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Solving a Cauchy Problem for a 3D Elliptic PDE with Variable Coefficients by a Quasi-Boundary-Value Method*

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Abstract

An ill-posed Cauchy problem for a 3D elliptic PDE with variable coefficients is considered. A well-posed quasi-boundary-value (QBV) problem is given to approximate it. Some stability error estimates are given. For the numerical implementation, a large sparse system is obtained from the discretizing the QBV problem using finite difference method (FDM). A Left-Preconditioner Generalized Minimum Residual (GMRES) method is used to solve the large system effectively. For the preconditioned system, a fast solver using the Fast Fourier Transform (FFT). Numerical results show that the method works well.

Key words. Elliptic equation; Ill-Posed; Cauchy problem; Finite difference method; Quasi-boundary-value method; Left-Preconditioned GMRES; Fast solver; Variable coefficients; Three dimensions; Fast Fourier Transform

1 Introduction

Let $\Omega = \{(y_1, y_2) | 0 < y_1 < 1, 0 < y_2 < 1\}$ and consider the following ill-posed Cauchy problem for an elliptic PDE,

$$(au_x)_x + (bu_{y_1})_{y_1} + (cu_{y_2})_{y_2} = f(x, y_1, y_2), \quad (x, y_1, y_2) \in (0, 1) \times \Omega, \quad (1.1)$$

$$u(x, y_1, y_2) = \phi(x, y_1, y_2), \quad x \in [0, 1], (y_1, y_2) \in \partial\Omega, \quad (1.2)$$

$$u(0, y_1, y_2) = \psi(y_1, y_2), \quad (y_1, y_2) \in \overline{\Omega}, \quad (1.3)$$

$$u_x(0, y_1, y_2) = g(y_1, y_2), \quad (y_1, y_2) \in \overline{\Omega}, \quad (1.4)$$

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where the coefficients are assumed to be piecewise differentiable satisfying

$$\begin{aligned} a(x, y_1, y_2) &\geq a_0 > 0, & b(x, y_1, y_2) &\geq b_0 > 0, & c(x, y_1, y_2) &\geq c_0 > 0, \\ -a_1 &\leq a_x \leq a_2, & -b_1 &\leq b_x, & -c_1 &\leq c_x. \end{aligned} \quad (1.5)$$

The constants a_1 , b_1 , and c_1 are assumed to be non-negative. The problem is to compute $u(x, y_1, y_2)$ numerically for $0 < x \leq 1$.

The Cauchy problem for an elliptic equation is a classical ill-posed problem and occurs in several important applications, such as inverse scattering [17, 37], electrical impedance tomography [10], optical tomography [7], and thermal engineering [23]. The topic is treated in several monographs [16, 36, 37, 41, 42, 45], and in numerous papers, see [1, 3, 6, 8, 9, 18, 24, 25, 34, 47, 48, 51, 57, 61] and the references therein. Even if some of the theoretical investigations are quite general, the numerical procedures proposed are typically for the two dimensional case and often only valid for the problem with constant coefficients. To our knowledge there are no papers in the literature that treat the numerical solution of elliptic Cauchy problems in three dimensions with all three coefficients depending on (x, y_1, y_2) . In this paper, we propose to use a *quasi-boundary-value [QBV] method*¹ [2] to regularize the problem (1.1)-(1.5) as follows:

$$(av_x)_x + (bv_{y_1})_{y_1} + (cv_{y_2})_{y_2} = f^\delta(x, y_1, y_2), \quad (x, y_1, y_2) \in (0, 1) \times \Omega, \quad (1.6)$$

$$v(x, y_1, y_2) = \phi^\delta(x, y_1, y_2), \quad x \in [0, 1], (y_1, y_2) \in \partial\Omega, \quad (1.7)$$

$$v(0, y_1, y_2) = \psi^\delta(y_1, y_2), \quad (y_1, y_2) \in \overline{\Omega}, \quad (1.8)$$

$$v_x(0, y_1, y_2) + \alpha v(1, y_1, y_2) = g^\delta(y_1, y_2), \quad (y_1, y_2) \in \overline{\Omega}, \quad (1.9)$$

where the noisy data satisfy

$$\|f^\delta - f\| + \|\phi^\delta - \phi\| + \|\psi^\delta - \psi\| + \|g^\delta - g\| \leq \delta. \quad (1.10)$$

The notation $\|\cdot\|$ denotes L^2 - norm. For the numerical solution of well-posed problems for general elliptic PDE's in three dimensions usually only iterative methods are effective. For nonselfadjoint problems the Generalized Minimum Residual method (GMRES) [53] is a standard iterative method. However, without a preconditioner the GMRES method converges slowly or even does not work.

Our proposed method is the following. After discretization (1.6)-(1.10) is reduced to a nonsymmetric linear system, with a large and sparse matrix. We solve it using preconditioned GMRES. As preconditioner we use the discretization of a nearby QBV equation where the variable coefficients have been replaced by constants. Such a problem can be solved very efficiently, using Fast Fourier Transform (FFT) techniques. We demonstrate that problems with half a million unknowns can be solved using MATLAB in about 15 iterations and in less than 90 seconds on a standard PC.

¹Also called the modified boundary method, or non-local boundary value problem method.

To motivate our choice of solution procedure we first note that for partial differential equations with variable coefficients one cannot obtain fundamental solutions, and therefore classical regularization methods depending on the reformulation as an integral equation, such as Tikhonov method, cannot be used. Thus it is necessary to keep the equation in PDE form. We then recall that for well-posed PDE's iterative procedures are routinely used. This approach has also been applied to the Cauchy problem, where a certain energy functional is minimized [6]; unfortunately, in each iteration of that procedure four well-posed elliptic equations would have to be solved over the whole three-dimensional domain. Some iterative methods, e.g. based on the alternating procedure of [40], often converge very slowly. Another approach [25] based on the Krylov subspace method for the cylindrical case requires the solution of only one two-dimensional problem at each iteration. However, it can not deal with the problem (1.1)-(1.5) with variable coefficient $a(x, y_1, y_2)$.

QBV-type methods have been used before for ill-posed problems [4, 5, 21, 22, 32–34, 43, 54, 58–60]. In [27], we applied the method to a Cauchy problem for an elliptic equation, and studied its stability. We also made a preliminary numerical implementation for a slightly less general problem than the one in the present paper. Now we further develop the implementation from [27] and demonstrate that it is an efficient algorithm for solving the general problem (1.1)-(1.5) with variable coefficients.

Preconditioned GMRES is widely used not only for well-posed problems, see e.g. [12, 52], but also for ill-posed problems [11, 13–15, 31, 38, 39]. The regularizing properties of preconditioned Krylov methods were investigated in [30]. To the authors' knowledge, preconditioned GMRES applied to an ill-posed problem has mostly been used for the discretization of an integral equation of the first kind, stabilized by Tikhonov regularization. However, in [49, 50] an ill-posed parabolic problem was solved using GMRES with a singular preconditioner, see also [26]. In the present paper, we approximate the ill-posed elliptic PDE by a well-posed QBV problem, and then we use preconditioned GMRES to solve the linear system of equations obtained by discretizing the well-posed problem.

The paper is organized as follows. First, in Section 2, we give an explicit stability result for the Cauchy problem. Then we describe in Section 3 how the QBV problem (1.6)-(1.10) can be discretized and solved iteratively using GMRES. However, as in the well-posed case, a preconditioner is necessary in order for GMRES to be efficient. Our preconditioner is the same QBV method applied to a nearby Cauchy problem with constant coefficients. In Section 3.3, we describe a fast solver for problem (1.6)-(1.10) with the constant coefficients. The problem of choosing the regularization parameter is discussed in Section 4. Finally, in Section 5, we discuss the numerical implementation and give some experiments that demonstrate the efficiency of the proposed method.

2 An Explicit Stability Result

It is well known that the Cauchy problem for an elliptic equation is severely ill-posed. General stability estimates are given in, e.g., [3, 37]; see also [16, 34]. In the case of a rectangular geometry, more concrete results can be found [24]. In the numerical solution of a mathematical problem perturbations due to discretization and round-off in the floating point arithmetic are inevitably introduced. Therefore, it is necessary to have explicit and concrete stability results for the underlying mathematical problem [24]. By explicit we here mean estimates, given under the assumption that certain regularity conditions are satisfied, where the quantities are expressed in terms of the data and coefficients of the problem. Actually, such conditional stability results imply not only the uniqueness of the solutions of the problems but also the convergence rate of the regularized solutions [19].

We here give a stability result of Hölder type for the following special problem, which is inspired by results in [24, 44–46], and which is a slight generalization of that in [24].

$$(au_x)_x + (bu_{y_1})_{y_1} + (cu_{y_2})_{y_2} = 0, \quad (x, y_1, y_2) \in (0, 1) \times \Omega, \quad (2.1)$$

$$u(x, y_1, y_2) = 0, \quad x \in [0, 1], (y_1, y_2) \in \partial\Omega, \quad (2.2)$$

$$u(0, y_1, y_2) = 0, \quad (y_1, y_2) \in \bar{\Omega}, \quad (2.3)$$

$$u_x(0, y_1, y_2) = g(y_1, y_2), \quad (y_1, y_2) \in \bar{\Omega}. \quad (2.4)$$

Before giving the stability result, we present some notations. Define the family of rectangular regions, parameterized by

$$D_\beta = \{(x, y_1, y_2) \mid 0 \leq x \leq \beta, (y_1, y_2) \in \Omega\}, \quad 0 \leq \beta \leq 1. \quad (2.5)$$

Set

$$K_1 = \widetilde{C}_0 + 4\lambda \quad \text{and} \quad K_2 = 2\lambda(2\lambda + \widetilde{C}_0), \quad (2.6)$$

where the constant λ satisfies

$$\lambda \geq \max\left(\frac{a_2}{2a_0}, \frac{a_1}{a_0}\right),$$

and

$$\widetilde{C}_0 = \max\left(\frac{a_1}{a_0}, \frac{b_1}{b_0}, \frac{c_1}{c_0}\right).$$

We introduce also the function

$$\nu(\beta) = \frac{1 - e^{-K_1\beta}}{1 - e^{-K_1}}. \quad (2.7)$$

Theorem 1 Assume that the two functions u_1 and u_2 satisfy problem (2.1)-(2.4) with different data g_i , $i = 1, 2$, and the boundedness assumptions

$$\int_{D_1} a u_i^2 dx dy_1 dy_2 \leq E_2, \quad i = 1, 2,$$

for some constant E_2 . If the data error is bounded

$$\int_0^1 \int_0^1 a(0, y_1, y_2) (g_1(y_1, y_2) - g_2(y_1, y_2))^2 dy_1 dy_2 \leq \tilde{\delta},$$

then, for $0 \leq \beta \leq 1$,

$$\int_{D_\beta} a(u_1 - u_2)^2 dx dy_1 dy_2 \leq 4e^{(-\beta + \nu(\beta))K_2/K_1} E_3^{\nu(\beta)} \tilde{\delta}^{1-\nu(\beta)}, \quad (2.8)$$

where $E_3 = 2(\lambda + (1 + a_1/a_0)/2)E_2 + \tilde{\delta}$.

Proof. A sketch of the proof is given in the appendix. Although the boundary condition is different, there is no essential difference from that in [24].

Remark 1 In fact, the results hold also for a general domain Ω . For the problem nonhomogeneous Dirichlet data, we can also obtain the same result as in Theorem 1. For the Cauchy problem (1.1)-(1.5) with nonhomogeneous Cauchy and boundary data, we can use the linearity of the problem and divide it into an ill-posed problem and a well-posed one to obtain the stability estimate [24]. We can also get the similar result by using the technique of [44]. Unfortunately it is not easy to derive an error estimate for the QBV solution. This will be a topic of our future research.

Remark 2 Note that the stability estimate (2.8), depending explicitly on the coefficients, allows us to draw the conclusion that if a_x is negative then the stability becomes worse than in the case of positive a_x , in the sense that E_3 becomes larger in the first case.

3 Solving the QBV Problem by GMRES

In this section, we will consider the solution of the QBV problem (1.6)-(1.10) with variable coefficients by preconditioned GMRES. First we describe the finite difference discretization of the problem. In our presentation it is essential to use finite differences, since in that case the action of our preconditioner can be implemented very efficiently. However, also a finite element discretization could be used, as long as one can find a good enough preconditioner.

Before using the left-preconditioned GMRES method, a suitable value of the regularization parameter α must be chosen. We discuss this in Section 4.

3.1 Discretization

We here describe the discretization of the problem (1.6)-(1.10) using the finite difference method (FDM) with central differences.

Let the interval $[0, 1]$ in the x direction be divided into N_x segments of length h_x , and, similarly, the intervals in the y_1 and y_2 directions be divided into N_y segments of length h_y . Then the coefficient matrix $\tilde{A}$ has dimension $N_x(N_y - 1)^2 \times N_x(N_y - 1)^2$. In detail, the PDE (1.6) is discretized

$$\begin{aligned}
& a(i - \frac{1}{2}, j, k)v(i - 1, j, k) + rb(i, j - \frac{1}{2}, k)v(i, j - 1, k) \\
& + rc(i, j, k - \frac{1}{2})v(i, j, k - 1) - \left\{ a(i - \frac{1}{2}, j, k) + a(i + \frac{1}{2}, j, k) \right. \\
& + r[b(i, j - \frac{1}{2}, k) + b(i, j + \frac{1}{2}, k)] + r[c(i, j, k - \frac{1}{2}) + c(i, j, k + \frac{1}{2})] \left. \right\} v(i, j, k) \\
& + rb(i, j + \frac{1}{2}, k)v(i, j + 1, k) + rc(i, j, k + \frac{1}{2})v(i, j, k + 1) \\
& + a(i + \frac{1}{2}, j, k)v(i + 1, j, k) = h_x^2 f^\delta(i, j, k),
\end{aligned} \tag{3.1}$$

with $r = h_x^2/h_y^2$. For the quasi-boundary condition (1.9) we get

$$\frac{v(1, j, k) - v(-1, j, k)}{2h_x} + \alpha v(N_x, j, k) = g^\delta(j, k). \tag{3.2}$$

The linear system becomes

$$\tilde{A}V = F, \tag{3.3}$$

where $\tilde{A}$ has the structure

$$\tilde{A} = \begin{pmatrix} (A_0 + A_1)/2 & 0 & \dots & \dots & \alpha h_x A_0 \\ B_1 & A_2 & 0 & & \\ A_2 & B_2 & A_3 & & \\ & \ddots & \ddots & \ddots & \\ 0 & \dots & A_{N_x-1} & B_{N_x-1} & A_{N_x} \end{pmatrix}, \tag{3.4}$$

with block-diagonal matrices A_i ,

$$A_i = \text{diag}(\mathcal{A}_i^1, \mathcal{A}_i^2, \dots, \mathcal{A}_i^{N_y-1}).$$

The diagonal blocks are given by

$$\mathcal{A}_i^j = \text{diag}(a(i - 1/2, j, 1), a(i - 1/2, j, 2), \dots, a(i - 1/2, j, N_y - 1)),$$

while the matrices B_i are block-tridiagonal

$$B_i = \text{tridiag}(\mathcal{B}_i^j, \mathcal{C}_i^j, \mathcal{B}_i^j),$$

with tridiagonal blocks

$$\mathcal{C}_i^j = \text{tridiag}(rc(i, j, k+1/2), d(i, j, k), rc(i, j, k+1/2)), \quad \mathcal{B}_i^j = \text{diag}(rb(i, j+1/2, k)),$$

where

$$d(i, j, k) = - \left\{ a(i - \frac{1}{2}, j, k) + a(i + \frac{1}{2}, j, k) + r[b(i, j - \frac{1}{2}, k) + b(i, j + \frac{1}{2}, k)] \right. \\ \left. + r[c(i, j, k - \frac{1}{2}) + c(i, j, k + \frac{1}{2})] \right\}.$$

The structure of the linear system (3.3) is similar to that of a discretization of a 3D selfadjoint elliptic boundary value problem, with the important exception that here the matrix is nonsymmetric, due to the quasiboundary condition. In general, linear systems arising from 3D problems with variable coefficients can be solved efficiently only using iterative methods, see, [52] for an overview. Since $\tilde{A}$ is non-symmetric, we use the Generalized Minimum Residual Method (GMRES) [53] (described in the following subsection).

However, it turns out that GMRES *without preconditioning* does not converge fast enough.

Example 1 Consider a nonhomogeneous equation in the unit cube with $a(x, y_1, y_2) = x + y_1 + y_2 + 1$, $b(x, y_1, y_2) = xy_1y_2 + 1$, $c(x, y_1, y_2) = x(y_1 + y_2) + 1$, and an exact solution $u(x, y_1, y_2) = \sin(x + y_1 + y_2)$, i.e.,

$$\begin{cases} (au_x)_x + (bu_{y_1})_{y_1} + (cu_{y_2})_{y_2} = f(x, y_1, y_2), & (x, y_1, y_2) \in (0, 1)^3, \\ u(x, 0, y_2) = \sin(x + y_2), & (x, y_2) \in [0, 1]^2, \\ u(x, 1, y_2) = \sin(x + 1 + y_2), & (x, y_2) \in [0, 1]^2, \\ u(x, y_1, 0) = \sin(x + y_1), & (x, y_1) \in [0, 1]^2, \\ u(x, y_1, 1) = \sin(x + y_1 + 1), & (x, y_1) \in [0, 1]^2, \\ u(0, y_1, y_2) = \sin(y_1 + y_2), & (y_1, y_2) \in [0, 1]^2, \\ u_x(0, y_1, y_2) = \cos(y_1 + y_2), & (y_1, y_2) \in [0, 1]^2, \end{cases}$$

The right hand side becomes $f(x, y_1, y_2) = (1 + xy_2 + x) \cos(x + y_1 + y_2) - (x + y_1 + y_2 + xy_1y_2 + x(y_1 + y_2) + 3) \sin(x + y_1 + y_2)$.

For a finite difference discretization with 49 unknowns in each y -direction and 50 steps in x we get a 120050×120050 matrix $\tilde{A}$. We chose the regularization parameter² $\alpha = 0.0003$. The GMRES method applied to the QBV problem did not converge in 3430 iterations. Note that here we used restarted GMRES, with restart after every 30 iterations (for restarted GMRES, see the next subsection).

Apparently, the reason for the slow convergence is that even if the ill-posed problem is regularized, it is still quite ill-conditioned. In [27] the GMRES method

²Here the regularization parameter was chosen by the *a-priori* rule in [27].

did not work even for the two dimensional problem with constant coefficients, and we therefore asked whether *it is possible to solve the linear equations obtained in the QBV method using preconditioned GMRES*. We there successfully constructed a preconditioner for the 2D problem based on approximation by a circulant matrix. In the following subsection we first give a quick introduction to preconditioned GMRES, and then show how to construct a preconditioner for the variable coefficient case that leads to fast convergence also in the 3D case.

3.2 GMRES with Preconditioning

Preconditioning is a key ingredient for the success of Krylov subspace methods for linear systems [52, Chapter 9]. The main purpose of using a preconditioner in the iterative solution of a linear system of equations is to reduce the number of iterations and, at the same time, the computing time. In general, the efficiency of iterative techniques depends on the quality of the preconditioner much more than the particular Krylov subspace method used. In the case of the GMRES, or other nonsymmetric iterative solvers, three options for applying the preconditioning operation (i.e., left, split and right preconditioning) are available. The left-preconditioned GMRES algorithm is stated in Figure 1³. In statements 4-7

Figure 1: ALGORITHM: GMRES with Left Preconditioning

-
1. Compute $r_0 = M^{-1}(b - Ax_0)$, $\gamma = \|r_0\|_2$, and $v_1 = r_0/\gamma$
 2. For $j = 1, \dots, m$, Do
 3. Compute $w := M^{-1}Av_j$
 4. For $i = 1, \dots, j$, Do
 5. $h_{i,j} := (w, v_i)$
 6. $w := w - h_{i,j}v_i$
 7. EndDo
 8. Compute $h_{j+1,j} = \|w\|_2$ and $v_{j+1} = w/h_{j+1,j}$
 9. EndDo
 10. Define $V_m := [v_1, \dots, v_m]$, $\bar{H}_m = \{h_{i,j}\}_{1 \leq i \leq j+1, 1 \leq j \leq m}$
 11. Compute $y_m = \operatorname{argmin}_y \|\gamma e_1 - \bar{H}_m y\|_2$ and $x_m = x_0 + V_m y_m$
 12. If satisfied Stop, else set $x_0 := x_m$ and go to 1
-

the newly computed Krylov basis vector w is orthogonalized against $v_1, \dots, v_j$. In cases when the algorithm does not converge very quickly, the storage of the v_j vectors can become prohibitive, due to memory restrictions and the work for orthogonalization. In that case, one often uses *restarted* GMRES: after a predefined number of steps, all basis vectors are discarded except the most recently computed one, and the procedure is restarted. In our context restarted GMRES was only

³Of course, unpreconditioned GMRES corresponds to putting M equal to the identity.

used in Example 1.

As preconditioner we use the matrix for the QBV method given by the problem with the constant coefficients, chosen as the mean values of the respective variable coefficients. It turns out that the linear system with this matrix can be solved very efficiently using a direct solver.

3.3 Fast Solver for the Constant Coefficient Case

The QBV problem for the constant coefficient case is

$$av_{xx} + bv_{y_1y_1} + cv_{y_2y_2} = f^\delta(x, y_1, y_2), \quad (x, y_1, y_2) \in (0, 1) \times \Omega, \quad (3.5)$$

$$v(x, y_1, y_2) = \phi^\delta(x, y_1, y_2), \quad x \in [0, 1], (y_1, y_2) \in \partial\Omega, \quad (3.6)$$

$$v(0, y_1, y_2) = \psi^\delta(y_1, y_2), \quad (y_1, y_2) \in \overline{\Omega}, \quad (3.7)$$

$$v_x(0, y_1, y_2) + \alpha v(1, y_1, y_2) = g^\delta(y_1, y_2), \quad (y_1, y_2) \in \overline{\Omega}, \quad (3.8)$$

where the regularization parameter α is chosen the same as for non-constant coefficients. We will now briefly describe a fast solver for the discretization of this PDE problem, based on the FFT, in a manner analogous to that when solving well-posed problems for Poisson's equation [35, 56].

If we discretize (3.5)-(3.8) in exactly the same way as in Section 3.1, we obtain a linear system $AU = F$ of the same dimension as $\tilde{A}$ in (3.3), with

$$A = \begin{pmatrix} aI & 0 & \dots & \dots & -\alpha h_x aI \\ T & aI & 0 & & \\ aI & T & aI & & \\ & \ddots & \ddots & \ddots & \\ 0 & \dots & aI & T & aI \end{pmatrix}, \quad (3.9)$$

where the block T has the structure

$$T = T_2 \otimes I + I \otimes T_1, \quad (3.10)$$

with tridiagonal matrices T_1, T_2 ($\otimes$ denotes the Kronecker product).

We can block-diagonalize the system $AU = F$ by discrete trigonometric transforms. Let S be the $(N_y - 1) \times (N_y - 1)$ discrete sine transform matrix (DST) $S_{ij} = \sin(\pi ij/N_y)$. Then T can be diagonalized by the following transformation (which is equivalent to a 2D DST [20]),

$$(S^* \otimes S^*)T(S \otimes S) = (S^*T_2S) \otimes I + I \otimes (S^*T_1S) = \Lambda_2 \otimes I + I \otimes \Lambda_1 := \Lambda; \quad (3.11)$$

(here S^* is the conjugate transpose of S). The matrices Λ_1 and Λ_2 are diagonal with explicit expressions for the elements [55, p. 113]. After this transformation

the matrix A is replaced by

$$\begin{pmatrix} aI & 0 & \dots & \dots & -\alpha h_x aI \\ \Lambda & aI & 0 & & \\ aI & \Lambda & aI & & \\ & \ddots & \ddots & \ddots & \\ 0 & \dots & aI & \Lambda & aI \end{pmatrix}. \quad (3.12)$$

Since the linear system with the matrix (3.12) is block-diagonal, one can reorder it into $(N_y - 1)^2$ decoupled systems of dimension N_x . Each such system has a lower tridiagonal matrix with a non-zero upper right corner element, and it can be solved in $O(N_x)$ operations.

The fast solver is summarized below. For readability we omit some details mainly associated with reorderings.

1. Divide the data vector F into N_x blocks F_m of length $(N_y - 1)^2$, and multiply each block by the matrix $S^* \otimes S^*$.
2. Reorder the elements of the transformed vector and solve $(N_y - 1)^2$ systems, each of dimension N_x , with the matrices

$$\begin{pmatrix} a & 0 & \dots & \dots & -\alpha h_x a \\ \Lambda(i, i) & a & 0 & & \\ a & \Lambda(i, i) & a & & \\ & \ddots & \ddots & \ddots & \\ 0 & \dots & a & \Lambda(i, i) & a \end{pmatrix}, \quad (3.13)$$

where $\Lambda(i, i)$ denotes a diagonal element of Λ , see (3.11).

3. Reverse the reordering, and multiply each block of length $(N_y - 1)^2$ by the matrix $S \otimes S$.

It is well known that the 1D DST of a vector of length N_y can be computed in $O(\log(N_y))$ operations using the FFT. Note that in the implementation of the algorithm the matrix $S^* \otimes S^*$ in step 1 is never formed; instead the vector F_m is reorganized as a square matrix and a 2D DST is computed (similarly in step 3). Therefore, one can see that this algorithm requires $O(N_x N_y^2 \log(N_y))$ operations for solving the linear system $AU = F$.

4 Regularization Parameter Choice

No matter which regularization method is used for an ill-posed problem, one core problem is how to choose the regularization parameter. The same is the case for the QBV method.

Using the linearity of the problem (1.1)-(1.4), one can subdivide into one well-posed problem and another ill-posed problem only with the nonhomogeneous Neumann data case. This trick has been widely used to deal with the nonhomogeneous ill-posed problems, see, e.g., the appendix in [25].

For the ill-posed problem (1.1)-(1.4) with all data equal to zero except the nonhomogeneous Neumann Cauchy data, *a-priori* and *a-posteriori* parameter choice rules have been given in the [27]⁴. Thus, the regularization parameter can be chosen *a-posteriori* according to the following theorem.

Theorem 2 [27] *Let the problem (1.1)-(1.4) be given with $\phi = 0$, $\psi = 0$, and $f = 0$, and with the nonhomogeneous Neumann data only. Suppose there exists the a-priori bound*

$$\|u(1, \cdot, \cdot)\| \leq E_1, \quad (4.1)$$

and that the condition (1.10) holds. Choose $\tau > 1$ such that $0 < \tau\delta < \|g^\delta\|$ and the regularization parameter $\alpha = \alpha(\delta) > 0$ such that

$$\|v_x^{\alpha, \delta}(0, \cdot, \cdot) - g^\delta(\cdot, \cdot)\| = \tau\delta. \quad (4.2)$$

Then, for $0 < x < 1$, we have the following estimate

$$\|u(x, \cdot, \cdot) - v^{\alpha, \delta}(x, \cdot, \cdot)\| \leq CE_1^x \delta^{1-x}, \quad (4.3)$$

where $C = \left(1 + \sqrt{2 \frac{1+(\tau-1)^2}{(\tau-1)^2}}\right)^x (1 + \tau)^{1-x}$.

For the convenience of the numerical application, we here do not consider the *a-priori* choice rule but use the same Morozov's discrepancy principle (4.2) of the *a-posteriori* parameter choice directly without decomposing the original problem. Some numerical results given later will show that this choice rule is rational and works efficiently.

5 Numerical implementation and experiments

In this section, we illustrate the method by solving 2D and 3D problems with variable coefficients. To obtain the regularization parameter α , we choose $\tau = 1.1$ in (4.2), as suggested by Hanke and Hansen [28, 29].

⁴In [27], the equation has the coefficient $a = 1$, which is not essentially different, since we can divide the coefficients a, b, c by a .

All our computations were performed using MATLAB 7.9 on a PC (Intel Core i5 with clock frequency 2GHz).

As is customary in the numerical solution of ill-posed test problems, we add normally distributed random perturbations to the data. Thus the perturbed right hand side is computed in MATLAB as $F_{\text{pert}} = F + \epsilon * \text{randn}(\text{size}(F))$, where the parameter ϵ determines the magnitude of the perturbation.

In order to compare our preconditioner with the one in [27], we start with the 2D case, and then consider 3D problems.

5.1 Two dimensional case

Naturally discretization of a 2D problem is less complicated than that in Section 3.1. Consider

$$(au_x)_x + (bu_y)_y = f(x, y), \quad (x, y) \in (0, 1) \times (0, 1), \quad (5.1)$$

$$u(x, 0) = \phi_1(x), \quad x \in [0, 1], \quad (5.2)$$

$$u(x, 1) = \phi_2(x), \quad x \in [0, 1], \quad (5.3)$$

$$u(0, y) = \psi(y), \quad y \in [0, 1], \quad (5.4)$$

$$u_x(0, y) = g(y), \quad y \in [0, 1]. \quad (5.5)$$

For this problem, the finite difference discretization of the QBV problems gives a linear system that we denote $\hat{A}U = F$. To construct the preconditioner M_1 we replace the variable coefficients $a(x, y), b(x, y)$ by the constants a, b obtained by computing the average over the unit square,

$$a := \int_0^1 \int_0^1 a(x, y) dx dy, \quad (5.6)$$

$$b := \int_0^1 \int_0^1 b(x, y) dx dy, \quad (5.7)$$

The preconditioner becomes

$$M_1 = \begin{pmatrix} aI & 0 & \dots & \dots & \alpha h_x aI \\ T_1 & aI & 0 & & \\ aI & T_1 & aI & & \\ & \ddots & \ddots & \ddots & \\ 0 & \dots & aI & T_1 & aI \end{pmatrix}, \quad (5.8)$$

where T_1 is tridiagonal,

$$T_1 = \begin{pmatrix} -2(a+br) & br & 0 & \cdots & 0 \\ br & -2(a+br) & br & \cdots & 0 \\ & & \ddots & & \\ & & & \ddots & \\ 0 & 0 & \cdots & br & -2(a+br) \end{pmatrix}.$$

Based on the discussion in Section 3.3, we see that the linear system $M_1 z = y$ can be solved in $N_x N_y \log(N_y)$ operations using the DST.

In fact, we can also divide the problem into a well-posed problem

$$\begin{aligned} (au^{(1)}_x)_x + (bu^{(1)}_y)_y &= f(x, y), & (x, y) &\in (0, 1) \times (0, 1), \\ u^{(1)}(x, 0) &= \phi_1(x), & x &\in [0, 1], \\ u^{(1)}(x, 1) &= \phi_2(x), & x &\in [0, 1], \\ u^{(1)}(0, y) &= \psi(y), & y &\in [0, 1], \\ u^{(1)}(1, y) &= (1-y)\phi_1(1) + y\phi_2(1), & y &\in [0, 1], \end{aligned}$$

and an ill-posed problem

$$\begin{aligned} (au^{(2)}_x)_x + (bu^{(2)}_y)_y &= 0, & (x, y) &\in (0, 1) \times (0, 1), \\ u^{(2)}(x, 0) &= 0, & x &\in [0, 1], \\ u^{(2)}(x, 1) &= 0, & x &\in [0, 1], \\ u^{(2)}(0, y) &= 0, & y &\in [0, 1], \\ u^{(2)}_x(0, y) &= g(y) - u^{(1)}_x(0, y), & y &\in [0, 1]. \end{aligned}$$

Then $u(x, y) = u^{(1)}(x, y) + u^{(2)}(x, y)$ is the solution of the original problem. For the derivative approximation of the same accuracy $O(h_x^2)$ as the general discretization, we give a three-point approximation for u_x as $u_x(0, y) = (3u(0, y) - 4u(h_x, y) + u(2h_x, y))/(-2h_x)$. Since it needs to compute two problems, the time takes almost twice.

Example 2 Consider an example with the exact solution $u(x, y) = \sin(0.4x + y)$, which satisfies

$$\begin{cases} ((0.4x + y + 1)/0.16u_x)_x + ((0.4xy + 1)u_y)_y = f(x, y), & (x, y) \in (0, 1) \times (0, 1), \\ u(x, 0) = \sin(0.4x), & x \in [0, 1], \\ u(x, 1) = \sin(0.4x + 1), & x \in [0, 1], \\ u(0, y) = \sin(y), & y \in [0, 1], \\ u_x(0, y) = 0.4 \cos(y), & y \in [0, 1], \end{cases}$$

Figure 2: Example 2: Numerical solution computed by left-preconditioned GMRES at $x = 0.6$. The regularization parameter was chosen equal to $\alpha = 0.01$ (left), and $\alpha = 0.001$ (right).

with $f(x, y) = (1 + 0.4x) \cos(0.4x + y) - (0.4x + y + 0.4xy + 2) \sin(0.4x + y)$.

Discretizing with $N_x = 100$ and $N_y = 250$, the QBV matrix $\hat{A}$ has dimension 24900×24900 . We solved the linear system $\hat{A}U = F_{\text{pert}}$ with $\epsilon = 10^{-3}$, using GMRES with the left-preconditioner (5.8). GMRES, with residual tolerance 10^{-6} converged in 12 iterations and 10.9 seconds. To study the sensitivity to the regularization parameter α , we chose several values and compared the solutions. The results for two representative values are illustrated in Figure 2.

In [27] we solved a 2D problem with constant coefficients, using left-preconditioned GMRES, where the preconditioner was a circulant matrix. There we performed 30 iterations, restarted, and then performed another 25 iterations before the procedure converged. The same convergence criterion was used.

From the results illustrated in Figure 2, we see that the solution is not very sensitive to the choice of regularization parameter α .

5.2 Three dimensional case

Now let us use the same idea for a 3D problem to see if our method works.

To see if the QBV method works well for the case of constant coefficients, we use MATLAB 7.9 to do some tests in this subsection. We divide the interval of x into $N_x = 50$ segments and the interval of y_1 and y_2 directions both into $N_y = 100$ segments. The coefficient matrix A in (3.9) is a large sparse matrix having the size 490050×490050 . In (3.10), $T_1 = \text{tridiag}(r * c, -2 * (a + r * b + r * c), r * c)$ and $T_2 = \text{tridiag}(r * b, 0, r * b)$, where $r = (h_x/h_y)^2$.

Example 3 We consider a homogeneous case with an exact solution $u(x, y_1, y_2) = \sinh(2\sqrt{2}\pi x) \sin(2\pi y_1) \sin(2\pi y_2)$, i.e.,

$$\begin{cases} u_{xx} + u_{y_1 y_1} + u_{y_2 y_2} = 0, & (x, y_1, y_2) \in (0, 1)^3, \\ u(x, 0, y_2) = 0, & (x, y_2) \in [0, 1]^2, \\ u(x, 1, y_2) = 0, & (x, y_2) \in [0, 1]^2, \\ u(x, y_1, 0) = 0, & (x, y_1) \in [0, 1]^2, \\ u(x, y_1, 1) = 0, & (x, y_1) \in [0, 1]^2, \\ u(0, y_1, y_2) = 0, & (y_1, y_2) \in [0, 1]^2, \\ u_x(0, y_1, y_2) = 2\sqrt{2}\pi \sin(2\pi y_1) \sin(2\pi y_2), & (y_1, y_2) \in [0, 1]^2. \end{cases}$$

Example 4 We consider a nonhomogeneous case with an exact solution $u(x, y_1, y_2) = \exp(x + y_1 + y_2)$, i.e.,

$$\begin{cases} u_{xx} + u_{y_1 y_1} + u_{y_2 y_2} = 3 \exp(x + y_1 + y_2), & (x, y_1, y_2) \in (0, 1)^3, \\ u(x, 0, y_2) = \exp(x + y_2), & (x, y_2) \in [0, 1]^2, \\ u(x, 1, y_2) = \exp(x + 1 + y_2), & (x, y_2) \in [0, 1]^2, \\ u(x, y_1, 0) = \exp(x + y_1), & (x, y_1) \in [0, 1]^2, \\ u(x, y_1, 1) = \exp(x + y_1 + 1), & (x, y_1) \in [0, 1]^2, \\ u(0, y_1, y_2) = \exp(y_1 + y_2), & (y_1, y_2) \in [0, 1]^2, \\ u_x(0, y_1, y_2) = \exp(y_1 + y_2), & (y_1, y_2) \in [0, 1]^2. \end{cases}$$

Figure 3 shows the results of Example 3 for $x_0 = 0.5$ with $\epsilon = 10^{-3}$.⁵ Figure 3(a) is the exact solution and Figure 3(b) is the approximation whose regularization parameter $\alpha = 4.68753 \times 10^{-7}$ chosen by Morozov's discrepancy principle (4.2). Figure 4 illustrates the solutions of Example 4 for $x_0 = 0.4$ with $\epsilon = 10^{-2}$. Figure 4(a) is the exact solution and Figure 4(b) is the approximated solution with $\alpha = 3 \times 10^{-5}$. From the tests, it is seen that our method works efficiently.

On the basis of the above fast solver for constant coefficient case, in the following, we will consider the variable coefficient case. Similar as the preconditioner $\widetilde{M}_1$, we construct a preconditioner $\widetilde{M}_2$ for 3D as following

$$\widetilde{M}_2 = \begin{pmatrix} \widetilde{a}I & 0 & \dots & \dots & \alpha h_x \widetilde{a}I \\ \widetilde{T}_2 & \widetilde{a}I & 0 & & \\ \widetilde{a}I & \widetilde{T}_2 & \widetilde{a}I & & \\ & \ddots & \ddots & \ddots & \\ 0 & \dots & \widetilde{a}I & \widetilde{T}_2 & \widetilde{a}I \end{pmatrix},$$

⁵For a vector v , we construct the corresponding noisy data by adding a distributed perturbation to the data v , i.e., $v^\delta = v + \epsilon \text{ randn}(\text{size}(v))$.

Figure 3: Example 3 at $x_0 = 0.5$: (a) Exact solution; (b) The error between the exact solution and approximation with $\epsilon = 10^{-3}$ and $\alpha = 4.68753 \times 10^{-7}$.

Figure 4: Example 4 at $x_0 = 0.4$: (a) Exact solution; (b) The error between the exact solution and approximation with $\epsilon = 10^{-2}$ and $\alpha = 3 \times 10^{-5}$.

where the block

$$\tilde{T}_2 = \tilde{T}_2^2 \otimes I + I \otimes \tilde{T}_2^1 \quad (5.9)$$

and $\tilde{T}_2^1 = \text{tridiag}(r\tilde{c}, -2(\tilde{a} + r\tilde{b} + r\tilde{c}), r\tilde{c})$, $\tilde{T}_2^2 = \text{tridiag}(r\tilde{b}, 0, r\tilde{b})$ with

$$\begin{aligned} \tilde{a} &:= \int_0^1 \int_0^1 \int_0^1 a(x, y_1, y_2) dx dy_1 dy_2, \\ \tilde{b} &:= \int_0^1 \int_0^1 \int_0^1 b(x, y_1, y_2) dx dy_1 dy_2, \\ \tilde{c} &:= \int_0^1 \int_0^1 \int_0^1 c(x, y_1, y_2) dx dy_1 dy_2. \end{aligned}$$

We also give two examples (Example 1 and Example 5) to verify our method.

For both examples, we have a finite difference grid of dimension $50 \times 100 \times 100$, i.e., the matrix $\tilde{A}$ in (3.3) has dimension 490050×490050 . Using the Left-Preconditioned GMRES method with the preconditioner $\tilde{M}_2$, solving the 3D Examples 1 and 5 only needs 15 and 13 iteration steps. The total time spent in the function GMRES for Examples 1 and 5 is 86 and 69 seconds, respectively. This means we can solve the 3D problems within reasonable time. The results given in Figures 5 and 6 show that our method works efficiently and the preconditioner $\tilde{M}_2$ is good.

Example 5 *We consider a case with $a(x, y_1, y_2) = xy_1y_2 + 1$, $b(x, y_1, y_2) = x(y_1 + y_2) + 1$, $c(x, y_1, y_2) = x + y_1 + y_2 + 1$, and an exact solution $u(x, y_1, y_2) = \exp(x + y_1 + y_2)$, i.e.,*

$$\left\{ \begin{array}{ll} (au_x)_x + (bu_{y_1})_{y_1} + (cu_{y_2})_{y_2} = f(x, y_1, y_2), & (x, y_1, y_2) \in (0, 1)^3, \\ u(x, 0, y_2) = \exp(x + y_2), & (x, y_2) \in [0, 1]^2, \\ u(x, 1, y_2) = \exp(x + 1 + y_2), & (x, y_2) \in [0, 1]^2, \\ u(x, y_1, 0) = \exp(x + y_1), & (x, y_1) \in [0, 1]^2, \\ u(x, y_1, 1) = \exp(x + y_1 + 1), & (x, y_1) \in [0, 1]^2, \\ u(0, y_1, y_2) = \exp(y_1 + y_2), & (y_1, y_2) \in [0, 1]^2, \\ u_x(0, y_1, y_2) = \exp(y_1 + y_2), & (y_1, y_2) \in [0, 1]^2, \end{array} \right.$$

with $f(x, y_1, y_2) = xy_1y_2 + xy_1 + xy_2 + y_1y_2 + 2x + y_1 + y_2 + 4$.

6 Conclusion

We have proposed a QBV method for solving a Cauchy problem for a 3D elliptic PDE with variable coefficients. Some stability error estimates are given. A large sparse linear system obtained from the QBV problem has been dealt with by a Left-Preconditioned GMRES method. A good preconditioner is constructed and

Figure 5: Example 1: The results solved by the Left-Preconditioned GMRES method at $x_0 = 0.3$ with $\epsilon = 10^{-3}$ and $\alpha = 0.001$. (a). The exact solution (b). The error between the exact solution and approximation

Figure 6: Example 5: The results solved by the Left-Preconditioned GMRES method at $x_0 = 0.2$ with $\epsilon = 10^{-3}$ and $\alpha = 0.001$. (a). The exact solution (b). The error between the exact solution and approximation

a fast solver using the FFT is given to solve the preconditioned system. When using the fast solver, time and memory are also saved. Numerical results show that the method works effectively. The proposed method is effective for the rectangular parallelepiped using FDM. It should be more interesting to construct a good preconditioner for the general domain using finite element method, which is our future work.

Appendix: Proof of Theorem 1

Here we just outline the framework. One can refer to paper [24] for more detail.

We use the logarithmic convexity method to obtain the stability result Theorem 1. Therefore, we want to get an energy functional. After some complicated computation, one can use the similar technique given in [24] to get the following energy functional as

$$F(\beta) = \int_{D_\beta} (\beta - x)aw(\beta w + w_x)dxdy_1dy_2, \quad (6.1)$$

where the domain D_β is defined by (2.5), and w satisfies the following problem

$$\begin{aligned} \lambda a(\lambda w + w_x) + (a(\lambda w + w_x))_x + (bw_{y_1})_{y_1} + (cw_{y_2})_{y_2} &= 0, & (x, y_1, y_2) \in (0, \beta) \times \Omega, \\ w(x, 0, y_2) = w(x, 1, y_2) = w(x, y_1, 0) = w(x, y_1, 1) &= 0, & x \in [0, \beta], (y_1, y_2) \in \partial\Omega, \\ w(0, y_1, y_2) &= 0, & (y_1, y_2) \in \overline{\Omega}, \\ \lambda w(0, y_1, y_2) + w_x(0, y_1, y_2) &= g(y_1, y_2), & (y_1, y_2) \in \overline{\Omega}. \end{aligned}$$

Here $\lambda \geq 0$ is to be chosen later.

From some derivation, one can get the following three Lemmas:

Lemma 1 *Assume that w satisfies the above problem, and that for all $(x, y_1, y_2) \in D_1$, a_x satisfies (1.5). Then, if λ is chosen such that $\lambda \geq a_2/(2a_0)$, the following estimates hold:*

$$\frac{1}{2} \int_{D_\beta} aw^2dxdy_1dy_2 \leq F(\beta) \leq \tilde{c} \int_{D_\beta} aw^2dxdy_1dy_2, \quad \tilde{c} = \frac{1}{2} + \lambda + \frac{a_1}{2a_0},$$

and

$$FF'' - (F')^2 \geq F\left[\int_{D_\beta} (bw_{y_1}^2 + cw_{y_2}^2 - a(\lambda w + w_x)^2)dxdy_1dy_2 - 2\lambda F'\right].$$

Lemma 2 *The following identity holds:*

$$\int_{D_\beta} (bw_{y_1}^2 + cw_{y_2}^2 - a(\lambda w + w_x)^2)dxdy_1dy_2$$

$$\begin{aligned}
&= -2\lambda \int_{D_\beta} (\beta - x)(bw_{y_1}^2 + cw_{y_2}^2 - a(\lambda w + w_x)^2) dx dy_1 dy_2 \\
&\quad + \int_{D_\beta} (\beta - x)(b_x w_{y_1}^2 + c_x w_{y_2}^2 + a_x(\lambda w + w_x)^2) dx dy_1 dy_2 \\
&\quad - \beta \int_0^1 \int_0^1 (a(\lambda w + w_x)^2)(0, y_1, y_2) y_1 dy_2.
\end{aligned}$$

Lemma 3 Assume that for all $(x, y_1, y_2) \in D_1$, a_x, b_x and c_x satisfy (1.5). Let

$$\tilde{c}_0 = \max\left(\frac{a_1}{a_0}, \frac{b_1}{b_0}, \frac{c_1}{c_0}\right).$$

Then

$$\int_{D_\beta} (\beta - x)(b_x w_{y_1}^2 + c_x w_{y_2}^2 + a_x(\lambda w + w_x)^2) dx dy_1 dy_2 \geq -\tilde{c}_0(F' + 2\lambda F),$$

and

$$-\int_{D_\beta} (\beta - x)(bw_{y_1}^2 + cw_{y_2}^2 - a(\lambda w + w_x)^2) dx dy_1 dy_2 \geq -(F' + 2\lambda F).$$

According to the above lemmas, we can get the following important result:

Theorem 3 Assume that

$$\lambda \geq \max\left(\frac{a_2}{2a_0}, \frac{a_1}{a_0}\right),$$

and that the coefficients satisfy (1.5). Then the stability functional satisfies the inequality

$$FF'' - (F')^2 \geq -K_1 FF' - K_2 F^2,$$

where K_1 and K_2 satisfy (2.6).

Now we define

$$\sigma = e^{-K_1 \beta},$$

and regard F as a function of σ . We introduce the auxiliary function

$$G(\sigma) = \log[F(\beta(\sigma))\sigma^{-K_2/K_1^2}].$$

Thus Theorem 3 shows that $G(\sigma)$ is convex on the interval $\sigma_1 \leq \sigma \leq 1$, with $\sigma_1 = e^{-K_1}$. Therefore,

$$G(\sigma) \leq \frac{\sigma - \sigma_1}{1 - \sigma_1} G(1) + \frac{1 - \sigma}{1 - \sigma_1} G(\sigma_1),$$

which is equivalent to

$$F(\beta) \leq e^{(-\beta + \nu(\beta)K_2/K_1)} [F(0)]^{1-\nu(\beta)} [F(1)]^{\nu(\beta)},$$

where $\nu(\beta)$ is defined by (2.7).

Now it is easy to prove Theorem 1.

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