Preconditioning the Jacobian system of the extreme type II Ginzburg Landau problem

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This presentation considers the extreme type–II Ginzburg–Landau equations that model vortex patterns in superconductors. The nonlinear PDEs are solved using Newton's method where preconditioning the solution method of the Jacobian system is crucial for the performance of the solver. Some of the properties of the Jacobian operator will be highlighted, emphasizing on how it is possible to make use of them to construct a good preconditioner.

For a general superconductor, given an open, bounded domain Ω, the unknowns that need to be solved for are the complex-valued *order parameter* $\psi \in H^2_{\mathbb{C}}(\Omega)$ as well as the vector-valued induced magnetic vector potential $\mathbf{A} \in H^2_{\mathbb{R}^n}(\Omega)$. We will study extreme type–II superconductors for which magnetic vector potential $\mathbf{A}$ can be considered given. The approximation is valid, for example, for all all high-temperature superconductors.

With

$$\begin{aligned} X &:= \big\{\psi \in H^2(\Omega) : \text{there is a defining sequence } \psi_k \text{ with} \\ &\qquad\qquad \lim_{k\to\infty} \mathbf{n} \cdot (-\mathrm{i}\nabla - \mathbf{A})\psi_k = 0 \text{ on } \partial\Omega\big\}, \\ Y &:= L^2(\Omega), \end{aligned}$$

the celebrated Ginzburg–Landau problem is to solve

$$\left\{ 0 = (-\mathrm{i}\nabla - \mathbf{A})^2 \psi - \psi \left(1 - |\psi|^2\right) \quad \text{on } \Omega \right\} \tag{1}$$

for $\psi \in X$. Here, for any applied magnetic field $\mathbf{H}_0$ the magnetic vector potential $\mathbf{A} = \mathbf{A}(\mathbf{H}_0)$ is given by the relations

$$\begin{cases} \nabla \times (\nabla \times \mathbf{A}) = 0, \\ \lim\limits_{\|x\|\to\infty} \nabla \times \mathbf{A} = \mathbf{H}_0. \end{cases}$$

Every solution ψ directly corresponds to the physical observable of the density of electron (Cooper) pairs, $\rho_{\mathrm{C}} = |\psi|^2$.

The discretization of (1) needs to be constructed with care to preserve certain properties that are physically desirable. For example, there exists a variant of finite volume discretizations which is well-behaving in this sense [2].

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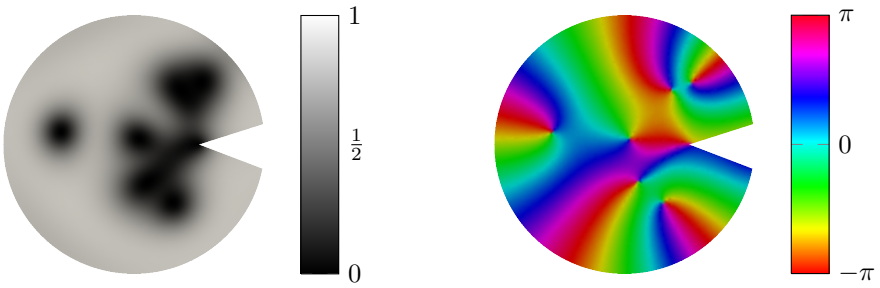

$|\psi|^2$ (Cooper pair density) $\arg\psi$

Figure 1: A solution ψ of the Ginzburg–Landau equation on a two-dimensional cut-circle domain with a magnetic field applied perpendicular to the sample. The typical *vortices* are exhibited around which the complex argument changes by multiples of 2π.

The solution of the Ginzburg–Landau equations is numerically challenging first and foremost due to their nonlinearity which suggests Newton's method to be used for the approximation of solutions. A typical application of numerical calculations with the Ginzburg–Landau equations however would not only involve the solution of the equation for *one* particular domain and vector potential. It is rather more interesting to get a complete overview over the whole set of possible vortex configurations. An important tool for exploring the energy landscape is numerical continuation with, e.g., the strength of the applied magnetic field as continuation parameter. In this context, thousands of nonlinear systems will need to be solved subsequently. That is why it is important to come up with efficient ways of solving the Newton system; the key to this of course lies in the solution of the linear Jacobian system that needs to performed in each Newton step.

The Jacobian operator of (1) is

$$\begin{aligned} &\mathcal{J}(\psi;\mathbf{A}) : X \to Y, \\ &\mathcal{J}(\psi;\mathbf{A})\varphi := \left((-\mathrm{i}\nabla - \mathbf{A})^2 - 1 + 2|\psi|^2\right)\varphi + \psi^2\overline{\varphi}. \end{aligned} \tag{2}$$

Note that $\mathcal{J}(\psi;\mathbf{A})$ is indeed linear when defined over X and Y as $\mathbb{R}$-vector spaces.

Although this particular form of the operator sets it aside from the more common case of operators not acting on $\overline{\varphi}$, this special structure does not have a large impact on iterative solution methods which merely assume a well-defined matrix-vector product. On the other hand, methods that make direct use of the entries of the discretized operator will require more effort to fit into the framework of operators like (2).

The Jacobian operator $\mathcal{J}$ has certain convenient properties such as the fact that

- For any given $\psi \in Y$, $\mathbf{A} \in H^2_{\mathbb{R}^n}(\Omega)$, the Jacobian operator $\mathcal{J}(\psi;\mathbf{A})$ is self-adjoint with respect to the inner product $\Re\langle\cdot,\cdot\rangle$.

Note that $\Re\langle\cdot,\cdot\rangle$ is in fact the natural inner product in the $\mathbb{R}$-vector space Y. In any case, this makes sure that the spectrum of $\mathcal{J}$ is purely real. Another interesting thing to note about the spectrum is that

- Let ψ_0 be a solution of the Ginzburg–Landau equations with given $\mathbf{A}_0$. Then
$$\mathcal{J}(\psi_0; \mathbf{A}_0)(\mathrm{i}\psi_0) = 0,$$
so for non-trivial solution states, $\mathcal{J}$ has a non-trivial kernel.

This is direct consequence of the fact that (1) is invariant under the gauge transformation $\widetilde{\psi} = \exp\{\mathrm{i}\chi\}\psi$ for any $\chi \in \mathbb{R}$.

Besides the fact that there is always a degenerate eigenvalue and that all eigenvalues are real, not much more can be said about the spectrum; in general, $\mathcal{J}(\psi)$ is indefinite. The definiteness depends entirely on the state ψ; if ψ is a solution to (1), it in turn is said to be stable or unstable depending whether or not $\mathcal{J}(\psi)$ has positive eigenvalues.

The default solving methods for self-adjoint, indefinite linear systems include MINRES and SYMMLQ, but also the CG method will converge after the negative eigenvalues have been deflated.

Generic entry-based preconditioners like the diagonal part or ILU are not readily available but can be constructed to leverage the unusual structure of $\mathcal{J}$. Equation-based preconditioners on the other hand can be derived as usual. Consider for example that

- The kinetic energy operator
$$K(\mathbf{A}) : X \to Y,$$
$$K(\mathbf{A})\varphi := (-\mathrm{i}\nabla - \mathbf{A})^2\varphi$$
is self-adjoint with respect to the regular inner product $\langle\cdot,\cdot\rangle$, positive semidefinite, and has an eigenvalue $\lambda_0 = 0$ if and only if $\mathbf{A} = 0$.

These nice properties help in coming up with an efficient solver for K. For example, linear systems with K could be solved with CG, preconditioned with, e.g., a multigrid strategy. Consequently, K^{-1} is an appropriate candidate for preconditioning $\mathcal{J}(\psi)$.

The talk will highlight more properties of K in conjunction with $\mathcal{J}$, as well as compare its performance as a preconditioner with various other choices. Numerical results for finite volume discretizations of the operator for various domains in two and three dimensions will be presented.

References

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