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Abstract:
A fast iterative solver for the variable coefficient diffusion equation on a disk

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Abstract

We present an efficient iterative method for solving the variable coefficient diffusion equation on a unit disk. The equation is written in polar coordinates and is discretized by the standard centered difference approximation under the grid arrangement of shifting half radial mesh away from the origin so that the coordinate singularity can be handled naturally without pole conditions. The resultant matrix is symmetric positive definite so the preconditioned conjugate gradient (PCG) method can be applied. Some different preconditioners have been tested for comparison, in particular, a preconditioner arising from the modified equation has been derived and shown to be the most efficient one. The present elliptic solver has been applied to study the vortex dynamics of the Ginzburg-Landau equation with a variable diffusion coefficient.

Key Words: variable diffusion equation; polar coordinates; iterative method; Ginzburg-Landau vortices.

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1 Introduction

The variable coefficient elliptic equation arises from many situations of physical applications. The heat transfer in heterogeneous material where the thermal conductivity depends on the position is one of the classical example. Another example comes from the Ginzburg-Landau theory for superconductivity. When a superconductor contains impurities, it is quite natural to consider the inhomogeneous coherence length in the Ginzburg-Landau equation. Thus, a nonlinear variable elliptic-type equation must be solved where the variable coefficient represents the coherence length for superconducting electrons in a material [4]. Motivated by the above problems, in this paper, we consider the following variable coefficient diffusion equation written in polar coordinates on a 2D unit disk $\Omega = \{(r, \theta) | 0 < r < 1, 0 \leq \theta < 2\pi\}$ as

$$-\frac{1}{r} \left[ \frac{\partial}{\partial r} \left( \beta r \frac{\partial u}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \frac{\beta u}{r} \frac{\partial}{\partial \theta} \right) \right] = f(r, \theta) \quad \text{in} \quad \Omega, \quad (1)$$

$$u(1, \theta) = g(\theta), \quad \text{on} \quad \partial \Omega, \quad (2)$$

where the diffusion coefficient $\beta(r, \theta) > 0$ is inhomogeneous in the disk.

When we solve the equation (1) numerically, the first issue called the coordinate singularity arises. This is because the equation is not valid at $r = 0$ when it is written in polar coordinates. In [11], the first author discretized the Poisson equation (a special case of $\beta(r, \theta) = 1$ in Eq. (1)) by using the standard centered difference scheme under a polar grid of shifting a half radial mesh away from the origin. It was found that the method handles the coordinate singularity without special treatment and the resultant matrix equation is simpler than the traditional method described in [16]. Furthermore, the desired accuracy has been preserved. Mohseni and Colonius [13] have used the similar grid arrangements to handle the coordinate singularities in finite difference and pseudo-spectral methods and have applied to the Bessel's equation and compressible Navier-Stokes equations.

Another standard technique to solve the Poisson equation on a disk is as follows. We first write the solution as a truncated Fourier series in $\theta$ direction and obtain a set of Fourier mode equations. Then those ordinary differential equations of Fourier coefficients are solved by either finite difference or spectral methods. Once again, in order to have the desired regularity and accuracy, most of the numerical methods including finite difference method [9], or spectral method [6, 8, 15] need to impose appropriate conditions for the
solution at the coordinate singularity. The accuracy of the numerical methods depends greatly on the choice of those pole conditions. Until recently, different numerical methods without pole conditions have been proposed as well [5, 7, 12].

The numerical solution of the variable coefficient diffusion equation (1) is another different story. Since now the elliptic equation has a variable diffusion coefficient, we are unable to write the solution as Fourier series expansion. Thus, the Fast Fourier Transform (FFT) cannot be called directly. Furthermore, the equation (1) is not a separable type, the resultant linear system after the discretization cannot be solved directly by the fast direct solvers such as those provided in public software package - FISHPACK [2]. The goal of this paper is to develop an efficient iterative method for solving the variable coefficient diffusion equation (1). The equation is first discretized by the standard centered difference approximation under the grid arrangement of shifting half mesh away from the origin so that the coordinate singularity can be easily handled without pole conditions. The resultant matrix is symmetric positive definite so some different preconditioned conjugate gradient (PCG) methods can be applied. In particular, a preconditioner arising from the modified equation will be derived and shown to be an efficient one. The present elliptic solver has been applied to study the vortex dynamics of the Ginzburg-Landau equation with a variable diffusion coefficient.

2 Finite difference discretization

We use the same grid points in the radial direction as in [13, 11] by
\[ r_i = (i - 1/2) \Delta r \quad r_{i-1/2} = r_i - \Delta r/2, \quad r_{i+1/2} = r_i + \Delta r/2 \] (3)
and the azimuthal direction
\[ \theta_j = (j - 1/2) \Delta \theta \quad \theta_{j-1/2} = \theta_j - \Delta \theta/2, \quad \theta_{j+1/2} = \theta_j + \Delta \theta/2 \] (4)
where \( \Delta r = 2/(2M + 1) \) and \( \Delta \theta = 2\pi/N \). By the choice of the radial mesh width, the boundary values are defined on the grid points. Let the discrete values be denoted by \( u_{ij} \approx u(r_i, \theta_j) \), \( f_{ij} \approx f(r_i, \theta_j) \), and \( g_j \approx g(\theta_j) \). Using the centered difference method to discretize Eq. (1), we have
\[
-\frac{1}{r_i} \left[ (r_{i+1/2} \beta_{i+1/2,j} \frac{u_{i+1,j} - u_{i,j}}{\Delta r} - r_{i-1/2} \beta_{i-1/2,j} \frac{u_{i,j} - u_{i-1,j}}{\Delta r})/\Delta r \right]
+ \left( \frac{\beta_{i,j+1} u_{i,j+1} - u_{i,j}}{r_i} \frac{\Delta \theta}{\Delta \theta} - \frac{\beta_{i,j-1} u_{i,j} - u_{i,j-1}}{r_i} \frac{\Delta \theta}{\Delta \theta} \right)/\Delta \theta = f_{i,j}.
\] (5)
Among the above representations, the numerical boundary values are given by $u_{M+1,j} = g_j$, and $u_{i0} = u_{i,N}$, $u_{i1} = u_{i,N+1}$ since $u$ is $2\pi$ periodic in $\theta$. At $i = 1$, we have immediately observed from (3) that $r_{1/2} = 0$, so the coefficient of $u_{0j}$ is zero. This implies that the scheme does not need any extrapolation for the inner numerical boundary value $u_{0j}$ so that there is no pole condition needed. It is also easy to check that the matrix of linear equations (5) is symmetric and positive definite so the preconditioned conjugate gradient methods can be applied.

For the Neumann problem, we still use the same grid described in (3) but with different choice of $\Delta r = 1/M$. With the choice of this mesh width, the discrete values of $u$ are defined midway between boundary so that the first derivative can be centered on the grid points.

### 2.1 The fast direct solver as a preconditioner

In this subsection, we derive a preconditioner which can be applied to the conjugate gradient method to solve the linear system (5). Our intention is to construct a preconditioner $P$ such that the inversion of the matrix $P$ can be done by available fast direct solvers such as FFT. One natural choice is to average the variable coefficient in the equation (1) so that a separable PDE is formed. More precisely, the preconditioner can be constructed from the equation

$$
-\frac{1}{r} \left[ \frac{\partial}{\partial r} \left( \tilde{\beta} \frac{\partial u}{\partial r} \right) + \frac{\partial}{\partial \theta} \left( \frac{\tilde{\beta}}{r} \frac{\partial u}{\partial \theta} \right) \right] = f(r, \theta),
$$

where the coefficient

$$
\tilde{\beta}(r) = \frac{1}{2\pi} \int_0^{2\pi} \beta(r, \theta) \, d\theta.
$$

Since the new diffusion coefficient $\tilde{\beta}$ is a function of $r$, the above PDE is separable. Thus, the inversion of the preconditioner can be efficiently done by fast direct solvers such as FFT or block cyclic reduction algorithm [1].

### 2.2 Numerical results

In this subsection, we perform several numerical tests for the presented method. Table 1 shows the maximum errors of the method for three different test examples as

1. $u = e^{r(\cos \theta + \sin \theta)}$, \quad $\beta = r^2 \sin^2 \theta + r \cos \theta + 1.1$
2. $u = \sin(r \cos \theta) \sin(r \sin \theta), \quad \beta = e^{r(\cos \theta + \sin \theta)}$

3. $u = r^5 \cos^3 \theta \sin^2 \theta / 3 + r^3 \cos^2 \theta \sin \theta + r \cos \theta + 1,$
   $\beta = 0.1 (r^2 \cos \theta \sin \theta + 1)$.

The right-hand side functions are obtained by substituting the solutions into the equation (1).

In all our tests, we use $M$ grid points in the radial direction and $N = 2M$ points in the azimuthal direction. The rate of convergence is computed by the formula $\log_2 \left( \frac{E_M}{E_M^2} \right)$, where $E_M$ is the relative maximum error with radial resolution $M$. All the results are obtained by solving the linear system (5) using PCG with the fast direct solver (6) as the preconditioner. The initial guess of the iteration is set to be $u_{ij} = 1$ everywhere, and the tolerance of residual is $10^{-8}$. One can see from Table 1 that indeed our scheme preserves clean second-order accuracy.

Table 2 shows the number of iterations needed for solving the solution of Example 1 by PCG method with different preconditioners. Those preconditioners include block Jacobi (BJ), symmetric successive over relaxation (SSOR), incomplete Cholesky factorization (IC), and the fast direct solver (FDS) described in (6). Indeed, the fast direct solver preconditioner turns out to be the most efficient one since it has the least number of iterations, and the iterations are kept to be a constant when we increase the grid points. The CPU time in seconds for different preconditioners are also listed in Table 2. Again, one can easily see that the fast direct solver (FDS) outperforms the other preconditioners.

3 Simulation of Ginzburg-Landau equation with a variable diffusion coefficient

In this section, we apply the present iterative elliptic solver to study the stable solutions of the following Ginzburg-Landau equation (GLE) with a variable diffusion coefficient in a unit disk $\Omega = \{r^2 = x^2 + y^2 < 1\}$

$$\frac{\partial u}{\partial t} = \frac{1}{a(\mathbf{x})} \nabla \cdot (a(\mathbf{x}) \nabla u) + \frac{1}{\varepsilon^2} (1 - |u|^2) u \quad \text{in} \quad \Omega, \quad \text{(8)}$$

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}) \quad \text{in} \quad \Omega, \quad \text{(9)}$$

$$\frac{\partial u}{\partial r} = 0 \quad \text{on} \quad \partial \Omega. \quad \text{(10)}$$
<table>
<thead>
<tr>
<th></th>
<th>M</th>
<th>16</th>
<th>32</th>
<th>64</th>
<th>128</th>
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<td>error rate</td>
<td>1.160E-03</td>
<td>-</td>
<td>2.828E-04</td>
<td>2.04</td>
</tr>
<tr>
<td>Ex.2</td>
<td>error rate</td>
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<td>-</td>
<td>7.043E-04</td>
<td>2.07</td>
</tr>
<tr>
<td>Ex.3</td>
<td>error rate</td>
<td>1.089E-03</td>
<td>-</td>
<td>2.742E-04</td>
<td>1.99</td>
</tr>
</tbody>
</table>

Table 1: The maximum errors of three different solutions $u$ with different diffusion coefficients $\beta$ for Eq. (1).

<table>
<thead>
<tr>
<th></th>
<th>M</th>
<th>CG (iteration)</th>
<th>BJ (iteration)</th>
<th>SSOR (iteration)</th>
<th>IC (iteration)</th>
<th>FDS (iteration)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>167 (0.20)</td>
<td>70 (0.23)</td>
<td>39 (0.22)</td>
<td>28 (0.09)</td>
<td>28 (0.16)</td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>450 (0.84)</td>
<td>133 (0.58)</td>
<td>60 (0.48)</td>
<td>53 (0.24)</td>
<td>33 (0.40)</td>
<td></td>
</tr>
<tr>
<td>64</td>
<td>1332 (9.11)</td>
<td>240 (4.61)</td>
<td>93 (3.19)</td>
<td>103 (2.12)</td>
<td>36 (1.04)</td>
<td></td>
</tr>
<tr>
<td>128</td>
<td>3924 (142.0)</td>
<td>478 (43.39)</td>
<td>147 (25.35)</td>
<td>195 (20.21)</td>
<td>36 (4.43)</td>
<td></td>
</tr>
</tbody>
</table>

Table 2: The performance comparison for using different preconditioners. The first number represents the number of iterations while the number in parenthesis represents the CPU time in seconds.

This 2D model approximates the three-dimensional Ginzburg-Landau equation with constant coherence length in a very thin variable superconducting film which the positive coefficient $a(x)$ characterizes the variable thickness [4]. The solution $u$ is a complex-valued function representing the order parameter and the parameter $\varepsilon$ is a small positive number. Note that, we use the Cartesian shorthand $\nabla \cdot (a(x) \nabla u)$ to represent the variable diffusion operator described as (1) in polar coordinates.

In this simulation, we want to study the steady equilibrium solutions of GLE (8). In particular, we will focus on seeking the stable solutions with vortices. The vortices are the topological defects which are zeros of the complex scalar field $u$ with nonzero integer winding numbers. Readers who are interested in the theory of Ginzburg-Landau vortices can refer to the book [3].

Throughout this section, we use the backward difference in time to dis-
cretize the Ginzburg-Landau equation (8)
\[
\frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{a(x)} \nabla \cdot (a(x) \nabla u^{n+1}) + \frac{1}{\varepsilon^2} (1 - |u^n|^2) u^{n+1} \text{ in } \Omega, \quad (11)
\]
\[
\frac{\partial u^{n+1}}{\partial r} = 0 \text{ on } \partial \Omega. \quad (12)
\]

Thus, at each time step, a variable diffusion coefficient elliptic equation with Neumann boundary on a disk arises and can be solved by the efficient iterative solver described in the previous section. In the following tests, we choose the initial condition as
\[
u_0(r, \theta) = \tanh \left( \frac{r}{\varepsilon} \right) e^{im\theta}, \quad (13)
\]
which is an approximate vortex solution with winding number \(m\). As mentioned before, we like to investigate the dynamics of this vortex solution and its final equilibrium.

In all runs, we use 64 \times 128 grid points in the radial and azimuthal directions, and the time step \(\Delta t = 1/320\). The parameter \(\varepsilon = 0.1\) and the winding number of initial vortex is \(m = 3\). Figure 1 shows the contour plots of the magnitude \(|u|\) for the constant diffusion case \(a(x) = 1\) at different times. One can observe that the initial vortex with winding number \(m = 3\) at the center splits into three vortices with winding number one and then migrate to the boundary gradually. At later time, those three vortices are completely absorbed by the boundary and the solution becomes a constant state \(|u| = 1\) eventually. This vortex dynamics is not new and has been confirmed, for instance, theoretically [10] and numerically [14]. One should also note that this final equilibrium state is nothing but the global minimizer of the Ginzburg-Landau free energy
\[
E(u) = \int_\Omega \left\{ \frac{1}{2} \nabla u^2 + \frac{1}{4\varepsilon^2} (1 - |u|^2)^2 \right\} a(x) \, dx, \quad (14)
\]
where the term \(|\nabla u|^2\) in polar coordinates has the form
\[
|\nabla u|^2 = \frac{\partial u}{\partial r}^2 + \frac{1}{r^2} \left( \frac{\partial u}{\partial \theta} \right)^2. \quad (15)
\]

Figure 2 shows that the Ginzburg-Landau energy is decreasing in time and becomes zero finally.
Figure 1: The contour plots of $|u|$ at different times for the constant diffusion $a(x) = 1$ case.
Figure 2: The time evolution of Ginzburg-Landau energy for the constant diffusion case.

For the variable diffusion coefficient case, the vortex dynamics and stability are completely different from the constant diffusion case. Figure 3 shows the different time contour plots of the magnitude $|u|$ for the case of variable diffusion $a(r, \theta) = (r^2 \cos \theta \sin \theta + 1) e^r$. The initial condition is still as in (13) with winding number $m = 3$. Unlike the constant diffusion case, the central vortex now splits into five vortices in which one vortex stays at the center and four of them migrate to the boundary. Later, those surrounding four vortices are completely absorbed by the boundary while the vortex at the center remains. Figure 4 shows that the free energy is decreasing in time and becomes a nonzero constant eventually. Therefore, by choosing the variable coefficient appropriately, we are able to stabilize the Ginzburg-Landau vortex which is exactly the same phenomena predicted by the theory [4]. In physics, this is called the pinning effect when a vortex is trapped by some defect of the conductor.

It is very interesting to mention that during the transition the winding number of the central vortex becomes $m = -1$ while the winding number of the surrounding four vortices are all $m = 1$. To see this, we plot the vector fields of real and imaginary parts for $u/|u|$ at $T = 0.5$ in Figure 5-(a). The final plots for the real and imaginary parts of $u/|u|$ near the vortex center (along the circle $r = 5 \Delta r/2$) are shown in Figure 5-(b). The graphs of real
Figure 3: The contour plots of $|u|$ at different times for the variable diffusion $a(r, \theta) = (r^2 \cos \theta \sin \theta + 1) e^r$.

and imaginary parts are exactly the functions $-\cos \theta$ and $\sin \theta$, respectively. Since we have

$$\frac{u}{|u|} = -\cos \theta + i \sin \theta = e^{i[(-1)\theta + \pi]}.$$ (16)

one can immediately concludes that the winding number of the stable vortex is indeed $m = -1$.

4 Conclusions

In this paper, we present a fast iterative method for solving the variable coefficient diffusion equation on a unit disk. The equation is written in polar coordinates and is discretized by the standard centered difference approx-
Figure 4: The time evolution of Ginzburg-Landau energy for the variable diffusion case.

Figure 5: (a) The vector fields of real and imaginary parts of $u/|u|$ at $T = 0.5$ for the variable diffusion case. (b) The graphs of the real and imaginary parts for $u/|u|$ along the circle near the vortex center at $T = 1$. The real part is denoted by the solid line and the imaginary part is denoted by the dash line.
imation under the grid arrangement of shifting half mesh away from the origin so that the coordinate singularity can be easily handled without pole conditions. The resultant matrix is symmetric positive definite so the preconditioned conjugate gradient (PCG) method can be applied. Some different preconditioners have been tested for comparison, in particular, a preconditioner arising from the modified equation has been derived and shown to be the most efficient one. The present elliptic solver has been applied to study the vortex dynamics of the Ginzburg-Landau equation with a variable diffusion coefficient. Meanwhile, the present numerical scheme can be extended straightforwardly to the similar equation in spherical coordinates and three-dimensional problems.

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References


[1]1 \{1\} \{1\} Eq. (1) [2] Eqs. (1) + (2)