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SuperScreen: An open-source package for simulating the magnetic response of two-dimensional superconducting devices

Logan Bishop-Van Horn[a,c,*], Kathryn A. Moler[a,b,c]

[a] *Department of Physics, Stanford University, Stanford, California 94305, USA*
[b] *Department of Applied Physics, Stanford University, Stanford, California 94305, USA*
[c] *Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, USA*

Abstract

Quantitative understanding of the spatial distribution of magnetic fields and Meissner screening currents in two-dimensional (2D) superconductors and mesoscopic thin film superconducting devices is critical to interpreting the results of magnetic measurements of such systems. Here, we introduce SuperScreen, an open-source Python package for simulating the response of 2D superconductors to trapped flux and applied time-independent or quasi-DC magnetic fields for any value of the effective magnetic penetration depth, Λ. Given an applied magnetic field, SuperScreen solves the 2D London equation using an efficient matrix inversion method [1, 2] to obtain the Meissner currents and magnetic fields in and around structures composed of one or more superconducting thin films of arbitrary geometry with spatially nonuniform magnetic penetration depth. SuperScreen can be used to model screening effects and calculate self- and mutual-inductance in superconducting devices, and simulate the magnetic response of inhomogeneous 2D superconductors.

Keywords: superconductivity, Meissner screening, London equation, inductance

PROGRAM SUMMARY

SuperScreen
CPC Library link to program files: (to be added by Technical Editor)
Developer's repository link: www.github.com/loganbvh/superscreen
Code Ocean capsule: (to be added by Technical Editor)
Licensing provisions: MIT License
Programming language: Python
Nature of problem: SuperScreen solves for Meissner screening currents in structures composed of 2D or thin film superconductors in the presence of an applied magnetic field, pinned vortices, and trapped flux.
Solution method: This package solves the 2D London equation for superconducting thin films using a matrix inversion method [1, 2].

*Corresponding author.
Email addresses: lbvh@stanford.edu (Logan Bishop-Van Horn), kmoler@stanford.edu (Kathryn A. Moler)

1. Introduction

SuperScreen is a Python package developed to simulate the static magnetic response of structures composed of one or more layers containing superconducting thin films characterized by a London penetration depth λ that is large compared to the film thickness d. SuperScreen solves the coupled Maxwell's and London's equations in and around superconducting films with spatially-varying penetration depth in the presence of inhomogeneous applied magnetic fields, pinned vortices, and trapped flux using a matrix inversion method introduced by Brandt and Clem [1, 2] and subsequently used by Kirtley, *et al.* to model the magnetic response of scanning superconducting quantum interference device (SQUID) sensors [3, 4].

There have been many previous numerical studies of magnetic screening and inductance extraction in thin film and two-dimensional (2D) superconducting devices [5, 6, 7, 8, 9, 10, 11, 12, 1, 2, 13, 14, 15]. However, few software tools for this task exist and those that are available are closed-source, are written in low-level compiled languages like C, and/or require the use of specialized file formats or separate computer aided

design (CAD) software for defining device geometries and model configurations.[1] Most of these tools are intended for use in the design of superconducting integrated circuits for single flux quantum (SFQ) logic and are primarily used for inductance extraction [16]. `SuperScreen` is an open-source, user-friendly, portable research tool designed to lower the barrier to entry to quantitative modeling of 2D superconductors, and to help interpret and inform measurements of superconducting thin films and devices.

This introduction to `SuperScreen` is organized as follows: In Section 2 we outline the model and its assumptions, and in Section 3 we describe its numerical implementation. In Section 4 we provide an overview of the structure of the `SuperScreen` package and discuss some important development details. In Section 5 we demonstrate how to perform several types of simulations using `SuperScreen` and compare the results to analytical solutions and experimental results. Finally, in Section 6 we conclude by discussing applications, limitations, and possible extensions of the package. Python scripts and Jupyter notebooks used to generate all figures presented below can be found in the GitHub repository accompanying this manuscript [17].

2. The Model

The goal of `SuperScreen` is to model the magnetic response of a thin superconducting film, or a structure composed of multiple superconducting films (which may or may not lie in the same plane), to an applied inhomogeneous out-of-plane magnetic field $H_{z,\,\mathrm{applied}}(x, y, z)$. Given $H_{z,\,\mathrm{applied}}(x, y, z)$ and information about the geometry and magnetic penetration depth of all films in a superconducting structure, we aim to calculate the thickness-integrated current density $\vec{J}(x, y)$ at all points inside the films, from which one can calculate the vector magnetic field $\vec{H}(x, y, z)$ at all points both inside and outside the films.

A convenient method for solving this problem was introduced by Brandt and Clem in Ref. [1], expanded by Brandt in Ref. [2], and subsequently used to model the magnetic response of scanning SQUID susceptometers [3, 4]. In the London model of superconductivity, the magnetic field $\vec{H}(\vec{r})$ and 3D current density $\vec{j}(\vec{r})$ in a superconductor with London penetration depth $\lambda(\vec{r})$ obey the second London equation: $\nabla \times \vec{j}(\vec{r}) = -\vec{H}(\vec{r})/\lambda^2(\vec{r})$, where $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)$. The 2D London model assumes that the current density $\vec{j}$ is approximately independent of z, such that $\vec{j}(\vec{r}) = \vec{j}(x, y, z) \approx \vec{j}_{z_0}(x, y)$ for a film lying parallel to the $x - y$ plane at vertical position z_0. Working now with the thickness-integrated current density $\vec{J}(x, y) = \vec{j}_{z_0}(x, y) \cdot d$, where d is the thickness of the film, the second London equation reduces to

$$\nabla \times \vec{J}(x, y) = -\vec{H}(x, y)/\Lambda(x, y), \tag{1}$$

where $\Lambda(x, y) = \lambda^2(x, y)/d$ is the effective penetration depth of the superconducting film (equal to half the Pearl length [18]).

It is important to note that the assumption $\vec{j}(x, y, z) \approx \vec{j}_{z_0}(x, y)$ is valid for only films that are thinner than their London penetration depth ($d \ll \lambda$, such that $\Lambda = \lambda^2/d \gg \lambda$). However the model has been applied with some success in structures with $\lambda \lesssim d$, for example by Kirtley, *et al.* in modeling the magnetic response of scanning SQUID susceptometers [3, 4]. Aside from this limitation, the method described below can be used to model films with any effective penetration depth $0 \leq \Lambda < \infty$.

Because the current density has zero divergence inside the superconducting film ($\nabla \cdot \vec{J} = 0$) except at small terminals where current can be injected, one can express $\vec{J}$ in terms of a scalar potential $g(x, y)$, called the stream function:

$$\vec{J}(x, y) = -\hat{z} \times \nabla g = \nabla \times (g\hat{z}) = \left(\frac{\partial g}{\partial y}, -\frac{\partial g}{\partial x}\right). \tag{2}$$

The stream function g can be thought of as the local magnetization of the film, or the area density of magnetic dipole sources (see Ref. [2] for more interesting properties of the stream function). We can rewrite Eq. 1, which gives the magnetic field inside of a 2D film, in terms of g:

$$\begin{aligned} \vec{H}(x, y) &= -\Lambda\left[\nabla \times \vec{J}(x, y)\right] \\ &= -\Lambda\left[\nabla \times (\nabla \times (g\hat{z}))\right] \\ &= -\Lambda\left[\nabla(\nabla \cdot (g\hat{z})) - \nabla^2(g\hat{z})\right] \\ &= \Lambda\nabla^2 g(x, y)\hat{z}, \end{aligned} \tag{3}$$

where $\nabla^2 = \nabla \cdot \nabla$ is the Laplace operator. (The last line follows from the fact that $\nabla \cdot [g(x, y)\hat{z}] = 0$). From Ampere's Law, the three components of the magnetic field $\vec{H}(\vec{r})$ at position $\vec{r} = (x, y, z)$ due to a sheet of current lying in the $x-y$ plane (at vertical position z') with stream

[1] A brief summary of existing tools can be found in Appendix A, and a more thorough overview in Ref. [16].

function $g(x', y')$ are given by:

$$\begin{aligned} H_x(\vec{r}) &= \int_F Q_x(\vec{r}, \vec{r}\,')g(x', y')\,\mathrm{d}^2r' \\ H_y(\vec{r}) &= \int_F Q_y(\vec{r}, \vec{r}\,')g(x', y')\,\mathrm{d}^2r' \\ H_z(\vec{r}) &= H_{z,\,\mathrm{applied}}(\vec{r}) + \int_F Q_z(\vec{r}, \vec{r}\,')g(x', y')\,\mathrm{d}^2r'. \end{aligned} \tag{4}$$

Here we assume a static out-of-plane applied magnetic field $\vec{H}_{\mathrm{applied}}(\vec{r}\,') = H_{z,\,\mathrm{applied}}(\vec{r}\,')\hat{z}$. F is the film area (with $g = 0$ outside of the film), and $Q_x(\vec{r}, \vec{r}\,')$, $Q_y(\vec{r}, \vec{r}\,')$, and $Q_z(\vec{r}, \vec{r}\,')$ are dipole kernel functions which give the respective component of the magnetic field at position $\vec{r} = (x, y, z)$ due to a dipole of unit strength at position $\vec{r}\,' = (x', y', z')$:

$$\begin{aligned} Q_x(\vec{r}, \vec{r}\,') &= 3\frac{(x - x')(z - z')}{4\pi[(z - z')^2 + \rho^2]^{5/2}} \\ Q_y(\vec{r}, \vec{r}\,') &= 3\frac{(y - y')(z - z')}{4\pi[(z - z')^2 + \rho^2]^{5/2}} \\ Q_z(\vec{r}, \vec{r}\,') &= \frac{2(z - z')^2 - \rho^2}{4\pi[(z - z')^2 + \rho^2]^{5/2}}, \end{aligned} \tag{5}$$

where $\rho = \sqrt{(x - x')^2 + (y - y')^2}$. Eq. 4 can also be seen as the Biot-Savart Law formulated in terms of the stream function g.

Comparing Eq. 3 and Eq. 4, we have in the plane of the film:

$$\begin{aligned} &\underbrace{\vec{H}(\vec{r}) \cdot \hat{z} = H_z(\vec{r}) = \Lambda\nabla^2 g(x, y)}_{z\text{−component of the total field}} = \\ &\underbrace{H_{z,\,\mathrm{applied}}(\vec{r})}_{\text{applied field}} + \underbrace{\int_F Q_z(\vec{r}, \vec{r}\,')g(\vec{r}\,')\,\mathrm{d}^2r'}_{\text{screening field}}, \end{aligned} \tag{6}$$

where now $\vec{r}$ and $\vec{r}\,'$ are 2D vectors, i.e. $z - z' = 0$ since the film is in the same plane as itself. From Eq. 6, we arrive at an integral equation relating the stream function g for points inside the superconductor to the applied field $H_{z,\,\mathrm{applied}}$:

$$\begin{aligned} &H_{z,\,\mathrm{applied}}(\vec{r}) = \\ &-\int_F \left[Q_z(\vec{r}, \vec{r}\,') - \delta(\vec{r} - \vec{r}\,')\Lambda(\vec{r}\,')\nabla^2\right] g(\vec{r}\,')\,\mathrm{d}^2r', \end{aligned} \tag{7}$$

where δ is the 2D Dirac delta function.

The goal, then, is to solve (invert) Eq. 7 for a given $H_{z,\,\mathrm{applied}}$ and film geometry F to obtain g for all points inside the film (with the boundary condition $g = 0$ enforced outside the film). Once $g(\vec{r})$ is known, the full vector magnetic field $\vec{H}(\vec{r})$ can be calculated at any point $\vec{r}$ from Eqs. 4 and 5.

2.1. Films with holes

In films that have holes (regions of vacuum completely surrounded by superconductor), each hole h can contain a trapped flux associated a current $I_{\mathrm{circ},\,h}$ circulating around the hole. The applied field that would cause such a circulating current is given by Eq. 7 if we set $g = I_{\mathrm{circ},\,h}$ for all points lying inside hole h:

$$\begin{aligned} &H_{z,\,\mathrm{eff},\,h}(\vec{r}) = \\ &-\int_{\text{hole } h} [Q_z(\vec{r}, \vec{r}\,') - \delta(\vec{r} - \vec{r}\,')\Lambda(\vec{r}\,')\nabla^2]I_{\mathrm{circ},\,h}\,\mathrm{d}^2r'. \end{aligned} \tag{8}$$

In this case, we modify the left-hand side of Eq. 7 as follows:

$$\begin{aligned} &H_{z,\,\mathrm{applied}}(\vec{r}) - \sum_{\text{holes } h} H_{z,\,\mathrm{eff},\,h}(\vec{r}) = \\ &-\int_F \left[Q_z(\vec{r}, \vec{r}\,') - \delta(\vec{r} - \vec{r}\,')\Lambda(\vec{r}\,')\nabla^2\right] g(\vec{r}\,')\,\mathrm{d}^2r'. \end{aligned} \tag{9}$$

The circulating current $I_{\mathrm{circ,\,h}}$ is defined as the total current crossing any curve that connects the interior of the hole h (where $g = I_{\mathrm{circ,\,h}}$ to the exterior of the film (where $g = 0$) [11, 2].

2.2. The fluxoid

The fluxoid Φ_S^f for a 2D region S with 1D boundary ∂S is given by the sum of magnetic flux through S and the line integral of the supercurrent density $\vec{J}$ around ∂S [2, 13, 19]:

$$\Phi_S^f = \underbrace{\int_S \mu_0 H_z(\vec{r})\,\mathrm{d}^2r}_{\text{“flux part”}} + \underbrace{\oint_{\partial S} \mu_0\Lambda(\vec{r})\vec{J}(\vec{r}) \cdot \mathrm{d}\vec{r}}_{\text{“supercurrent part”}}. \tag{10}$$

The fluxoid vanishes for a region S completely contained within a superconducting film that contains no holes or vortices, and has the same value for any region containing a given hole or collection of vortices in a superconducting film. This path-independence of the fluxoid follows from the static London equation (Eq. 1) on which the present model is based. Fluxoid quantization—the requirement that the fluxoid $\Phi_S^f = n\Phi_0$ where n is an integer and $\Phi_0 = h/2e$ is the magnetic flux quantum—is not automatically enforced by Eq. 1 for multiply-connected films, however it can be included as an external constraint.

2.3. Vortices

In addition to being trapped in holes (see Section 2.1), flux may be trapped in a superconducting film in the

form of vortices. The presence of vortices trapped in a film at positions $\vec{r}_v$ modifies Eq. 9 as follows:

$$H_{z,\,\mathrm{applied}}(\vec{r}) - \sum_{\mathrm{holes}\,h} H_{z,\,\mathrm{eff},\,h}(\vec{r}) - \sum_{\mathrm{vortices}\,v} \frac{\Phi_v}{\mu_0}\delta(\vec{r}-\vec{r}_v) = \\ -\int_F \left[Q_z(\vec{r},\vec{r}\,') - \delta(\vec{r}-\vec{r}\,')\Lambda(\vec{r}\,')\nabla^2\right] g(\vec{r}\,')\,\mathrm{d}^2r', \tag{11}$$

where δ is the 2D Dirac delta function and each vortex v is associated with a flux Φ_v (typically $\Phi_v = n\Phi_0 = nh/2e$, where n is an integer, Φ_0 is the magnetic flux quantum, h is the Planck constant, and e is the elementary charge). By solving Eq. 11 to obtain $g(\vec{r})$, one can compute the supercurrent density in the film due to an applied field and flux trapped in both holes and vortices. For a simply-connected region S containing a set of vortices v each associated with a flux Φ_v, the fluxoid is equal to $\Phi_S^f = \sum_{\mathrm{vortices}\,v} \Phi_v$. The numerical solution to Eq. 11 is described at the end of Section 3.

2.4. Multi-layer structures

For structures with multiple films lying in different planes or layers, with layer ℓ lying in the plane $z = z_\ell$, the stream functions and fields for all layers can be computed self-consistently using the following recipe:

1. Calculate the stream function $g_\ell(\vec{r})$ for each layer ℓ by solving Eq. 11 given an applied field $H_{z,\,\mathrm{applied}}(\vec{r}, z_\ell)$.
2. For each layer ℓ, calculate the z-component of the field due to the currents in all other layers $m \neq \ell$ (encoded in the stream function $g_m(\vec{r})$) using Eq. 4.
3. Re-solve Eq. 11 taking the new applied field at each layer to be the original applied field plus the sum of screening fields from all other layers. This is accomplished via the substitution

$$H_{z,\,\mathrm{applied}}(\vec{r}, z_\ell) \to H_{z,\,\mathrm{applied}}(\vec{r}, z_\ell) \\ + \sum_{m\neq\ell} \int_{F_m} Q_z(\vec{r},\vec{r}\,')g_m(\vec{r}\,')\,\mathrm{d}^2r', \tag{12}$$

   where F_m is surface of all films in layer m and g_m is the stream function for layer m.
4. Repeat steps 1-3 until the solution converges.

Convergence can be quantified by, for example, calculating the total magnetic flux though all films and holes in the model at the end of each iteration. In general, the more layers there are in a structure the more iterations are required to reach a given level of convergence.

3. Numerical Implementation

In order to numerically solve Eq. 4 and Eq. 9, we have to discretize the films, holes, and the vacuum regions surrounding them. We use a triangular (Delaunay) mesh, consisting of p points (or vertices) which together form t triangles. Below we denote column vectors and matrices using bold font. $\mathbf{AB}$ denotes matrix multiplication, with $(\mathbf{AB})_{ij} = \sum_{k=1}^{\ell} A_{ik}B_{kj}$ (ℓ being the number of columns in $\mathbf{A}$ and the number of rows in $\mathbf{B}$). Column vectors are treated as matrices with ℓ rows and 1 column. On the other hand, we denote element-wise multiplication with a dot: $(\mathbf{A}\cdot\mathbf{B})_{ij} = A_{ij}B_{ij}$ for two matrices and $(\mathbf{A}\cdot\mathbf{v})_{ij} = (\mathbf{v}\cdot\mathbf{A})_{ij} = A_{ij}v_i$ for a matrix $\mathbf{A}$ and a column vector $\mathbf{v}$. $\mathbf{A}^T$ denotes the transpose of matrix $\mathbf{A}$.

The discrete version of Eq. 4 is

$$\underbrace{\mathbf{h}_z}_{\text{total field}} = \underbrace{\mathbf{h}_{z,\,\mathrm{applied}}}_{\text{applied field}} + \underbrace{(\mathbf{Q}\cdot\mathbf{w}^T)\mathbf{g}}_{\text{screening field}} \\ h_{z,i} = h_{z,\,\mathrm{applied},i} + \sum_j Q_{ij}w_j g_j, \tag{13}$$

where for clarity we show both the matrix version of Eq. 4 (top line) and the equivalent discrete sum version (bottom line).

The $p\times p$ kernel matrix $\mathbf{Q}$ represents the kernel function $Q_z(\vec{r},\vec{r}\,')$ for all points lying in the plane of the film, and the $p\times 1$ weight vector $\mathbf{w}$, which assigns an effective area to each vertex in the mesh, represents the differential element d^2r'. Both $\mathbf{Q}$ and $\mathbf{w}$ are solely determined by the geometry of the mesh, so they only need to be computed once for a given device. $\mathbf{h}_z$, $\mathbf{h}_{z,\,\mathrm{applied}}$, and $\mathbf{g}$ are all $p\times 1$ vectors, with each row representing the value of the quantity at the corresponding vertex in the mesh. The vector $\mathbf{w}$ is equal to the diagonal of the "lumped mass matrix" $\mathbf{M}$: $w_i = M_{ii} = \frac{1}{3}\sum_{t\in\mathcal{N}(i)} \mathrm{area}(t)$, where $\mathcal{N}(i)$ is the set of triangles t adjacent to vertex i. The kernel matrix $\mathbf{Q}$ is given by

$$Q_{ij} = (\delta_{ij}-1)q_{ij} + \delta_{ij}\frac{1}{w_{ij}}\left(C_i + \sum_{l\neq i} q_{il}w_{il}\right), \tag{14}$$

where $q_{ij} = \left(4\pi|\vec{r}_i - \vec{r}_j|^3\right)^{-1}$ (which is $\lim_{\Delta z\to 0} Q_z(\vec{r},\vec{r}\,')$ cf. Eq. 5), and δ_{ij} is the Kronecker delta function. The diagonal terms involving the $p\times 1$ vector $\mathbf{C}$ are meant to work around the fact that q_{ii} diverge (see Ref. [2] for more details), and $\mathbf{C}$ is given by

$$C_i = \frac{1}{4\pi}\sum_{p,q=\pm 1} \sqrt{[\Delta x - p(x_i-\bar{x})]^{-2} + [\Delta y - q(y_i-\bar{y})]^{-2}}, \tag{15}$$

where $\Delta x = (x_{\max} - x_{\min})/2$ and $\Delta y = (y_{\max} - y_{\min})/2$ are half the side lengths of a rectangle bounding the modeled film and $(\bar{x}, \bar{y})$ are the coordinates of the center of the rectangle.

The matrix version of Eq. 9 is

$$\mathbf{h}_{z,\,\text{applied}} - \sum_{\text{holes } h} \mathbf{h}_{z,\,\text{eff},\,h} = -(\mathbf{Q} \cdot \mathbf{w}^T - \nabla^2 \cdot \mathbf{\Lambda}^T)\mathbf{g}, \quad (16)$$

where we exclude points in the mesh lying outside of the superconducting film but keep points inside holes in the film. $\mathbf{\Lambda}$ is either a scalar or a vector defining the effective penetration depth at every included vertex in the mesh, and ∇^2 is the Laplace operator, a $p \times p$ matrix defined such that $\nabla^2 \mathbf{f}$ computes the Laplacian $\nabla^2 f(x, y)$ of a function $f(x, y)$ defined on the mesh (see Appendix B).

Eq. 16 is a matrix equation relating the applied field to the stream function inside a superconducting film, which can efficiently be solved (e.g. by Cholesky or LU decomposition) for the unknown vector $\mathbf{g}$, the stream function inside the film. Since the stream function outside the film and inside holes in the film is already known, solving Eq. 16 gives us the stream function for the full mesh. Defining $\mathbf{K} = \left(\mathbf{Q} \cdot \mathbf{w}^T - \nabla^2 \cdot \mathbf{\Lambda}^T\right)^{-1}$, we have

$$\mathbf{g} = \begin{cases} -\mathbf{K}\left(\mathbf{h}_{z,\,\text{applied}} - \sum_{\text{holes } h} \mathbf{h}_{z,\,\text{eff},\,h}\right) & \text{inside the film} \\ I_{\text{circ},\,h} & \text{inside hole } h \\ 0 & \text{elsewhere} \end{cases} \quad (17)$$

If there is a vortex containing flux Φ_j located in a film at position $\vec{r}_j$ indexed as mesh vertex j, then for each position $\vec{r}_i$ within that film, we add to the stream function g_i the quantity $\mu_0^{-1} \Phi_j K_{ij} / w_j$, where K_{ij} is an element of the inverse matrix defined above, and w_j is an element of the weight matrix which assigns an effective area to the mesh vertex at which the vortex is located. This process amounts to numerically inverting Eq. 11 as described in Ref. [2].

Once the stream function $\mathbf{g}$ is known for the full mesh, the supercurrent flowing in the film can be computed from Eq. 2, the z-component of the total field in the plane of the film can be computed from Eq. 13, and the full vector magnetic field $\vec{H}(x, y, z)$ at any point in space can be computed from Eqs. 4 and 5. Multi-layer structures are solved iteratively as described in Section 2.4.

4. Package Overview

In this section we give a high-level overview of the `SuperScreen` package. Further details can be found in the online documentation [20]. The specific version of the package corresponding to this manuscript is `v0.4.0`.

4.1. Development Details

At the time of writing, `SuperScreen` requires Python version 3.7–3.9. The package is located in a public repository on GitHub [21, 22], and a suite of unit tests is run automatically via the GitHub Actions continuous integration (CI) tool whenever a change or proposed change (Pull Request) is made to the `main` branch of the repository. At the time of writing, the test suite is executed using Python versions 3.7 through 3.9, and the test coverage is $> 95\%$. Any changes to the `main` branch of the repository also trigger an automatic re-build of the online documentation [20]. Stable versions of the package are tagged on GitHub and uploaded to PyPI, the Python Package Index. The source code and documentation are provided under the MIT License.[2]

`SuperScreen` has several important dependencies beyond the Python standard library: `numpy` [23] and `scipy` [24] for numerics, `matplotlib` [25] for visualization, `pint` [26] for handling physical units, `shapely` [27] for creating and manipulating device geometries, `meshpy` [28, 29, 30] and `optimesh` [31] for mesh generation, and `Ray` [32, 33] for parallel processing with shared memory (see Appendix E).

4.2. Devices

Information about the geometry and penetration depth of a superconducting structure is described by an instance of the `superscreen.Device` class. A `Device` is made up of one or more superconducting layers, each represented by an instance of `superscreen.Layer`. Each layer sits in a specified plane parallel to the $x - y$ plane and has its own effective penetration depth Λ, which can either be a constant or a `superscreen.Parameter` that defines $\Lambda(x, y)$, the effective penetration depth as a function of position (see Appendix C). Alternatively, the effective penetration depth Λ can be defined in terms of a layer's London penetration depth λ and its thickness d: $\Lambda = \lambda^2/d$, in which case the London penetration depth can be either a constant or a `superscreen.Parameter`.

Each layer can contain one or more superconducting `films` which may have one or more `holes` in them. Films and holes are represented by instances of the `superscreen.Polygon` class. All polygons in a device must be simply-connected; a hole in a film is modeled as

[2] https://opensource.org/licenses/MIT

SuperScreen	Set-theoretic	Boolean
`polygonA.union(polygonB)`	$A \cup B$	`OR`
`polygonA.intersection(polygonB)`	$A \cap B$	`AND`
`polygonA.difference(polygonB)`	$A \setminus B$	`AND NOT`
`polygonA.difference(polygonB, symmetric=True)`	$(A \setminus B) \cup (B \setminus A)$	`XOR`

Table 1: Methods for combining `superscreen.Polygon` objects, along with their corresponding set-theoretic and boolean logic operations.

one `Polygon` instance whose coordinates all lie within the `Polygon` representing the film. `Polygons` can constructed and combined using set-theoretic operations. Table 1 shows the four methods available for combining a `supercreen.Polygon` instance `polygonA`, whose vertices lie in set A, with a polygon `polygonB`, whose vertices lie in set B. Note that `polygonB` can be a `superscreen.Polygon`, an $n \times 2$ `numpy` array of vertex coordinates, or a `LineString`, `LinearRing`, or `Polygon` from the `shapely` package [27].

In addition to superconducting films and holes, one may define "abstract regions," which are polygons that do not necessarily correspond to a physical feature in the structure, but will still be meshed. Abstract regions can be used to define a "bounding box" around a structure to be modeled, or to locally increase the density of the computational mesh in a given region. The `superscreen.geometry` module provides functions for generating the underlying polygon vertices for simple shapes (ellipses and rectangles), which can be combined as described above to create more complicated geometries.

Once the layers, films, holes, and abstract regions have been defined, one can generate the computational mesh by calling `Device.make_mesh()`. The region that is meshed is defined by the convex hull of the union of all polygons in the device. Mesh generation is a two step process. First, an initial Delaunay mesh is created using `meshpy` [28], which is a Python interface to Triangle [30, 29], a fast compiled 2D mesh generation tool. Second (and optionally), the mesh is further optimized using `optimesh` [31]. The goal of the mesh optimization step is to improve the "quality" of each triangular element in the mesh, where quality measures how close a triangle is to equilateral (quality ≤ 1, with equality for equilateral triangles). In practice, the more `optimesh` steps are performed, the more uniform in size and spatial density the triangles in the mesh become. The local density of triangles in the mesh is determined by the density of vertices in the device's polygons and the total number of triangles. Regions where there are many polygon vertices will be meshed more densely than regions with few polygon vertices. If no `optimesh` optimization is performed, then every polygon vertex is guaranteed to be a mesh vertex. See Code Block 1 for a demonstration of the process of creating a `Device`, and Figure 1(**a**) to view the resulting geometry and mesh. After the mesh has been generated, the geometry-dependent matrices and vectors described in Section 3 are computed and one can begin solving models.

4.3. Solvers

A `SuperScreen` model consists of 1) a `Device` with a mesh, 2) a function or `Parameter` that defines the applied magnetic field as a function of position $H_{z,\,\mathrm{applied}}(x, y, z)$, 3) a value for the current circulating around each hole in the device due to trapped flux, and 4) a collection of vortices v located at positions $\vec{r}_v$ and carrying flux Φ_v. These items serve as the inputs to `SuperScreen`'s main solver function, `superscreen.solve()`, which implements the calculation outlined in Section 3. When simulating a device with more than one layer, one can specify the number of times to implement the iterative calculation described in Section 2.4 in order to solve for the response of all layers self-consistently. One can also skip the iterative portion of the calculation entirely and only solve for the response of each layer to the applied field, assuming no interaction between layers. The `device.solve_dtype` attribute determines the `numpy` floating point data type used by `solve()`. The default data type is `float64` (64-bit double-precision float, equivalent to Python's `float` type), but one can, for instance, set `device.solve_dtype = "float32"` to use 32-bit single-precision floats in order to save memory.

The output of `superscreen.solve()` is a `list` of `superscreen.Solution` objects, with a length of 1 plus the number of iterations used for the iterative portion of the calculation. A `Solution` encapsulates all of the information about a solved model: the `Device`, applied field, circulating currents, vortices, and calculated stream functions and magnetic fields for all layers in the

```python
import superscreen as sc
from superscreen.geometry import circle, box

# Define the device geometry.
length_units = "um"
ro = 3  # outer radius
ri = 1  # inner radius
slit_width = 0.25
Lambda = 1  # effective penetration depth
# circle() and box() generate arrays of polygon (x, y) coordinates.
ring = circle(ro)
hole = circle(ri)
slit = box(slit_width, 1.5 * (ro - ri), center=(0, -(ro + ri) / 2))
# Define the Polygon representing the superconductor.
layer = sc.Layer("base", Lambda=Lambda)
film = sc.Polygon.from_difference(
    [ring, slit, hole], name="ring_with_slit", layer="base"
)
bounding_box = sc.Polygon("bounding_box", layer="base", points=circle(1.2 * ro))
# Create a Device and generate and plot the computational mesh.
device = sc.Device(
    film.name,
    layers=[layer],
    films=[film],
    abstract_regions=[bounding_box],
    length_units=length_units,
)
device.make_mesh(min_points=3500, optimesh_steps=None)
device.plot(mesh=True)
# Calculate the device's response to a uniform applied field.
applied_field = sc.sources.ConstantField(10)
solution = sc.solve(device, applied_field=applied_field, field_units="uT")[-1]
# Visualize the solution.
# Plot the current density evaluated at each layer in the Device.
solution.plot_currents()
# Plot the magnetic field evaluated at each layer in the Device.
solution.plot_fields()
# Plot the field evaluated at any points in space.
solution.plot_field_at_positions(device.points, zs=0.5)
```

Code Block 1: The typical workflow for a `SuperScreen` simulation: 1) Define the device geometry and materials properties, 2) generate the computational mesh, 3) solve the model for a given applied field and/or trapped flux, and 4) visualize the results.

device. A `Solution` also has methods for processing the simulation results, including:

- `Solution.grid_data()`: Interpolates the calculated stream functions $g(x, y)$, magnetic fields $\mu_0 H_z(x, y)$, or current densities $\vec{J}(x, y)$, for each layer from the triangular mesh to a rectangular grid.
- `Solution.field_at_position()`: Calculates the vector magnetic field at any point(s) in space due the applied field and the currents flowing the in the device using Eqs. 4 and 5.
- `Solution.interp_current_density()`: Evaluates the 2D current density $\vec{J}(x, y)$ in each layer at arbitrary (x, y) coordinates via interpolation.
- `Solution.polygon_flux()`: Calculates the total flux through each polygon in the device.

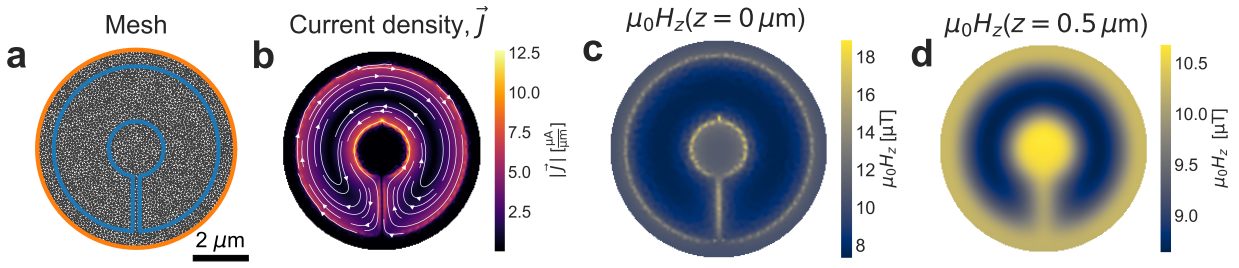

Figure 1: The output of Code Block 1: Meissner screening of a uniform $10\,\mu$T out-of-plane field by a ring with inner diameter $1\,\mu$m, outer diameter $3\,\mu$m, and effective penetration depth $\Lambda = 1\,\mu$m, interrupted by a slit of width $0.25\,\mu$m. (**a**) Plot of the boundary of the ring (blue), circular bounding box (orange), and the computational mesh (gray), generated with `Device.plot()`. (**b**) The current density $\vec{J}$ in the ring, generated with `Solution.plot_currents()`. (**c**) The z-component of the magnetic field $\mu_0 H_z$ evaluated at the plane of the ring, generated with `Solution.plot_fields()`. (**d**) The z-component of the magnetic field evaluated $z = 0.5\,\mu$m above the ring (generated using `Solution.plot_field_at_positions()`).

- `Solution.polygon_fluxoid()`: Calculates the fluxoid for a specified polygonal region in the device. See Section 5.1 for more details.

`Solutions` also have several visualization methods built in (see Code Block 1, Figure 1, and Section 4.4).

One may wish to solve many models involving the same device while varying other aspects of the model, for example sweeping the applied field, circulating currents, vortex properties, or some parameter of one or more layers in the device. Fortunately, the mesh, Laplace operator, kernel matrix, etc. (described in Section 3) depend only on the geometry of the device parallel to the $x-y$ plane. This means that the same mesh and matrices can be re-used for models with different applied fields, circulating currents, vortex properties, layer z-positions, and penetration depths.

The `superscreen.solve_many()` function manages the setup and execution of such a sweep. One can provide a sequence of `Parameter` objects defining different applied fields and/or a sequence of circulating current values over which to sweep and/or a "layer updater" function that modifies each layer in the device according to some set of keyword arguments, which can also be swept. The latter option can be used to sweep layer heights or penetration depths. Given these inputs, `superscreen.solve_many()` will generate and solve all of the corresponding models. The models can either be solved in series in a single Python process (the default), or in parallel in multiple Python processes running across multiple CPUs, or even across multiple nodes in a cluster (see Appendix E).

4.4. Visualization

`SuperScreen` offers several functions for visualizing the results of simulations (which are also aliased as methods on `superscreen.Solution`):

- `superscreen.plot_streams()`: Given a `Solution`, plots the stream function $g(x, y)$ for one or more layers in the device.
- `superscreen.plot_currents()`: Given a `Solution`, plots the current density $\vec{J}(x, y)$ for one or more layers in the device.
- `superscreen.plot_fields()`: Given a `Solution`, plots the total field $H_z(x, y)$ or the screening field $H_z(x, y) - H_{z,\,\mathrm{applied}}(x, y)$ for one or more layers in the device.
- `superscreen.plot_field_at_positions()`: Given a `Solution`, plots the total field $\vec{H}(x, y, z)$ or $H_z(x, y, z)$ at an arbitrary set of positions (x, y, z).

See Code Block 1 and Figure 1 for an example of the usage and output of `plot_fields()` and `plot_currents()`.

4.5. Comparison & Persistence

`Parameters`, `Layers`, `Polygons`, `Devices`, and `Solutions` all implement the equality operator, `==`. Two `Parameters` are considered equal if the Python bytecode of their underlying functions is the same and their keyword arguments are the same. Two `Layers` are equal if their name, penetration depth, thickness, and vertical position are all equal. Two `Polygons` are equal if they are in the same layer and their name and polygon vertices are equal. Two `Devices` are equal if their name, layers, films, holes, and abstract regions are all equal. Two `Solutions` are equal if their device, applied field, circulating currents, list of trapped vortices, timestamp (time at which the solution was created), and all stream function and magnetic field arrays are equal.

Two `Solutions` created at different times can also be compared using the `solution.equals()` method.

Instances of `superscreen.Device` and `superscreen.Solution` can be saved to and loaded from disk using their respective `to_file()` and `from_file()` methods, making it straightforward to store and share models and simulation results. `Layers`, `Polygons`, and all metadata are serialized to JSON, a widely-used, human-readable plain text format. Functions and `Parameters`, such as those that compute the applied field or penetration depth, are serialized in binary form using the `dill` package [34]. `Numpy` arrays, such as the mesh itself and the computed stream functions and fields, are saved in the `numpy npz` file format. A `list` of `Solutions`, such as that returned by `superscreen.solve()` can be saved/loaded all at once using `save_solutions()` and `load_solutions()`.

5. Examples

5.1. Calculating the fluxoid

`SuperScreen` allows one to calculate the fluxoid Φ_S^f for any polygonal region S whose boundary ∂S lies completely within a superconducting film using the method `Solution.polygon_fluxoid()` (see Section 2.2, Eq. 10). The "flux part" $\int_S \mu_0 H_z(\vec{r})\, \mathrm{d}^2 r$ is calculated using `Solution.polygon_flux()`, which computes the flux through a polygon representing a region S as $\Phi_S = \sum_{i \in S} \mu_0 H_{z,i} w_i$, where $H_{z,i}$ is the magnetic field at vertex i (recall that w_i assigns an effective area to mesh vertex i). The "supercurrent part" $\oint_S \mu_o \Lambda(\vec{r}) \vec{J}(\vec{r}) \cdot \mathrm{d}\vec{r}$ is calculated by evaluating the vector current density $\vec{J}$ at each point in the path ∂S using `Solution.interp_current_density()`, then computing the line integral along the path using the trapezoid rule. The sum of these two terms gives the fluxoid Φ_S^f.

While the 2D London model doesn't "know" about fluxoid quantization, in the sense that the quantization condition $\Phi_S^f = n\Phi_0$ is not automatically satisfied by solutions to Eq. 1 for multiply-connected films, we can nevertheless calculate current and field distributions for different fluxoid states in multiply-connected superconductors by adjusting the currents circulating around each hole to realize a prescribed set of fluxoid values. For a structure with N_h holes, we can specify N_h fluxoids Φ_h^f and find the circulating currents I_h by minimizing the deviation of each fluxoid from its desired value. This calculation is implemented in the `superscreen.find_fluxoid_solution()` function.

```python
import superscreen as sc
# Assume that we have already created a
# superscreen.Device with one or more
# holes, and generated the mesh.
# Specify the desired fluxoid for each
# hole in the device:
fluxoids = {
    hole_name: 0
    for hole_name in device.holes
}
applied_field = sc.sources.ConstantField(1)
field_units = "mT"

result = sc.find_fluxoid_solution(
    device=device,
    fluxoids=fluxoids,
    applied_field=applied_field,
    field_units=field_units,
)
solution, opt_result = result
```

Code Block 2: Calculating the field and current distributions for fluxoid states in a multiply-connected superconducting film. Given a `Device` with $N_h \geq 1$ holes and a desired fluxoid Φ_h^f for each hole, `superscreen.find_fluxoid_solution()` optimizes the current I_h circulating around each hole to realize the desired fluxoid state. The function returns a `tuple` of length 2, the first element being the final optimized `superscreen.Solution` and the second element being an instance of either `scipy.optimize.RootResults` (if $N_h = 1$) or `scipy.optimize.OptimizeResult` (if $N_h > 1$), which contains information about the optimization that was performed. See Figure 2 for an example of the results for a film with two holes, both in the $n = 0$ fluxoid state.

For $N_h = 1$, it is treated as a root-finding problem, which can be solved with typically only three calls to `superscreen.solve()`. For $N_h > 1$, it is a least-squares minimization problem with N_h free parameters. Code Block 2 demonstrates how to model a device with one or more holes, each in the $n = 0$ fluxoid state, subject to a uniform applied field, and Figure 2 shows the field and current distributions for a rectangular superconducting film with $\Lambda = 0.25\,\mu$m, which has one rectangular and one elliptical hole. The least-squares minimization for the model shown in Figure 2, with $N_h = 2$, required 18 total calls to `superscreen.solve()`. It is important to note that while `SuperScreen` can calculate the field and current distributions or a given fluxoid state, the model does not capture transitions between fluxoid states.

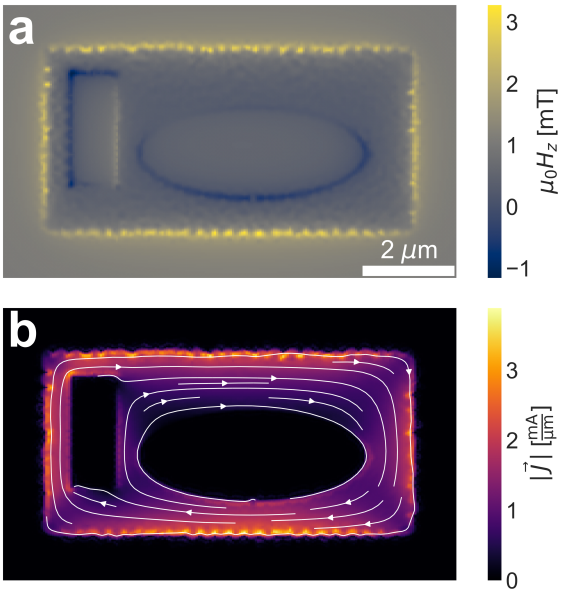

Figure 2: (**a**) Magnetic field and (**b**) current density distributions generated by Code Block 2 for a rectangular superconducting film with $\Lambda = 0.25\,\mu$m, which has one rectangular and one elliptical hole. The film is subject to a uniform applied out-of-plane field of 1 mT, and both holes are set to be in the $n = 0$ fluxoid (i.e. Meissner) state. The resulting ciruclating currents are $I_{\text{rectangle}} = -1.071$ mA and $I_{\text{ellipse}} = -1.589$ mA, and the residual fluxoid for each hole is smaller than $10^{-7}\,\Phi_0$. These results were computed using a mesh with approximately 5,000 vertices and 10,000 triangles.

5.2. *Pearl vortices in thin films*

Vortices trapped in 2D superconductors ($d \ll \lambda$, where d is the film thickness and λ is the London penetration depth), i.e. "Pearl vortices," are associated with different current and magnetic field distributions than Abrikosov vortices trapped in bulk type-II superconductors [18]. The 2D Fourier transform $\tilde{H}_z(\vec{k}, z)$ of the out-of-plane component of the magnetic field $H_z(\vec{r}, z)$ from a Pearl vortex located at the origin $x = y = z = 0$ is given by

$$\tilde{H}_z(\vec{k}, z) = \mathcal{F}\{H_z(\vec{r}, z)\} = \frac{1}{\mu_0} \frac{\Phi_0 e^{-|\vec{k}|z}}{1 + 2\Lambda|\vec{k}|}, \qquad (18)$$

where $\mathcal{F}\{\cdot\}$ is the 2D Fourier transform, $\vec{k} = (k_x, k_y)$ are in-plane spatial frequencies, z is the out-of-plane position at which the field is evaluated, and $2\Lambda = 2\lambda^2/d$ is the Pearl length [18, 35]. The real-space magnetic field distribution near a Pearl vortex can be calculated by taking the inverse Fourier transform of Eq. 18: $H_z(\vec{r}, z) = \mathcal{F}^{-1}\{\tilde{H}_z(\vec{k}, z)\}$.

To include vortices in a `SuperScreen` model, one can simply input a `list` of `superscreen.Vortex` objects when calling `superscreen.solve()`. A `Vortex` object specifies the x, y position for the vortex core, the name of the superconducting layer in which the vortex is pinned, and the number of flux quanta Φ_0 contained in the vortex (which is 1 by default). The field distributions generated by `SuperScreen` in the presence of vortices as described in Sections 2.3 and 3 agree to within a few percent with the distributions obtained using this Fourier transform method, as demonstrated in Figure 3. Figure 3(**e**) shows the fluxoid for a circular region S with radius $r = 1\,\mu$m enclosing a Pearl vortex trapped in a film as a function of the film's effective penetration depth, Λ. When $\Lambda = 0$, the screening currents decay very quickly away from the center of the vortex, so the "supercurrent part" of the Φ_S^f vanishes. With increasing Λ, the "supercurrent part" accounts for an increasing fraction of the total fluxoid. See Ref. [2] for a method to compute the self-energy and interaction energies of vortices in thin films.

5.3. *Calculating inductance*

As shown in Ref. [2], the mutual inductance M_{ij} between holes i and j in a superconducting structure is given by

$$M_{ij} = \frac{\Phi_{S_i}^f}{I_j}, \qquad (19)$$

where $\Phi_{S_i}^f$ is the fluxoid for a region S_i containing the hole i, and I_j is the current circulating around hole j. The mutual inductance values for a set of holes form a mutual inductance matrix. The diagonals of the mutual inductance matrix are the hole self-inductances ($M_{ii} = L_i$, the self-inductance of hole i), and the matrix is symmetric ($M_{ij} = M_{ji}$) due to the reciprocity theorem. In this context, the flux and supercurrent parts of the fluxoid correspond to the geometric and kinetic inductance respectively [1]. If the penetration depth of the film containing hole i is $\Lambda = 0$, then no field penetrates the film, the fluxoid $\Phi_{S_i}^f$ is equal to the flux through hole i, and the total inductance is equal to the geometric inductance. For a device with N_h holes, the $N_h \times N_h$ mutual inductance matrix $\mathbf{M}$ can be computed using the `Device.mutual_inductance_matrix()` method. For example, the mutual inductance matrix for the device shown in Figure 2 is:

$$\mathbf{M} = \begin{pmatrix} 10.319 & -1.536 \\ -1.527 & 7.130 \end{pmatrix} \text{pH},$$

where the matrix is indexed as

$$\begin{pmatrix} \text{ellipse} \\ \text{rectangle} \end{pmatrix},$$

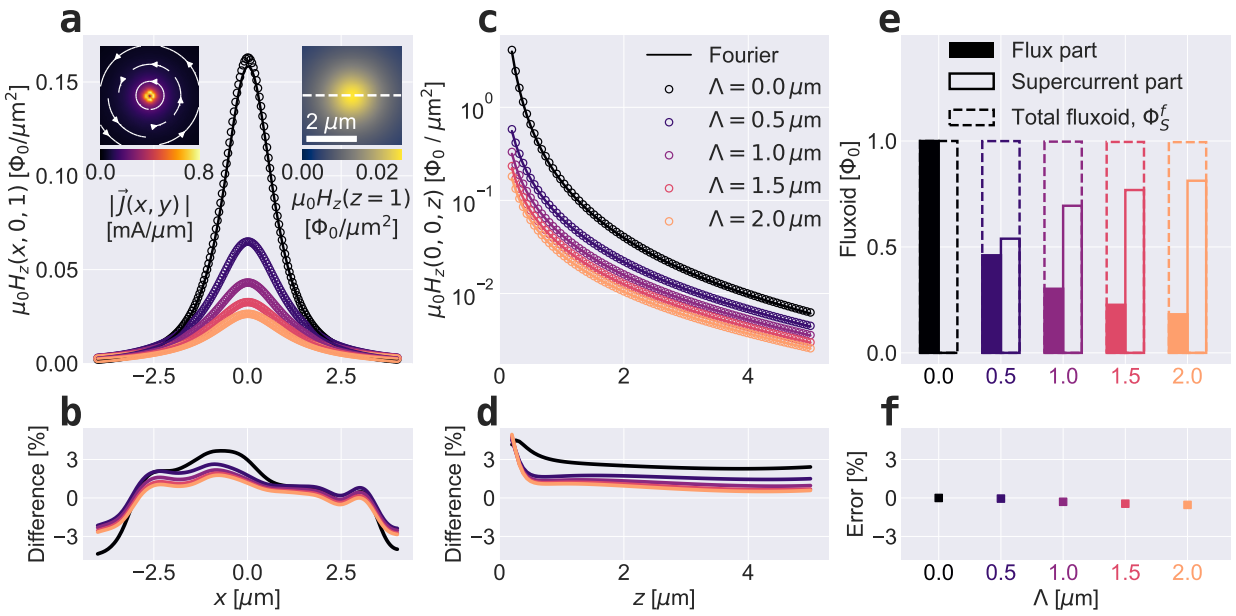

Figure 3: Vortex field profiles calculated using `SuperScreen` agree with the analytical solution (Eq. 18) to within a few percent. Here, we model a vortex trapped at the center of a square superconducting film lying in the $x-y$ plane with side length $20\,\mu$m as a function of the film's effective penetration depth, Λ. (**a**) Cross section along the x-axis of the out-of-plane magnetic field $\mu_0 H_z$ from the vortex, evaluated at a vertical distance $z = 1\,\mu$m above the film. The left inset shows the current density in the plane for film for $\Lambda = 2\,\mu$m, and the right inset shows the corresponding magnetic field evaluated at $z = 1\,\mu$m, with a dashed white line indicating the cross-section axis. (**b**) Percentage difference between the $\mu_0 H_z$ calculated with `SuperScreen` and the Fourier transform method for the x-axis cut shown in (**a**). (**c**) Cross-section along the z-axis of $\mu_0 H_z$ directly above the center of the vortex (logarithmic y axis scale). (**d**) Percentage difference between the $\mu_0 H_z$ calculated with `SuperScreen` and the Fourier transform method for the z-axis cut shown in (**c**). In (**a**) and (**c**), the results from `SuperScreen` are shown as open circles and the results from the Fourier transform method are shown as solid lines. (**e**) The fluxoid Φ_S^f for a circular region in the film with radius $r = 1\,\mu$m centered on the vortex core. As Λ increases, so to does the supercurrent contribution to the fluxoid. (**f**) Error in the total simulated fluxoid relative to Φ_0: error $= (\Phi_S^f(\Lambda) - \Phi_0)/\Phi_0$.

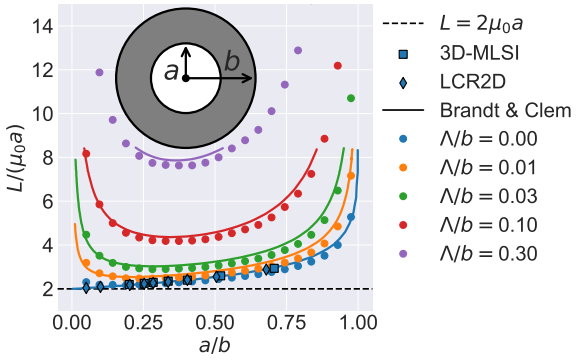

Figure 4: Self-inductance L of a circular ring with inner radius a and outer radius b (see inset), as a function of the ratio a/b and the ring's effective penetration depth Λ. Filled circles indicate results from `SuperScreen`, solid lines show numerical results from Figure 2 of Ref. [1], blue squares and diamonds show numerical results from Figure 1 of Ref. [9], and the dashed line indicates the analytical solution, $L = 2\mu_0 a$, for $\Lambda = 0$ in the limit $a/b \to 0$[7, 12]. The `SuperScreen` results were generated using a mesh with approximately 4,000 vertices and 8,000 triangles.

and the "fractional asymmetry" of $\mathbf{M}$ is $|M_{01} - M_{10}|/\min(|M_{01}|, |M_{10}|) \approx 0.6\%$.

The self-inductance L of a 2D circular ring with inner radius a and outer radius b (see inset of Figure 4) has been used as an informal benchmark for superconducting inductance calculations. For a ring with effective penetration depth $\Lambda = 0$, it has been shown analytically that $L \to 2\mu_0 a$ in the limit $a/b \to 0$ [7, 12]. Khapaev calculated the inductance for $\Lambda = 0$ as a function of a/b [9], and Brandt and Clem calculated the inductance as a function of both Λ and a/b [1]. Figure 4 shows a comparison between these previous numerical results and the results from `SuperScreen`. Note that the models used by Brandt and Clem (solid lines) and by the LCR2D software (blue diamonds) require a circularly symmetric superconducting film, whereas `SuperScreen` (filled circles) and 3D-MLSI [9, 10, 11] (blue squares) support arbitrary 2D geometry.

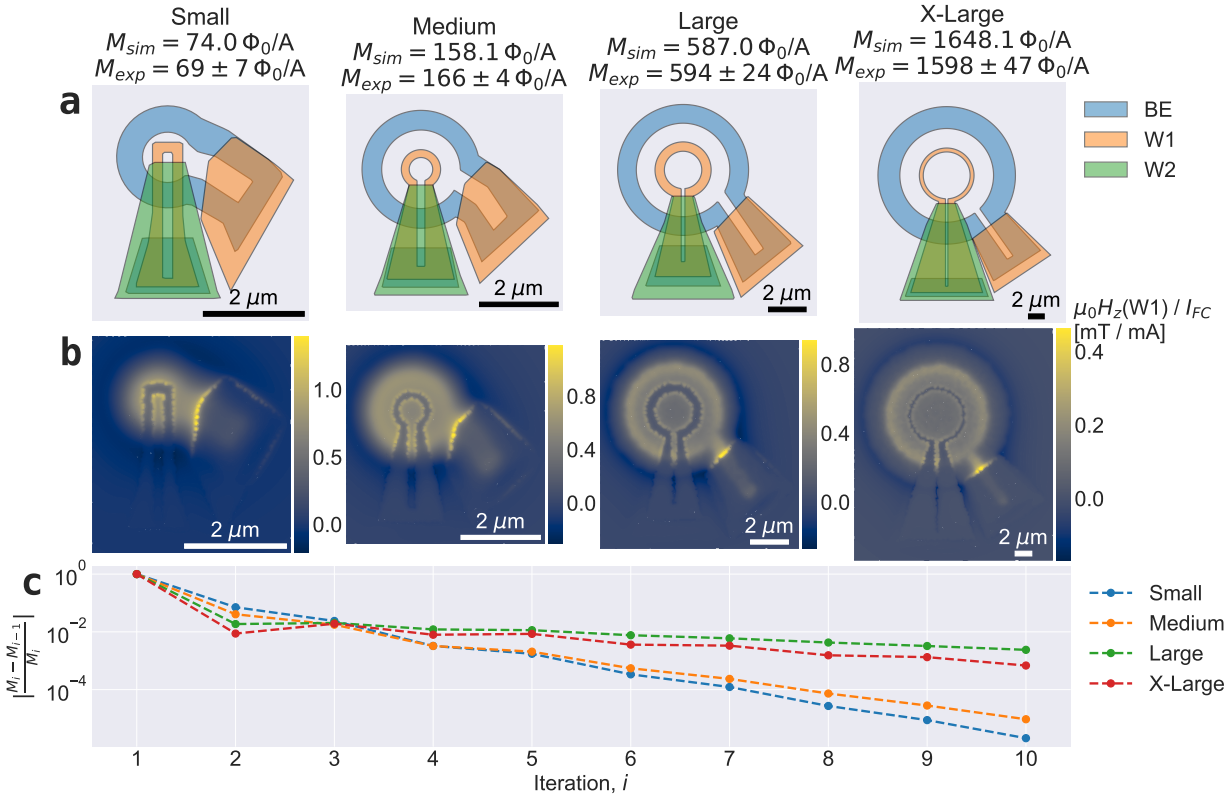

Figure 5: Calculating SQUID susceptometer mutual inductance, defined as the fluxoid induced in the SQUID pickup loop per unit current flowing in the field coil: $M_{\mathrm{PL-FC}} = \Phi^f_{\mathrm{PL}}/I_{\mathrm{FC}}$. Top row (**a**): Schematics of `SuperScreen` models for the field coil and pickup loop region of four sizes of scanning SQUID susceptometer (generated using `Device.draw()`) with pickup loop inner radii ranging from 0.1 μm ("Small") to 3 μm ("X-Large"). Middle row (**b**): Simulated magnetic field $\mu_0 H_z$ evaluated at the plane of layer W1, which contains the pickup loop, normalized by the current I_{FC} flowing in the field coil (which is located in layer BE). Bottom row (**c**): Convergence of the four models, defined as the fractional change in mutual inductance between subsequent iterations i. For all four models, the simulated mutual inductance, M_{sim}, falls within the range of mutual inductance values measured in real devices, M_{exp}, which were reported in Table 1 of Ref. [3]. The mutual inductance values are shown in units of Φ_0/A, where $1\,\Phi_0/\mathrm{A} \approx 2.068 \times 10^{-3}$ pH. The meshes for the "Small," "Medium," and "Large" models consisted of approximately 7,000 vertices and 14,000 triangles, whereas the mesh for the "X-Large" model consisted of about 8,000 vertices and 15,000 triangles. The two smaller models converge more quickly than the two larger models for reasons discussed in Appendix D. Note that for the "X-Large" model, we set the thicknesses of layers I1 and I2 both to 400 nm (instead of the nominal values of 150 nm and 130 nm respectively), to ensure convergence (see Appendix D and Figure D.8).

5.4. Application: scanning SQUID susceptometry

As an example application, we consider scanning SQUID microscopy, a technique in which a superconducting sensor is used to study superconducting or magnetic samples on micron length scales [3]. In scanning SQUID susceptometry, the magnetic susceptibility of a sample is measured by bringing the sample close to a pair of superconducting loops [36, 37, 38]. The first loop, called the "pickup loop" (PL) is attached to a SQUID circuit that sensitively measures the magnetic flux threading the loop. The second loop, called the "field coil" (FC), carries a known current I_{FC} and applies a known magnetic field to both the pickup loop and the sample. A superconducting sample will screen the magnetic field from the field coil, modifying the amount of flux threading the pickup loop and reducing the mutual inductance $M_{\mathrm{PL-FC}}$. The magnitude of this reduction in $M_{\mathrm{PL-FC}}$ is a measure of the sample's penetration depth and therefore its superfluid density.

Figure 5(**a**) shows `SuperScreen Device` models of the field coil and pickup loop region of four types of real SQUID susceptometers, with geometry taken from the layout artwork (GDS) files. In addition to the field coil and pickup loop, there are superconducting shields that limit the amount of magnetic flux that can penetrate the leads connecting the loops to the rest of the circuit (the rest of the circuit is not modeled). There are three relevant layers of superconducting films: the base

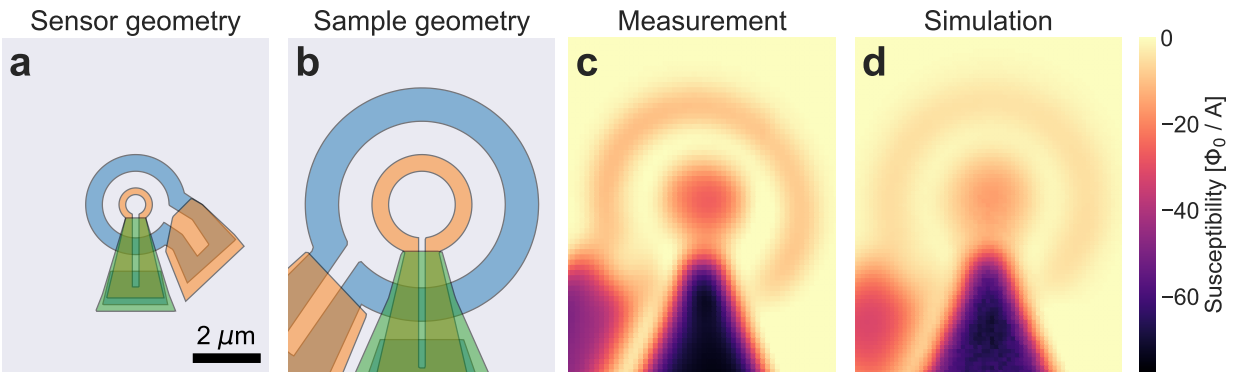

Figure 6: Simulation of a scanning SQUID susceptometry measurement. (**a**) Geometry of the `Device` representing the "sensor" SQUID. (**b**) Geometry of the `Device` representing the "sample" SQUID. (**c**) Susceptibility of the sample SQUID measured at a temperature of 4.0 K. (**d**) Simulated susceptibility, calculcated using the method described in Section 5.4. The pickup loop of the sample, which in reality is connected to a SQUID circuit that has a non-linear magnetic response, is modeled as a continuous superconducting loop in the zero-fluxoid (i.e. Meissner) state. The susceptibility signal is defined as $M_{\text{PL-FC}} - M_{\text{PL-FC, no sample}}$, where $M_{\text{PL-FC, no sample}} \approx 163\,\Phi_0/\text{A}$ (see Figure 5(**a**), second column). The scale bar in (**a**) applies to all four panels.

electrode (BE), which is furthest from the sample contains the field coil; the first wiring layer (W1), which contains the pickup loop and a shield covering the field coil leads; and the second wiring layer (W2), which is closest to the sample and contains a shield covering the pickup loop leads. There are two insulating layers: I1, which separates BE and W1, and I2, which separates W1 and W2. For the superconducting layers, which are made of Nb, we take the London penetration depth to be $\lambda = 80\,\text{nm}$, and the layer thicknesses correspond to the real device design (see Table 1 of Ref. [4] and Figure 8 of Ref. [3]). It is important to note that because $\lambda < d$ for all three layers, the susceptometers are not in the 2D limit in which the model described in Section 2 is technically valid. Nevertheless, as shown in Figure 5, the field coil - pickup loop mutual inductances, M_{sim}, computed by `SuperScreen` lie within the range of mutual inductances measured in real devices, M_{exp} (taken from Table 1 of Ref. [3]), for all four sizes of susceptometer, indicating that variation in current density along the thickness of each film is not critical in determining the mutual inductance in this case. Figure 5(**c**) shows the convergence of $M_{\text{PL-FC}}$ as a function of solver iteration (see Section 2.4).

Having established the value of the field coil - pickup loop mutual inductance in the absence of a sample, $M_{\text{PL-FC, no sample}}$, we can simulate a scanning SQUID susceptometry measurement by calculating $M_{\text{PL-FC}}$ in the presence of a superconducting sample as a function of the relative position of the pickup loop and the sample, (x_s, y_s). For example, in Figure 6 we simulate a SQUID susceptometry measurement of a "Large" susceptometer (the sample) measured with a "Medium" susceptometer (the sensor). Given a `Device` representing the sensor and a `Device` representing the sample, this calculation is performed in three steps:

1. Simulate the sensor with some known current I_{FC} circulating in the field coil to obtain `field_coil_solution` and $M_{\text{PL-FC, no sample}}$.
2. For a given relative position (x_s, y_s) between the sensor and sample, simulate the sample with an applied field given by `field_coil_solution.field_at_position()` to obtain `sample_solution`.
3. Simulate the sensor again, this time with the applied field given by `sample_solution.field_at_position()`, evaluate the fluxoid Φ_{PL}^f for the hole representing the sensor's pickup loop, and calculate the mutual inductance: $M_{\text{PL-FC}}(x_s, y_s) = \Phi_{\text{PL}}^f / I_{\text{FC}}$.

These three steps are repeated for every desired (x_s, y_s) to build up a susceptometry image. The susceptibility signal is reported as $M_{\text{PL-FC}}(x_s, y_s) - M_{\text{PL-FC, no sample}}$, where values that are more negative indicate a stronger diamagnetic response from the sample. Note that in principle it is possible to combine the sensor and sample into a single `Device` with 6 superconducting layers, however this is impractical because it would require generating a new mesh for each (x_s, y_s) and, as discussed in detail in Appendix D, the problem scales unfavorably with the number of layers in a device and with the total lateral extent of a device.

6. Conclusion

The ability to model and visualize screening effects in inhomogeneous 2D superconductors and devices constructed from superconducting thin films can help to build intuition about these systems, aid in interpretation of measurement results, and enable optimization of measurement and device design. `SuperScreen` is an open-source, user-friendly, portable, and efficient tool that solves this problem. Applications of the package include calculating self- and mutual-inductance in planar and multi-planar superconducting circuits, and modeling the magnetic interaction between inhomogeneous superconducting samples and superconducting sensors such as scanning SQUID susceptometers [3].

There are several important limitations to the applicability of `SuperScreen` and the matrix inversion method on which it is based [1, 2]. First, strictly speaking all superconducting films should be in the 2D limit, with London penetration depth λ large compared to the film thickness d, such that the current density is approximately constant along the thickness of the film. There are cases where the model reproduces experimental results despite violation of this condition (e.g. the calculations and in Refs. [3, 4] and Section 5.4), but care must be taking in interpreting results in these cases. Second, the model assumes that all superconducting films behave linearly and without dissipation, and that the applied magnetic field and current density are well below the critical field and critical current density of all films in a device. Third, `SuperScreen` does not support "terminal currents," i.e. currents flowing in one terminal of a device and out another terminal. This means that inductance calculations are limited to structures with holes, in which all applied currents are circulating currents associated with trapped flux. Terminal currents can, however, be included in stream function-based models by setting appropriate boundary conditions [9, 10, 11, 14]. An extension to the model described above that treats the magnetic response of a superconducting ring interrupted by two Josephson junctions (i.e. a SQUID) with trapped vortices and terminal currents is given in Ref. [13]. Finally, care should be taken to ensure that for a given model the mesh is of sufficient density that, to within the desired precision, the results of simulations do not depend on mesh size (see Appendix D).

Potential improvements to `SuperScreen` include: support for terminal currents as discussed above, automated determination of solution convergence for models with multiple layers, more sophisticated mesh generation (e.g. automated local mesh refinement based on device geometry or adaptive mesh refinement based on solution convergence), integration with standard integrated circuit layout software or file formats, and further numerical optimization, including GPU acceleration.

7. Acknowledgements

We acknowledge useful discussions with John R. Kirtley. This work is supported by the Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515. Some of the computing for this project was performed on the Sherlock cluster. We would like to thank Stanford University and the Stanford Research Computing Center for providing computational resources and support that contributed to these research results.

Appendix A. Existing tools

Here, we briefly describe existing software tools for modeling the magnetic response of superconducting devices, most of which are specifically designed for inductance extraction for superconducting integrated circuits. FastHenry, a widely-used 3D (normal metal) inductance extraction tool from MIT [39], has been extended to support superconducting elements [40, 41]. This modified version of FastHenry has been used for inductance extraction in the commercial software InductEx [42]. While FastHenry is open-source, it is written in C and must be compiled for a specific computer architecture and operating system. FastHenry executables compiled for several common operating systems are available as part of the open-source XicTools superconducting integrated circuit design suite from Whiteley Research, Inc [40, 41]. A 2D London model based on a scalar stream function, much like the model used by `SuperScreen` [1, 2], forms the basis of the 3D-MLSI software package [9, 10, 11], which is also written in C and is not open-source. For a more thorough overview and comparison of inductance extraction tools, see Ref. [16].

Appendix B. Laplace operator

The definition of the discrete Laplace operator ∇^2 (also called the Laplace-Beltrami operator) deserves special attention, as it reduces the problem of solving a partial differential equation $\nabla^2 g(x, y) = f(x, y)$ to the problem of solving a matrix equation $\nabla^2 \mathbf{g} = \mathbf{f}$ [43]. As described in Ref. [44], the Laplace operator ∇^2 for a

mesh is defined in terms of two matrices, the mass matrix $\mathbf{M}$ and the weak Laplacian matrix $\mathbf{L}$: $\nabla^2 = \mathbf{M}^{-1}\mathbf{L}$.

In a 2D mesh, the mass matrix $\mathbf{M}$ gives an effective area to each vertex in the mesh. Here we use a "lumped" mass matrix, which is diagonal with elements $M_{ii} = \frac{1}{3}\sum_{t\in\mathcal{N}(i)} \text{area}(t)$, where $\mathcal{N}(i)$ is the set of triangles t adjacent to vertex i. The weak Laplacian matrix $\mathbf{L}$ is defined in terms of a symmetric weight matrix $\mathbf{W}$, which assigns a weight to every edge in the mesh. $\mathbf{W}$ may be defined in a number of ways:

1. Uniform weighting: In this case, $\mathbf{W}$ is simply the adjacency matrix for the mesh vertices:

$$W_{ij} = \begin{cases} 0 & \text{if } i = j \\ 1 & \text{if } i \text{ is adjacent to } j \\ 0 & \text{otherwise} \end{cases}$$

2. Inverse-Euclidean weighting: Each edge is weighted by the inverse of its length: $|\vec{r}_i - \vec{r}_j|^{-1}$, where $\vec{r}_i$ is the position of vertex i.

$$W_{ij} = \begin{cases} 0 & \text{if } i = j \\ |\vec{r}_i - \vec{r}_j|^{-1} & \text{if } i \text{ is adjacent to } j \\ 0 & \text{otherwise} \end{cases}$$

3. Half-cotangent weighting: Each edge is weighted by the half the sum of the cotangents of the two angles opposite to it.

$$W_{ij} = \begin{cases} 0 & \text{if } i = j \\ \frac{1}{2}\left(\cot\alpha_{ij} + \cot\beta_{ij}\right) & \text{if } i \text{ is adjacent to } j \\ 0 & \text{otherwise} \end{cases}$$

By default, `SuperScreen` uses half-cotangent weighting. The Laplacian matrix $\mathbf{L}$ is defined in terms of the weight matrix $\mathbf{W}$: $L_{ij} = W_{ij} - \delta_{ij}\sum_\ell W_{i\ell}$. Finally, the Laplace operator is given by $\nabla^2 = \mathbf{M}^{-1}\mathbf{L}$.

Appendix C. Spatially inhomogeneous Λ

As mentioned in Section 4.2, the effective penetration depth Λ of each layer can be specified as a numeric constant or as a `superscreen.Parameter` that computes $\Lambda(x, y)$, the effective penetration depth as a function of position. As a (somewhat contrived) example, Code Block 3 demonstrates how to modify the model of a ring with a slit from Code Block 1 and Figure 1 such that the ring's penetration depth $\Lambda(x, y)$ increases linearly as a function of the angle between the vector $\vec{r} = (x, y)$ and the $-y$ axis (along which the slit lies). The resulting current and field distributions are shown in Figure C.7. Note that $\Lambda(x, y)$ must vary slowly on the scale of the spacing between mesh vertices in order for results to be reliable. For example, the simulated supercurrent density near a point-like defect (i.e small compared to the triangles in the mesh) associated with a penetration depth Λ_{defect} in an otherwise uniform film with penetration depth $\Lambda_0 \ll \Lambda_{\text{defect}}$ will depend strongly on the specifics of the mesh near the defect. One can avoid this problem by increasing the density of the mesh in regions of fast-varying Λ by adding one or more "abstract regions" to the `Device` as described in Section 4.2.

Appendix D. Numerical considerations

While the numerical method described in Section 3 is generally quite robust, it can break down for certain extreme geometries. The stream function $g(x, y)$ represents the local magnetization or density of infinitesimal current loops. The z-component of the magnetic field at position $\vec{r} = (x, y, z)$ from a film F with stream function g lying in a plane parallel to the $x - y$ plane at vertical position z' is given by (see Equations 4 and 5):

$$\begin{aligned} H_z(\vec{r}) &= \int_F Q_z(\vec{r}, \vec{r}')g(x', y')\,\mathrm{d}^2r', \text{ where} \\ Q_z(\vec{r}, \vec{r}') &= \frac{2(z - z')^2 - \rho^2}{4\pi[(z - z')^2 + \rho^2]^{5/2}} \end{aligned} \tag{D.1}$$

and $\rho = \sqrt{(x - x')^2 + (y - y')^2}$. Eq. D.1 is exact for a continuous stream function g. However, the discretized version of Eq. D.1, in which the double integral over the film area F is replaced by a sum over triangular mesh elements, is only valid if $\delta z = z - z'$, the vertical distance between the film and the point at which the field is being evaluated, is large compared to the typical distance δr between vertices in the mesh representing the film. For $z - z' = \delta z \lesssim \delta r$, the field $H_z(\vec{r})$ resembles that of a discrete set of isolated dipoles located at the mesh vertex positions, rather than that of a continuous sheet of current (see Figure D.8(**b**)). This can lead to unphysical results when evaluating the field very close to the surface of a film (for example using `Solution.field_at_position()`), or when solving models involving multi-layer structures where the vertical spacing between layers is much smaller than the lateral extent of the films, in which case the iterative calculation (Section 2.4) may not converge.

The limitation described above can be seen in the model of the largest SQUID susceptometer described in Section 5.4, which has a field coil inner radius of

```python
def linear_vs_angle(
    x: np.ndarray, y: np.ndarray, *, min_val: float, max_val: float
) -> np.ndarray:
    # Rotate the input coordinates so that theta = 0
    # corresponds to the slit position (along the -y axis).
    x, y = sc.geometry.rotate(
        np.stack(np.atleast_1d(x, y), axis=1), np.degrees(-np.pi / 2)
    ).T
    # Calculate the angular position of each mesh vertex.
    angles = np.arctan2(y, x) + np.pi  # range: [0, 2 * pi]
    # Set Lambda to increase linearly from min_val to max_val
    # as a function of angular position.
    Lambdas = angles / (2 * np.pi) * (max_val- min_val) + min_val
    return Lambdas

# Define the Parameter and assign it as the Lambda of the superconducting layer.
Lambda = sc.Parameter(linear_vs_angle, min_val=0.1, max_val=1.0)
device.layers["base"].Lambda = Lambda
# Everything below is identical to Code Block 1:
# Calculate the device's response to a uniform applied field.
applied_field = sc.sources.ConstantField(10)
solution = sc.solve(device, applied_field=applied_field, field_units="uT")[-1]
# Visualize the solution.
# Plot the current density evaluated at each layer in the Device.
solution.plot_currents()
# Plot the magnetic field evaluated at each layer in the Device.
solution.plot_fields()
# Plot the field evaluated at any points in space.
solution.plot_field_at_positions(device.points, zs=0.5)
```

Code Block 3: Simulating an inhomogeneous superconducting device. Here we modify the superconducting ring with a slit from Code Block 1 and Figure 1 to have an effective penetration depth $\Lambda(x, y)$, which increases linearly from $0.1\,\mu$m to $1\,\mu$m as a function of the angle between the vector $\vec{r} = (x, y)$ and the $-y$ axis. See Figure C.7 for the resulting current and field distributions.

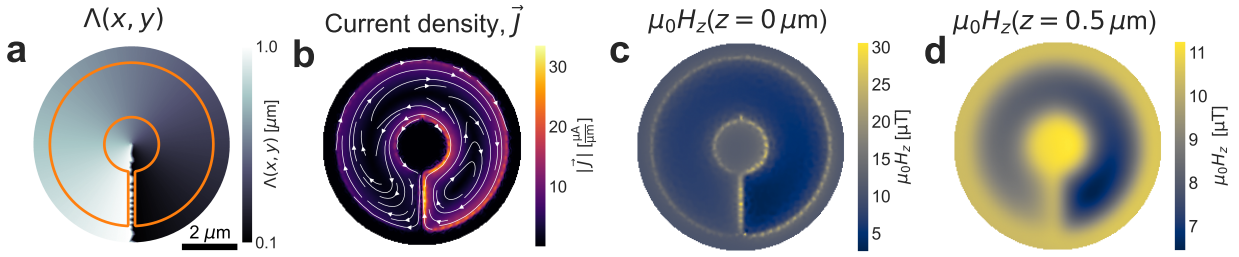

Figure C.7: The output of Code Block 3: Meissner screening of a uniform applied field of $10\,\mu$T by a ring with a slit in a superconducting film with inhomogeneous effective penetration depth $\Lambda(x, y)$. (**a**) The inhomogeneous effective penetration depth $\Lambda(x, y)$, with the ring's outline overlaid in orange. (**b**) The current density $\vec{J}$ in the ring, generated with `Solution.plot_currents()`. (**c**) The z-component of the magnetic field $\mu_0 H_z$ evaluated at the plane of the ring, generated with `Solution.plot_fields()`. (**d**) The z-component of the magnetic field evaluated $z = 0.5\,\mu$m above the ring (generated using `Solution.plot_field_at_positions()`).

$6\,\mu$m and a total modeled area of roughly $600\,\mu\text{m}^2$. As shown in Figure D.8, `SuperScreen` significantly overestimates the mutual inductance between the field coil and pickup loop when $\delta z < \delta r$ because, in that case, the discretized version of Eq. D.1 does not correctly compute the magnetic field due the stream functions of the

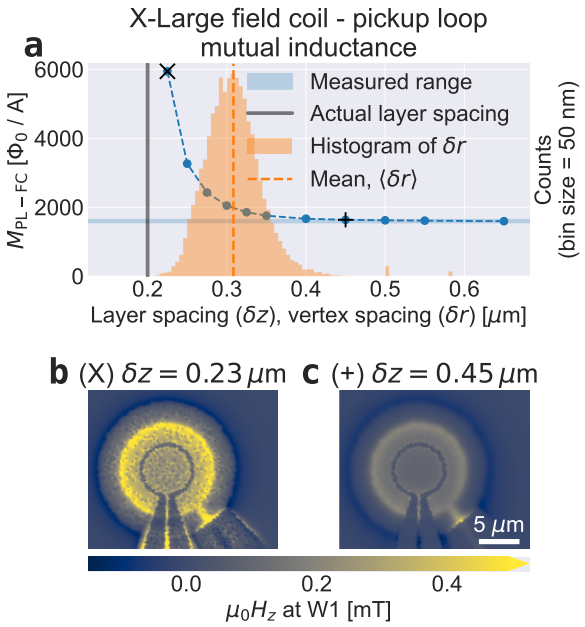

Figure D.8: `SuperScreen` results may be unreliable for multi-layer models where the spacing between layers is smaller than the typical vertex-to-vertex distance, δr. (**a**) Field coil - pickup loop mutual inductance for the largest SQUID suscepometer modeled in Section 5.4 as a function of the minimum vertical spacing between layers, δz. The simulated mutual inductance is shown with blue circles, and a histogram of the mesh vertex-to-vertex distances δr is shown in orange (arb. y axis units). When $\delta z \lesssim \delta r$, the model significantly overestimates the mutual inductance. (**b**) and (**c**): Out-of-plane magnetic field $\mu_0 H_z$ evaluated at the plane of the pickup loop (W1 layer) for (**b**) the nominal layer spacing with $\delta z < \delta 2$ (indicated with a black × in (**a**)) and (**c**) $\delta z > \delta r$ (indicated with a black + in (**a**)). For $\delta r \lesssim \delta z$, the magnet field calculated using Eq. D.1 resembles that of a discrete set of isolated dipoles rather than a continuous sheet of current. Note that (**b**) and (**c**) share the same color scale, which is saturated in (**b**).

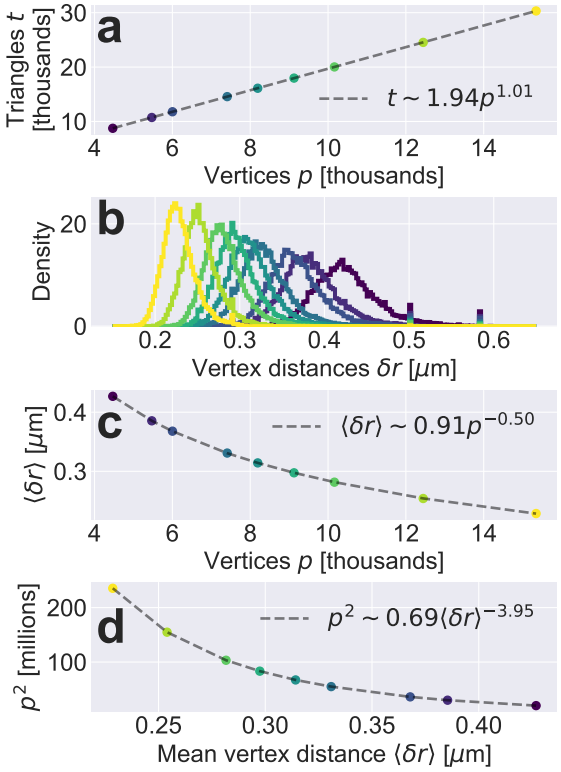

Figure D.9: Scaling of kernel matrix size p^2 with mesh vertex spacing δr for a mesh with p vertices and t triangles for the device shown in Figure D.8. (**a**) Typically the number of triangle t in the mesh is close to twice the number of vertices p. (**b**) Normalized histograms of vertex distances δr. The histogram bins are given by `numpy.linspace(0.15, 0.65, 201)`. (**c**) The mean vertex-to-vertex distance $\langle\delta r\rangle$ scales roughly as $p^{-1/2}$. (**d**). The size of each $p \times p$ kernel matrix (of which where are $\binom{L}{2}$ for a device with L layers) scales roughly as $\langle\delta r\rangle^{-4}$. Note that in each row the colors correspond to the number of vertices p in the mesh, as indicated in (**a**), with mesh size increasing from dark to light colors.

superconducting layers. For the sake of computing mutual inductance as in Section 5.4, it is physically reasonable to artificially increase the vertical spacing between layers such that $\delta z \geq \delta r$ because we expect the magnetic field at the pickup loop, a vertical distance δz away from the center of the field coil, to fall off roughly as $\left(\delta z^2 + R_{FC}^2\right)^{-3/2}$, where $R_{FC} \approx 6\,\mu\text{m} \gg \delta z$. However, in situations where δz is a critical dimension (in the sense that increasing it would invalidate the physical model), one's only option is to decrease δr by increasing the density of the mesh.

For this reason, mutli-layer structures with closely-spaced layers are the most challenging class of problem to solve. The iterative method used described in Section 2.4 is memory-intensive for models with a large mesh (many vertices p and triangles t, with typically $t \approx 2p$) and/or many layers L, because the average distance between vertices decreases slowly with increasing number of vertices, $\langle\delta r\rangle \sim p^{-1/2}$, whereas the size of the (dense floating-point) $p \times p$ matrix that represents the dipole kernel $Q_z(\vec{r}, \vec{r}')$ in Eq. D.1 increases as p^2. The end result is that the memory footprint of kernel matrix scales roughly as $\langle\delta r\rangle^{-4}$, so decreasing the mean distance between vertices by a factor of 2 increases the memory required by a factor of roughly 16 (see Figure D.9).

Furthermore, for a model with L layers there are $\binom{L}{2} = L(L-1)/2$ such kernel matrices needed for each iteration of the calculation outlined in Section 2.4. In `superscreen.solve()`, these $\binom{L}{2}$ matrices are computed during the first iteration and then cached in memory for use in subsequent iterations.

One can force the kernel matrices to be cached to disk if they would otherwise occupy too large a fraction of the available system memory using the `cache_kernel_memory_cutoff` argument, but this comes at a significant performance cost. In many cases, one can use lower-precision floating point numbers (e.g. using 32-bit single-precision floats instead of the default 64-bit double-precision floats by setting `device.solve_dtype = "float32"`) to reduce memory requirements without significantly impacting solution accuracy.

Appendix E. Parallel processing

As discussed above, one can solve many models involving the same `Device` in parallel across multiple CPUs using the `superscreen.solve_many()` function. There are two methods available for process-based parallelism in `SuperScreen`: `parallel_method="multiprocessing"`, which uses the `multiprocessing` package from the Python standard library, and `parallel_method="ray"`, which uses the third-party distributed computing framework `Ray`[3] [32, 33]. Both approaches utilize shared memory so that only a single copy is made of the large arrays required to solve a `Device` (the mesh, kernel matrix $\mathbf{Q}$, Laplace operator ∇^2, etc.), rather than `num_cpus` copies, where `num_cpus` is the number of worker processes.

There are three ways to invoke `Ray` from `SuperScreen` when running on a single machine, e.g. a multi-core CPU. The first is to simply pass the keyword argument `parallel_method="ray"` when calling `solve_many()` (see Code Block 4). This will automatically create a `Ray` cluster using (by default) all available physical CPU cores, solve the models in parallel, and then shut down the cluster before returning. The second method is to manually create a `Ray` cluster using the `Ray` Python application programming interface (API) prior to calling `solve_many(..., parallel_method="ray")`, as demonstrated in Code Block 5. The third method is to start a `Ray` cluster using the command line interface (CLI), then connect to the existing cluster using the Python API prior to calling `solve_many(..., parallel_method="ray")`, as demonstrated in Code Block 6. One of the latter two methods should be used for finer control over the `Ray` cluster. For example, if calling `solve_many()` many times in a single session, one can use these methods to avoid the overhead of starting and stopping a `Ray` cluster multiple times.

```
parallel_method = "multiprocessing"
# parallel_method = "ray"

# Specify number of worker processes:
num_cpus = 4
# Or automatically use all
# available physical CPUs:
# num_cpus = None

_ = superscreen.solve_many(
    device=device,
    parallel_method=parallel_method,
    num_cpus=num_cpus,
    **solve_kwargs,
)
```

Code Block 4: Utilizing process-based parallelism in `SuperScreen` given a `superscreen.Device` and solver options stored in a dictionary `solve_kwargs`.

Running `superscreen.solve_many()` in parallel across multiple nodes in a computing cluster is a simple extension to the method outlined in Code Block 6, although the specifics depend upon the infrastructure of the cluster, e.g. job management software. See the "Multi-Node Ray" section of the `Ray` documentation for more details [33].

[3] Note that at the time of writing, `Ray` support for Windows is experimental and under active development.

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```python
# Assume that we have already created a Device and put all other inputs
# to superscreen.solve_many() into a dictionary called other_kwargs.
import psutil
import ray

# Specify the number of CPUs/cores to allocate.
num_cpus = 3
# Use at most N processes for a machine with N physical CPUs.
num_cpus = min(num_cpus, psutil.cpu_count(logical=False))

# Start a ray cluster
ray.init(num_cpus=num_cpus)
# Solve the models
solutions, paths = superscreen.solve_many(
    parallel_method="ray",
    **other_kwargs,
)
# Potentially call solve_many() again using the same ray cluster...
# Finally, shutdown the ray cluster
ray.shutdown()
```

Code Block 5: Starting and stopping `Ray` outside of `superscreen.solve_many()` using the Python API. See the "API and Package Reference" section of the `Ray` documentation for additional options in `ray.init()` [33].

```
# Start a ray cluster from the command line, e.g. bash
ray start --head --num-cpus=3
```

```python
# Assume that we have already created a Device and put all other inputs
# to superscreen.solve_many() into a dictionary called other_kwargs.
import ray
# Connect to the existing ray cluster.
# If more than one ray cluster is running, specify
# which to connect to using address="{ip}:{port}".
ray.init(address="auto")
# Solve the models.
solutions, paths = superscreen.solve_many(
    parallel_method="ray",
    **other_kwargs,
)
# Potentially call solve_many() again using the same ray cluster...
```

```
# Shut down the ray cluster from the command line
ray stop
```

Code Block 6: Starting and stopping `Ray` outside of `superscreen.solve_many()` using the command line interface. See the `Ray` documentation for additional options in `ray start` [33].

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