

Modeling and Simulating Vortex Pinning and Transport Currents for High Temperature Superconductors

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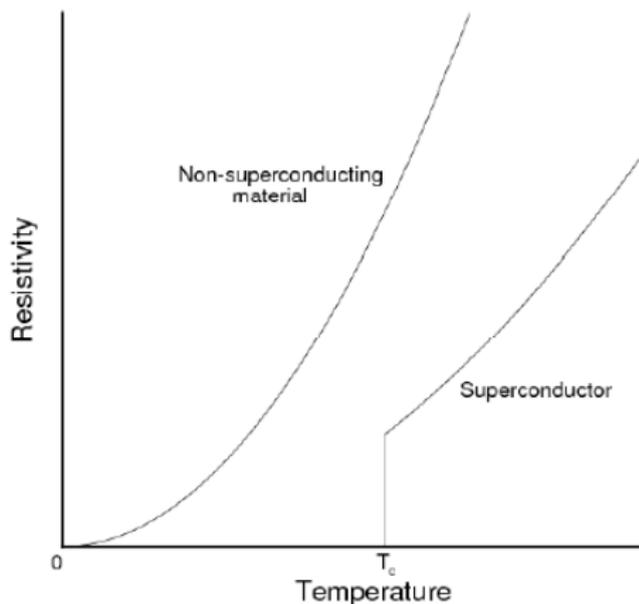
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Superconductivity and Motivation

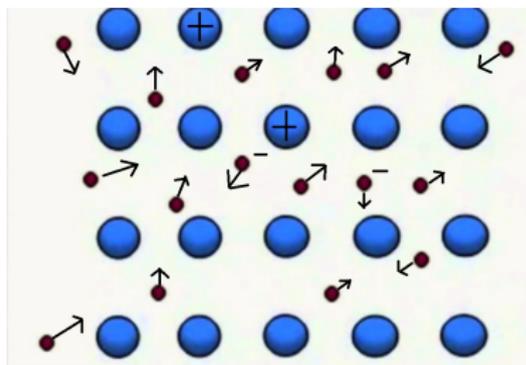
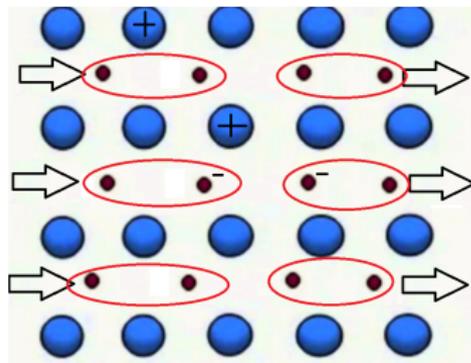
What is Superconductivity?

- Two Hallmark Properties:
 - 1. Zero Electrical Resistance
 - 2. The Meissner Effect
- The first property was discovered by Onnes in 1911.
- Only occurs below critical temperature T_c .
- Normal Metal Vs. Superconductor:



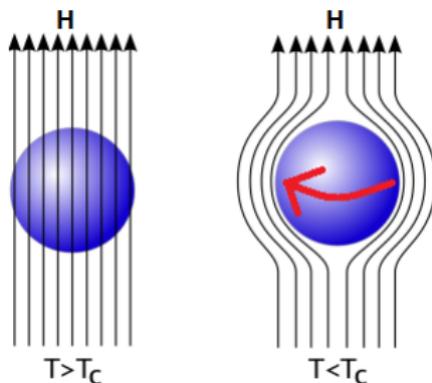
How does this Occur

- Below T_c the electrons form pairs (top).
- Movement is orderly.
- No waste heat!
- Above T_c things break down (bottom).



The Meissner Effect

- Occurs when a superconductor (SC) is in a magnetic field.
- A resistance free current (**super current**) is induced.
- The current prevents penetration.
- This persists until the field reaches a critical strength H_c .
- Magnetic Field Penetration = NO Superconductivity.



Type I and Type II

- Type I SC are not penetrated at all (Meissner Effect) (top right).
- Type II SC are only penetrated by tubes of magnetic flux (**Vortices**) (bottom).
- Two critical H values, H_{c1} and H_{c2} .
- Vortex state: $H_{c1} < H < H_{c2}$.

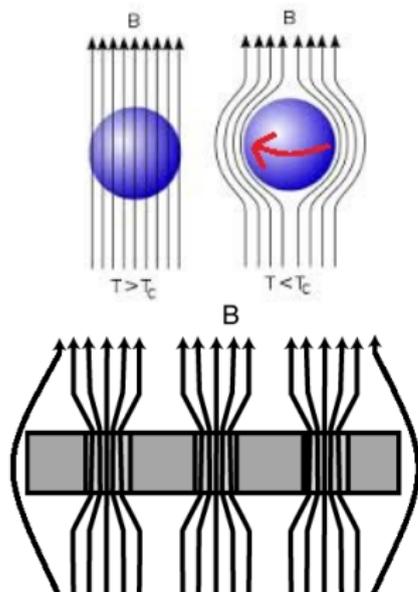


Figure : Normal and Type I (top).
Type II (bottom)

Why You Should Care: Applications

Possible Superconducting Technology:

- Efficient Current Carriers
- Powerful Magnets (by magnetization)
- MRI
- Efficient Mag Lev

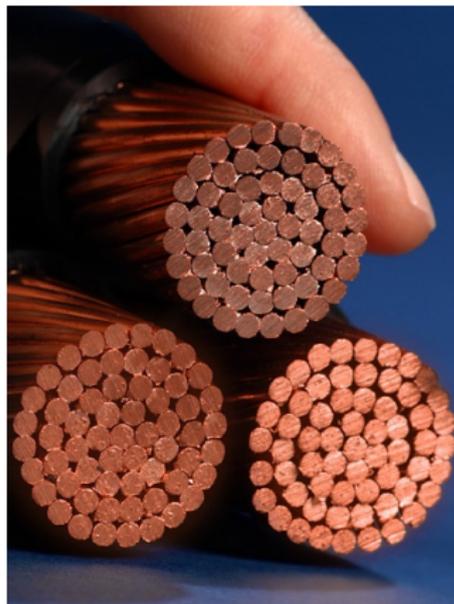


The Catch

- There is no free lunch.
- T_c is close to 0 K for most metals.
- Liquid helium is expensive.
- This rules out many applications such as power wires.
- Thankfully recent discoveries have overcome this.

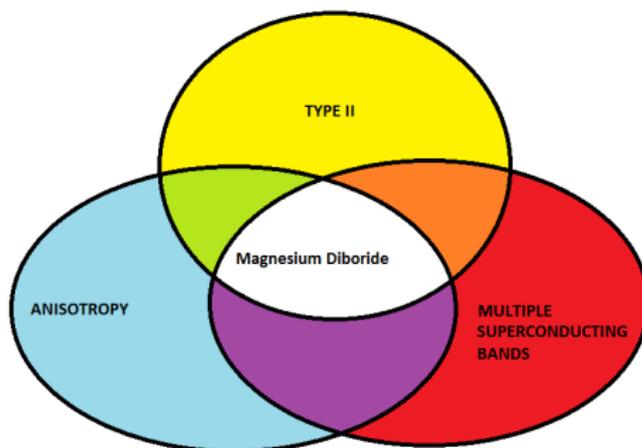
High Temperature Superconductors (HTS)

- New materials have revitalized superconductivity.
- Higher T_c values allow the use of liquid N or O coolants.
- Magnesium Diboride (MgB_2) is cheap and ductile ($T_c = 39$ K or -234° C).
- $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_8$ is used in MRIs ($T_c = 135$ K or -138° C).
- Hydrogen Sulfide under 150 G. Pascals of pressure ($T_c = 203$ K or -70° C).



High Temperature Superconductors (HTS)

- These materials come with new odd properties:
- Odd temperature dependencies in quantities.
- All of are **Type II** S.C.
- This complicates the modeling process.



Visualizing Vortices

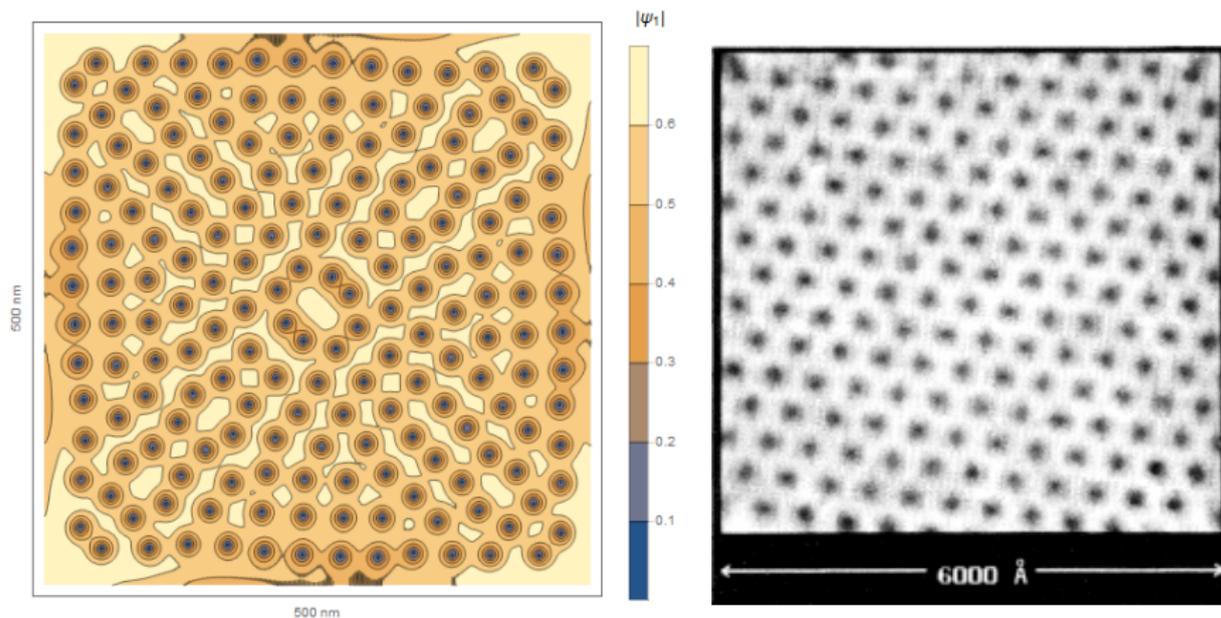


Figure : Simulation

Figure : SEM image of vortices

Applied Currents

- So far we have T_c and H_c .
- What happens when we apply a current to a SC?
- Can it be carried without Resistance?
- Only below J_c !

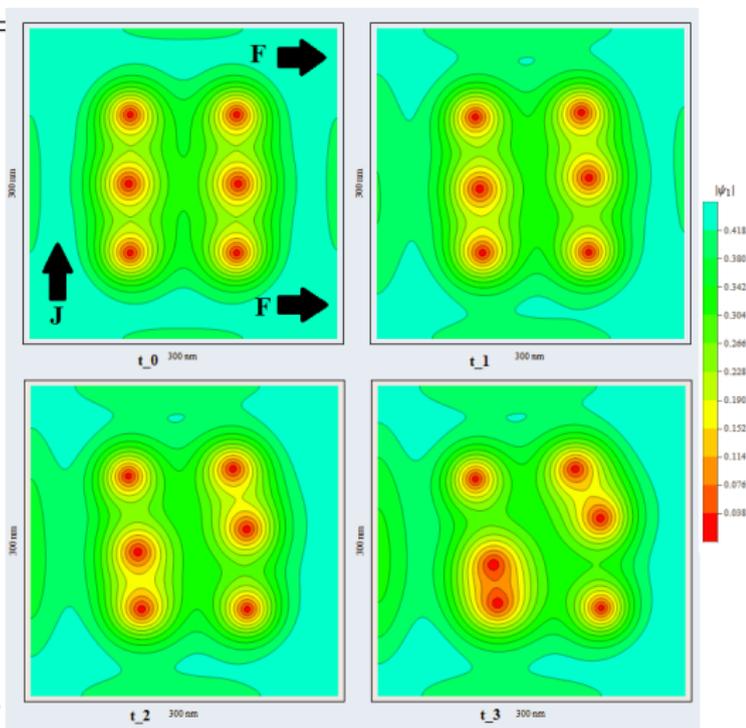
Why Vortex Dynamics are Important

- **Vortices** (B) and Current (J) = Flux Flow.
- Moving Vortices (flux flow) creates Resistance.

$$f \hat{x} = J \hat{y} \times B \hat{z}$$

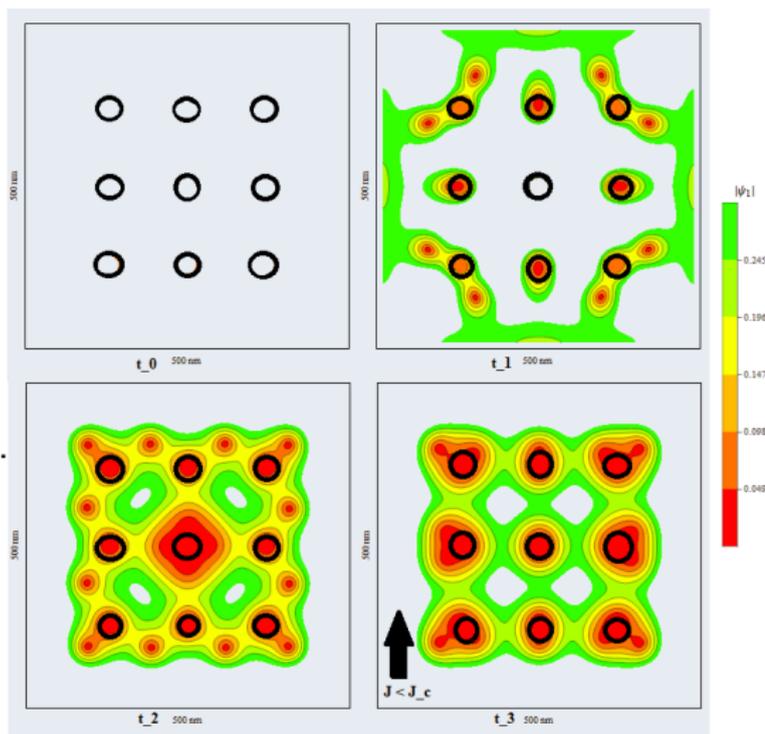
$$E \hat{y} = B \hat{z} \times u \hat{x}$$

- Flux Flow induces Electric Field (E) and Voltage (V).
- Resistance now exists ($\frac{V}{I} = R$).



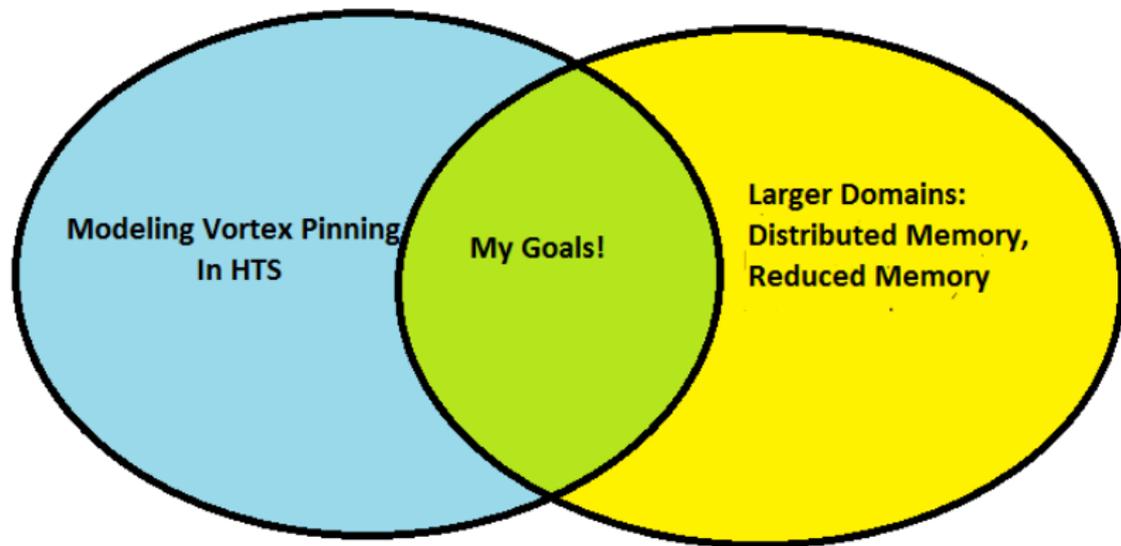
Vortex Pinning Comes to the Rescue

- Immobilizing the **Vortices** Is Crucial.
- Non Superconducting Metal = Normal Metal = Pinning Sites. (Outlined in Black)
- **Vortices** “Stick” To impurities.
- Limited increase In J_c .



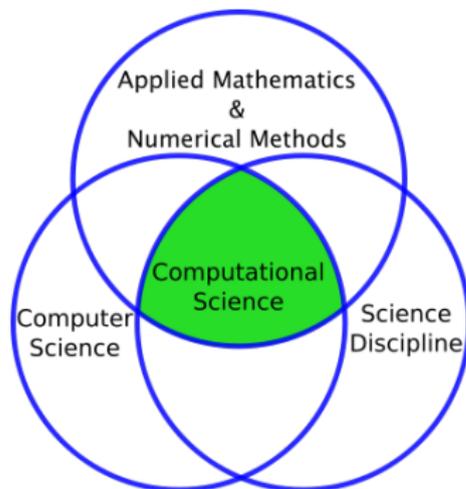
Simulations

- Simulations are critical to modeling new technology.
- No models for two-band SC and vortex pinning by impurities.
- Larger domains to avoid boundary effects.



The Framework

- A model: the Ginzburg-Landau model.
- Modify it for HTS and vortex pinning.
- Specify a material and model it.
- Modify for large scale simulations.



Ginzburg-Landau

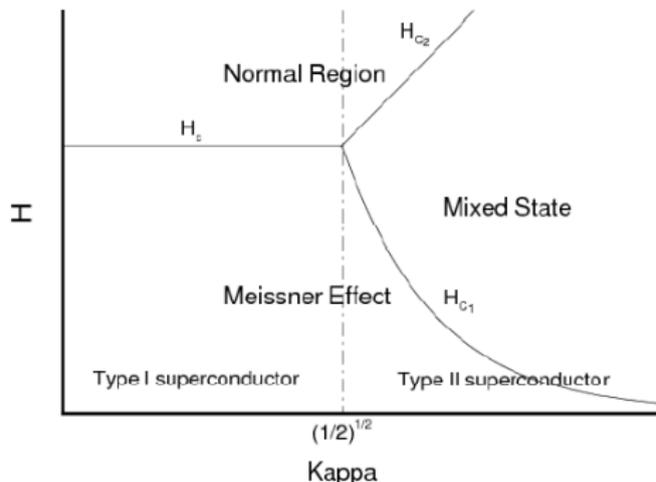
Ginzburg-Landau (GL) Theory

- The G-L theory (or model) describes superconductivity as a phase transition for a valid temperature range.
- A free energy functional is formed.
- Its minimum is given by the G-L equations.
- This is done using calculus of variations.
- Gauge invariance.
- The model is non-dimensionalized using important material parameters.

Important Quantities

- Two variables:
 - ψ - The complex order parameter, describes the density of superconducting electrons.
 - \mathbf{A} - The magnetic vector potential, $\nabla \times \mathbf{A} = \mathbf{B}$.
- Three material parameters:
 - λ - The penetration depth.
 - ξ - The coherence length.
 - κ - The G-L parameter
$$\kappa = \frac{\lambda}{\xi}.$$

- Type I & II Revisited:



The Time Dependent G-L Model (TDGL)

- The solution (ψ, \mathbf{A}) minimizes the free energy.
- CGS units (no ϵ_0 or μ_0).

$$\Gamma\left(\frac{\partial\psi}{\partial t}\right) + i\kappa\Phi\psi + (|\psi|^2 - (1 - \frac{T}{T_c}))\psi + (-i\frac{\xi}{x_0}\nabla - \frac{x_0}{\lambda}\mathbf{A})^2\psi = 0 \quad (1)$$

$$\sigma\left(\frac{1}{\lambda^2}\frac{\partial\mathbf{A}}{\partial t} + \nabla\Phi\right) + \nabla(\nabla\cdot\mathbf{A}) + \nabla\times\nabla\times\mathbf{A} + \frac{i}{2\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^*) + \frac{1}{\lambda^2}|\psi|^2\mathbf{A} = \nabla\times\mathbf{H} \quad (2)$$

+ B.C.s and I.C.s

- \mathbf{H} is the applied magnetic field.
- Note $\mathbf{H} = \mathbf{B} - \mathbf{M}$; \mathbf{M} =magnetization.
- σ is the normal conductivity. T is temperature. Γ is relaxation constant.
- x_0 is scaling factor; Φ the potential is 0 by gauge choice.

Super and Normal Current

- Two components of the electrical current.

Normal Current Density

The resistive, normal current.

$$\mathbf{J}_n = \sigma \mathbf{E} = \sigma \left(\frac{1}{\lambda} \frac{\partial \mathbf{A}}{\partial t} + \nabla \Phi \right)$$

Super Current Density

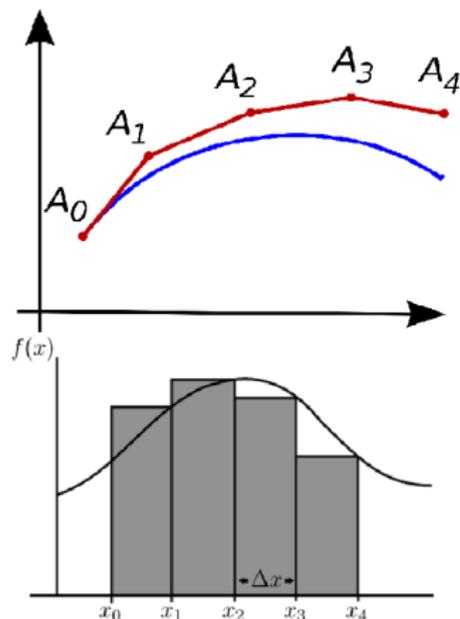
The resistance free super current.

This is the current that gives rise to the Meissner effect.

$$\mathbf{J}_s = -\frac{i}{2\kappa} (\psi \nabla \psi^* - \psi^* \nabla \psi) - \frac{1}{\lambda^2} |\psi|^2 \mathbf{A}$$

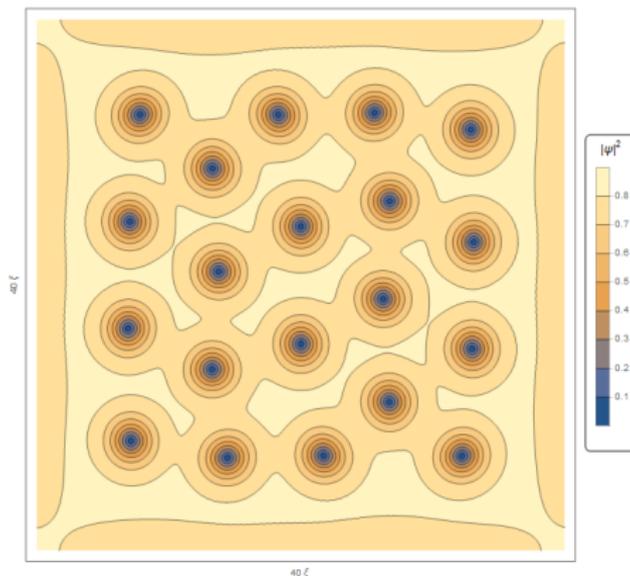
Solving The TDGL system

- Non-linear, time dependent, coupled system of PDEs.
- FEM for space. Quadratic triangular elements.
- Quadrature for integrals.
- Adaptive backward Euler for time.
- Newton for non-linearities.
- Direct or Krylov Solver? (SUPERLU_DIST at first)



TDGL Simulation

- $\psi \rightarrow 0$ where the material is normal (vortices or impurities).
- $\lambda = 60$ nm, $\xi = 5$ nm, $(1 - \frac{T}{T_c}) = 0.7$, $\frac{T}{T_c} = 0.3$, $\mathbf{H} = 1.5 = 1.5H_c$, and $\kappa = 12$.



TDGL Simulation

Anisotropy

Anisotropy can be modeled by assuming electrons have directional dependent masses \rightarrow Effective mass model.

It also creates quantities for each direction: $\xi^x, \lambda^x, \kappa^x, H_{c2}^x + [\cdot]^y$

Normal Inclusion

Impurities (Normal Inclusion model) can be modeled as well by solving a second set of equations. This is done by setting the reduced temperature $(1 - \frac{T}{T_c}) = -1$ and removing the $|\psi|^2\psi$ term.

Applied Current

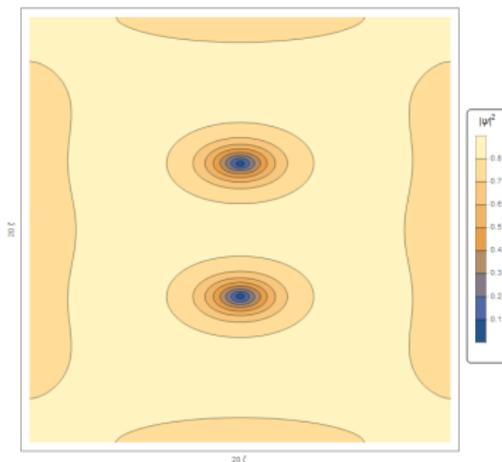
Applied currents can modeled by modifying the potential Φ .

$$-\sigma \nabla \Phi = \mathbf{J}$$

- Modeling Vortex Pinning = Applied Current + Normal Inclusions.

Anisotropy

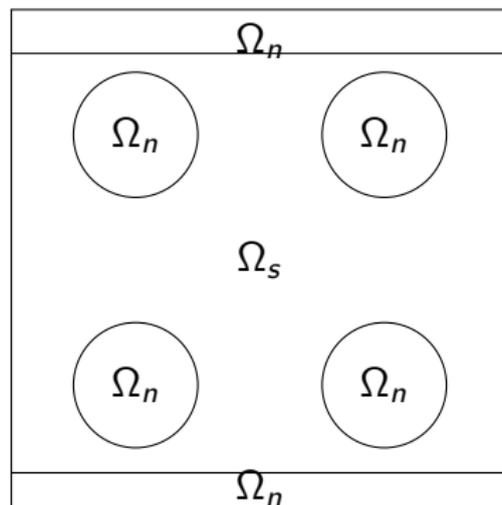
- Anisotropy distorts the shape of vortices.
- $\lambda^x = 60$ nm, $\xi^x = 5$ nm, $(1 - \frac{T}{T_c}) = 0.7$, $\frac{T}{T_c} = 0.3$,
 $\mathbf{H} = 1.5 = 1.5\sqrt{2}\mathbf{H}_c^x$ and $m_y = \frac{1}{4}m_x$.



Anisotropy

G-L Variants: Normal Inclusion Model

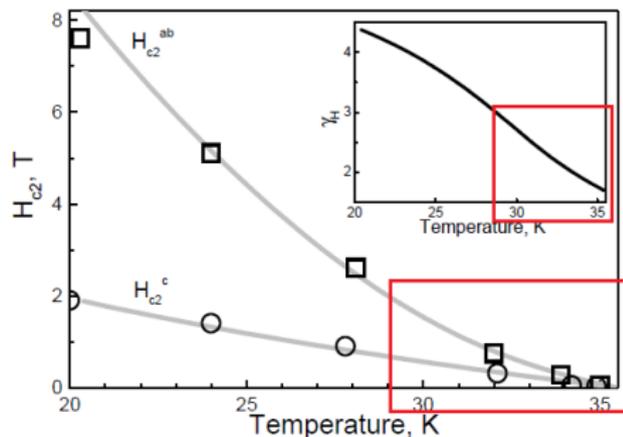
- Superconducting (Ω_s), Normal (Ω_n).



Two-Band Superconductivity

Two-Band Superconductivity

- Some HTS come with odd properties.
- Magnesium Diboride (MgB_2) ($T_c = 39 \text{ K}$) is no exception.
- Anisotropic direction ab .
- Isotropic direction c .
- Upward curvature in T dependence of H_{c2} .



Two-Band Superconductivity

- Addition of second superconducting band explained behavior. Bands are “pathways”.
- Two-band TDGL model (2B-TDGL) $\rightarrow \psi_1$ and ψ_2 .
- $\lambda_i, \xi_i, \kappa_i, H_{i,c2}, T_{i,c}$
- Composite T_c, H_{c2} above each band's value from Coupling.
- Peculiarity: $T > T_{2,c}$, but $T < T_{1,c}$ and Superconductivity persists.
- Other HTS (Iron Pnictides) possess similar behavior.

Modified 2B-TDGL (M2B-TDGL) for HTS

- We would like to model HTS and all their odd properties.
- This composite model includes:
 - Two-band Behavior
 - Anisotropy
 - Applied Currents
 - Novel Strategy for Normal Inclusion
- How to ensure normal behavior?

Ensuring Normal Behavior

- For SC $(1 - \frac{T}{T_c}) > 0$
- One-band normals $(1 - \frac{T}{T_c}) \rightarrow -1$
- Two-band for MgB₂ $(1 - \frac{30K}{T_{2,c}}) \approx -1.5$
- No coupling in normal regions and $(1 - \frac{T}{T_{i,c}}) \rightarrow$.

$$\alpha_i(x, y)|_{\Omega_n} < \min\left\{\left(1 - \frac{T}{T_{1,c}}\right), \left(1 - \frac{T}{T_{2,c}}\right)\right\} < 0$$

$$\alpha(x, y) = -2 \in \Omega_n.$$

$$\left(\frac{\partial \psi_1}{\partial t} - i \frac{J_y}{\sigma} \kappa_1 \psi_1 \right) - \alpha_1(x, y) \psi_1 + b(x, y) |\psi_1|^2 \psi_1 + \left(\hat{\mathbf{D}}_1 \cdot \Lambda_1(x, y) \cdot \hat{\mathbf{D}}_1 \right) \psi_1 + \eta(x, y) \psi_2 = 0 \quad (3)$$

$$\Gamma \left(\frac{\partial \psi_2}{\partial t} - i \frac{J_y}{\sigma} \kappa_1 \psi_2 \right) - \alpha_2(x, y) \psi_2 + b(x, y) |\psi_2|^2 \psi_2 + \left(\hat{\mathbf{D}}_2 \cdot \Lambda_2(x, y) \cdot \hat{\mathbf{D}}_2 \right) \psi_2 + \eta(x, y) \nu^2 \psi_1 = 0 \quad (4)$$

$$\begin{aligned} \nabla \times \mathbf{H} + \mathbf{J} &= \sigma \frac{\partial \mathbf{A}}{\partial t} + \nabla \times \nabla \times \mathbf{A} \\ &+ \Lambda_1(x, y) \cdot \left[\frac{i}{2\kappa_1} (\psi_1^* \nabla \psi_1 - \psi_1 \nabla \psi_1^*) + \frac{x_0^2}{\lambda_{1,c}^2} \mathbf{A} |\psi_1|^2 \right] \\ &+ \Lambda_2(x, y) \cdot \left[\frac{i}{2\nu\kappa_2} (\psi_2^* \nabla \psi_2 - \psi_2 \nabla \psi_2^*) + \frac{x_0^2}{\lambda_{2,c}^2} \mathbf{A} |\psi_2|^2 \right] \end{aligned} \quad (5)$$

$$\hat{\mathbf{D}}_1 = -i \frac{\xi_{1,c}}{x_0} \nabla - \frac{x_0}{\lambda_{1,c}} \mathbf{A}$$
$$\hat{\mathbf{D}}_2 = -i \frac{\xi_{2,c}}{x_0} \nabla - \nu \frac{x_0}{\lambda_{2,c}} \mathbf{A}$$
$$\nu = \frac{\lambda_{2,c} \xi_{2,c}}{\lambda_{1,c} \xi_{1,c}}$$

Modeling MgB_2 .

Modeling MgB_2

- MgB_2 is an ideal candidate for our model.
- MgB_2 is cheap and ductile, being ideal for wires.
- Superconducting wires \rightarrow Transport currents.
- Validating our model and it's simulation?
- Flux flow, vortex pinning, and transport currents.

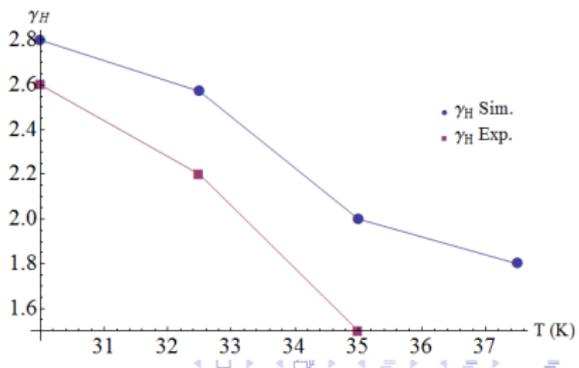
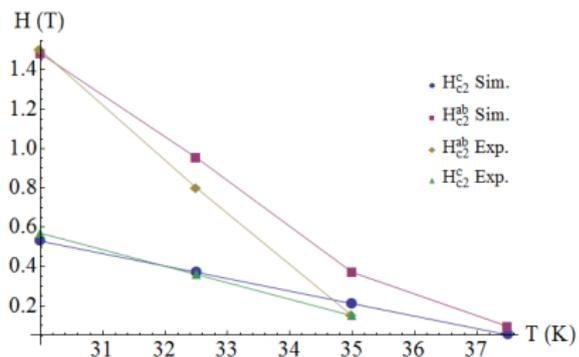
Material Parameters

- The material parameters for MgB₂.
- Notice one band is Type II, the other is Type I.
- Γ_i and ϵ (or η) derived.

$\xi_{1,c}=13.0$ nm	$\lambda_{1,c}=47.8$ nm	$\kappa_1=3.62$
$\xi_{2,c}=51.0$ nm	$\lambda_{2,c}=33.6$ nm	$\kappa_2=0.66$
$\Gamma_1=0.0288\hbar$	$\Gamma_2=0.001875\hbar$	$\epsilon(0K)=-2.7016\times 10^{-17}$ J
$T_{c1}=35.6$ K	$T_{c2}=11.8$ K	$T_c=39.0$ K
$H_{1,c}(0K)=0.3745$ T	$H_{2,c}(0K)=0.1358$ T	$\rho_n=0.7$ $\mu\Omega/cm$
$\gamma_1(0K)=4.55$	$\gamma_2(0K)=1.0$	

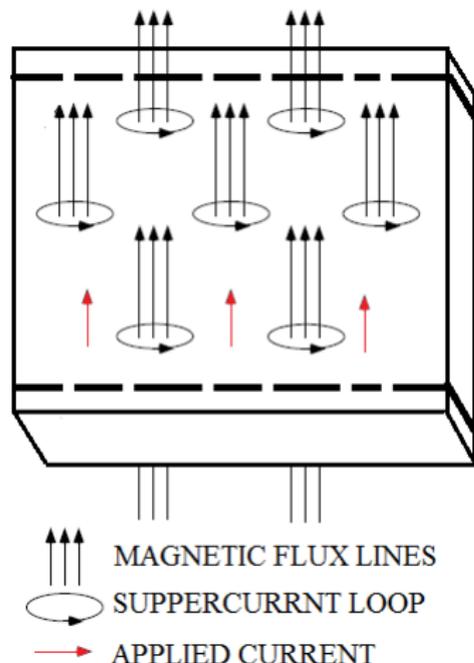
Validation: Curvature in H_{c2}

- One of the well known properties is the curvature in H_{c2} .
- Can we reproduce this in simulations?
- Our coupling is simplified.
- Qualitative behavior.



Vortex Pinning and Transport Currents

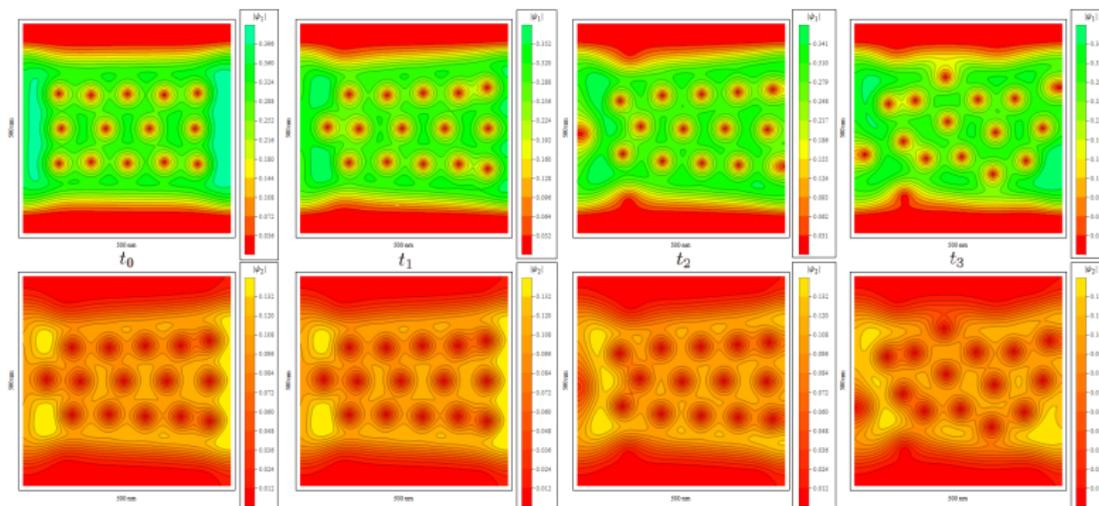
- Now we model vortex pinning.
- Our numerical domain.
(Current $+y$, Field $+z$)
- Normal bands (dashed lines) are metal leads.
- We can see how much current is transported resistance free.



- 1. Flux flow with field.
- 2. Vortex pinning.
- 3. Are the normal inclusions pinning?

Simulation 1: Flux Flow in Field

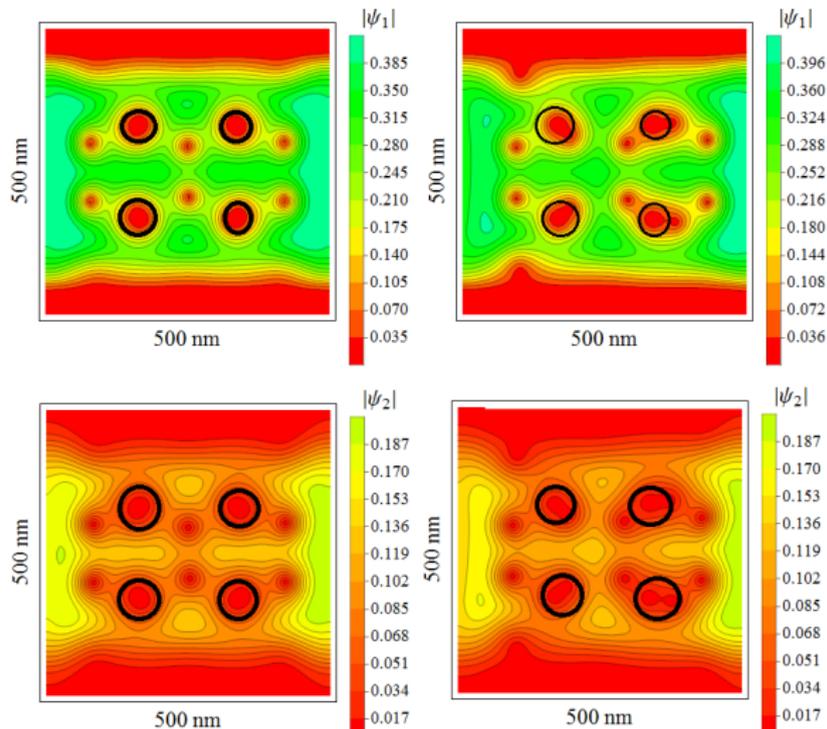
- Now $\mathbf{H} = 0.2648 \text{ T}$, $\mathbf{J} = 33.717 \text{ MA cm}^{-2}$, $T = 30\text{K}$
- Movie time frame: 1203.84 ps (1.2 ns)



Simulation 1: Flux Flow in Field

Simulation 2: Flux Flow and Normal inclusions

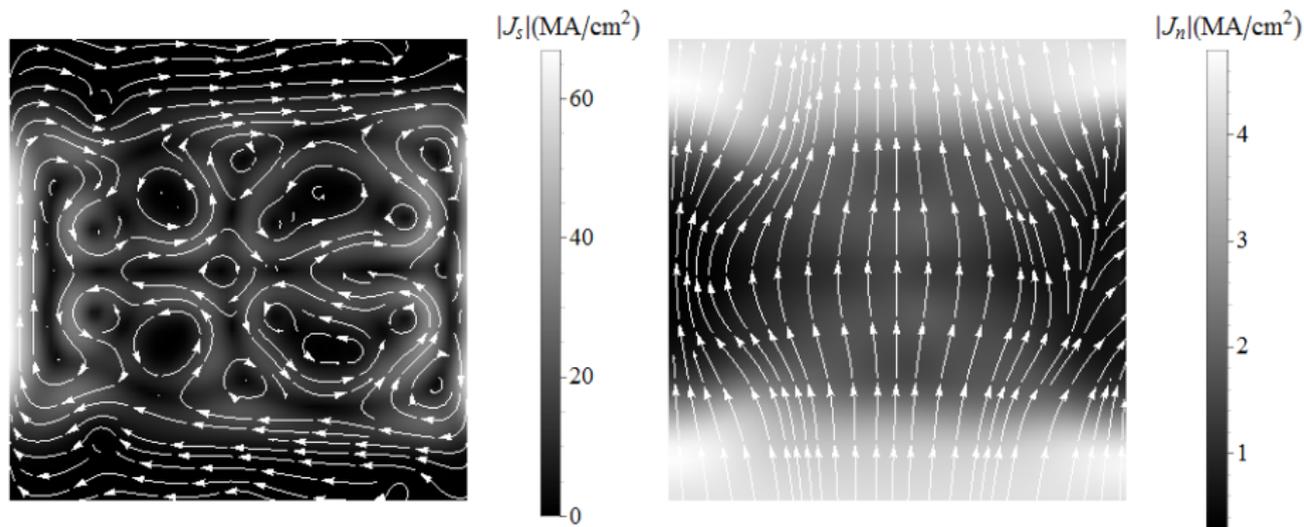
- $\mathbf{H} = 0.2648 \text{ T}$ $\mathbf{J} = 4.214 \text{ MA cm}^{-2}$, $T = 30\text{K}$.
- 4 Normal Inclusion, outlined in black.



Simulation 2: $\mathbf{J}=4.214 \text{ MA cm}^{-2}$

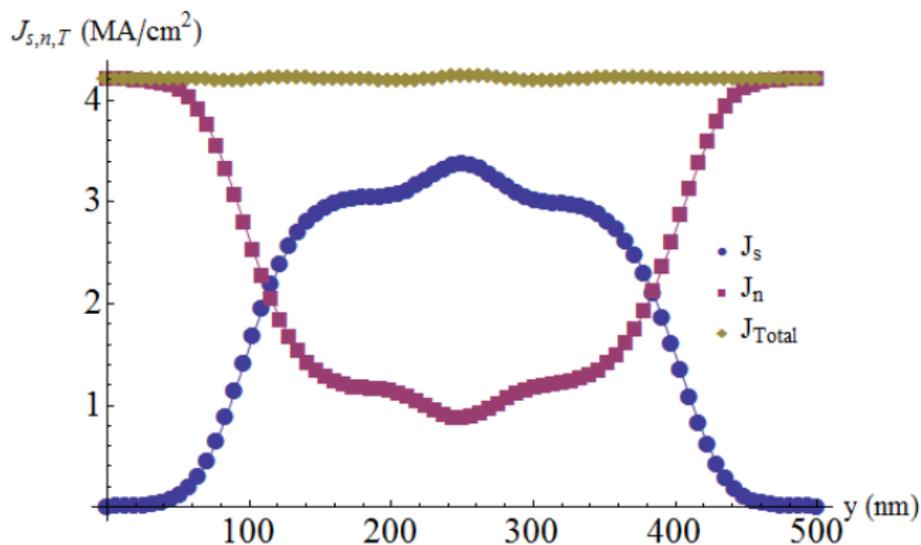
Simulation 2: Resistance Free Current?

- Super and normal current stream density plots.
- Hard to determine!



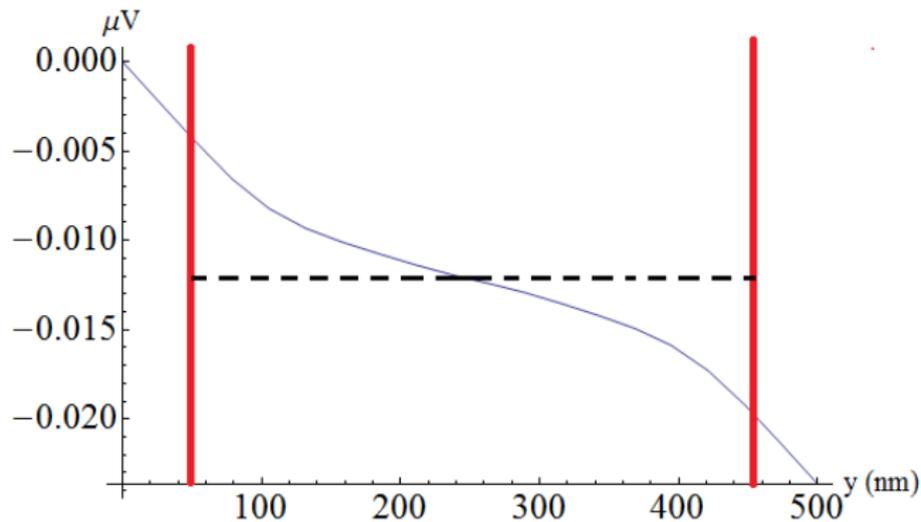
Average Currents

- We can also look at values in the y-direction averaged over x.
- There is a large minimum in J_n .



Resistance By Voltage

- Can the voltage be used as a proxy to resistance?
- No Resistance = No Voltage in S.C.! $V(y) = V(0) - \int_0^y E_{y,avg}(y')y'$

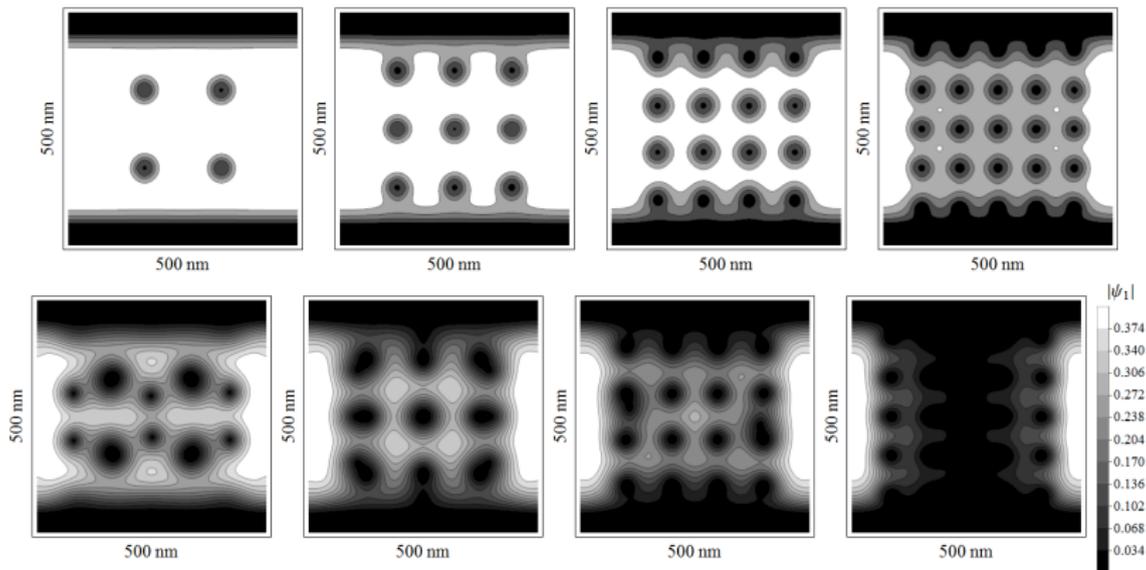


Resistance By Voltage

- J_c is hard to find. Envelope of simulations.
- How can you tell if normal inclusions are working?
- If the vortices are pinned, the voltage change should be small (Metric).
- Implies less flux flow and resistance.

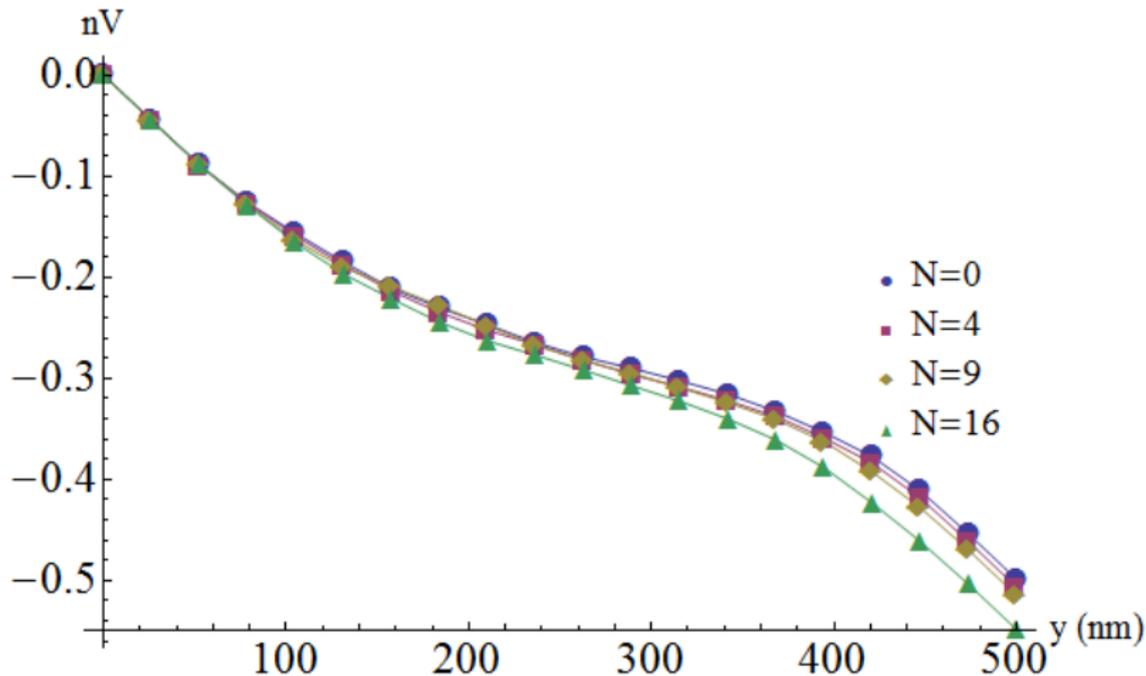
Vortex Pinning

- The normal inclusion arrangement (top) for $N=4, 9, 16, 25$ normal inclusions.
- Their respective steady state solutions with $\mathbf{H} = 0.2648$ T and $T = 30$ K. (bottom)



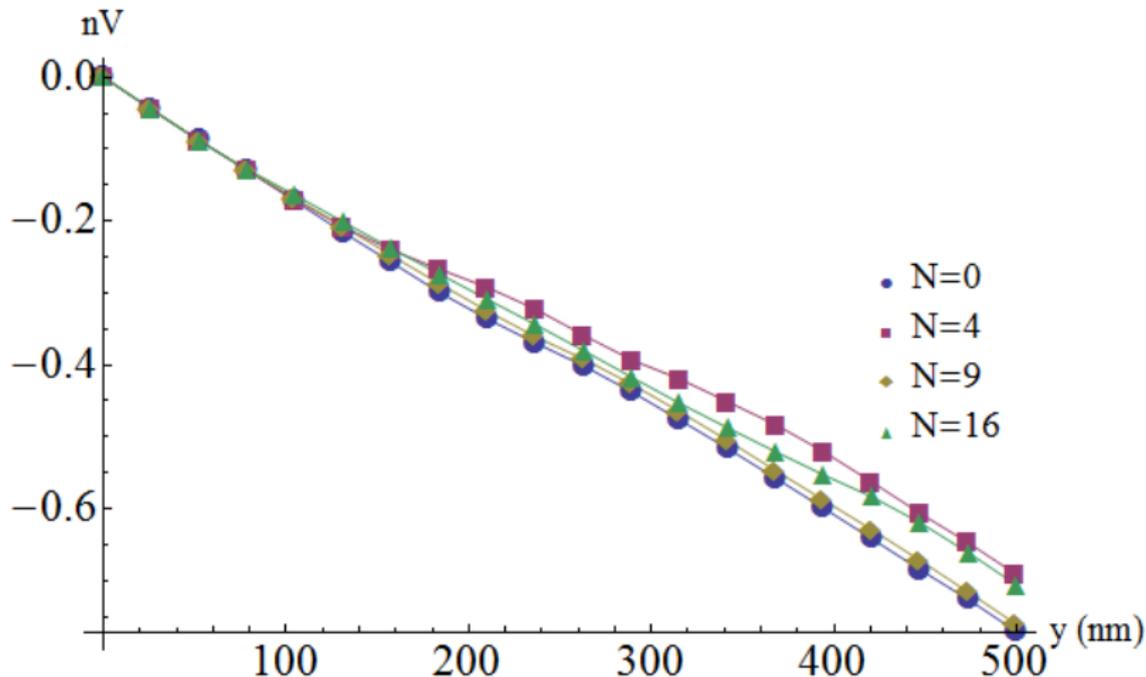
$$J = 0.0843 \text{ MA cm}^{-2} \text{ at } t = 0$$

- $N=0$ has the smallest voltage change at first. Notice the trend with N ?



$J = 0.0843 \text{ MA cm}^{-2}$ at 100 TS.

- Now $N = 4$ and $N = 16$ have the smallest change due to pinning.



Various Applied Currents

- While the exact pattern is not known, the normal inclusions pin vortices for mild current densities.

- ΔV in nV

N	$J=33.717 \text{ MA cm}^{-2}$	$J=0.08429 \text{ MA cm}^{-2}$	$J= 0.8429 \text{ KA cm}^{-2}$
0	-326.656 nV	-0.793243 nV	$-5.16257 \times 10^{-3} \text{ nV}$
4	-326.954 nV	-0.714098 nV	$-6.37429 \times 10^{-3} \text{ nV}$
9	-337.007 nV	-0.782900 nV	$-4.33417 \times 10^{-3} \text{ nV}$
16	-335.168 nV	-0.728167 nV	$-6.97961 \times 10^{-3} \text{ nV}$

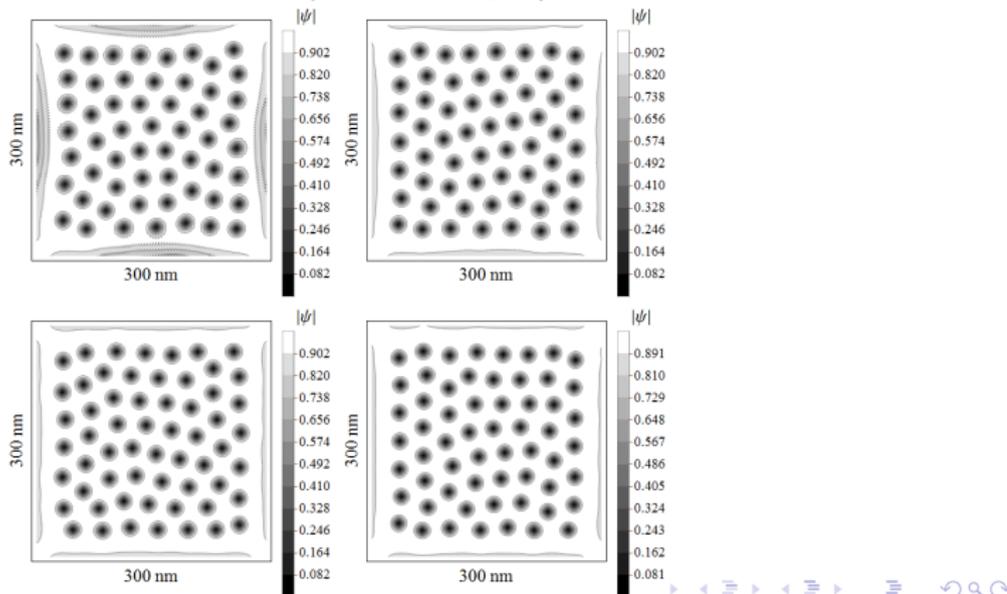
Computational Issues

Computational Issues

- HTS modeling is only part of the endeavor.
- To simulate superconducting technology, large domains are needed.
- Limited computational resources call for superior methods.
- The needed resolution also grows non-linearly with domain size.
- In this second endeavor, we to hope find ways to improve storage and shorten solve times.
- One-band: $\lambda = 50$ nm, $\xi = 5$ nm, $(1 - \frac{T}{T_c}) = 1.0$, $\frac{T}{T_c} = 0.0$,
 $\mathbf{H} = .15\kappa H_c$, and $\kappa = 10$.

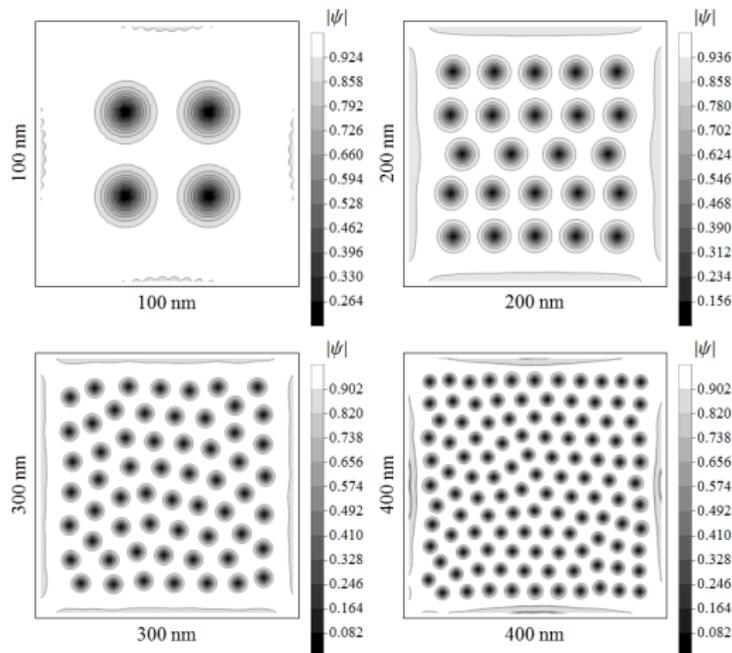
Resolution Issues

- A 300 nm by 300 nm domain. The number of vortices changes with resolution.
- 103040 DOFs and 56 vortices (top left), 231360 DOFs and 59 vortices (top right), 410880 DOFs and 60 vortices (bottom left), and 641600 DOFs and 60 vortices (bottom right)



Non-Linear Growth in Resolution

- Domain sizes of $(100 \text{ nm})^2$, $(200 \text{ nm})^2$, $(300 \text{ nm})^2$, $(400 \text{ nm})^2$
- $h = 4.761 \text{ nm}$ for $(100 \text{ nm})^2$, $h = 3.278 \text{ nm}$ for $(200 \text{ nm})^2$, $h = 2.127 \text{ nm}$ for $(300 \text{ nm})^2$, and $h = 1.990 \text{ nm}$ for $(400 \text{ nm})^2$.



- Banded solver and symmetric Cholesky solver.
- CSR and SuperLU gave storage improvements.
- Parallelization through Trilinos and distributed matrices.
- Geometry is still a problem.
- Trilinos provides vast suite of solvers (and preconditioners).

- Decoupling methods can reduce memory.
- Decoupling large systems \rightarrow Reducing in DOFs.
- Decoupling ψ and \mathbf{A} equations?
- This give one non-linear system $(\mathcal{R}\{\psi\}, \mathcal{I}\{\psi\})$ and one linear systems $(\mathbf{A}_x, \mathbf{A}_y)$.

Decoupling of Type I Vs Full Equations

- The storage advantage is clear!
- Going to steady state may take longer with decoupling.
- Global transient behavior.
- Is it more appropriate for dynamic studies?

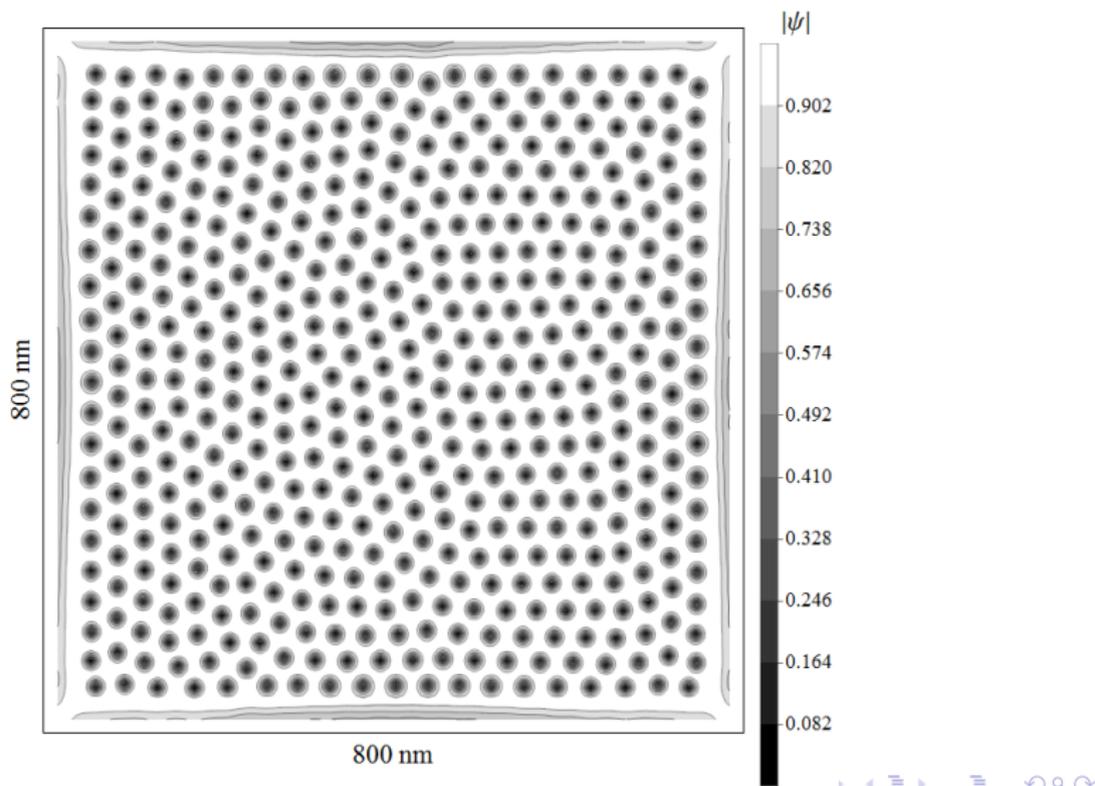
Domain Expansion

- Now we can see what the improvements have done for us.
- The serial Banded solver limited us to 24 vortices.
- Now we have ≈ 450 when the geometry routine maxed out the memory.

Implementation	Method Max	Domain (nm ²)	Domain (ξ^2)	DOFs*	Vortices
		50 ²	(10 ξ) ²	1,680	0
		100 ²	(20 ξ) ²	6,560	4
		150 ²	(30 ξ) ²	58,080	12
Serial	Banded	200 ²	(40 ξ) ²	58,080	24
		300 ²	(60 ξ) ²	314,720	60
Serial	CSR Full Eq.	400 ²	(80 ξ) ²	641,600	116
Serial	CSR Decoup. Type 1	500 ²	(100 ξ) ²	1,640,960	172
Parallel	Serial Geom max	800 ²	(160 ξ) ²	23,049,600	≈ 450

A Small Hurdle

120 processors for 96 hours (11520 CPU hours)

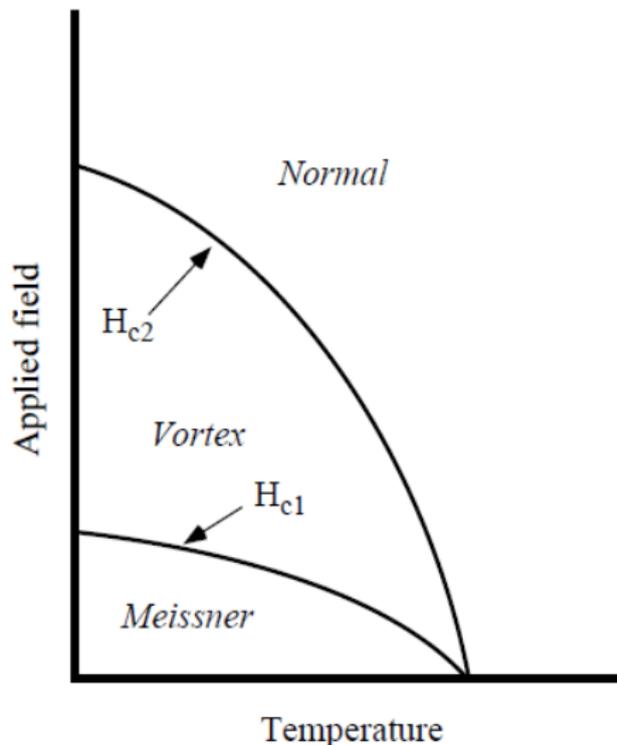


- Improve some aspects of the M2B-TDGL.
- More realistic modeling: Normal inclusion metals.
- Apply computational methods to two-band model.

Back Up Slides

Type II

- Type II SC have 2 critical values for \mathbf{H} .
- H_{c1} : Transition form Meissner to Vortex state.
- H_{c2} : Transition form Vortex to Normal state.
- H_c is still used for ND in Type II calculations.



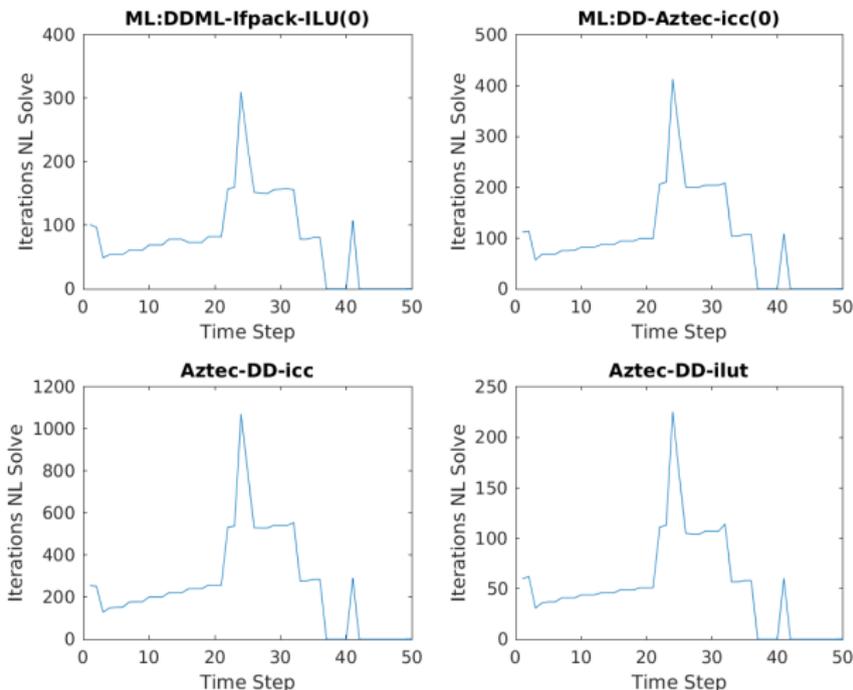
Preconditioning

- Several we tested on 100 time steps, with 25921 degrees of freedom on a 20 nm by 20 nm domain.
- $\lambda = 50$ nm, $\xi = 5$ nm, $\kappa = 10$, $(1 - \frac{T_c}{T_c}) = 1.0$, $\mathbf{H} = 0.15\kappa\sqrt{2}H_c \hat{z}$

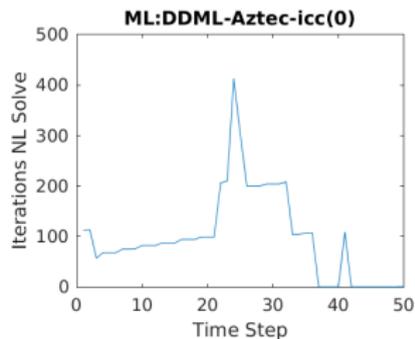
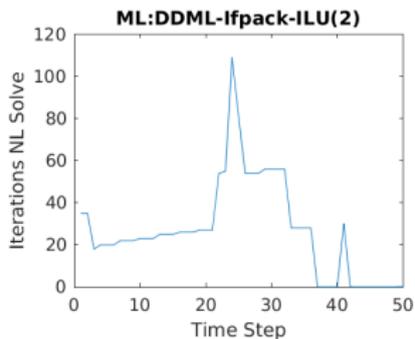
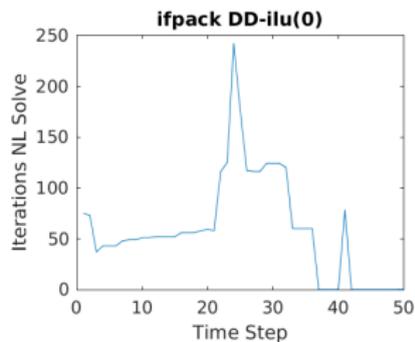
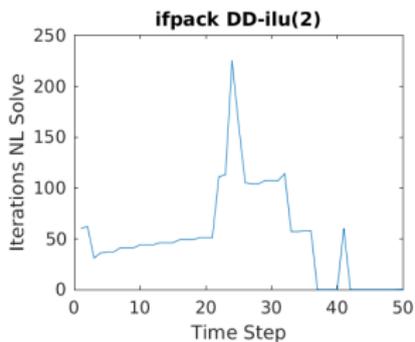
Preconditioner	NL solver Timing (sec)
Aztec-DD-icc(0)	1193.74
Aztec-DD-ilut(0)	1319.49
ifpack DD-ilu(0)	1332.03
ifpack DD-ilu(2)	1411.68
ML:DD-Aztec-icc(0)	3118.95
ML:DDML-Aztec-icc(0)	3325.07
ML:DDML-Ifpack-ILU(2)	4108.58
ML:DDML-Ifpack-ILU(0)	4319.17

Preconditioning

- GMRES iterations for each non-linear solve.
- Aztec-DD-icc has the shortest run time but largest iteration count.
- Iteration count before non-linear tolerance tightened.



Preconditioning



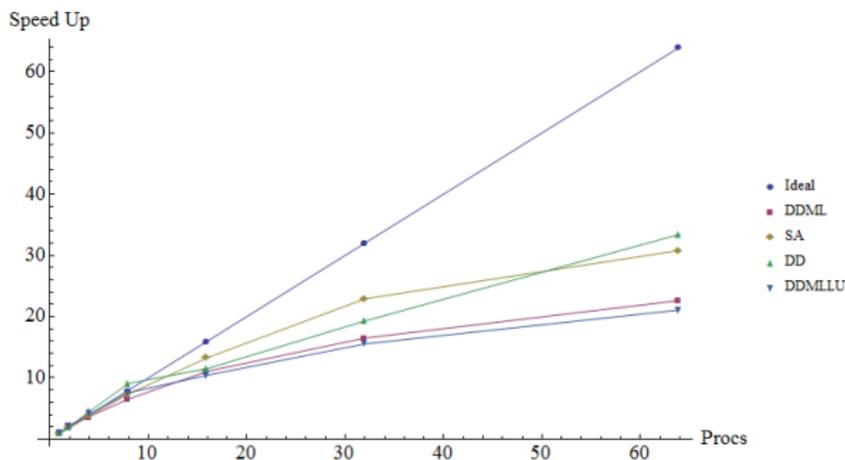
Preconditioning

- Iteration counts and solve times?
- How do they perform with more DOFs?

Preconditioner	DOFs	wall time	avg iters per GMRES solve
Aztec-DD-icc(0)			
	103040	1193.74	540.9
	1640960	123479.0	859.0
ifpack DD-ilu(0)			
	103040	1411.68	204.6
	1640960	220355.2	103.3
ML:DD-Aztec-icc(0)			
	103040	3118.95	237.14
	1640960	106508.0	261.6
ML:DDML-Aztec-icc(0)			
	103040	3325.07	237.14
	1640960	47905.8	91.457

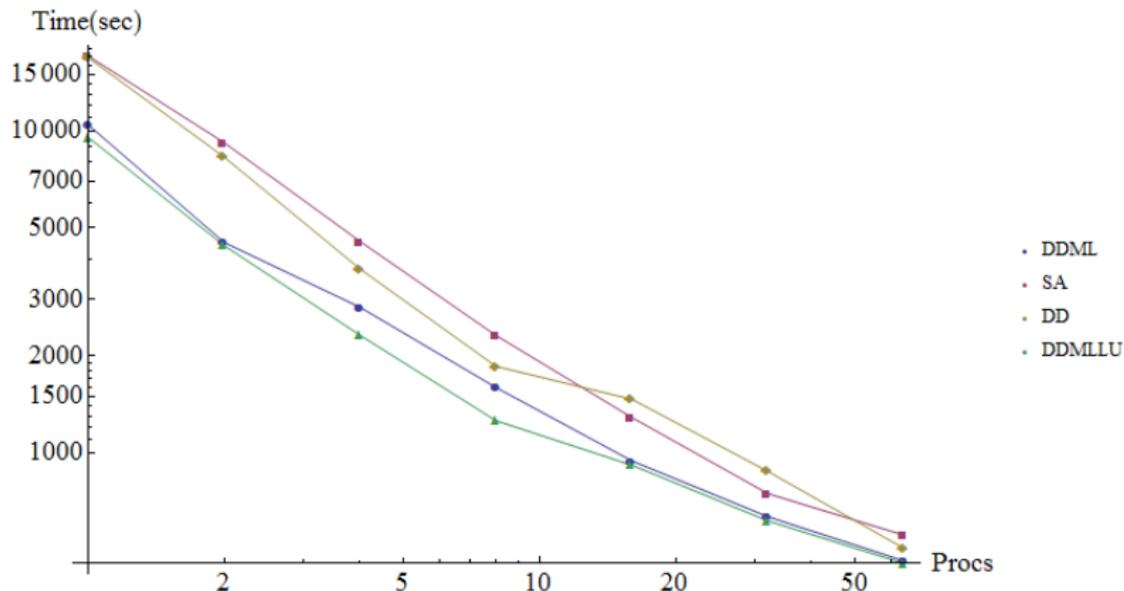
Preconditioning

- Clearly the ML preconditioners perform well for large domains.
- How do they scale for a small set of processors? (103041 DOFS)



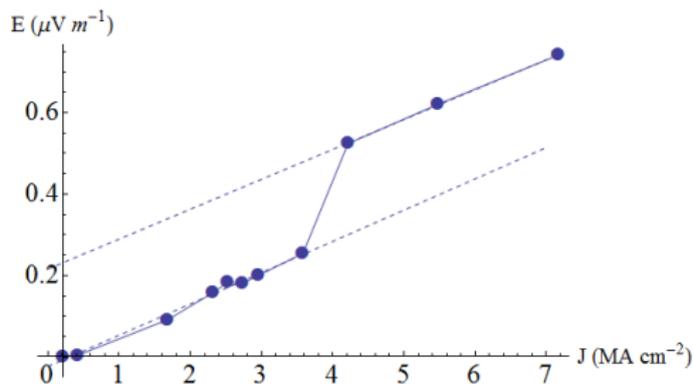
Preconditioning

- The Domain Decomposition (DD) and Smooth Aggregation (SA) scale well.
- But have the worst timings.



$E - J$ Curve

- The $E - J$ curve helps characterize J_c in Materials.
- Finding J_c numerically can be a chore!
- However this observable is still important.
- Flux Flow!



```
initialization of time;  
set initial time step;  
Newton iterates,  $\psi(0) = \psi_{0,0}$  and  $\mathbf{A}(0) = \mathbf{A}_{0,0}$ ;  
set  $\text{tol} = 10^{-8}$ ;  
for each time step  $i$  do  
| Non Linear Solve;  
| if steady state then  
| | STOP;  
| else  
| | update solution and continue;  
| end  
end
```

Algorithm 1: General TDGL Algorithm

Let: $G(\psi, \mathbf{A})$ be the G-L equation

Let: $M(\psi, \mathbf{A})$ be the Maxwell equation

for $k = 1, \dots, k_{max}$ *iterate between equations do*

Solve: $\text{Jac}[G(\psi_{k,i}, \mathbf{A}_{k,i})] \delta \psi_{k+1,i} = -\text{Resid}[G(\psi_{k,i}, \mathbf{A}_{k,i})];$

$\psi_{k+1,i} = \psi_{k,i} + \delta \psi_{k+1,i};$

Solve: $M(\psi_{k+1,i}, \mathbf{A}_{k,i}) \mathbf{A}_{k+1,i} = \nabla \times \mathbf{H};$

Calculate: $R_1 = \text{Resid}[G(\psi_{k,i+1}, \mathbf{A}_{k,i+1})];$

Calculate: $R_2 = \text{Resid}[M(\psi_{k+1,i}, \mathbf{A}_{k,i+1})];$

set $\text{Max } R = \max\{R_1, R_2\};$

if $\text{Max } R < \text{tol}$ **then**

 | go to next time step;

else

 | continue iterating;

end

end

Algorithm 2: The decoupling of type 1 algorithm for the TDGL system

Decoupling of Type I Vs Full Equations

- Performance test to steady state.
- Full Equations DOFs: 25920, Decoupling of Type 1 DOFs: 13122.
- Since our matrix size has been reduced by $1/2$, our storage is cut by $1/4$.
- At the cost of more time steps and non-linear iterations.

Method	Storage	Time steps	Horizon	Wall Time
Full	1165896	145	5002.05	526.226 s
Decoupl. type 1	296964	328	5477.00	1463.32 s

Method	NL time (sec)	NL time Avg. (sec)	Avg NL steps
Full	522.459	3.60	1.55
Decoupl. type 1	1463.32	4.461	3.71

Decoupling of Type I Vs Full Equations

- The adaptive time step does not give a fair comparison.
- For a fixed non-dimensionalized time step of 0.5.
- Full Equations DOFs: 410,880, Decoupling of type 1 DOFs: 206,082.
- The Decoupling Method gives a shorter solve time! (2 small vs 1 big)

Method	Time steps	NL. Time (sec)	NL time Avg. (sec)	Avg NL steps
Full Eq.	1000	63733.7	63.733	1.455
Decoup. type 1	1000	44974.0	44.974	2.128

Decoupling

- The next clear step is to decouple the TDGL system into 4 four systems.
- This would cut the matrix storage by $1/16$ when compared to the full equations.
- Possibly more time steps to steady state.
- What if we just want the steady state?

Decoupling of Type 2

- What if we decouple and linearize using previous time steps (ψ_n, \mathbf{A}_n) .
- Now we have 4 decoupled linear equations.
- Best case scenario?

$$\frac{\partial \psi}{\partial t} - \Delta \psi^{n+1} = -(|\psi^n|^2 - (1 - \frac{T}{T_c})\psi^n - \frac{i}{\kappa} \psi^n \nabla \cdot \mathbf{A}^n - \frac{i}{\kappa} \mathbf{A}^n \cdot \nabla \psi^n - \frac{1}{\lambda^2} \psi^n |\mathbf{A}^n|^2) \text{ in } \Omega \times (0, T), \quad (6)$$

$$\begin{aligned} \sigma \left(\frac{1}{\lambda^2} \frac{\partial \mathbf{A}}{\partial t} \right) + \nabla \times \nabla \times \mathbf{A}^{n+1} - \nabla (\nabla \cdot \mathbf{A}^{n+1}) &= \sigma \left(\frac{1}{\lambda^2} \frac{\partial \mathbf{A}}{\partial t} \right) - \Delta \mathbf{A}^{n+1} \\ &= -\frac{i}{2\kappa} (\psi^n \nabla \psi^{*n} - \psi^{*n} \nabla \psi) - \frac{1}{\lambda^2} |\psi^n|^2 \mathbf{A}^n + \nabla \times \mathbf{H} \text{ in } \Omega \times (0, T). \end{aligned} \quad (7)$$

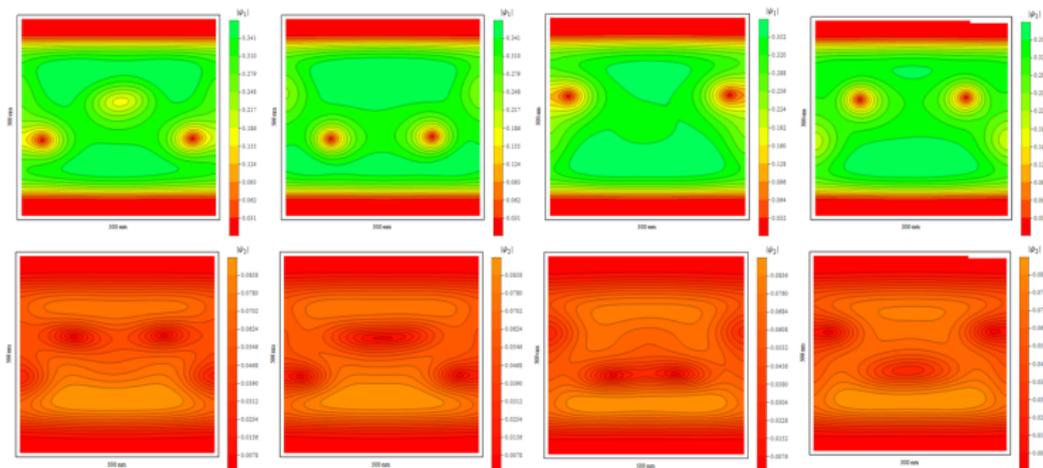
Decoupling of Type 2

- Time step size restriction for “backward Euler”.
- The restriction has some relations to resolution.
- Could another time method help (Exponential Integrators?)

DOFs	Domain Size (nm ²)	Acceptable Time Step size (ND units)
6561	10 ²	0.5
25921	20 ²	0.3
103041	20 ²	0.3
103041	30 ²	0.0625
410881	50 ²	<0.0625

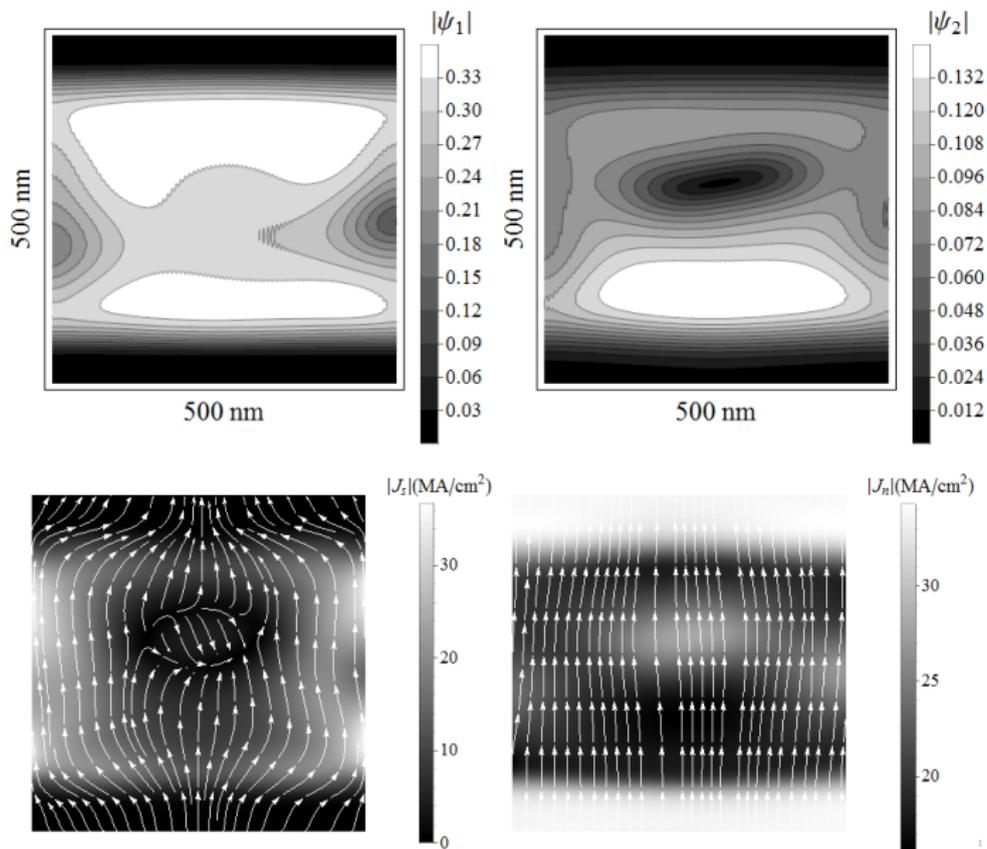
Simulation 1: Flux Flow

- $\mathbf{H} = 0$, $J = 33.717 \text{ MA cm}^{-2}$, $T = 30 \text{ K}$, ψ_1 (top), ψ_2 (bottom).
- $t = 0.6912 \text{ ns}$, $t = 0.6933 \text{ ns}$, $t = 0.6974 \text{ ns}$, $t = 0.6992 \text{ ns}$.



$$J = 33.717 \text{ MA cm}^{-2}$$

Resistance Free Current?



Resistance Free Current?

- \mathbf{J}_s and \mathbf{J}_n in y -direction averaged over x .
- 1/2 of the current is Normal! ($J = 33.717 \text{ MA cm}^{-2}$)
- Flux flow is a problem!

