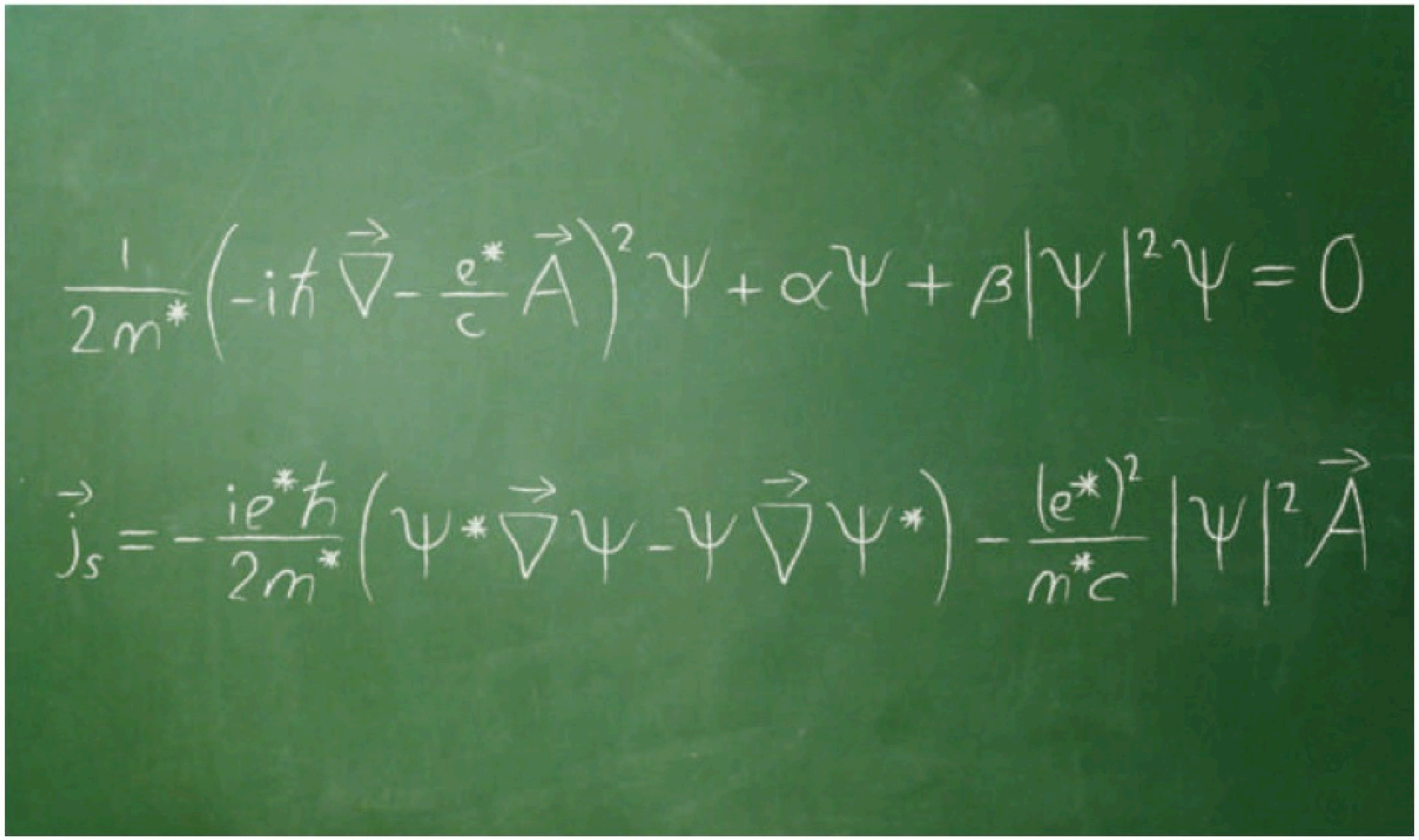
2003 Nobel prize



1962 Nobel prize



Ginzburg and Landau, 1950



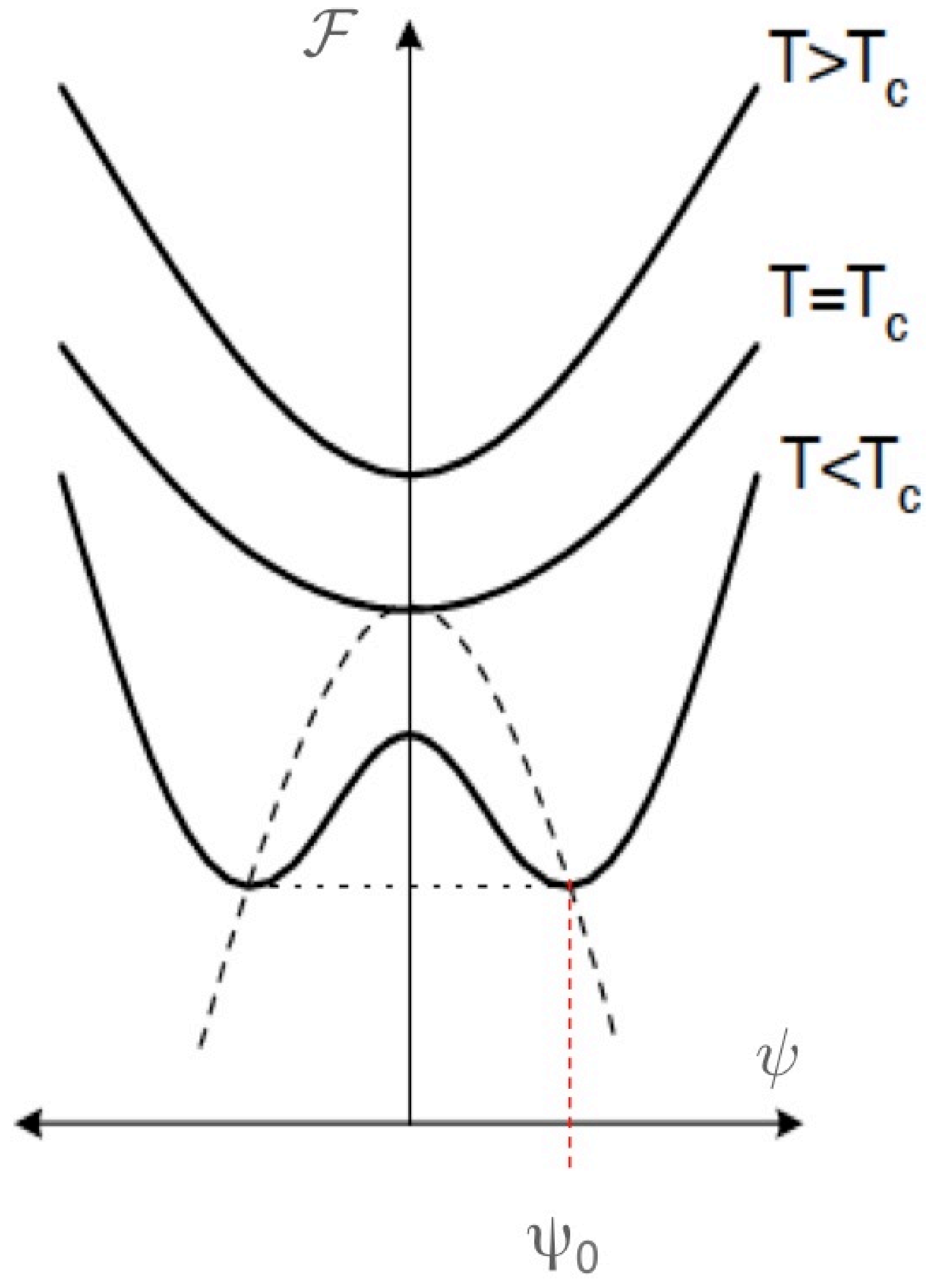
- describes vast variety of phenomena: from *nonlinear waves to second-order phase transitions, from superconductivity, superfluidity, and Bose-Einstein condensation to liquid crystals and strings in field theory*
- often even on a quantitative level

Phenomenological description

- (complex) order parameter ψ(r,t)
- expansion of the free energy in low order of ψ
- general theory of 2nd order phase transitions

$$\mathcal{F}_s = \mathcal{F}_n + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 \text{ (local)}$$

$$\alpha \propto (T - T_c) \qquad \beta > 0$$



We also need interaction:
→ consider (real) local order parameter on a grid

$$\mathcal{H}_{\text{int}} = -\gamma \sum_{\langle i,j \rangle} \psi_i \psi_j a^{d-2}$$

going over to the continuum results in the additional term to the free energy:

$$\gamma|\nabla\psi|^2$$

Ginzburg-Landau theory for superconductors

- Superconducting order parameter

  Microscopic origin: Coherent state of Cooper pairs

$$\begin{aligned} \psi(\mathbf{r}) &= |\psi| e^{i\varphi(\mathbf{r})} \\ n_s &= |\psi|^2 \\ \mathbf{p} &= \hbar \nabla \varphi \end{aligned}$$

- free energy of a superconductor in magnetic field

$$\mathcal{F}_{GL} = \frac{1}{2} \int d^d x \left\{ \beta \left(\frac{\alpha}{\beta} + |\psi|^2 \right)^2 + \frac{\hbar^2}{m} \left| \left(i\nabla - \frac{2\pi}{\phi_0} \mathbf{A} \right) \psi \right|^2 + \frac{1}{4\pi} (\nabla \times \mathbf{A} - \mathbf{H})^2 \right\}$$

$\alpha(T) \sim (T_c - T)$

Scientific Meso Challenge: Transport governed by phenomena on the *mesoscale*

Problem: the “glass-ceiling” for J_c is only 20-30% of the theoretical limit (depairing current)

- Origin not known and not explainable in small arrays or continuum approximations

→ vortex motion in large systems with large number of vortices needs to be studied

GL model bridges the micro (single vortex) to the macro scale (vortex matter)

Emerging phenomena in large-scale arrays

- mutual long-range repulsion among vortex lines
- flexibility of vortex lines → simultaneously seek and attach to many pinning defects
- resulting in intricate dynamic configurations as vortex segments detach from one pinning defect and attach to another
- interruption of superconducting current pathways by non-superconducting pinning defects reducing the cross-sectional supercurrent flow area
- possibility of vortices cutting and reconnecting during motion

Prediction of the behavior of large-scale vortex arrays of is a fundamental challenge of high practical value

→ remained out of reach of analytical theory and conventional numerical simulation.

Simulations

Time dependent GL equations:

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

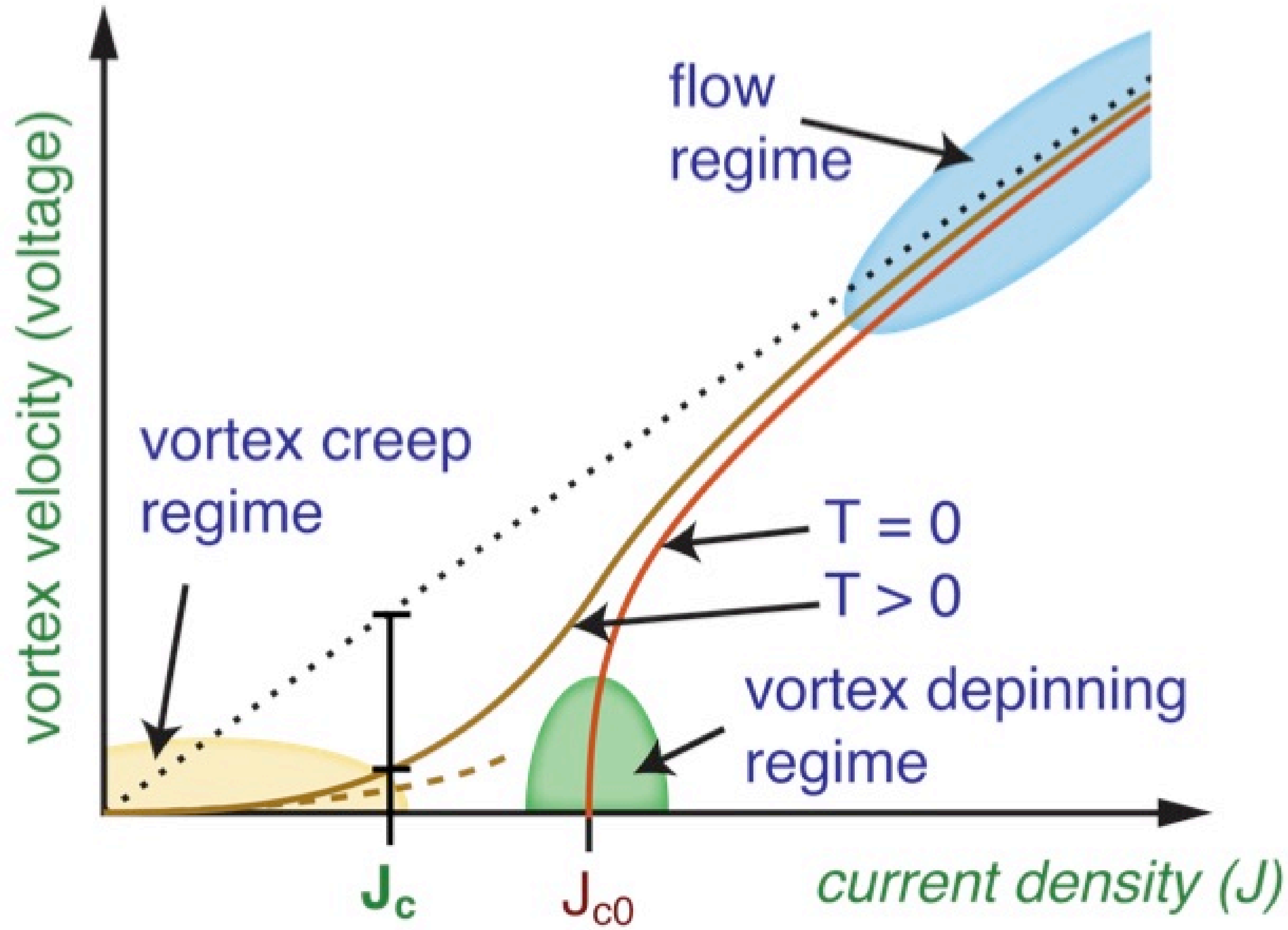
$$u(\partial_t + i\mu)\psi = \epsilon(\mathbf{r})\psi - |\psi|^2\psi + (\nabla - i\mathbf{A})^2\psi + \zeta(\mathbf{r}, t)$$
$$\kappa^2 \nabla \times (\nabla \times \mathbf{A}) = \mathbf{J}_n + \mathbf{J}_s + \mathcal{I},$$

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

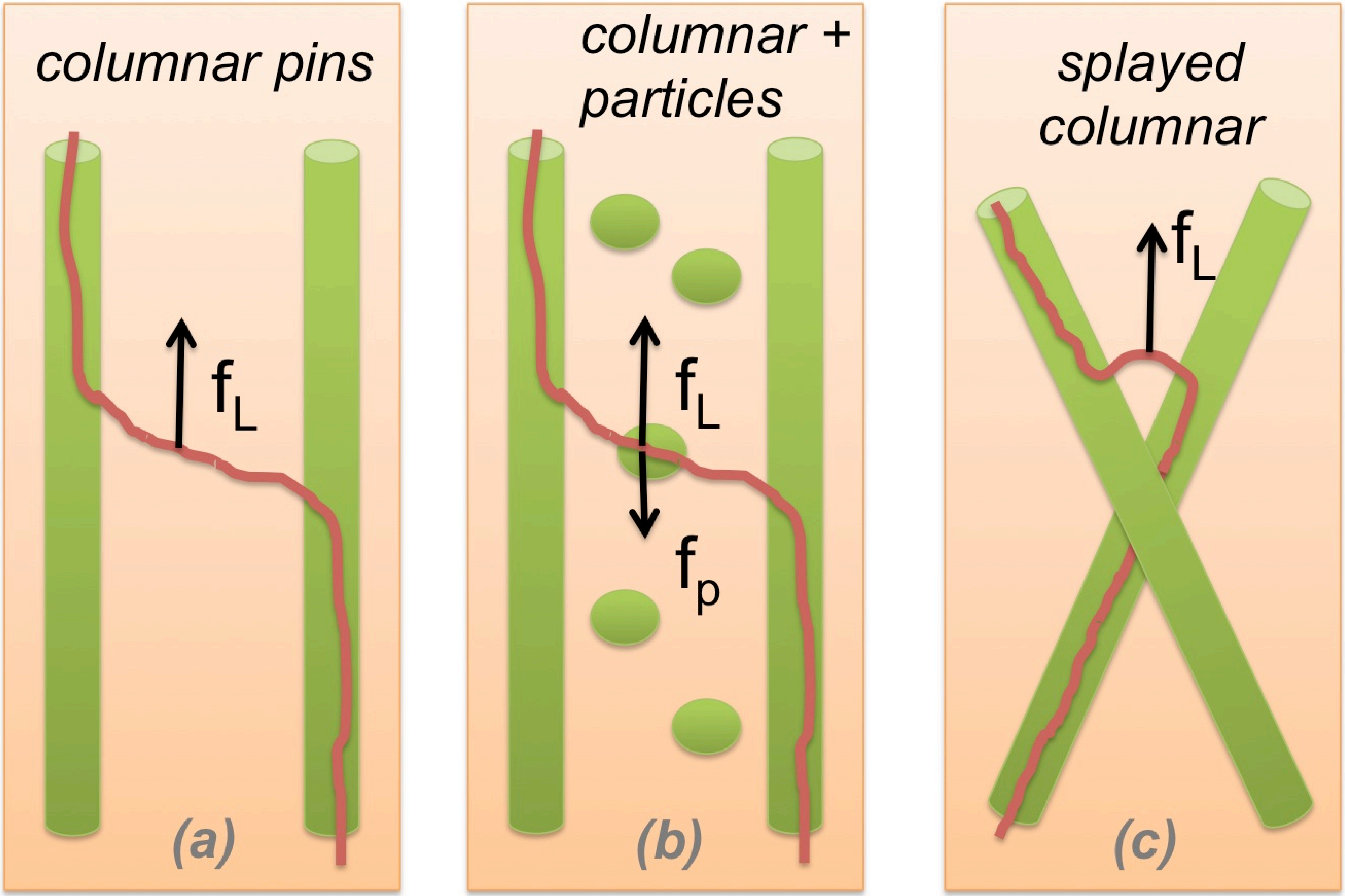
$$\mathbf{J} = \mathrm{Im}\left[\psi^*(\nabla - i\mathbf{A})\psi\right] - (\nabla\mu + \partial_t \mathbf{A})$$

critical current J_c:

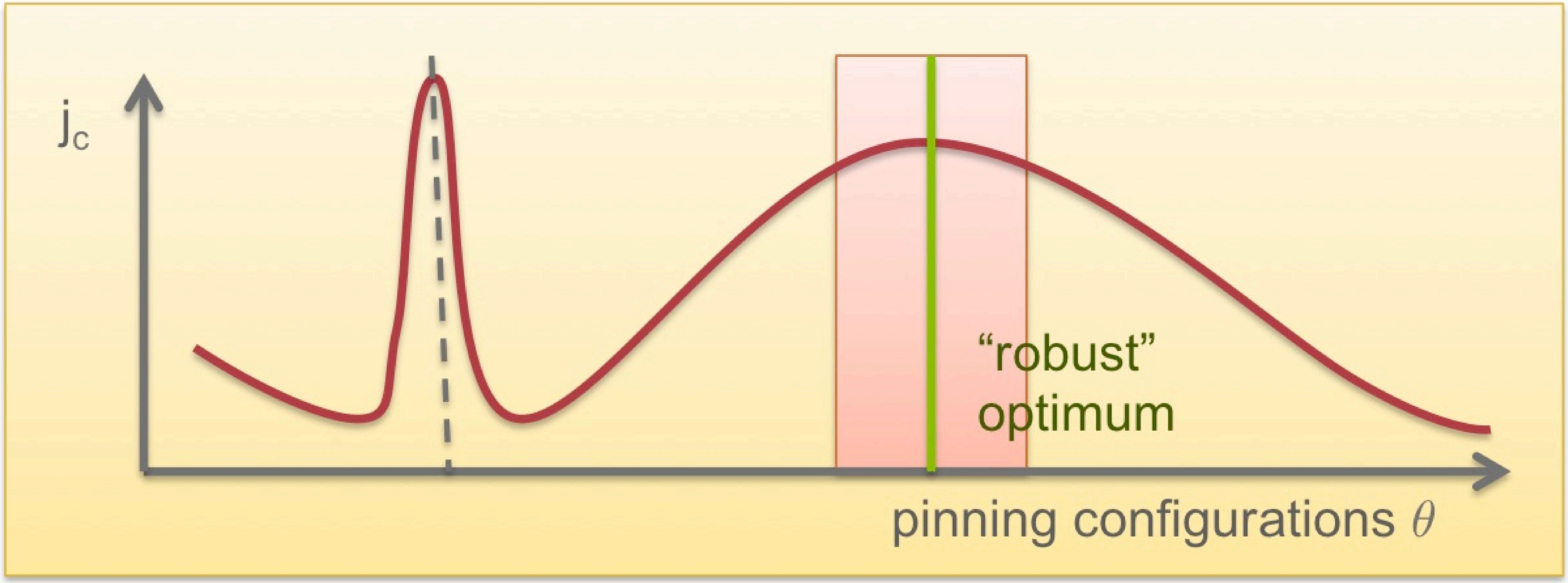
- no unique definition
- usually defined when voltage V is a small percentage δ (here 1%) of the free flow value V_{ff}
- ***J_c calculated by a bisection method***



Pinning configurations - improvement of the critical current



Optimization of pinning for maximal current



Determining optimal pinning landscape:

- ***Optimize critical current***
- ***Minimize deviations from best case***
- ***Min-max or min rms***

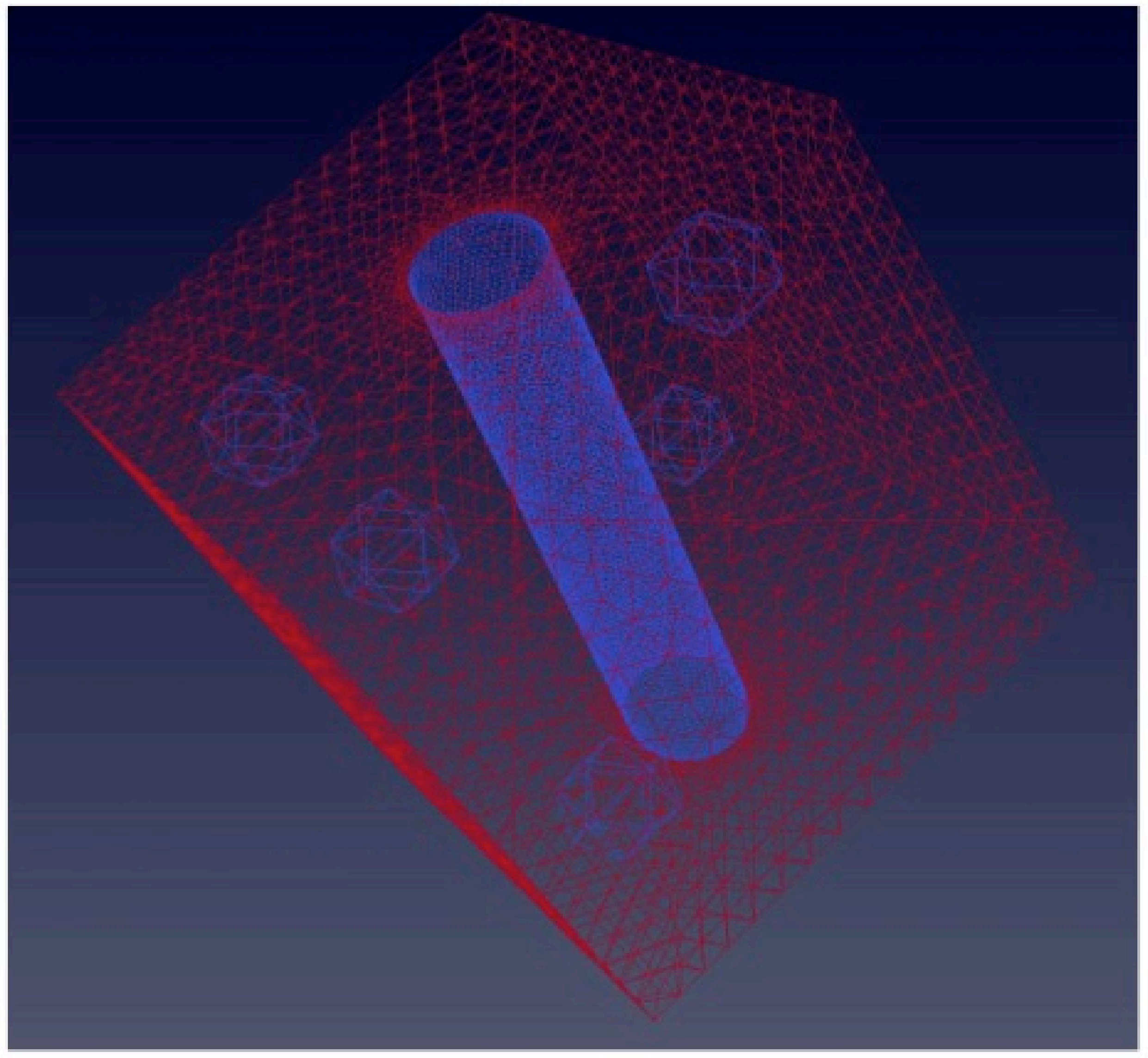
$$\begin{aligned} \max_{\theta} \quad & J_c(\theta) \\ \text{such that} \quad & J_c(\theta) = \max_{J} \left\{ J : V_\theta(J) \leq \delta V_{\mathrm{ff}}(J) \right\}, \\ & \theta \in \Theta, \end{aligned}$$

Computational Challenge: Complexity

Typical simulation complexity

- Simulations of $\mathcal{O}(10^6)$ timesteps for reliable V values
- Sample volumes $\mathcal{O}(10^6)\xi^3$ + with cell mesh size $\mathcal{O}(10^{-1})\xi$

  → *$\mathcal{O}(10^9)$ degrees of freedom (DoF) per realization of pinning configuration θ.*



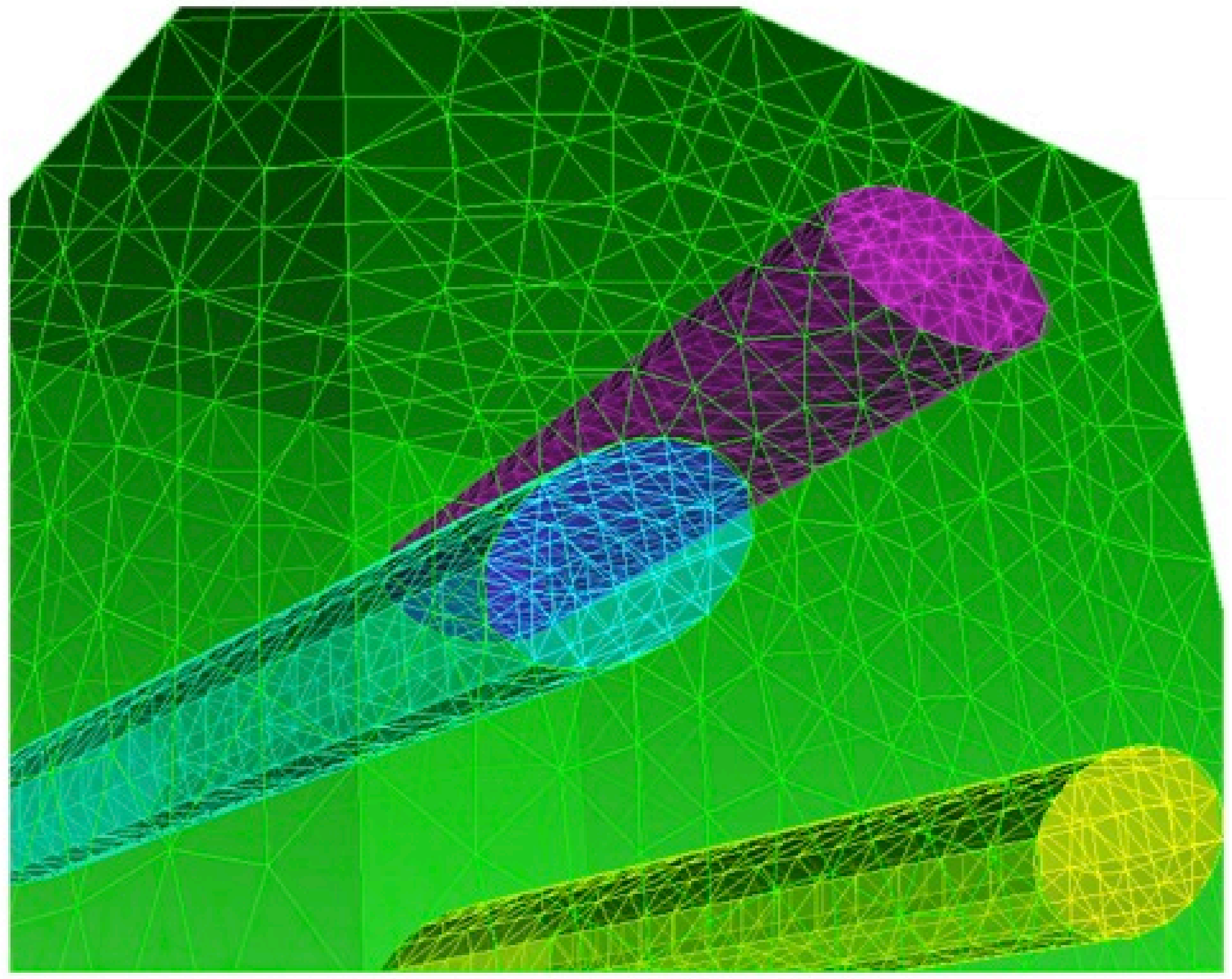
Computational demand for 10^3 flops per DoF per timestep

- 10 - 100h on full 100TFlop/s machine *at peak* for single θ
- Optimization increases demand by $\mathcal{O}(100)$-$\mathcal{O}(1000)$ x

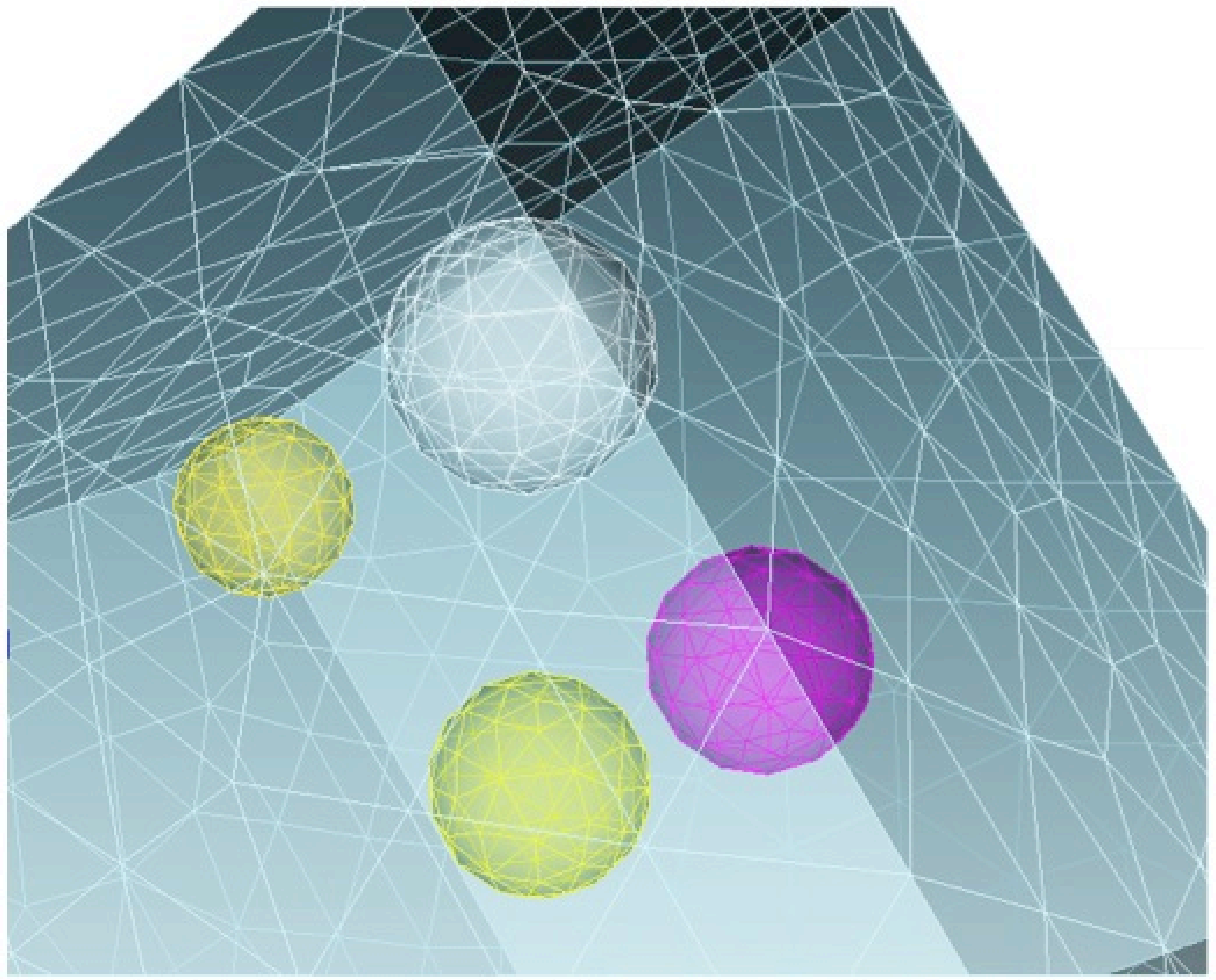
→ **Computational requirements**

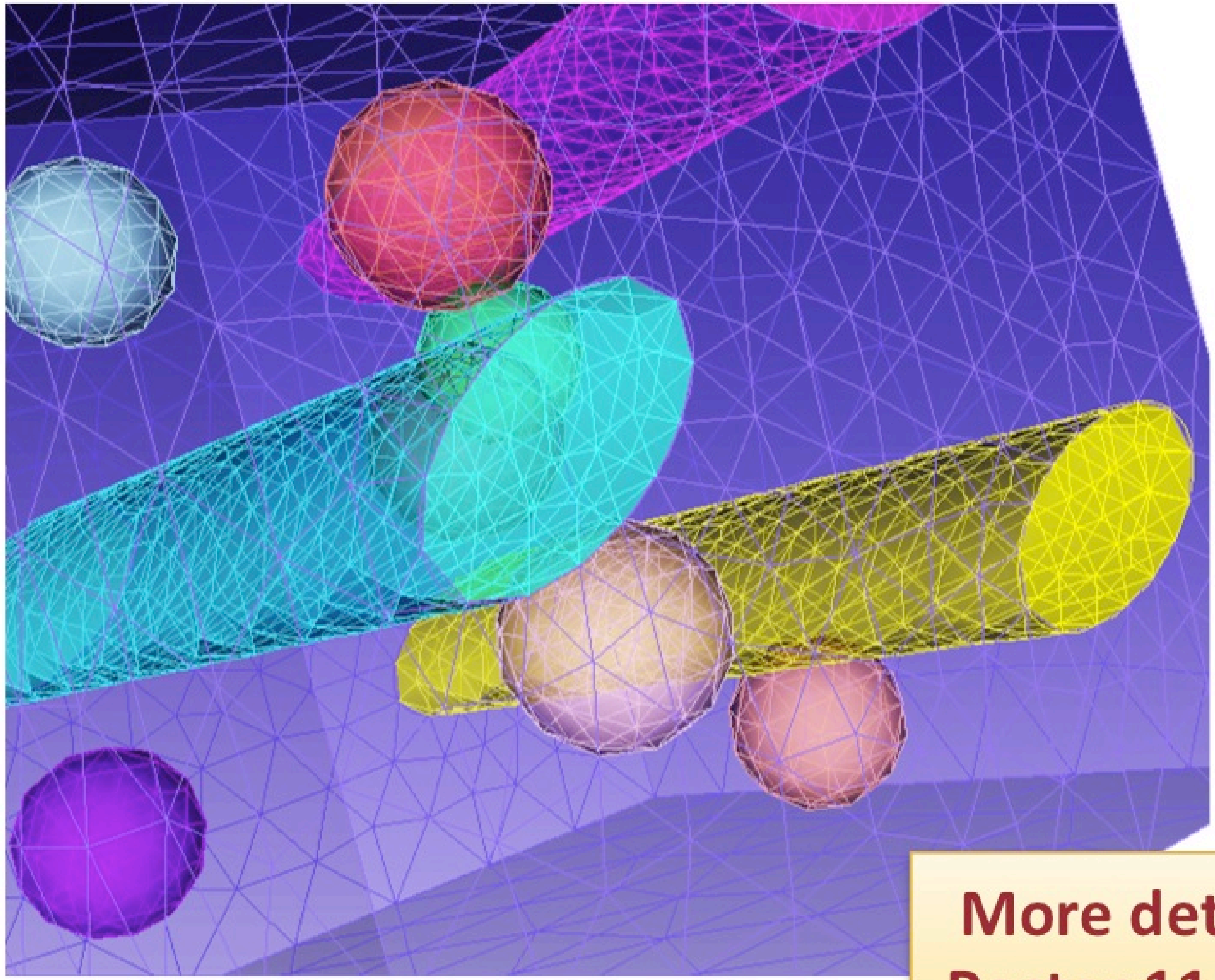
- Leadership-class hardware for computational optimization of pinning structures
- State-of-the-art sampling techniques to minimize the number of probed θ
- Automated meshing of materials with embedded pinning structures
- Fully implicit time-integration to circumvent the timestep size limitation
- Modern iterative methods to solve $\mathcal{O}$(1B) system at each timestep in optimal time.

Computational Challenge: Meshing



- mesh size needs to be smaller than the coherence length to capture order parameter variations
- near inclusions and defects mesh needs to be finer
  → *Adaptive meshing*
- increased precision by adaptive mesh refinement near vortices





More details on Poster 11 on Tue

Broader Impact

The results and methods obtained and developed have significant impact beyond the scientific knowledge

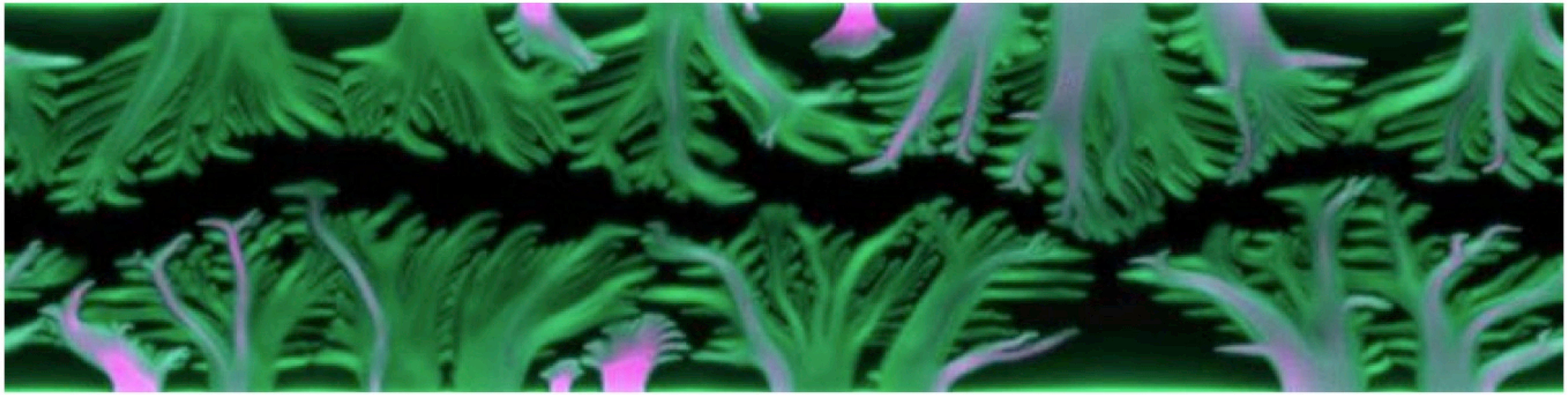
→ increased J_c for applications in power-transmission & magnets

Applicable and related to many other mesoscopic models & systems:

- phase-field models
- granular materials
- **self-propelled swimmers**
- fluid and fracture dynamics
- ***cold atoms***
- solidification from a melt or solution

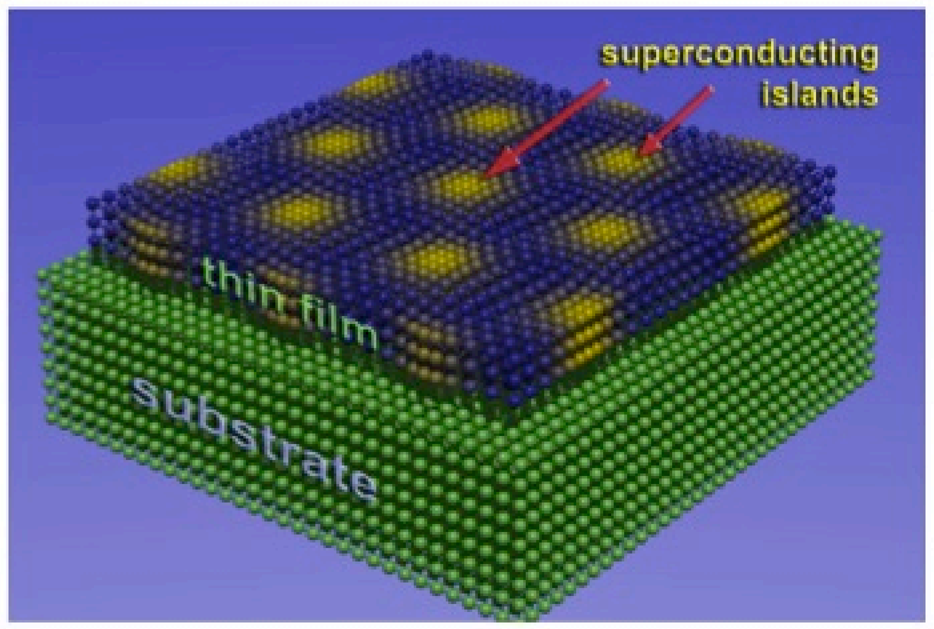
Extension of the TDGL formalism

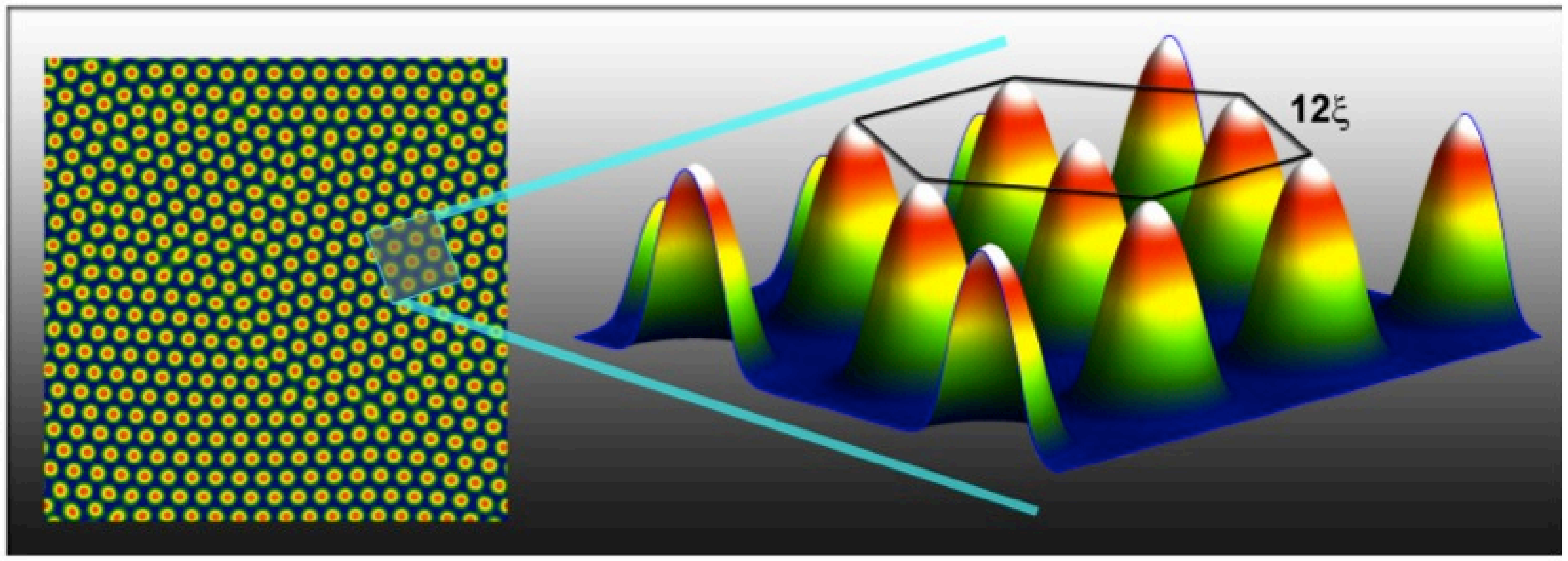
- Modeling of thermomagnetic avalanches



nonlinear magnetic flux diffusion equation coupled to thermal diffusion in 2D

- Coupling to elastic strain



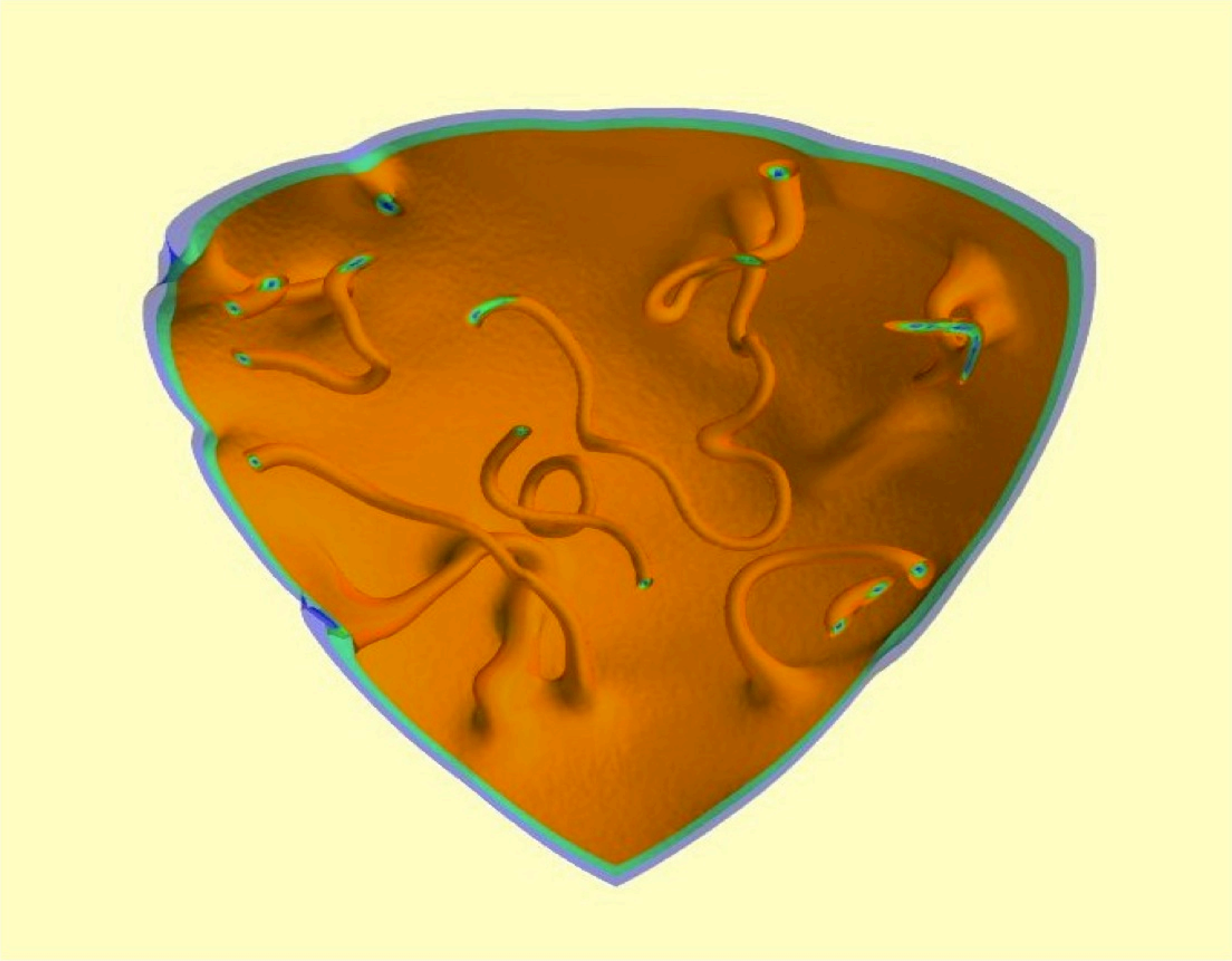


inclusion of elastic interaction (intrinsic or external) leads to spatial variations of T_c

- Magnetic inclusions for enhanced pinning

magnetic inclusions have long-range interaction
→ could strongly suppress thermal creep

Application to other areas (I): Evaporative cooling of a Bose-Einstein Condensate

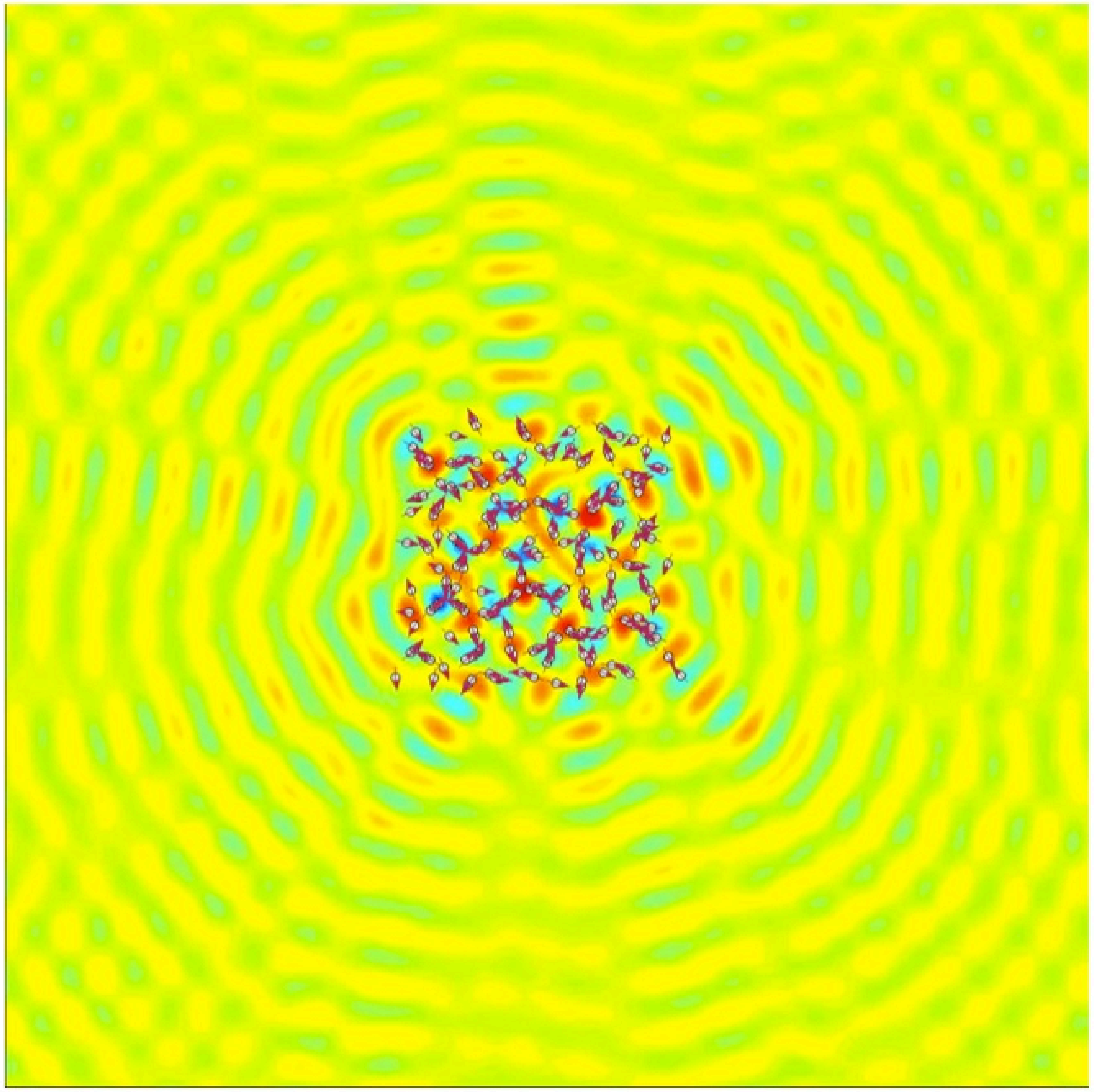


time dependent ***complex*** Ginzburg-Landau equation coupled to diffusion equations

Simulation volume: **512^3 grid points**, up to 10^5 time steps

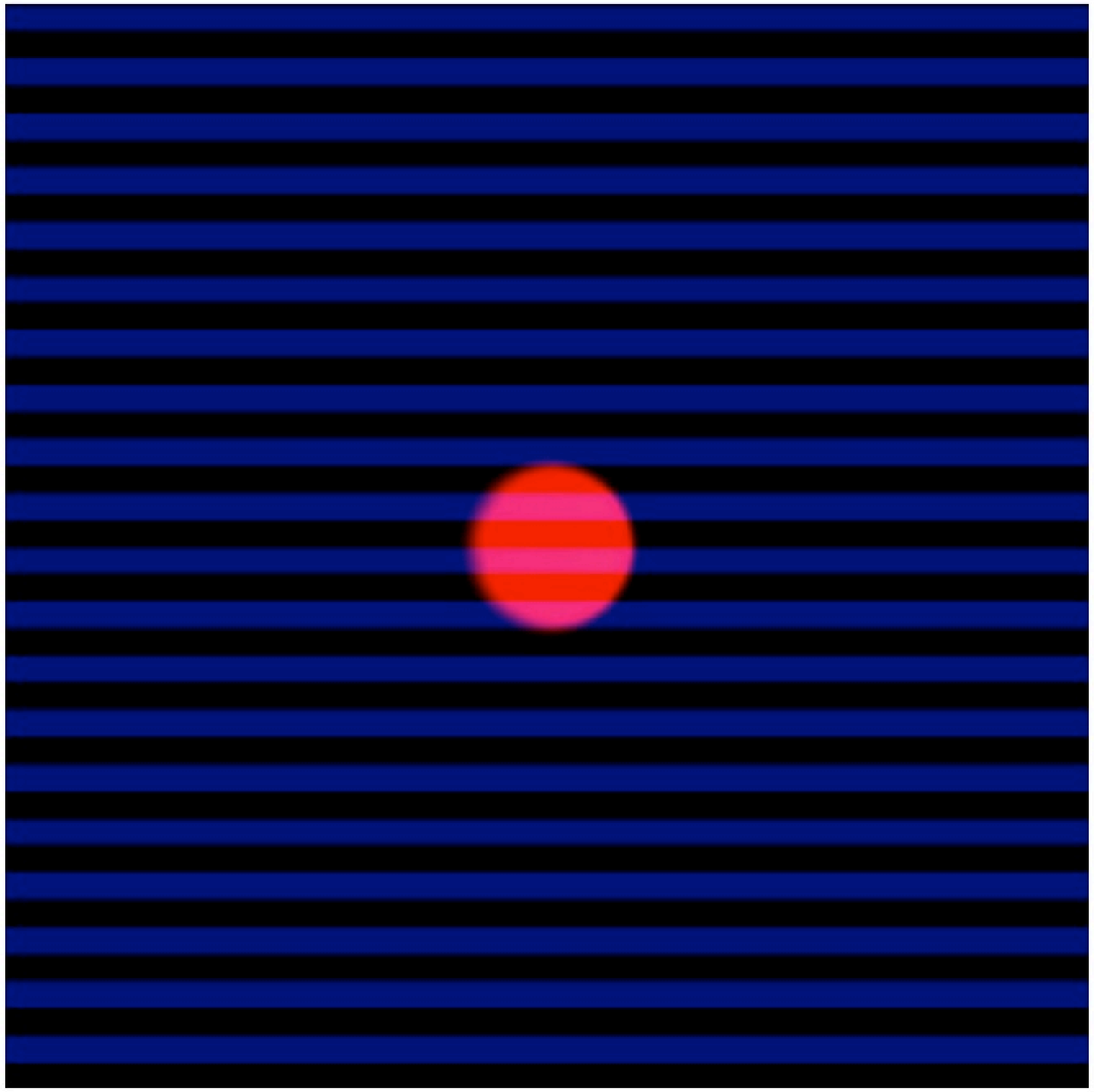
Example (II): Self-assembly and cell dynamics

Self-Assembled Magnetic Surface Microswimmers



Model: Magnetic particles coupled to surface described by shallow water fluid dynamics

Cell Motion: e.g. a keratocyte cell crawling on patterned substrate



Model: Phase-field similar to GLE coupled to additional fields (density of actin filaments, concentration of linkers) and elastic deformations of the substrate

OSCon Organization Structure & Key Collaborations