Scientific Computing

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Main Points

- What is Scientific Computing (SC)?
- Agreement Between SC and Experiment
- SC complementing Experiments
- SC complementing Theory
- The SC department and program

What is Scientific Computing?

- Scientific Computing (SC) or Computational Science is an **Interdisciplinary Science**.
- Combining Mathematics, Computer Science, Engineering, and Natural Sciences to solve problems.
- Scientific Computing $\neq$ Computer Science

How is it used?

- Typically Computational Scientist fall into two groups.
- Using algorithms and **Improving** / **Implementing** algorithms.
- The second group shares the true spirit of Scientific Computing.
- Scientific Computing is aimed at finding ways to improve problem solving and solving new problems

How is it used? (Cont.)

- Physical phenomena can be modeled by numerical algorithms to take advantage of what **computers do best**.
- Some of these advantages are seen in:
    - Complicated domains and non-linearities in PDE's.
    - Large statical analysis or Monte Carlo methods.
    - Large matrix equations or eigenvalue problems

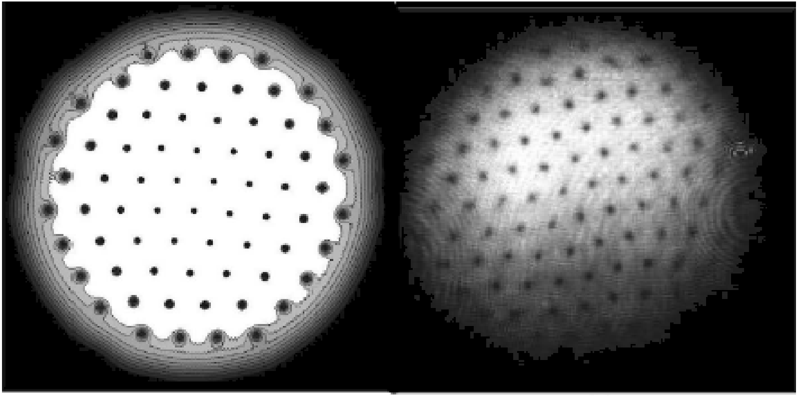
Why Should You Care?

- Computers are becoming more powerful.
- FSU's RCC HPC has 403 nodes, 6464 CPU cores and 109.5 Tflops (10^{12} operations per second).
- Symbiotic relation with Science.
- Numerical simulations can complement experiments.
- Complementing complicated theories.

SC Agreeing With Experiment

- Verification and Validation are critical
- Some may say nothing new was done.
- Some also are suspect of the numerical error associated with the algorithm, but this is were verification comes in.
- Experimental uncertainty and numerical error

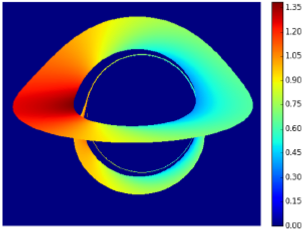
- Qiang Du, shows that his algorithm for the Gross-Pitaevskii equations. This a BEC of an alkali-metal gas. The voctices are nucleated by laser stirring and rotating magnetic traps. His results for the vortices in the substance are shown in (a). Experimental results from MIT are shown in (b).



(a) (b)

Gravitational Lensing

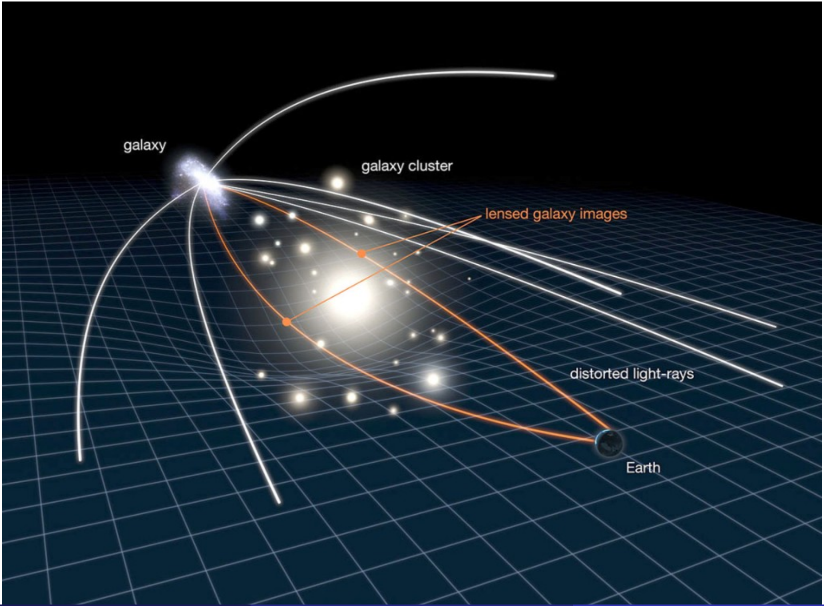
- Bin Chen of FSU's RCC uses his Linearized backward gravitational lensing code to reproduce a scene from a movie. All though the movie is pretty graphic art, Bin's algorithm reproduces a similar realistic simulation.



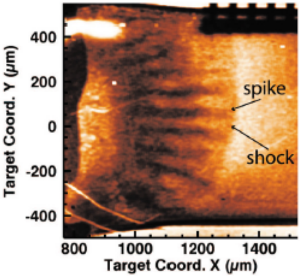
Chen et al. **2015**, ApJS, 218, 4

Picture from movie **"interstellar"**

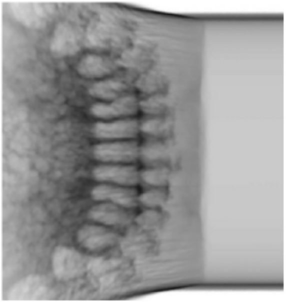
Gravitational Lensing



- The experiment (left) Simulates shock in a Super Nova.
- The simulation (right) tries to replicate it but is slightly off.

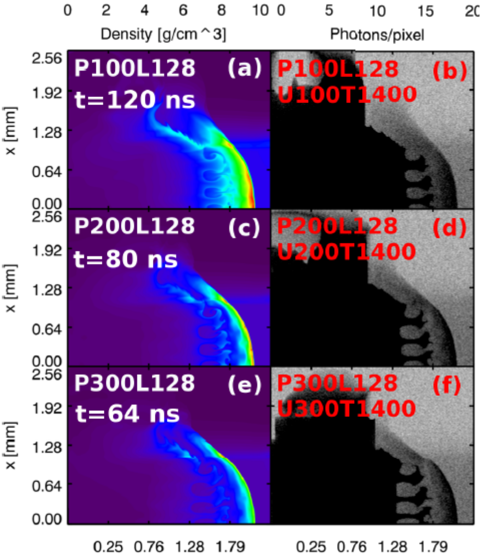


(a) An x-ray radiographic image of an experiment that used a 3D, single-mode perturbation. Time $t = 21$ ns. Adopted from Kuranz et. al [10]



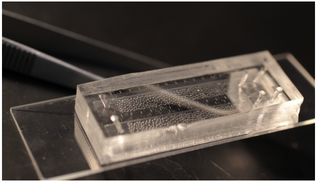
(b) The results from a 3D FLASH simulation with 3D, single-mode initial conditions. Time $t = 21$ ns. Adopted from Fryxell et. al [6]

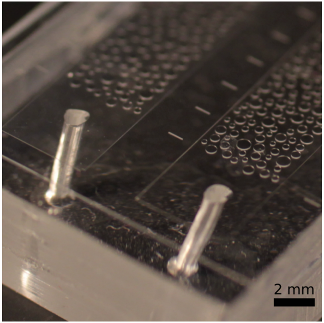
Omega Laser and Super Nova



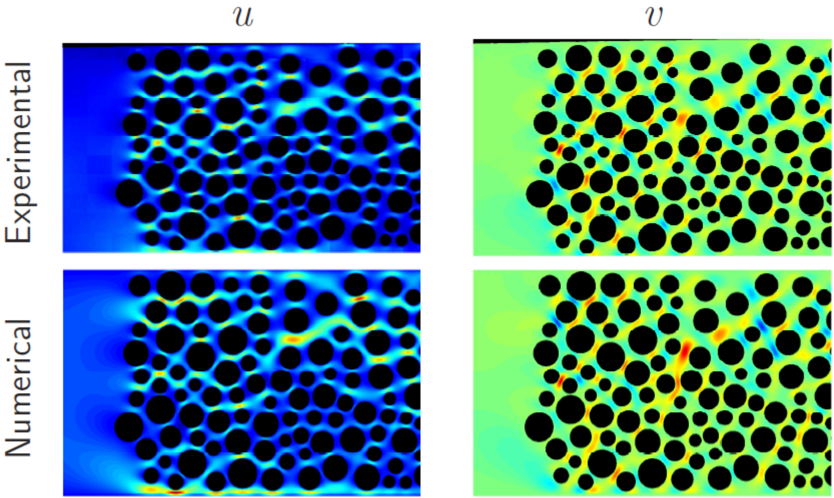
Experimental setup

- Channel has dimensions $5.2mm \times 45mm \times 0.1mm$
- Water injected at $0.01mm^3/s$
- $Re = 0.005$
- Particle Image Velocimetry (PIV) applied to 8 million neutrally buoyant spherical particles (diameter $= 1\mu m$)

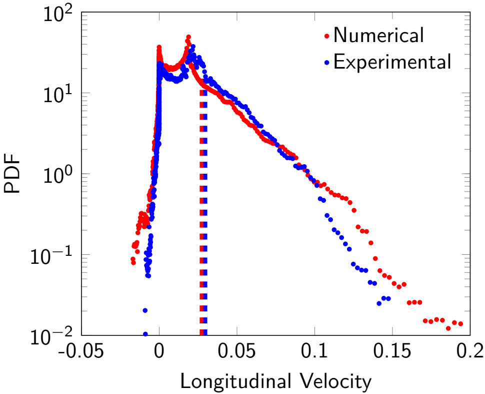




Velocity Field

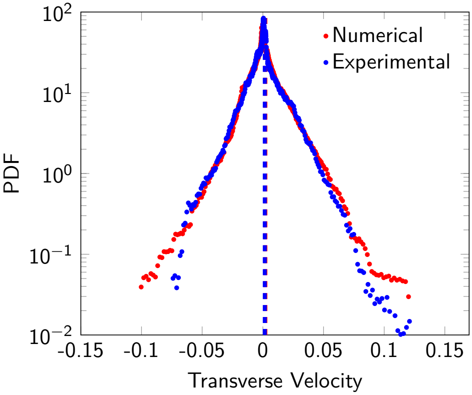


PDF of **v**

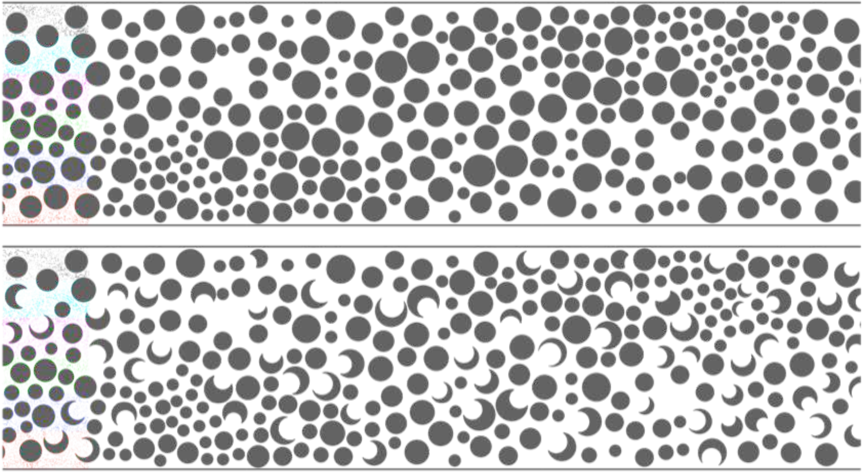


Numerical
Experimental
PDF
10^2
10^1
10^0
10^{-1}
10^{-2}
-0.05
0
0.05
0.1
0.15
0.2
Longitudinal Velocity

PDF of **v**


10^2
10^1
10^0
10^{-1}
10^{-2}
PDF
-0.15
-0.1
-0.05
0
0.05
0.1
0.15
Transverse Velocity
Numerical
Experimental

Mixing

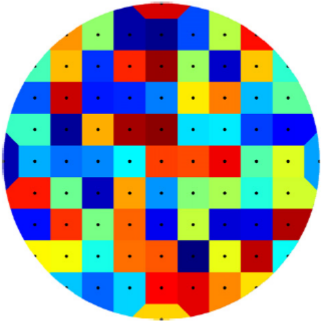


SC Complementing Experiment

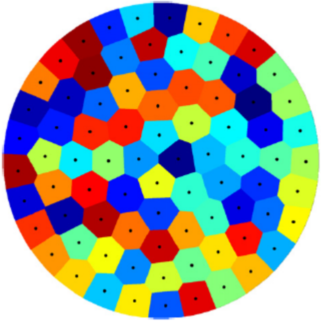
- After verification and validation, we can simulate experiments
- SC be can used where experiments are too expensive or not feasible.
- Simulations can used to filter through experiential situations

- FSU's Dr. Shanbhag and Steve Henke, developed a simulation of a projectile crashing into a brittle material.
- The aim of the study was to show how the setup of the numerical grid affects the results.

S.F. Henke, S. Shanbhag / Computer Physics Communications 185 (2014) 181–193



(a) Square grid.



(b) Centroidal Voronoi generators.

Projectile Impact

- This Simulation could used to test materials ballistic strength without destroying precious materials

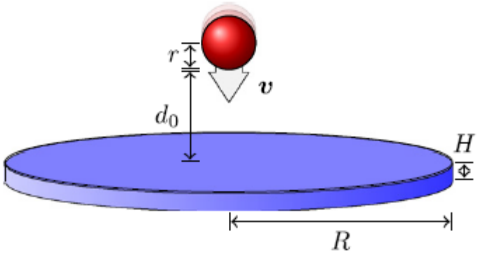
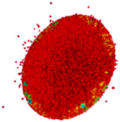
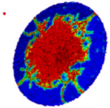
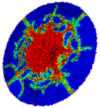
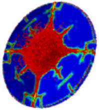
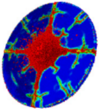
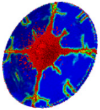
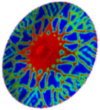
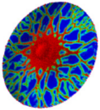
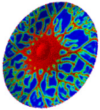


Fig. 6. The initial problem geometry consists of a high speed spherical projectile incident upon a cylindrical plate of the same composition.

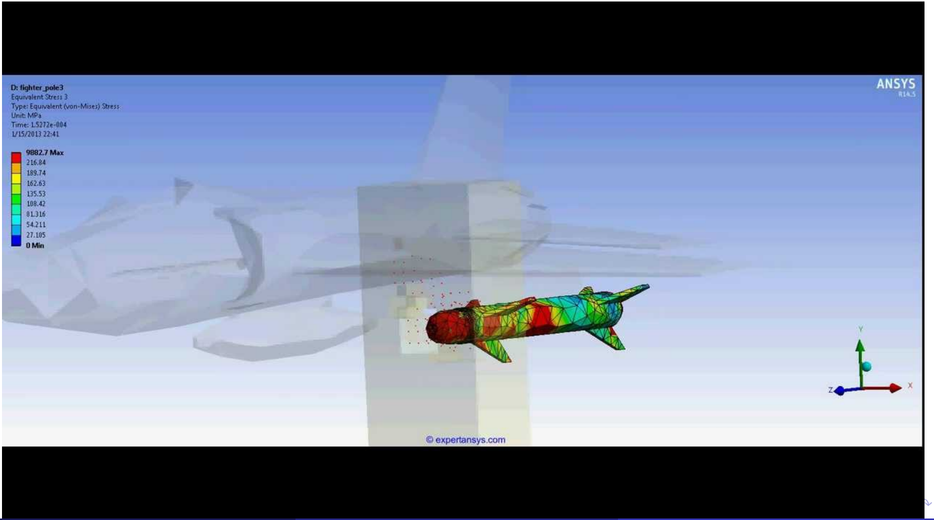
Projectile impact

Table 5
Effects of spatial and temporal refinement on damage patterns in the brittle impact problem. All simulations use a simple cubic grid and an impact velocity of 100 m/s.

	$\Delta t = 2.0 \times 10^{-8}$	$\Delta t = 1.0 \times 10^{-8}$	$\Delta t = 0.5 \times 10^{-8}$
$m = 2$	 Avg. Damage 0.9739	 Avg. Damage 0.4808	 Avg. Damage 0.3646
$m = 3$	 Avg. Damage 0.2985	 Avg. Damage 0.2493	 Avg. Damage 0.2386
$m = 4$	 Avg. Damage 0.4054	 Avg. Damage 0.4065	 Avg. Damage 0.4090

Jet crash

- Another example of precious materials is a billion dollar fighter jet.



SC Complementing Theory.

- Solving theories analytically can call for crafty approximations
- Simple domains, dimensional reduction, and asymptotic behavior
- Numerical methods on computers can crank out complicated calculations
- SC aims at improving algorithms that can handle complicated models
- These algorithms can used to make through theoretical predictions.

Ginzburg Landau Equations for Superconductivity

$$\Gamma\left(\frac{\partial\psi}{\partial t} + i(\frac{Jy}{\sigma})\kappa\psi\right) + \left(|\psi|^2 - 1\right)\psi + (\frac{i}{\kappa}\nabla - \mathbf{A})^2\psi = 0$$

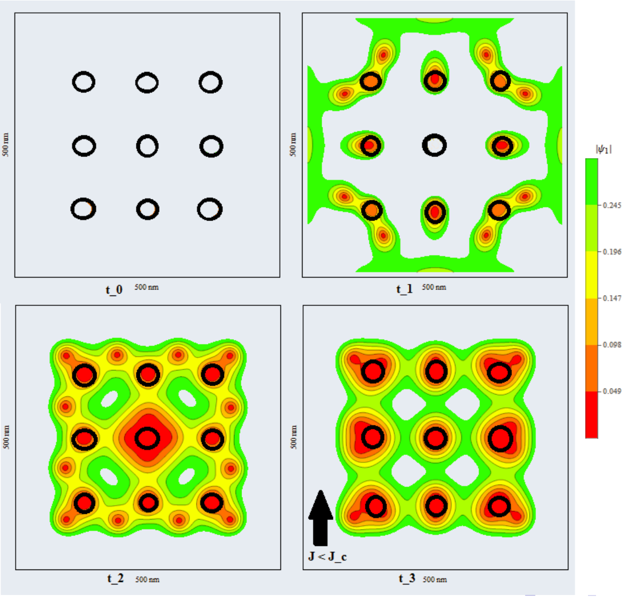
$$\nabla \times \mathbf{H} + \mathbf{J} = \sigma\frac{\partial \mathbf{A}}{\partial t} + \nabla \times \nabla \times \mathbf{A}$$
$$+\frac{i}{2\kappa}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) + \mathbf{A}|\psi|^2$$

where

$$\sigma\nabla\phi = \mathbf{J}$$

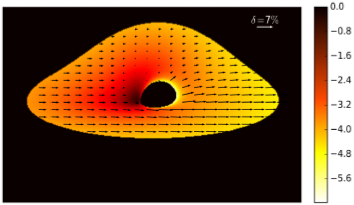
$$\mathbf{A}\cdot\mathbf{n} = 0\ ,\ \frac{i}{\kappa_\mu}\nabla\psi_\mu\cdot\mathbf{n} = 0\ ,\ (\nabla\times\mathbf{A})\times\mathbf{n} = (\mathbf{H}_e - \mathbf{H}_J)\times\mathbf{n} \text{ on } \partial\Omega$$

GL

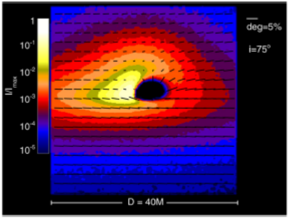


Faraday Rotation

- Bin also reproduced the results of another research group
- They are looking for Gravitational Faraday rotation from a Galaxy
- This can seen in the X-ray polarization. This simulation can tell astronomers what to look for.



Gravitational Faraday Rotation
(Chen et al. 2015 ApJS)



Schnittman & Krolik 2010, ApJ 701, 1175

The Scientific Computing Department

- Located on the 4th floor of Dirac (Secret Elevator)
- We specialize in implementing and improving algorithms
- www.sc.fsu.edu
- Advisor: Mark Howard, 403, mlhoward@fsu.edu
- Double Major (47 Credits) or Minor?
- Skills are valuable for research and grad school.
- TEA AND COOKIES, Wednesdays at 3:00

Courses

- ISC 3313(0) Intro to SC
- ISC 3222 (3) Symbolic and Numerical Computations
- ISC 4304 (4) Programming for Scientific Applications
- ISC 4220 (4) Algorithms for Science Applications I
- ISC 4221 (4) Algorithms for Science Applications II
- ISC 4223 (4) Computational Methods for Discrete Problems
- ISC 4232 (4) Computational Methods for Continuous Problems
- ISC 4943 (3) Practicum in Computational Science

Second Major

- All core courses
- 3 seminars
- 6 hours of SC electives
- 12 hours of other electives

Prerequisites

- Calc I and II
- Basic programming: COP 3014 or ISC 3313
- Science with lab
- Collateral: Linear algebra and Stats (3000 +)
- Double count electives

Minor

- Both
  - ISC 3222 (3) Symbolic and Numerical Computations
  - ISC 4304 (4) Programming for Scientific Applications
- and one of
  - ISC 4220 (4) Algorithms for Science Applications I
  - ISC 4221 (4) Algorithms for Science Applications II
- and 1 more elective (14 hours total)

Skills

- Interpolation
- Approximation (Least Squares)
- Numerical Linear Algebra
- Numerical Differentiation and Integration (Quadrature)
- Non-Linearities and Optimization
- Game theory applications
- Statistics and Probabilities
- ODE's and PDE's

Programming Languages

- MATLAB
- Mathemitca
- Python
- Fortran
- C / C++
- Java

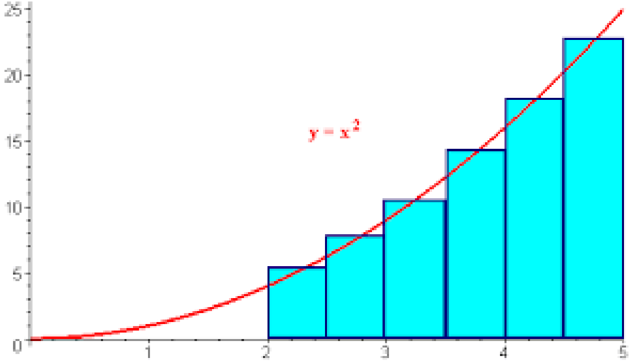
Why SC is Useful to a Physicist

- Simulating experiments.
- SC can help explore problems deeper.
- Computing skills are valuable for grad school and industry.
- SC teaches how to implement math problems on computers.

Quadrature Example

- A Riemann Sum is descried as

$$\int_a^b f(x)\,dx \approx \sum_{k=1}^{N} f(x_k^*)\Delta x$$

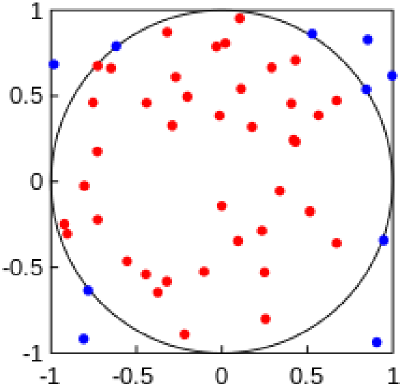


Quadrature Example

- Consider the integral that yields the area of the unit circle.

$$A = \int_0^R \int_0^{2\pi} r \, d\theta \, dr$$

- We can throw darts instead, known as the Monte Carlo method.



Monte Carlo

- For a given N_{in} and N_{total}.

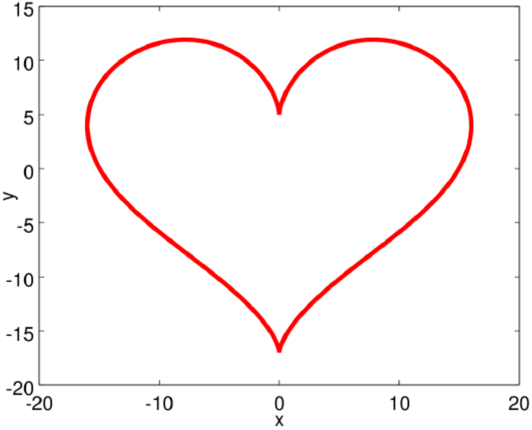
$$A \approx \frac{N_{in}}{N_{total}} A_{total}$$

- $4*0.8 = 3.2 \approx \pi$.
- Why should you care?
- Error $\propto \sqrt{N_{total}}$
- In the Riemann Sum (or any analytic quadrature), Error $\propto (\Delta x)^n$
- What happens as n grows? Monte Carlo wins.

Monte Carlo

- Now consider a complicated domain.

$$\mathbf{h}(t) = \left(16\sin^3 t,\ 13\cos t - 5\cos 2t - 2\cos 3t - \cos 4t\right), \quad 0 \le t < 2\pi.$$



My story

- I do physics, math and SC
- Started with Superconductivity (physics)
- I wanted to understand vortex dynamics

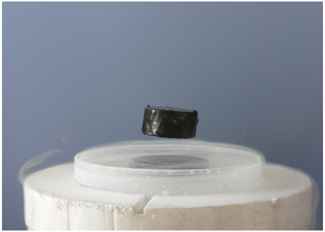


Figure : A magnet floating on top of Superconductor.

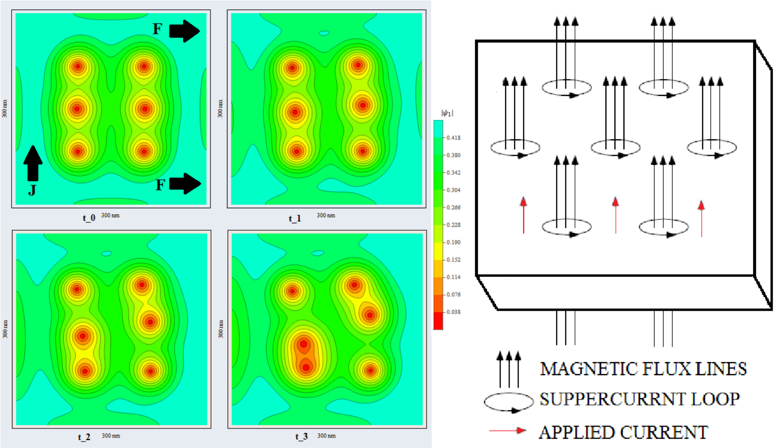


Figure : Vortex Dynamics with applied current and field (left), the set up (right).

Ginzburg Landau Model (Physics and Math)

- I had to understand the GL model (math)

$$G_s = \int f_n + \alpha(T)|\psi|^2 + \frac{1}{2}\beta(T)|\psi|^4 + \frac{1}{2m_s}|(-i\hbar\nabla - \frac{e_s}{c}\mathbf{A})\psi|^2$$
$$+\frac{1}{2}\frac{\mathbf{B}\cdot(\mathbf{B}-\mathbf{H}_e)}{4\pi}\, d\Omega$$

- I learned Calculus of variations and how to rescale equations.

$$-\psi + |\psi|^2\psi + (\frac{i}{\kappa}\nabla - \mathbf{A})^2\psi = 0 = \frac{\delta G}{\delta\psi} \text{ in } \Omega$$

$$\mathbf{J}_s = \nabla\times(\nabla\times\mathbf{A} - \mathbf{H}_e) = -\frac{i}{2\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^2) - |\psi|^2\mathbf{A} \text{ in } \Omega$$

$$(\frac{i}{\kappa}\nabla - \mathbf{A})\psi\cdot\mathbf{n} = 0 \text{ on } \Gamma$$

$$\nabla\times\mathbf{A}\times\mathbf{n} = \mathbf{H}\times\mathbf{n} \text{ on } \Gamma$$

Gauge invariance (Physics Math)

- Including time demanded an understanding of gauge invariance.

$$\phi \to \phi - \frac{1}{c}\frac{\partial f}{\partial t}, \quad \mathbf{A} \to \mathbf{A} + \nabla f, \quad \psi \to \psi e^{if}$$

$$\mathbf{E} = (-\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi), \quad \mathbf{B} = \nabla \times \mathbf{A}$$

- Now we disturb the system and account for the total current.

$$\Gamma(\frac{\partial \psi}{\partial t} + i\kappa\phi\psi) = \frac{\delta G}{\delta \psi}$$

$$\mathbf{J} = \mathbf{J}_n + \mathbf{J}_s = \sigma\mathbf{E} + \mathbf{J}_s$$

GL equations (Physic and Math)

$$\Gamma\left(\frac{\partial\psi}{\partial t}+i(\frac{Jy}{\sigma})\kappa\psi\right)+\left(|\psi|^2-1\right)\psi+(\frac{i}{\kappa}\nabla-\mathbf{A})^2\psi=0$$

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

where

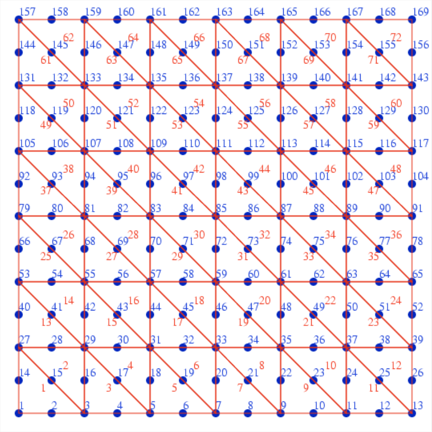
$$\sigma\nabla\phi=\mathbf{J}$$

$$\mathbf{A}\cdot\mathbf{n}=0\ ,\ \frac{i}{\kappa_\mu}\nabla\psi_\mu\cdot\mathbf{n}=0\ ,(\nabla\times\mathbf{A})\times\mathbf{n}=(\mathbf{H}_e-\mathbf{H}_J)\times\mathbf{n}\text{ on }\partial\Omega$$

Numerical Analysis (NA)

- I have a system of non-linear, time dependent, PDE's
- Now I had to learn how to solve PDE's on a computer (NA)
- I used my skills to convert math to code
- The Finite element Method was used to solve the PDE.

- Discretization was needed



- Implementing derivatives, integrals, non-linearities, and the time domain. (NA)

$$x_{n+1} = x_n - \frac{f'(x_n)}{f(x_n)} \rightarrow J(x_n)(x_{n+1} - x_n) = -F(x_n)$$

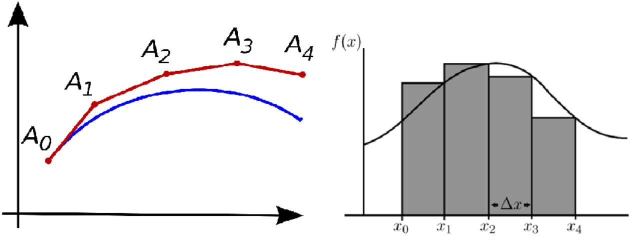


Figure : Newton's method (top), Euler's method (left), Riemann sum (right)

Numerical Analysis (NA)

- Now I'm ready solve my matrix equation!

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

- I run the code and....

Compression (CS)

- I ran out of space, so i quit storing 0's. (CS)

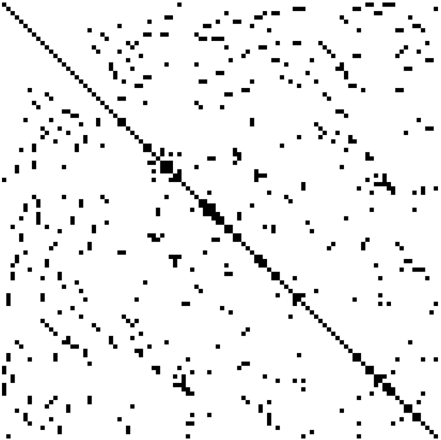


Figure : The black dots are non zero values in the matrix

Compression (CS)

- Compressed Spare Row storage did the trick

$$A = \begin{pmatrix} \underset{(0,0)}{10} & 0 & 0 & \underset{(0,3)}{12} & 0 \\ 0 & 0 & \underset{(1,2)}{11} & 0 & \underset{(1,4)}{13} \\ 0 & \underset{(2,1)}{16} & 0 & 0 & 0 \\ 0 & 0 & \underset{(3,2)}{11} & 0 & \underset{(3,4)}{13} \end{pmatrix}$$

$$\begin{aligned} val &= \begin{pmatrix} \underset{(0,0)}{10} & \underset{(0,3)}{12} & \underset{(1,2)}{11} & \underset{(1,4)}{13} & \underset{(2,1)}{16} & \underset{(3,2)}{11} & \underset{(3,4)}{13} \end{pmatrix} \\ colInd &= \begin{pmatrix} \underset{(0}{0} & \underset{)}{3} & \underset{(1}{2} & \underset{)}{4} & \underset{(2)}{1} & \underset{(3}{2} & \underset{)}{4} \end{pmatrix} \\ rowPtr &= \begin{pmatrix} \underset{(0)}{0} & \underset{(1)}{2} & \underset{(2)}{4} & \underset{(3)}{5} & \underset{(4)}{7} \end{pmatrix} \end{aligned}$$

Parallel Computing (CS)

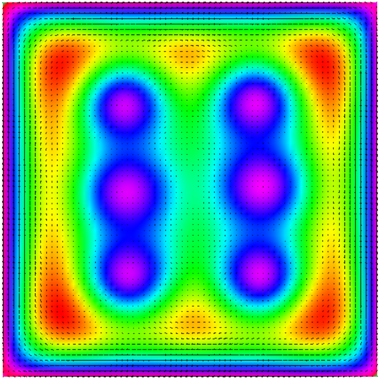
- The I ran out out time... I need Parallel computing (HPC)

Parallel Computing Problems (CS)

- I need a linear algebra solver, SuperLU
- I learned how to use make files and link libraries (CS)
- Lots of debugging.

Finally

- I got my Data!!!!
- Then I had use plotting software (CS) to make my plots and poster



Pinning Effects in Two-Band Superconductors

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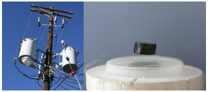
Objectives

- Numerically simulate the vortex dynamics in the superconducting material MgB_2.
- Devise a way to raise the maximum amount of current carried in the superconductor.
- Simulate how impurities raise the maximal current in MgB_2.

Introduction

Most are familiar with the waste heat produced by resistance in an electrical wire. This wasted energy can be avoided by using resistance free superconductors. However superconductors posses critical (maximum) values for their temperature, magnetic field, and current, only below which they operate as resistance free. Introducing impurities can raise the critical current by preventing flux flow. Practical superconducting devices could revolutionize technology but numerical simulations are needed to give insight.



MgB_2

- Magnesium Diboride (MgB_2) is a two band superconductor that can carry resistance free current under a temperature of 39K (-389.47 ° F).
- The bands act as pathways for electrons, each possessing their own properties seen in Table 1 .
- The bands interact to give composite direction and temperature dependent magnetic properties.

λ_1=47.8 nm	λ_2= 36.6 nm	ξ_1=13 nm	ξ_2=51 nm
κ_1=3.61	κ_2=0.658	$\nu = 2.757$	$\eta = -0.1701$

Table 1: The material parameters for MgB_2.

Flux Flow

- In the presence of a external magnetic field, normal materials are completely penetrated by the field. However superconductors such as MgB_2 are only penetrated by small magnetic flux vortices.
- The flux vortices interact with the applied current, **J** to produce a Lorentz force, **F**, perpendicular to **J**.
- The movement of the vortices, known as flux flow, induces an electric field, **E**, parallel to the applied current, creating an effective resistance.
- Figure 3 shows how the force moves the vortices (red) as time increases.

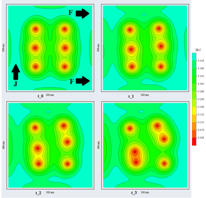


Figure 1: The vortices can be seen where ψ_1 is at is smallest (red). They are pushed to the right by the Lorentz force. At later times (t_3) the vortices rearrange themselves.

Mathematical Model

The Modified 2B-TDGL model describes superconductivity and contains ψ_1 and ψ_2, the density functions for the current carriers, the magnetic vector potential, **A**, and takes the parameters from Table 1 as input. The vortices can be seen where ψ_1 is at its smallest. Numerical simulations of vortex dynamics from the model are seen in Figures 1, 4

Methods

The finite element, Euler, and Newton methods were used together to solve the model equations. Supercomputers were used at F.S.U.'s R.C.C. for calculations.

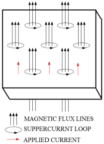


Figure 2: The set up for the numerical simulations. The magnetic field penetrates the sample as flux vortices and an applied current is transported across the sample.

Results

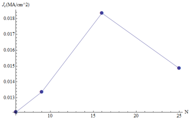


Figure 3: The critical current for different numbers of impurity sites. This under a temperature of 30 K and magnetic field of 0.106 Tesla.

Impurities were successfully modeled in the material. The pinning effects are shown in Figure 4. The impurity sites are outlined by the open black circles. A raise in the critical current J_c was found by increasing the normals N (Figure 3). However too many impurities degraded the superconducting material and lower J_c, as seen where N=25.

Conclusion

MgB_2 was successfully modeled using the simulation. Figure 5 shows directional dependence on the critical magnetic fields, comparable to experiments. An algorithm to model impurities in the sample was successful in raising the critical current.

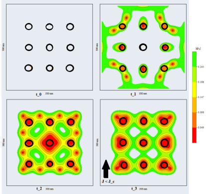


Figure 4: From top left to bottom right, vortices (red) are generated from a magnetic field. They become pinned to the normal site (black circles). When a current **J** is applied, the vortices remained pinned, unlike Figure 2.

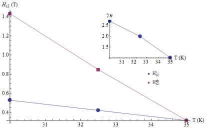


Figure 5: Magnetic properties comparable to experiment, $\gamma_H = H_{c2}^{ab}/H_{c2}^{c}$.

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Put It All Together

- Physics + Math+ NA+ CS =SC
- I didn't know I could do it.
- The SC and Physics departments prepared me well!

Why You Should SC

- Now we see how SC is useful
- You can expand your research
- Computer's play a huge role today and you can do it too!
- www.sc.fsu.edu
- Advisor: Mark Howard, 403, mlhoward@fsu.edu
- Tea and cookies Wednesday 3:00 (colloquium after)!

References

- Max Gunzburger for his insightful comments on the subject.
- Qiang Du, Penn State
- Sachin Shanbahg, FSU, Department of Scientific Computing
- Bin Chen, FSU Research Computing Center
- https://www.youtube.com/watch?v=bPvQ48gIa6U

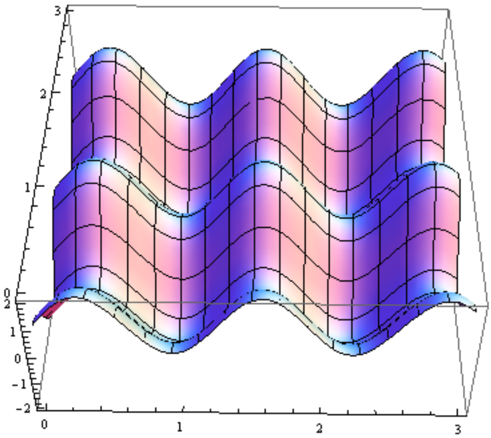
References

- Bryan Quaife for his Fluid dynamics examples.

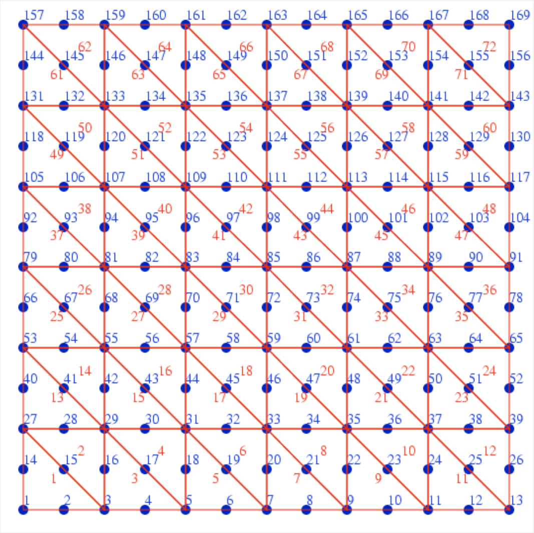
- Tomasz Plewa, Tim Handy and Dr. Plewa's post docs for their Omega laser examples.

Finite Elements

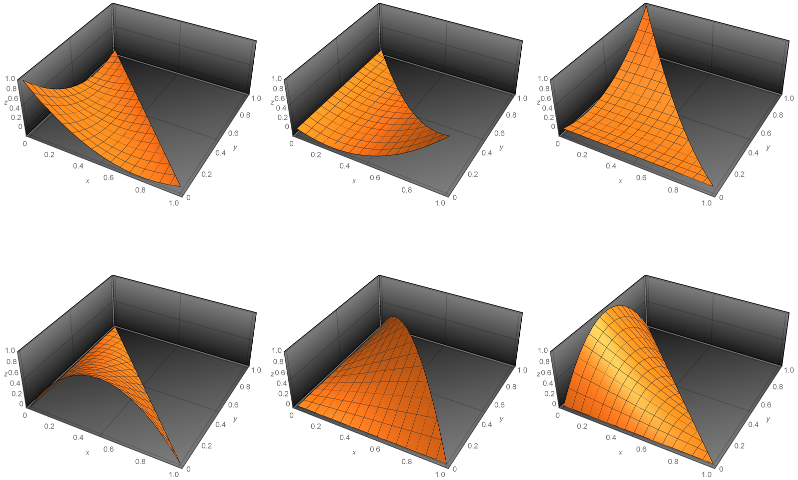
- FEM is a method used to solve PDE's
- Discretization and Basis Functions
- Consider a surface plot from a function u(x,y)



- Now the Domain is discretized.

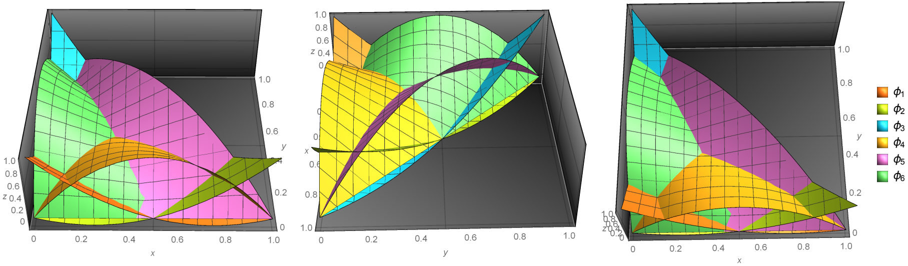


- Basis Functions



Finite Elements

- Basis Functions



- Consider Poisson's equation

$$-\Delta u = f(x,y) \text{ in } \Omega;\ u{=}0 \text{ on } \Gamma_x \text{ and } \nabla u \cdot n = g(x) \text{ on } \Gamma_y$$

- Multiply by a smooth bound test function, ϕ, and IBP

$$-\int (\Delta u)\phi \, d\Omega = -\int \nabla u \cdot n\phi \, d\Gamma_y + \int \nabla u \cdot \nabla\phi \, d\Omega = \int f(x,y)\phi \, d\Omega$$

- Derivative BC

$$\int \nabla u \cdot \nabla\phi \, d\Omega = \int f(x,y)\phi \, d\Omega + \int g(x)\phi \, d\Gamma_y$$

Finite Elements

- Now test for ALL basis function in our set, ϕ_i

$$\int \nabla u \cdot \nabla \phi_i \, d\Omega = \int f(x,y)\phi_i \, d\Omega + \int g(x)\phi_i \, d\Gamma_y$$

- Expand u in terms of ϕ_i since it is a complete basis.

$$u(x,y) = \sum_j^N c_j \phi_j(x,y)$$

- Now we have a matrix equation

$$c_j \int \nabla \phi_j \cdot \nabla \phi_i \, d\Omega = \int f(x,y)\phi_i \, d\Omega + \int g(x)\phi_i \, d\Gamma_y$$

- if ϕ_i is Γ_x node, set ij term to 1 and RHS i term to 0

Non-dimensionalization ND

- We can rescale with familiar quantities.
- We can close the magnitude gap.
- Let's introduce

$$\tilde{\mathbf{x}} = \lambda \mathbf{x}, \quad \tilde{\psi} = \psi\sqrt{\frac{-\alpha}{\beta}}, \quad \tilde{\mathbf{A}} = \sqrt{2}H_c\lambda, \quad \tilde{\mathbf{H}} = \sqrt{2}H_c\mathbf{H}$$

$$\lambda(T) = \sqrt{-\frac{m_s\beta(T)c^2}{4\pi\alpha(T)e^{2*}}}, \quad \xi(T) = \sqrt{-\frac{\hbar^2}{2m_s\alpha(T)}}, \quad \kappa = \frac{\lambda}{\xi}$$

ND

- Inserting $\tilde{\mathbf{x}}, \tilde{\psi}, \tilde{\mathbf{A}}, \tilde{\mathbf{H}}$ and forming λ and ξ.
- We divide through by the common term.
- The ND gives us a much cleaner form (with the tilde's dropped).

$$g_s = f_n + |\psi|^2 + \frac{1}{2}|\psi|^4 + \frac{1}{2m_s}|(-i\hbar\nabla - \frac{e_s}{c}\mathbf{A})\psi|^2 + \frac{1}{2}\frac{(\nabla \times \mathbf{A}) \cdot (\nabla \times \mathbf{A} - \mathbf{H}_e)}{4\pi}$$

- (Several lines of algebra)

$$g_s = f_n - |\psi|^2 + \frac{1}{2}|\psi|^4 + |(\frac{i}{\kappa}\nabla - \mathbf{A})\psi|^2 + \frac{1}{2}(\nabla \times \mathbf{A}) \cdot (\nabla \times \mathbf{A} - \mathbf{H}_e)$$

What We Do with the Free Energy?

- We want the Free energy minimized
- Functions ψ and **A** must minimize it.
- Calculus of Variations!!!

Calculus of Variations

- We want the path that minimizes $\int g(\psi, \mathbf{A})\, d\Omega$ for ψ and $\mathbf{A}$.

- We vary these two variables instead of x and $\dot{x}$.

- Starting with ψ^* (the complex conjugate), lets take a functional derivative (not ψ).

$$\frac{\delta g_s}{\delta \psi} = \lim_{\eta \to 0} \frac{1}{\eta} \int_\Omega g_s(\psi + \eta\phi) - g_s(\psi)\, d\Omega = 0$$

- Now we're only left with terms with a ψ factor

$$\frac{\delta g_s(\psi,\psi^*,\mathbf{A})}{\delta\psi} = \lim_{\eta\to 0}\frac{1}{\eta}\int_\Omega g_s(\psi,\psi^*+\eta\phi,\mathbf{A}) - g_s(\psi,\psi^*,\mathbf{A})\ d\Omega = 0$$

$$= \lim_{\eta\to 0}\frac{1}{\eta}\int -(\psi^*+\eta\phi)\psi+\frac{1}{2}((\psi^*+\eta\phi)\psi)^2+(\frac{-i}{\kappa}\nabla-\mathbf{A})(\psi^*+\eta\phi)\cdot(\frac{i}{\kappa}\nabla-\mathbf{A})\psi$$

$$-(|\psi|^2+\frac{1}{2}|\psi|^4+|(\frac{i}{\kappa}\nabla-\mathbf{A})\psi|^2)\ d\Omega$$

The Variational form

- After some simplification, we have the Variational form.
- This coincides with the weak from of the Finite element method.
- To get the EL equations, we need Integration by parts.

$$G_s = \int -\psi\phi + |\psi|^2\psi\phi + (\frac{-i}{\kappa}\nabla - \mathbf{A})\phi \cdot (\frac{i}{\kappa}\nabla - \mathbf{A})\psi \, d\Omega = 0$$

$$G_s = \int -\psi\phi + |\psi|^2\psi\phi + \mathbf{D}^*\phi \cdot \mathbf{D}\psi \, d\Omega = 0$$

IBP

- We need to use IBP on the derivative term to get rid of ϕ
- The i's change a few things

$$\int \mathbf{D}^*\phi \cdot \mathbf{D}\psi \; d\Omega = \int \mathbf{D}\psi\phi \cdot \mathbf{n} \; ds + \int (\mathbf{D}^2\psi)\phi \; d\Omega$$

- A Boundary Condition can eliminate the surface integral

$$\mathbf{D}\psi \cdot \mathbf{n} = (\frac{i}{\kappa}\nabla - \mathbf{A})\psi \cdot \mathbf{n} = 0$$

The EL equation for ψ

$$G_s = \int (-\psi + |\psi|^2\psi + (\frac{i}{\kappa}\nabla - \mathbf{A})\psi)^2 \phi \; d\Omega = 0$$

- The Integrand must be zero,

- The EL equation for ψ is, with the boundary condition

$$-\psi + |\psi|^2\psi + (\frac{i}{\kappa}\nabla - \mathbf{A})^2\psi = 0$$

$$(\frac{i}{\kappa}\nabla - \mathbf{A})\psi \cdot \mathbf{n} = 0$$

The EL equation for $\mathbf{A}$

- Using the same process and a lot few vector calculus identities.

$$\frac{\delta g_s}{\delta \mathbf{A}} = \lim_{\eta \to 0} \frac{1}{\eta} \int_\Omega g_s(\mathbf{A} + \eta\phi) - g_s(\mathbf{A}) \, d\Omega = 0$$

- The EL equation of $\mathbf{A}$ is found to be, with a boundary condition to cancel the surface integrals.

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

$$\nabla \times \mathbf{A} \times \mathbf{n} = \mathbf{H} \times \mathbf{n}$$

The ND GL equations

- Putting everything together, we have a nonlinear system of PDE's

$$-\psi + |\psi|^2\psi + (\frac{i}{\kappa}\nabla - \mathbf{A})^2\psi = 0 \text{ in } \Omega$$

$$\nabla \times \nabla \times \mathbf{A} + \frac{i}{2\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^2) + |\psi|^2\mathbf{A} = \nabla \times \mathbf{H} \text{ in } \Omega$$

$$(\frac{i}{\kappa}\nabla - \mathbf{A})\psi \cdot \mathbf{n} = 0 \text{ on } \Gamma$$

$$\nabla \times \mathbf{A} \times \mathbf{n} = \mathbf{H} \times \mathbf{n} \text{ on } \Gamma$$