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Numerical Solution of a Cauchy Problem for an Elliptic Equation by Krylov Subspaces

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Abstract.

We study the numerical solution of a Cauchy problem for a self-adjoint elliptic partial differential equation $u_{zz} - Lu = 0$ in three space dimensions (x, y, z) , where the domain is cylindrical in z . Cauchy data are given on the lower boundary and the boundary values on the upper boundary are sought. The problem is severely ill-posed. The formal solution is written as a hyperbolic cosine function in terms of the two-dimensional elliptic operator L (via its eigenfunction expansion), and it is shown that the solution is stabilized (regularized) if the large eigenvalues are cut off. We suggest a numerical procedure based on the rational Krylov method, where the solution is projected onto a subspace generated using the operator L^{-1} . This means that in each Krylov step a well-posed two-dimensional elliptic problem involving L is solved. Furthermore, the hyperbolic cosine is evaluated explicitly only for a small symmetric matrix. A stopping criterion for the Krylov recursion is suggested based on the relative change of an approximate residual, which can be computed very cheaply. Two numerical examples are given that demonstrate the accuracy of the method and the efficiency of the stopping criterion.

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1. Introduction: A Cauchy Problem on a Cylindrical Domain

Let Ω be a connected domain in $\mathbb{R}^2$ with smooth boundary $\partial\Omega$, and assume that L is a linear, self-adjoint, and positive definite elliptic operator defined in Ω . We consider the ill-posed Cauchy problem,

$$\begin{aligned} u_{zz} - Lu &= 0, & (x, y, z) &\in \Omega \times [0, z_1], \\ u(x, y, z) &= 0, & (x, y, z) &\in \partial\Omega \times [0, z_1], \\ u(x, y, 0) &= g(x, y), & (x, y) &\in \Omega, \\ u_z(x, y, 0) &= 0, & (x, y) &\in \Omega. \end{aligned} \tag{1}$$

The problem is to determine the values of u on the upper boundary, $f(x, y) = u(x, y, z_1)$, $(x, y) \in \Omega$.

This is an ill-posed problem in the sense that the solution (if it exists), does not depend continuously on the data. It is a variant of a classical problem considered originally by Hadamard, see e. g. [23], and it is straightforward to analyze it using an eigenfunction expansion. In Appendix B we discuss the ill-posedness of the problem and derive a stability result.

Since the domain is cylindrical with respect to z , we can use a separation of variables approach, and write the solution of (1) formally as

$$u(x, y, z) = \cosh(z\sqrt{L})g. \tag{2}$$

The operator $\cosh(z\sqrt{L})$ can be expressed in terms of the eigenvalue expansion of L , cf. Appendix B. Due to the fact that L is unbounded, the computation of $\cosh(z\sqrt{L})$ is unstable and any data errors or rounding errors would be blown up, leading to a meaningless approximation of the solution.

The problem can be stabilized (regularized) if the operator L is replaced by a bounded approximation. In a series of papers [11, 12, 13, 31, 32, 33] this approach has been used for another ill-posed Cauchy problem, the sideways heat equation, where wavelet and spectral methods were used for approximating the unbounded operator (in that case the time derivative). A similar procedure for a Cauchy problem for the Laplace equation was studied in [5]. However, for such an approach to be applicable, it is required that the domain is rectangular or can be mapped conformally to a rectangular region. It is not clear to us how a spectral or wavelet approximation of derivatives can be used in cases when the domain is complicated so that, e.g., a finite element procedure is used for the numerical approximation of the 2-D operator L .

Naturally, since it is the large eigenvalues of L (those that tend to infinity) that are associated with the ill-posedness, it would be natural to devise the following regularization method:

- Compute approximations of the smallest eigenvalues of L and the corresponding eigenfunctions, and discard the components of the solution (2) that correspond to large eigenvalues.

It is straightforward to prove that such a method is a regularization method in the sense that the solution depends continuously on the data (Theorem 3). However, in

the direct implementation of such a method one would use unnecessarily much work to compute eigenvalue-eigenfunction approximations that are not needed for the particular data function g . Thus the main contribution of this paper is a numerical method for approximating the regularized solution that has the following characteristics:

- The solution (2) is approximated by a projection onto a subspace computed by means of a Krylov sequence generated using the operator L^{-1} . The hyperbolic cosine of the restriction of the operator L^{-1} to that subspace is computed.
- At each step of the Krylov recursion, dealing with L^{-1} corresponds to solving a well-posed two-dimensional elliptic problem involving L . Any standard (black box) elliptic solver, derived from the discretization of L , can be used.
- The method takes advantage of the fact that the regularized solution operator is applied to the particular data function g_m .

We will demonstrate that the proposed method requires considerably fewer solutions of two-dimensional elliptic problems, than the approach based on the eigenvalue expansion.

A recent survey of the literature on the Cauchy problem for the Laplace equation is given in [2], see also [4]. There are many engineering applications of ill-posed Cauchy problems, see [25, 26, 36] and the references therein. A standard approach for solving Cauchy problems of this type is to apply an iterative procedure, where a certain energy functional is minimized; a recent example is given in [1]. Very general (non-cylindrical) problems can be handled, but if the procedure from [1] were to be applied to our problem, then at each iteration four well-posed elliptic equations would have to be solved over the whole three-dimensional domain. In contrast, our approach for the cylindrical case requires the solution of only *one two-dimensional* problem at each iteration[‡].

We are not aware of any papers in the literature that treat the numerical solution of elliptic Cauchy problems in three dimensions. Those in the reference list of [2] all discuss less general problems.

Krylov methods with explicit regularization have been used before for ill-posed problems. For instance, [6, 27] describe *regularized* Lanczos (Golub-Kahan style) bidiagonalization procedures for the solution of integral equations of the first kind. Our approach is different in that it uses a Krylov method for approximating the regularized solution operator.

We conclude by noticing that the procedure described in this paper can be generalized in a straightforward way to problems in more than three space dimensions.

The paper is organized as follows. In Section 2 we give a brief review of the ill-posedness and stabilization of the problem. More details of this are given in Appendix B. The Krylov method is described in Section 3, and the stopping criterion and implementation details are discussed Sections 4 and 5. In Section 6 we describe a

[‡] In one of our examples the two-dimensional problem had 8065 degrees of freedom and the three-dimensional one had 250015.

couple of numerical experiments. In Appendix A we show that the assumption that the Cauchy data are $u_z(x, y, 0) = 0$ is no restriction: the general case can be transformed to this special case by solving a 3-D well-posed problem.

Throughout we will use an $L_2(\Omega)$ setting with inner product and norm,

$$\langle f, g \rangle = \int_{\Omega} f(x, y)g(x, y)dxdy, \quad \|f\| = \langle f, f \rangle^{1/2}, \quad (3)$$

and their finite-dimensional counterparts.

2. Ill-posedness and Stabilization of the Cauchy Problem

Let the eigenvalues and eigenfunctions of the operator L be $(\lambda_{\nu}^2, s_{\nu}(x, y))_1^{\infty}$; the eigenfunctions are orthonormal with respect to the inner product (3), and the system of eigenfunctions is complete; see, e.g., [10, XIV.6.25], [15, Chapter 6.5]. Further, we assume that the eigenvalues are ordered as $0 < \lambda_1 \leq \lambda_2 \leq \dots$. In analogy to the case when Fourier analysis can be used, we will refer to the eigenvalues as frequencies.

It is a standard exercise (see Appendix B) in Hilbert space theory to show that the formal solution (2) can be understood as an expansion in terms of eigenfunctions,

$$u(x, y, z) = \sum_{\nu=1}^{\infty} \cosh(\lambda_{\nu} z) \langle s_{\nu}, g \rangle s_{\nu}(x, y). \quad (4)$$

The unboundedness of the solution operator is evident: a high-frequency perturbation of the data, $g_m = g + e$, will cause the corresponding solution to blow up.

It is customary in ill-posedness problems to incorporate the data perturbation in the problem formulation and stabilize the problem by assuming that the solution is bounded. Thus we define the *stabilized problem*,

$$u_{zz} - Lu = 0, \quad (x, y) \in \Omega, \quad z \in [0, z_1], \quad (5)$$

$$u(x, y, z) = 0, \quad (x, y) \in \partial\Omega, \quad z \in [0, z_1], \quad (6)$$

$$u_z(x, y, 0) = 0, \quad (x, y) \in \Omega, \quad (7)$$

$$\|u(\cdot, \cdot, 0) - g_m(\cdot, \cdot)\| \leq \epsilon, \quad (8)$$

$$\|u(\cdot, \cdot, z_1)\| \leq M. \quad (9)$$

It is again a standard exercise (and for this reason we relegate it to Appendix B) to demonstrate that the solution of (5)-(9) is stable, but not unique.

Proposition 1. *Any two solutions, u_1 and u_2 , of the stabilized problem (5)-(9) satisfy*

$$\|u_1(\cdot, \cdot, z) - u_2(\cdot, \cdot, z)\| \leq 2\epsilon^{1-z/z_1} M^{z/z_1}, \quad 0 \leq z < z_1. \quad (10)$$

Given the non-uniqueness of the solution of the stabilized problem (5)-(9), its numerical treatment is not straightforward. However, one can define approximate solutions in other ways (i.e., not referring to the stabilized problem), and it is possible to prove approximation results in terms of any solution of (5)-(9).

Definition 2. For $\lambda_c > 0$, a regularized solution is given by

$$v(x, y, z) = \sum_{\lambda_\nu \leq \lambda_c} \cosh(\lambda_\nu z) \langle s_\nu, g_m \rangle s_\nu(x, y). \quad (11)$$

The quantity λ_c is referred to as a *cut-off frequency*. It is easy to show that the function v satisfies an error bound that is optimal in the sense that it is of the same type as that in Proposition 1. A proof is given in Appendix B.3.

Theorem 3. Suppose that u is a solution defined by (4) (with exact data g), and that v is a regularized solution (11) with measured data g_m , satisfying $\|g - g_m\| \leq \epsilon$. If $\|u(\cdot, \cdot, 1)\| \leq M$, and if we choose $\lambda_c = (1/z_1) \log(M/\epsilon)$, then we have the error bound

$$\|u(\cdot, \cdot, z) - v(\cdot, \cdot, z)\| \leq 3\epsilon^{1-z/z_1} M^{z/z_1}, \quad 0 \leq z \leq z_1. \quad (12)$$

The result above indicates that if we can solve approximately the eigenvalue problem for the operator L , i.e. compute good approximations of the eigenvalues and eigenfunctions for $\lambda_\nu \leq \lambda_c$, then we can compute a good approximation of the regularized solution. The solution of the eigenvalue problem for the smallest eigenvalues and eigenfunctions by a modern eigenvalue algorithm for sparse matrices [3] requires us to solve a large number of well-posed 2-D elliptic problems with a discretization of L .

If we use the eigenvalue approach then we do not take into account that we actually want to compute not a good approximation of the solution operator itself but rather *the solution operator applied to the particular right-hand side* g_m . We will now show that it is possible to obtain a good approximation of (11) much more cheaply by using a Krylov subspace method initialized with g_m .

Remark Theorem 3 only gives continuity in the interior of the interval, $[0, z_1)$. In the theory of ill-posed Cauchy problems one often can obtain continuous dependence on the data for the closed interval $[0, z_1]$ by assuming additional smoothness and using a stronger norm, see e.g. [30, Theorem 3.2]. We are convinced that this can be done also here, but we have not pursued this.

3. A Krylov Subspace Method

From now on we assume that the problem has been discretized with respect to (x, y) , and that the operator $L \in \mathbb{R}^{N \times N}$ is a symmetric, positive definite matrix. The details of the discretization are unimportant for our presentation, we only assume that it is fine enough so that the discretization errors are small compared to the uncertainty ϵ of the data; this means that L is a good approximation of the differential operator, whose unboundedness is reflected in a large norm of L . In the following we use small roman letters to denote vectors that are the discrete analogs of the continuous quantities. Thus the solution vector $u(z)$ is a vector-valued function of z .

For a given z , the discrete analogs of the formal and regularized solutions in (2) and in (11) are given by

$$u(z) = \cosh(z\sqrt{L})g = \sum_{j=1}^N (\cosh(z\lambda_j) s_j^\top g) s_j, \quad (13)$$

$$v(z) = \sum_{\lambda_j \leq \lambda_c} (\cosh(z\lambda_j) s_j^\top g_m) s_j, \quad (14)$$

respectively, where (λ_j^2, s_j) are the eigenpairs of L , such that $0 < \lambda_1^2 \leq \dots \leq \lambda_N^2$.

We will now discuss how to compute an approximation of (14) using a Krylov subspace method, which is an iterative method. An error estimate for the Krylov approximation is given in Proposition 4, and a stopping criterion is derived in Section 4.

Krylov subspace approximations of matrix functions have been extensively employed in the solution of certain discretized partial differential equations, see, e.g., [16, 34, 20, 35, 19, 21, 8], while more recently attention has been devoted to acceleration procedures, see, e.g., [9, 24, 22, 29], where shift-invert type procedures are explored. The standard approach consists in generating the Krylov subspace $K_k(L, g) = \text{span}\{g, Lg, \dots, L^{k-1}g\}$ by a step-wise procedure (for details, see Section 5). Let $(\hat{q}_i)_{i=1}^k$ be an orthonormal basis of $K_k(L, g)$, with $\hat{q}_1 = g/\|g\|$. Letting $\hat{Q}_k = (\hat{q}_1, \hat{q}_2, \dots, \hat{q}_k)$ and $\hat{T}_k = \hat{Q}_k^\top L \hat{Q}_k \in \mathbb{R}^{k \times k}$ be the symmetric representation of L onto the space, an approximation to u in $K_k(L, g)$ may be obtained by projection,

$$u_k(z) = \hat{Q}_k \cosh(z\hat{T}_k^{1/2}) e_1 \|g\|. \quad (15)$$

Here and in the following, e_j denotes the j 'th canonical vector, of appropriate dimension. It may be shown that the error norm satisfies

$$\|u_k(z) - u(z)\| \approx \frac{\alpha}{2k} \exp\left(-\alpha \left(\frac{2k^2}{\alpha^2} + O\left(\left(\frac{2k}{\alpha}\right)^4\right)\right)\right), \quad (16)$$

where $\alpha = z\lambda_{\max}$ and $\lambda_{\max}^2$ is the largest eigenvalue of L . Convergence is superlinear, and the quality of the approximation depends on how small $\lambda_{\max}$ is. An approximation to the stabilized solution (14) in the approximation space $K_k(L, g_m)$ (note that g has been replaced by g_m) may be obtained by accordingly truncating the expansion of the solution u_k in terms of the eigenpairs of $\hat{T}_k$.

In our context, the smallest eigenvalues of L are the quantities of interest; cf. (14). Since the convergence of the Krylov subspace approximation is faster away from the origin (see, e.g., [3, Section 4.4.3]), a shift-invert procedure is commonly used to speed up convergence to the eigenvalues closest to a target value. More precisely, the spectral approximation is obtained in the Krylov subspace

$$K_k(L^{-1}, g_m) = \text{span}\{g_m, L^{-1}g_m, \dots, L^{-(k-1)}g_m\},$$

or more generally, in $K_k((L - \tau I)^{-1}, g_m)$ for some well selected value of τ . For simplicity of exposition, we assume in this section that $\tau = 0$, and let the orthonormal columns of

Q_k span such a space. If the Arnoldi process is employed to generate the orthonormal basis, we have the relation (see, e.g., [3])

$$L^{-1}Q_k = Q_k T_k + \beta_{k+1} q_{k+1} e_k^\top, \quad q_{k+1}^\top Q_k = 0.$$

Let $((\theta_j^{(k)})^2, y_j^{(k)})$, $j = 1, \dots, k$ be the eigenpairs of T_k^{-1} , so that $((\theta_j^{(k)})^2, Q_k y_j^{(k)})$, $j = 1, \dots, k$ approximate some of the eigenpairs of L . Using $\cosh(z T_k^{-1/2}) = \sum_{j=1}^k y_j^{(k)} \cosh(z \theta_j^{(k)}) (y_j^{(k)})^\top$, the truncated approximation can be obtained as

$$v_k(z) = Q_k \sum_{\theta_j^{(k)} \leq \lambda_c} y_j^{(k)} \cosh(z \theta_j^{(k)}) (y_j^{(k)})^\top e_1 \|g_m\|. \quad (17)$$

If our purpose were to first accurately approximate the small eigenvalues of L and then compute $v_k(z)$ above, then we would have made the problem considerably harder. Indeed, the convergence rate of eigenvalue and eigenvector approximations is in general significantly slower than that of the matrix function (cf. (16)). Following [28, Th. 12.4.1 and Th. 12.4.3], for each eigenpair (λ_j^2, s_j) of interest, one would obtain

$$\begin{aligned} |(\theta_j^{(k)})^2 - \lambda_j^2| &= O(2 \exp(-4k\sqrt{\gamma})) \\ \tan(s_j, K_k(L^{-1}, g_m)) &= O(2 \exp(-2k\sqrt{\gamma})), \end{aligned} \quad (18)$$

where γ is related to the gap between the sought after eigenvalues and the rest of the spectrum.

Fortunately, we can merge the two steps of the spectral approximation and the computation of $v_k(z)$, without first computing accurate eigenpairs. By computing the sought after solution while approximating the eigenpairs, the iterative process can be stopped as soon as the required solution is satisfactorily good (see section 5 for a discussion on the stopping criterion). In particular, the number of terms in the sum defining $v_k(z)$ can be chosen dynamically as k increases, since the number of eigenvalues $\theta_j^{(k)}$ less than λ_c may increase as k grows.

The value of λ_c depends on the data perturbation, (see Theorem 3), and it may be known approximately a priori. However, the number of eigenvalues smaller than λ_c is usually not known. As a consequence, it is not possible to fix a priori the number of summation terms neither in $v(z)$ (stabilized solution (14)) nor in $v_k(z)$ (Krylov approximation (17) of the stabilized solution). Clearly, these problems would dramatically penalize an approach that first computes accurate eigenvalues and then obtains v_k .

We would also like to stress that, although the convergence rate of $v_k(z)$ does depend on the eigenpairs and thus it is slower than that in (16), there is absolutely no need to get accurate spectral approximants; indeed, the final error norm $\|v_k(z) - u(z)\|$ stagnates at a level that depends on the data perturbation, much before accurate spectral approximation takes place. This fact is investigated in the next section.

3.1. Accuracy of the Stabilized Approximation

As a first motivation for the stopping criterion, we now look at an error estimate for the Krylov subspace solution. Note that it is possible to derive an error estimate of the

type (12) also for the problem that is discretized in Ω . Therefore we want to express the error estimate for the Krylov approximation in similar terms, as much as is possible.

Let $F(z, \lambda) = \cosh(z\sqrt{\lambda})$ and let L^c be the restriction of L onto the invariant subspace of eigenvalues less than the threshold λ_c . Let E^c be the orthogonal projector associated with the eigenvalues less than the threshold. Define $S_k = T_k^{-1}$ and adopt the corresponding notation for S_k^c . Given $u(z) = F(z, L)g$ and $v_k(z) = Q_k F(z, S_k^c) Q_k^\top g_m$, we want to estimate the error norm $\|u - v_k\|$ so that we can emphasize the stagnation level. We have

$$\begin{aligned} \|u(z) - v_k(z)\| &= \|F(z, L)g - Q_k F(z, S_k^c) Q_k^\top g_m\| \\ &\leq \|(F(z, L)g - Q_k F(z, S_k^c) Q_k^\top g)\| \\ &\quad + \|Q_k F(z, S_k^c) Q_k^\top (g - g_m)\| =: \alpha + \beta. \end{aligned}$$

As in Lemma 8 in Appendix B, β can be bounded as follows:

$$\beta \leq \|Q_k F(z, S_k^c) Q_k^\top\| \|g - g_m\| \leq \exp(z\lambda_c) \epsilon \leq \epsilon^{1-z/z_1} M^{z/z_1}.$$

Then we can estimate

$$\alpha = \|(F(z, L) - Q_k F(z, S_k^c) Q_k^\top)g\| \leq \alpha_1 + \alpha_2,$$

where, for the first term we use $g = (F(z_1, L))^{-1}f$,

$$\begin{aligned} \alpha_1 &= \|(I - E^c)(F(z, L) - Q_k F(z, S_k^c) Q_k^\top)(F(z_1, L))^{-1}f\|, \\ \alpha_2 &= \|E^c(F(z, L) - Q_k F(z, S_k^c) Q_k^\top)g\|. \end{aligned} \tag{19}$$

Since $(I - E^c)F(z, L^c) = 0$, we have

$$\alpha_1 \leq \|(I - E^c)F(z, L)(F(z_1, L))^{-1}f\| \tag{20}$$

$$+ \|(I - E^c)(F(z, L^c) - Q_k F(z, S_k^c) Q_k^\top)F(z_1, L))^{-1}f\|. \tag{21}$$

The first term (20) can be estimated as in the last part of the proof of Lemma 8, giving

$$\|(I - E^c)(F(z, L)(F(z_1, L))^{-1})\| M \leq 2\epsilon^{1-z/z_1} M^{z/z_1},$$

while the second term is bounded by $\|(F(z, L^c) - Q_k F(z, S_k^c) Q_k^\top)g\|$. Moreover,

$$\begin{aligned} \alpha_2 &= \|E^c(F(z, L) - Q_k F(z, S_k^c) Q_k^\top)g\| \\ &= \|E^c(F(z, L^c) - Q_k F(z, S_k^c) Q_k^\top)g\| \leq \|(F(z, L^c) - Q_k F(z, S_k^c) Q_k^\top)g\|. \end{aligned}$$

We have thus proved the following error estimate.

Proposition 4. *Let u be defined by (13) and assume that hypotheses corresponding to those in Theorem 3 hold. Let v_k be defined by (17). Then*

$$\|u(z) - v_k(z)\| \leq 3\epsilon^{1-z/z_1} M^{z/z_1} + 2\|(F(z, L^c) - Q_k F(z, S_k^c) Q_k^\top)g\|. \tag{22}$$

The two terms in the upper bound of Proposition 4 emphasize different stages of the convergence history. The error $\|u(z) - v_k(z)\|$ may be large as long as the approximate low frequencies are not sufficiently accurate, and this convergence is guided by (18). Once this accuracy has satisfactorily improved, then the error $\|u(z) - v_k(z)\|$ is dominated by the “intrinsic error”, due to the data perturbation. This behavior is confirmed by our numerical experiments; see Section 6.

4. Stopping Criterion

In a standard inverse problem framework, one would want to compute the residual

$$r_k = Kv_k - g, \quad (23)$$

where K is the operator that maps the function $f(x, y, z_1) = u(x, y, z_1)$, with data $u_z(x, y, 0) = 0$, and homogeneous boundary values on the lateral boundary $\partial\Omega \times [0, z_1]$, to the function values at the lower boundary, $u(x, y, 0)$. This is related to the *discrepancy principle* [14, p. 84], [18, p. 179]. A stopping criterion for an *iterative regularization procedure*, based on the discrepancy principle is usually of the type “stop iterating as soon as $\|r_k\| \leq C\epsilon$ ”, where C is of the order 2, say, and $\epsilon = \|g - g_m\|$ (the safety factor C is used to make up for the possible uncertainty concerning the knowledge of ϵ). Thus the number of iterations is the regularization parameter. If one continues the iterations further, then the solution will soon become unstable and blow up.

Our approach is different in the following two important aspects.

- (i) The cut-off value λ_c is the regularization parameter (Theorem 3), and the stopping criterion only determines when the numerical approximation to the regularized solution is good enough.
- (ii) In our setting, the computation of the residual would require the solution of a 3-D elliptic boundary value problem, which is much more costly than solving the 2-D elliptic problems. In general we cannot afford to compute the residual several times, and therefore it is not practical to use it in a stopping criterion. However, we can compute an approximate residual, which, in addition to being a good approximation of the true residual, is cheap to compute and gives information about the convergence of the Krylov process (Proposition 5).

4.1. Computing Approximate Residuals

Consider the approximate solution after k steps of the Krylov procedure:

$$v_k = Q_k w_k, \quad w_k = \cosh(z_1(S_k^c)^{1/2})Q_k^\top g_m,$$

where $S_k = T_k^{-1}$ denotes the projected representation of L , and S_k^c its truncated version. The vector w_k is the solution at $z = z_1$ of the projected Cauchy problem

$$\begin{aligned} w_{zz} - S_k^c w &= 0, \\ w(0) &= Q_k^\top g_m, \\ w_z(0) &= 0. \end{aligned} \quad (24)$$

The well-posed problem corresponding to (24) is

$$\begin{aligned} w_{zz} - S_k w &= 0, \\ w(z_1) &= \tilde{w}, \\ w_z(0) &= 0, \end{aligned} \quad (25)$$

and we can write its solution at $z = 0$ as

$$w(0) = (\cosh(z_1 S_k^{1/2}))^{-1} \tilde{w}.$$

Note that since the problem (25) is well-posed, it is not necessary to truncate the spectrum of S_k .

Given v_k we would like to compute the residual of the unprojected, well-posed problem,

$$r_k = (\cosh(z_1 L^{1/2}))^{-1} v_k - g_m, \quad (26)$$

which requires the solution of the well-posed 3D problem

$$\begin{aligned} u_{zz} - Lu &= 0, \\ u(z_1) &= v_k, \\ u_z(0) &= 0. \end{aligned} \quad (27)$$

We cannot use the projected well-posed problem (25) at step k to compute an approximation of the residual (26), because then we would only see the effect of the truncation. However, the well-posed problem (25) at step $k+p$, for some natural number p , can be expected to give a better approximation of the residual (26).

In order to use w_k as data for the well-posed problem at step $k+p$, we augment it with p zeros,

$$w_k^{(k+p)} = \begin{pmatrix} w_k \\ 0 \end{pmatrix} \in \mathbb{R}^{k+p}.$$

The approximate residual is then computed as

$$r_k^{(k+p)} = Q_{k+p} (\cosh(z_1 S_{k+p}^{1/2}))^{-1} w_k^{(k+p)} - Q_{k+p} Q_{k+p}^\top g_m, \quad (28)$$

and

$$\begin{aligned} \|r_k^{(k+p)}\| &= \|(\cosh(z_1 S_{k+p}^{1/2}))^{-1} w_k^{(k+p)} - Q_{k+p}^\top g_m\| \\ &= \|(\cosh(z_1 S_{k+p}^{1/2}))^{-1} w_k^{(k+p)} - \beta e_1\|. \end{aligned}$$

Clearly, as $k+p$ gets large, the approximate residual tends to the true residual in (26). However, only small values of $k+p$ are required to get a satisfactory approximate regularized solution.

Proposition 5. *With the previous notation, let $S_{k+p} = Y_{k+p} \Theta_{k+p} Y_{k+p}^\top$ be the eigenvalue decomposition of S_{k+p} , and split Y_{k+p} as $Y_{k+p} = (Y_{k+p}^c \ Y_{k+p}^\perp)$. Then the approximate residual in (28) satisfies*

$$\|r_k^{(k+p)}\| \leq \|F(z_1, S_{k+p})^{-1} (w_k^{(k+p)} - w_{k+p})\| + \|(Q_{k+p} Y_{k+p}^\perp)^\top g_m\|.$$

Proof. With the notation of Proposition 4 ($F(z, \lambda) = \cosh(z\sqrt{\lambda})$), we have

$$\begin{aligned}
 r_k^{(k+p)} &= Q_{k+p} \left(F(z_1, S_{k+p})^{-1} w_k^{(k+p)} - Q_{k+p}^\top g_m \right) \\
 &= Q_{k+p} F(z_1, S_{k+p})^{-1} \left(w_k^{(k+p)} - F(z_1, S_{k+p}) Q_{k+p}^\top g_m \right) \\
 &= Q_{k+p} F(z_1, S_{k+p})^{-1} \left(\begin{bmatrix} F(z_1, S_k^c) & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q_k^\top g_m \\ 0 \end{bmatrix} - F(z_1, S_{k+p}) Q_{k+p}^\top g_m \right) \\
 &= Q_{k+p} F(z_1, S_{k+p})^{-1} \left(\begin{bmatrix} F(z_1, S_k^c) & 0 \\ 0 & 0 \end{bmatrix} - F(z_1, S_{k+p}) \right) Q_{k+p}^\top g_m
 \end{aligned}$$

where in the last equality we have used $Q_{k+p}^\top g_m = \beta e_1$ and the fact that

$$\begin{bmatrix} Q_k^\top g_m \\ 0 \end{bmatrix} = Q_{k+p}^\top g_m.$$

With the eigenvalue decomposition $S_{k+p} = Y_{k+p} \Theta_{k+p} Y_{k+p}^\top$ we can write

$$\begin{aligned}
 \Theta_{k+p} &= \Theta_{k+p}^c + \Theta_{k+p}^\perp \\
 &:= \text{diag}(\theta_1^{(k+p)}, \dots, \theta_s^{(k+p)}, 0, \dots, 0) + \text{diag}(0, \dots, 0, \theta_{s+1}^{(k+p)}, \dots, \theta_{k+p}^{(k+p)}),
 \end{aligned}$$

where $\theta_1^{(k+p)} \leq \dots \leq \theta_s^{(k+p)} \leq \lambda_c < \theta_{s+1}^{(k+p)} \leq \dots \leq \theta_{k+p}^{(k+p)}$. We now have

$$\begin{aligned}
 F(z_1, S_{k+p}) &= Y_{k+p} \begin{bmatrix} F(z_1, \Theta_{k+p}^c) & 0 \\ 0 & 0 \end{bmatrix} Y_{k+p}^\top \\
 &\quad + Y_{k+p} \begin{bmatrix} 0 & 0 \\ 0 & F(z_1, \Theta_{k+p}^\perp) \end{bmatrix} Y_{k+p}^\top =: F_{k+p}^c + F_{k+p}^\perp,
 \end{aligned}$$

and we get

$$\begin{aligned}
 r_k^{(k+p)} &= Q_{k+p} F(z_1, S_{k+p})^{-1} \left(\begin{bmatrix} F(z_1, S_k^c) & 0 \\ 0 & 0 \end{bmatrix} - F_{k+p}^c \right) Q_{k+p}^\top g_m \quad (29) \\
 &\quad - Q_{k+p} F(z_1, S_{k+p})^{-1} F_{k+p}^\perp Q_{k+p}^\top g_m =: t_k^{(1)} + t_k^{(2)}.
 \end{aligned}$$

The vector $t_k^{(1)}$ in (29) can be written as $t_k^{(1)} = Q_{k+p} F(z_1, S_{k+p})^{-1} (w_k^{(k+p)} - w_{k+p})$, and its norm provides the first term in the requested bound. The vector $t_k^{(2)}$ simplifies to

$$t_k^{(2)} = -Q_{k+p} Y_{k+p} \begin{bmatrix} 0 & 0 \\ 0 & I_{k+p-s} \end{bmatrix} Y_{k+p}^\top Q_{k+p}^\top g_m.$$

With the partitioning $Y_{k+p} = (Y_{k+p}^c \quad Y_{k+p}^\perp)$ we have $\|t_k^{(2)}\| = \|(Q_{k+p} Y_{k+p}^\perp)^\top g_m\|$. $\square$

The quantity $\|F(z_1, S_{k+p})^{-1} (w_k^{(k+p)} - w_{k+p})\|$ measures the difference between the approximate solutions at steps k and $k+p$ transformed back to the data level, i.e. for $z = 0$. Of course, when the Krylov solution has stabilized so that the approximate solutions at $z = z_1$ are close, then this quantity is small. However, since $F(z_1, S_{k+p})^{-1}$ is

the discretization of a compact operator, we can expect $\|F(z_1, S_{k+p})^{-1}(w_k^{(k+p)} - w_{k+p})\|$ to be smoother than $\|w_k^{(k+p)} - w_{k+p}\|$ as functions of k .

The term $\|(Q_{k+p}Y_{k+p}^\perp)^\top g_m\|$ is the size of the projection of the data vector g_m onto the high frequency components that correspond to eigenvalues larger than λ_c . Based on the analysis in Appendix B, we can expect that for k sufficiently large, $\|(Q_{k+p}Y_{k+p}^\perp)^\top g_m\| \approx \epsilon$, provided that the cut-off λ_c is close to what it should be, cf. Theorem 3. When the Krylov approximation of the relevant eigenvalues and eigenvectors of L has stabilized somewhat, then the second term in the bound of Proposition 5 dominates the residual norm.

As stopping criterion we suggest

$$\frac{\left| \|r_{k-1}^{(k-1+p)}\| - \|r_k^{(k+p)}\| \right|}{\|r_k^{(k+p)}\|} \leq \text{tol}, \quad (30)$$

with $p = 2$ and $\text{tol} = 10^{-3}$, say. With this criterion the Krylov procedure is stopped when the decrease of the norm of the approximate residual has stagnated, which means that the quality of the solution will not improve if further steps are taken. If instead we were to base the criterion on the closeness of $\|r_k^{(k+p)}\|$ to ϵ , then there would be a risk that the condition might never be satisfied. In particular, if our estimate of ϵ is too small, then neither the true nor the approximate residual is likely to reach that value, as they are computed from the actual data vector g_m .

5. Implementation

The matrix Q_k , whose columns $q_1, \dots, q_k$ span the Krylov subspace $K_k(L^{-1}, g_m)$, may be obtained one vector at the time by means of the Lanczos procedure. Starting with $q_0 = 0$ and $q_1 = g_m/\|g_m\|$, this process generates the subsequent columns $q_2, q_3, \dots$ by means of the following short-term recurrence,

$$L^{-1}q_k = q_{k-1}\beta_{k-1} + q_k\alpha_k + q_{k+1}\beta_k, \quad k = 1, 2, \dots, \quad (31)$$

with $\alpha_k = q_k^\top L^{-1}q_k$ and $\beta_k = q_{k+1}^\top L^{-1}q_k$; see, e.g. [28, 3]. An analogous recurrence is derived when the shift-inverted matrix $(L - \tau I)^{-1}$ is employed. These coefficients form the entries of the tridiagonal symmetric matrix T_k , that is $T_k = \text{tridiag}(\beta_{k-1}, \alpha_k, \beta_k)$, with the α_k 's on the main diagonal. At each iteration k , the eigenpairs of T_k are computed, and the approximate solution v_k in (17) could be derived. An approximation to the theoretical quantity λ_c is determined a-priori (see Theorem 3), so that the partial sum in (17) is readily obtained. The process is stopped when the approximate solution is sufficiently accurate.

The overall algorithm can be summarized as follows.

Algorithm. Given $L, z, g_m, \text{tol}, \text{maxit}, \lambda_c$

$q_0 = 0, q_1 = g_m/\|g_m\|, Q_1 = q_1, \beta_0 = 0$

for $k = 1, 2, \dots, \text{maxit}$

 Compute $\tilde{q} = L^{-1}q_k - q_{k-1}\beta_{k-1}$

```

    Compute  $\alpha_k = q_k^\top \tilde{q}$ 
    Compute  $\tilde{q} = \tilde{q} - q_k \alpha_k$ 
    Compute  $\beta_k = \|\tilde{q}\|$  and  $q_{k+1} = \tilde{q}/\beta_k$ 
    Expand  $T_k$ 
    Compute eigenpairs  $((\theta_j^{(k)})^2, y_j^{(k)})$  of  $T_k^{-1}$ 
    Compute  $w_k = \sum_{\theta_j^{(k)} \leq \lambda_c} y_j^{(k)} \cosh(z\theta_j^{(k)})(y_j^{(k)})^\top e_1 \|g_m\|$ 
    If  $k > p$  then
        Compute the residual  $r_{k-p}^{(k)}$ 
        If  $k > p + 1$  and  $\left| \|r_{k-p-1}^{(k-1)}\| - \|r_{k-p}^{(k)}\| \right| / \|r_{k-p}^{(k)}\| \leq \text{tol}$ , then
            Compute  $v_{k-p} = Q_{k-p} w_{k-p}$  and stop
        endif
    endif
    Set  $Q_{k+1} = [Q_k, q_{k+1}]$ 
endfor
    
```

The recurrence above generates the new basis vector by means of a coupled two-term recurrence, which is known to have better stability properties than the three-term recurrence (31); see, e.g., [3, section 4.4]. In a practical implementation, additional safeguard strategies such as partial or selective reorthogonalization are commonly implemented to avoid well known loss of orthogonality problems in the Lanczos recurrence [3, section 4.4.4].

When procedures such as the finite element method are used to discretize the given equation over the space variables, equation (5) becomes

$$Hu_{zz} - Lu = 0, \quad (32)$$

where H is the $N \times N$ symmetric and positive definite matrix associated with the employed inner product; it is usually called the *mass* matrix. Clearly, using the Cholesky factorization of H , i.e. $H = R^\top R$, the equation in (32) may be reformulated in the original way as $\tilde{u}_{zz} - \tilde{L}\tilde{u} = 0$, where $\tilde{L} = R^{-\top}LR^{-1}$, and $\tilde{u} = Ru$. Such procedure entails performing the factorization of H and applying the factors and their inverses, whenever the matrix $\tilde{L}$ is employed.

To avoid the explicit use of the factorization of H , one can rewrite (32) as

$$u_{zz} + H^{-1}Lu = 0.$$

Since both H and L are symmetric and positive definite, the eigenvalues of $H^{-1}L$ are all real and equal to those of $\tilde{L}$. Moreover, the eigenvectors s_j of $H^{-1}L$ are H -orthogonal, and can be made to be H -orthonormal by a scaling, that is, $\tilde{s}_j = s_j / \sqrt{s_j^\top H s_j}$. Therefore, setting $\tilde{S} = [\tilde{s}_1, \dots, \tilde{s}_N]$ so that $H^{-1}L = \tilde{S}\Lambda\tilde{S}^{-1}$ and $\tilde{S}^{-1} = \tilde{S}^\top H$, we have that

$$\begin{aligned}
 u &= \cosh(z\sqrt{H^{-1}L})g = \tilde{S}\cosh(z\Lambda)\tilde{S}^{-1}g \\
 &= \tilde{S}\cosh(z\Lambda)\tilde{S}^\top Hg
 \end{aligned}$$

$$= \sum_{j=1}^N (\cosh(z\lambda_j) \tilde{s}_j^\top H g) \tilde{s}_j.$$

Hence, the stabilized approximation may be obtained by truncating the eigenvalue sum.

The approximation with the Lanczos algorithm may be adapted similarly. Following a procedure that is typical in the generalized eigenvalue context, see, e.g., [3, Chapter 5], the approximation to the stabilized solution may be sought after in the Krylov subspace $K_k((L - \tau H)^{-1}, g_m)$. The basis vectors are computed so as to satisfy an H -orthogonality condition, that is $q_{k+1}^\top H Q_k = 0$; see, e.g., [3, section 5.5].

It is important to remark that the use of the mass matrix also affects the norm employed throughout the analysis, and in particular, in the determination of the perturbation tolerance ϵ associated with the measured data g_m ; see Theorem 3. More precisely, we assume that g_m satisfies

$$\|g - g_m\|_H^2 := (g - g_m)^\top H (g - g_m) \leq \epsilon^2,$$

and the error is measured in the same norm.

6. Numerical Experiments

Example 1. In our numerical experiments we used MATLAB 7.5. In the first example we chose the region Ω to be the unit square $[0, 1] \times [0, 1]$, and the operator the Laplace operator. Thus the Cauchy problem was

$$\begin{aligned} u_{zz} + \Delta u &= 0, & (x, y, z) &\in \Omega \times [0, 0.1], \\ u(x, y, z) &= 0, & (x, y, z) &\in \partial\Omega \times [0, 0.1], \\ u(x, y, 0) &= g(x, y), & (x, y) &\in \Omega, \\ u_z(x, y, 0) &= 0, & (x, y) &\in \Omega. \end{aligned}$$

We wanted to determine the values at the upper boundary, that is $f(x, y) = u(x, y, 0.1)$, $(x, y) \in \Omega$.

In constructing our data we chose a solution, $f(x, y) = 30x(1 - x)^6y(1 - y)$; with this solution the Cauchy problem is not easy to solve, as $|\partial f / \partial x|$ is relatively large along $x = 0$. We computed the data function $g(x, y)$ by solving the well posed problem with boundary values $u(x, y, 0.1) = f(x, y)$ and $u_z(x, y, 0) = 0$, and evaluating the solution at the lower boundary $z = 0$. That solution was taken as the “exact data” g . The well-posed problem was solved by separation of variables: trigonometric interpolation of f (relative interpolation error of the order of the machine precision) on a grid with $h_x = h_y = 0.01$, and numerical evaluation of the hyperbolic cosine (i.e. MATLAB’s `cosh`). In Figure 1 we give the solution and the data function.

We then perturbed the data, and added normally distributed noise to each component, giving g_m . The relative data perturbation $\|g - g_m\| / \|g\|$ was of the order 0.0085. From the singular value expansion (B.3) we can deduce that the condition number of the discrete problem is $\cosh(\lambda_{\max} z_1) / \cosh(\lambda_{\min} z_1)$, where $\lambda_{\max}^2$, and $\lambda_{\min}^2$ are the largest and smallest eigenvalues of the matrix L . Here the condition number

Figure 1. Example 1. True solution (left) and data function (right).

is $8.7 \cdot 10^{11}$ (the largest and smallest eigenvalues of the matrix L are 80000 and 20, respectively), and therefore computing an unregularized solution with g_m is completely meaningless.

Using the actual value of the norm of the solution f , the cut-off frequency defined in Theorem 3 was 50, approximately. It turned out that a lower value of the cut-off frequency, $\lambda_c = 40$, gave a slightly more accurate solution; however, the difference was minor. To study the efficiency and the reliability of the stopping criterion, we plotted the norm of the true error, the residual r_k , and the norm of the approximate residual $r_k^{(k+2)}$ as functions of the iteration number k , see Figure 2.

Figure 2. Example 1. Norm of the true relative error (solid line), relative residual (dashed), relative approximate residual (dashed-dotted with squares), as functions of the iteration k . The lower straight line is $\epsilon/\|g_m\|$.

The stopping criterion (30), with $p = 2$ and $\text{tol} = 10^{-3}$ was first satisfied for $k = 18$. The approximate solution at $y = 1/2$ is given in Figure 3.

Figure 3. Example 1. The true solution (solid) and the approximate (dashed), evaluated at $y = 0.5$ for $k = 18$.

To demonstrate that we get a good enough approximation of the solution long before the eigenvalue approximations have stabilized, we illustrated the convergence of the eigenvalues. It is seen in Figure 4 that quite few of the eigenvalues that are smaller than $\lambda_c = 40$ have converged when the stopping criterion is satisfied. On the other hand, for $k = 30$ it seems that the eigenvalues smaller than $\lambda_c = 40/3$ have converged, but not those that are larger. Then, if we compute the approximate solution for the converged eigenvalues, we get a rather bad approximation, due to the fact that there are significant components of the solution for eigenvalues larger than $40/3$.

Example 2 Our second example illustrates the use of a finite element discretization, and our computations are based on the codes from the book [17]§. The region was defined as

$$\Omega = \{(x, y, z) \mid x^2 + y^2/4 \leq 1, 0 \leq z \leq z_1 = 0.6\}.$$

The operator L was defined

$$L = -(k(x, y)u_x)_x - (k(x, y)u_y)_y, \quad k(x, y) = 1 + 0.25x^2y,$$

and the two-dimensional problem was discretized using linear elements and six mesh refinements, giving mass and stiffness matrices of dimension 8065. We prescribed the

§ The codes are available at <http://www.math.mtu.edu/~msgocken/fembook/>

Figure 4. Example 1. Left: Ritz values (eigenvalue approximations) smaller than $\lambda_c = 40$ as functions of the number of Krylov steps k . Right: The exact solution (solid line), the approximate solution computed with $\lambda_c = 40$ and $k = 18$ (dashed), and for $\lambda_c = 40/3$ and $k = 30$ (dashed-dotted).

solution $u(x, y, z_1) = f(x, y) = (1 - x^2 - y^2/4) \exp(-(x - 0.2)^2 - y^2)$ on the upper boundary $z = z_1$, and $u_z(x, y, 0) = 0$ on the lower boundary. To generate the “exact data function” we solved the 3D problem, discretized in the z direction using a central difference, with a step length $z_1/30$ (a problem with 250015 unknowns; this boundary value problem was solved using the MATLAB function `pcg` with an incomplete Cholesky preconditioner with drop tolerance 10^{-3}). We then perturbed the data function by adding a normally distributed perturbation with standard deviation 0.03 giving the data function g_m illustrated in Figure 5.

Figure 5. Example 2. Exact data function (left) and perturbed data function, standard deviation 0.03 (right).

We computed the rational Krylov solution as in Example 1, with the modifications outlined in Section 5. Here we chose the cut-off level to be 0.6 times $(1/z_1) \log(M/\epsilon)$; thus we had $\lambda_c = 6.6$. In Figure 7 we illustrate the convergence history.

We also tested the stopping criterion, using the same parameters as in Example 1. The criterion was satisfied after nine Krylov steps. To compare the number of elliptic

Figure 6. Example 2. Convergence history: true relative error (solid), and the relative residual (dashed), and the approximate residual with $p = 2$. The straight line is $\epsilon/\|g_m\|$.

Figure 7. Example 2. Left: True solution. Right: approximate solution after nine Krylov steps.

solves to that in the solution based on the explicit eigencomputation in the eigenvalue expansion, we used the MATLAB function `eigs` to compute the 17 eigenvalues below the cut-off level; that required 74 elliptic solves.

To see if the problem was sufficiently ill-conditioned to be interesting as a test example, we computed the condition number, and it was equal to $7 \cdot 10^{69}$ (which means that in IEEE double precision it qualifies as a “a discrete ill-posed problem”).

7. Conclusions

We have proposed a truncated eigenfunction expansion method for solving an ill-posed Cauchy problem for an elliptic PDE in three space dimensions. The regularization parameter is the cut-off frequency. The method approximates the explicit regularized solution, involving a hyperbolic function on a low-dimensional subspace, by means of a rational Krylov method. A crucial part of the algorithm is to determine when to stop the recursion that increases the dimension of the Krylov subspace. We suggest a stopping criterion based on the relative change of an approximate, cheaply computable residual. The much more costly true residual for the three-dimensional problem, if needed, may be checked at a final stage. The criterion reflects the accuracy of the approximation of the required components in the solution rather than the accuracy of all the eigenvalues that are smaller than the cut-off value. As a consequence, the procedure dynamically improves the accuracy of the sought after solution, with no a-priori knowledge on the number of involved eigenpairs. This represents a particular feature of this method, because no explicit spectral information on the problem is required.

In the case when the a priori knowledge needed to determine the cut-off frequency λ_c is uncertain, it may be necessary to compute the solution for several different values of λ_c . That can be done very cheaply, since those computations can be performed with the already computed Krylov sequence, and probably in many cases without any additional elliptic solves.

Our preliminary experiments are very promising, and we plan to also adapt the strategy to more general problems.

8. Acknowledgements

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Appendix

Appendix A. Transforming a General Cauchy Problem

Consider the Cauchy problem,

$$\begin{aligned} u_{zz} - Lu &= 0, & (x, y, z) &\in \Omega \times [0, z_1], \\ u(x, y, z) &= b(x, y, z), & (x, y, z) &\in \partial\Omega \times [0, z_1], \\ u(x, y, 0) &= g(x, y), & (x, y) &\in \Omega, \\ u_z(x, y, 0) &= h(x, y), & (x, y) &\in \Omega. \end{aligned} \tag{A.1}$$

The problem is to determine the values of u on the upper boundary, $f(x, y) = u(x, y, z_1)$, $(x, y) \in \Omega$. We assume that

$$g(x, y) = b(x, y, 0) \text{ for } (x, y) \in \partial\Omega; \tag{A.2}$$

this is essential to avoid the Gibbs phenomenon [7, p. 197].

We can transform this problem to a simpler one by using linearity. Let u_1 satisfy the well-posed problem

$$\begin{aligned} u_{zz} - Lu &= 0, & (x, y, z) &\in \Omega \times [0, z_1], \\ u(x, y, z) &= b(x, y, z), & (x, y, z) &\in \partial\Omega \times [0, z_1], \\ u(x, y, z_1) &= \phi(x, y), & (x, y) &\in \Omega, \\ u_z(x, y, 0) &= h(x, y), & (x, y) &\in \Omega. \end{aligned}$$

The function ϕ is chosen as the solution of the two-dimensional boundary value problem

$$\begin{aligned} L\phi &= 0, \\ \phi(x, y) &= b(x, y, z_1), & (x, y) &\in \partial\Omega. \end{aligned}$$

Then, let u_2 be an approximate solution of the ill-posed Cauchy problem,

$$\begin{aligned} u_{zz} - Lu &= 0, & (x, y, z) &\in \Omega \times [0, z_1], \\ u(x, y, z) &= 0, & (x, y, z) &\in \partial\Omega \times [0, z_1], \\ u(x, y, 0) &= g(x, y) - u_1(x, y, 0), & (x, y) &\in \Omega, \\ u_z(x, y, 0) &= 0, & (x, y) &\in \Omega. \end{aligned} \tag{A.3}$$

Obviously, $u = u_1 + u_2$ is an approximate solution of the original ill-posed problem (A.1). Therefore, since, in principle, we can solve the well-posed problem with arbitrarily high accuracy, and since the stability analysis is usually considered as an asymptotic analysis as the data errors tend to zero, it makes sense to analyze the ill-posedness of the original problem in terms of the simplified problem (A.3).

Note that, due to the assumption (A.2), $u_2(x, y, 0) = 0$ at $\partial\Omega$, so no Gibbs phenomenon should occur there.

Appendix B. Ill-Posedness and Regularization

Appendix B.1. Singular Value Analysis

In order to study the ill-posedness of the Cauchy problem (1) we will first write it in operator form as

$$Kf = g,$$

for some (compact) operator K , and then determine the singular value expansion of K . Consider the well-posed problem

$$\begin{aligned} u_{zz} - Lu &= 0, & (x, y) &\in \Omega, \quad z \in [0, z_1], \\ u(x, y, z) &= 0, & (x, y) &\in \partial\Omega, \quad z \in [0, z_1], \\ u(x, y, z_1) &= f(x, y), & (x, y) &\in \Omega, \\ u_z(x, y, 0) &= 0, & (x, y) &\in \Omega. \end{aligned}$$

With the separation of variables ansatz

$$u(x, y, z) = \sum_{k=1}^{\infty} w^{(k)}(z) s_k(x, y),$$

where s_k are the (orthonormal) eigenfunctions of L (with zero boundary values), the equation $u_{zz} - Lu = 0$ becomes

$$\sum_{k=1}^{\infty} w_{zz}^{(k)}(z) s_k(x, y) - \sum_{k=1}^{\infty} \lambda_k^2 w^{(k)}(z) s_k(x, y) = 0,$$

where λ_k^2 are the eigenvalues of L .

Expanding the boundary values at $z = z_1$,

$$f(x, y) = \sum_{k=1}^{\infty} \langle s_k, f \rangle s_k(x, y),$$

we get a boundary value problem for an ordinary differential equation for each value of k ,

$$w_{zz}^{(k)} = \lambda_k^2 w^{(k)}, \quad w^{(k)}(z_1) = \langle s_k, f \rangle, \quad w_z^{(k)}(0) = 0,$$

with the unique solution

$$w^{(k)}(z) = \frac{\cosh(\lambda_k z)}{\cosh(\lambda_k z_1)} \langle s_k, f \rangle, \quad 0 \leq z \leq z_1.$$

Thus we can write the solution of the elliptic equation

$$u(x, y, z) = \sum_{k=1}^{\infty} \frac{\cosh(\lambda_k z)}{\cosh(\lambda_k z_1)} \langle s_k, f \rangle s_k(x, y), \quad 0 \leq z \leq z_1, \quad (x, y) \in \Omega. \quad (\text{B.1})$$

Now consider the solution at the lower boundary,

$$g(x, y) = u(x, y, 0) = \sum_{k=1}^{\infty} \frac{1}{\cosh(\lambda_k z_1)} \langle s_k, f \rangle s_k(x, y). \quad (\text{B.2})$$

Summarizing the derivation above, we see that the Cauchy problem (1) can be written as an integral equation of the first kind $g = Kf$, where the integral operator is defined in terms of the eigenvalue expansion,

$$g(x, y) = \sum_{k=1}^{\infty} \frac{1}{\cosh(\lambda_k z_1)} \langle s_k, f \rangle s_k(x, y). \quad (\text{B.3})$$

Obviously this is the singular value expansion of the operator, and since the operator is self-adjoint this is the same as the eigenvalue expansion. Thus, the singular values and singular functions are

$$\sigma_k = \frac{1}{\cosh(\lambda_k z_1)}, \quad u_k = v_k = s_k.$$

The λ_k will also be referred to as *frequencies*. The eigenvalues λ_k^2 of a self-adjoint elliptic operator satisfy $\lambda_k \rightarrow \infty$ as $k \rightarrow \infty$. Therefore we have exponential decay of the singular values to zero and the problem is *severely ill-posed*.

|| When L is the 1D Laplace operator on the interval $[0, \pi]$, then $\lambda_k = k$ and $s_k(x) = \sin(kx)$.

Appendix B.2. Stability in a z -Cylinder

We can use the concept of logarithmic convexity to prove a stability result for the Cauchy problem. Put

$$\begin{aligned} F(z) &= \int_{\Omega} |u(x, y, z)|^2 dx dy = \int_{\Omega} \left| \sum_k \frac{\cosh(\lambda_k z)}{\cosh(\lambda_k z_1)} \alpha_k s_k(x, y) \right|^2 dx dy \\ &= \sum_k \frac{\cosh^2(\lambda_k z)}{\cosh^2(\lambda_k z_1)} \alpha_k^2, \end{aligned}$$

where $\alpha_k = \langle s_k, f \rangle$, and where we have used the orthonormality of the eigenfunctions.

We will show that this function is log-convex. The first and second derivatives are

$$F'(z) = 2 \sum_k \frac{\cosh(\lambda_k z) \sinh(\lambda_k z)}{\cosh^2(\lambda_k z_1)} \lambda_k \alpha_k^2,$$

and

$$F''(z) = 2 \sum_k \frac{\sinh^2(\lambda_k z) + \cosh^2(\lambda_k z)}{\cosh^2(\lambda_k z_1)} \lambda_k^2 \alpha_k^2 \geq 4 \sum_k \frac{\sinh^2(\lambda_k z)}{\cosh^2(\lambda_k z_1)} \lambda_k^2 \alpha_k^2.$$

Then it follows that

$$\begin{aligned} F F'' - (F')^2 &\geq \\ &\geq 4 \left(\sum_k \frac{\cosh^2(\lambda_k z)}{\cosh^2(\lambda_k z_1)} \alpha_k^2 \right) \left(\sum_k \frac{\sinh^2(\lambda_k z)}{\cosh^2(\lambda_k z_1)} \lambda_k^2 \alpha_k^2 \right) \\ &\quad - 4 \left(\sum_k \frac{\cosh(\lambda_k z) \sinh(\lambda_k z)}{\cosh^2(\lambda_k z_1)} \lambda_k \alpha_k^2 \right)^2 \geq 0 \end{aligned}$$

by the Cauchy-Schwarz inequality. This implies that $\log F$ is convex.

Now consider the *stabilized problem*,

$$\begin{aligned} u_{zz} - Lu &= 0, & (x, y) \in \Omega, \quad z \in [0, z_1], \\ u(x, y, z) &= 0, & (x, y) \in \partial\Omega, \quad z \in [0, z_1], \\ u_z(x, y, 0) &= 0, & (x, y) \in \Omega, \\ \|u(\cdot, \cdot, 0) - g_m(\cdot, \cdot)\| &\leq \epsilon, \\ \|u(\cdot, \cdot, z_1)\| &\leq M. \end{aligned} \tag{B.4}$$

From logarithmic convexity it now follows that solutions of the stabilized problem depend continuously on the data (in an $L_2(\Omega)$ sense) for $0 \leq z < z_1$.

Proposition 6. *Any two solutions, u_1 and u_2 , of the stabilized problem satisfy*

$$\|u_1(\cdot, \cdot, z) - u_2(\cdot, \cdot, z)\| \leq 2\epsilon^{1-z/z_1} M^{z/z_1}, \quad 0 \leq z < z_1. \tag{B.5}$$

Proof. Put $F(z) = \|u_1(\cdot, \cdot, z) - u_2(\cdot, \cdot, z)\|^2$. Since $u_1 - u_2$ satisfies the differential equation $u_{zz} - Lu = 0$, with the Cauchy data, $F(z)$ is logarithmic convex. This implies that

$$\log F(z) \leq (1 - z/z_1) \log F(0) + z/z_1 \log F(z_1),$$

or, equivalently,

$$F(z) \leq F(0)^{1-z/z_1} F(1)^{z/z_1}.$$

Using the triangle inequality and the bounds in (B.4) we obtain (B.5). $\square$

Appendix B.3. Regularization by Cutting off High Frequencies

Taking the inner product with respect to s_k in the expansion (B.2) we get $\langle s_k, f \rangle = \cosh(\lambda_k z_1) \langle s_k, g \rangle$, and therefore, using (B.1), we can write the solution of the Cauchy problem with exact data g formally as

$$u(x, y, z) = \sum_{k=1}^{\infty} \cosh(\lambda_k z) \langle s_k, g \rangle s_k(x, y). \quad (\text{B.6})$$

This does not work for *inexact data* g_m (nor for numerical computations with exact data), since high frequency noise (including floating-point round-off) will be blown up arbitrarily. However, we can obtain a useful approximate solution by cutting off high frequencies. Thus, define

$$v(x, y, z) = \sum_{\lambda_k \leq \lambda_c} \cosh(\lambda_k z) \langle s_k, g_m \rangle s_k(x, y), \quad (\text{B.7})$$

where λ_c is the *cut-off frequency*. We will call such a solution a *regularized solution*.

We will now show that a regularized solution satisfies an almost optimal error bound of the type (B.5). A couple of lemmas are needed.

Lemma 7. *Assume that v_1 and v_2 are two regularized solutions defined by (B.7), with data g_1 and g_2 , respectively, satisfying $\|g_1 - g_2\| \leq \epsilon$. If we select $\lambda_c = (1/z_1) \log(M/\epsilon)$, then we have the bound*

$$\|v_1(\cdot, \cdot, z) - v_2(\cdot, \cdot, z)\| \leq \epsilon^{1-z/z_1} M^{z/z_1}, \quad 0 \leq z \leq z_1. \quad (\text{B.8})$$

Proof. Using the orthonormality of the eigenfunctions we have

$$\begin{aligned} \|v_1 - v_2\|^2 &= \sum_{\lambda_k \leq \lambda_c} (\cosh(\lambda_k z) \langle g_1 - g_2, s_k \rangle)^2 \\ &\leq (\cosh(\lambda_c z))^2 \sum_{\lambda_k \leq \lambda_c} (\langle g_1 - g_2, s_k \rangle)^2 \leq (\cosh(\lambda_c z))^2 \|g_1 - g_2\|^2 \\ &\leq \exp(2\lambda_c z) \epsilon^2. \end{aligned}$$

The inequality (B.8) now follows using $\lambda_c = (1/z_1) \log(M/\epsilon)$. $\square$

Lemma 8. *Let u be a solution defined by (B.1), and let v be a regularized solution with the same exact data g . Suppose that $\|u(\cdot, \cdot, 1)\| \leq M$. Then, if $\lambda_c = (1/z_1) \log(M/\epsilon)$,*

$$\|u(\cdot, \cdot, z) - v(\cdot, \cdot, z)\| \leq 2\epsilon^{1-z/z_1} M^{z/z_1}, \quad 0 \leq z \leq z_1. \quad (\text{B.9})$$

Proof. Using (B.2) we have

$$v(x, y, z) = \sum_{\lambda_k \leq \lambda_c} \cosh(\lambda_k z) \langle s_k, g \rangle s_k(x, y) = \sum_{\lambda_k \leq \lambda_c} \frac{\cosh(\lambda_k z)}{\cosh(\lambda_k z_1)} \langle s_k, f \rangle s_k(x, y),$$

where $f(x, y) = u(x, y, 1)$. Thus, from (B.1) we see that

$$\|u - v\|^2 = \sum_{\lambda_k > \lambda_c} \left(\frac{\cosh(\lambda_k z)}{\cosh(\lambda_k z_1)} \langle s_k, f \rangle \right)^2 \leq 4 \exp(-2\lambda_c(z_1 - z)) \sum_{\lambda_k > \lambda_c} (\langle s_k, f \rangle)^2,$$

where we have used the elementary inequality

$$\frac{1 + e^{-\lambda z}}{1 + e^{-\lambda z_1}} \leq 2, \quad \lambda \geq 0, \quad 0 \leq z \leq z_1.$$

The inequality (B.9) now follows from the assumptions $\|f\| \leq M$ and $\lambda_c = (1/z_1) \log(M/\epsilon)$. $\square$

Now the main error estimate can be proved.

Theorem 9. *Suppose that u is a solution defined by (B.1), and that v is a regularized solution with measured data g_m , satisfying $\|g - g_m\| \leq \epsilon$. Then, if $\|u(\cdot, \cdot, 1)\| \leq M$ and we choose $\lambda_c = (1/z_1) \log(M/\epsilon)$, we have the error bound*

$$\|u(\cdot, \cdot, z) - v(\cdot, \cdot, z)\| \leq 3\epsilon^{1-z/z_1} M^{z/z_1}, \quad 0 \leq z \leq z_1.$$

Proof. Let v_1 be a regularized solution with exact data g . Then using the two previous lemmas we get

$$\|u - v\| \leq \|u - v_1\| + \|v_1 - v\| \leq 3\epsilon^{1-z/z_1} M^{z/z_1}.$$

$\square$

References

- [1] S. Andrieux, T. N. Baranger, and A. Ben Abda. Solving Cauchy problems by minimizing an energy-like functional. *Inverse Problems*, 22:115–133, 2006.
- [2] M. Azaïez, F. B. Belgacem, and H. El Fekih. On Cauchy’s problem: II. completion, regularization and approximation. *Inverse Problems*, 22:1307–1336, 2006.
- [3] Z. Bai, J. Demmel, J. Dongarra, A. Ruhe, and H. van der Vorst, editors. *Templates for the Solution of Algebraic Eigenvalue Problems: A Practical Guide*. SIAM, Philadelphia, 2000.
- [4] F. B. Belgacem. Why is the Cauchy problem severely ill-posed? *Inverse Problems*, 23:823–836, 2007.
- [5] F. Berntsson and Lars Eldén. Numerical solution of a Cauchy problem for the Laplace equation. *Inverse Problems*, 17:839–854, 2001.
- [6] Å. Björck, E. Grimme, and P. Van Dooren. An implicit shift bidiagonalization algorithm for ill-posed systems. *BIT*, 34:510–534, 1994.
- [7] G. Cain and G. Meyer. *Separation of Variables for Partial Differential Equations: An Eigenfunction Approach*. Studies in Advanced Mathematics Volume: 46. Chapman & Hall/CRC, 2006.
- [8] V. Druskin and L. Knizhnerman. Krylov subspace approximation of eigenpairs and matrix functions in exact and computer arithmetic. *Numerical Linear Algebra with Appl.*, 2(3):205–217, 1995.

- [9] V. Druskin and L. Knizhnerman. Extended Krylov subspaces: Approximation of the matrix square root and related functions. *SIAM Journal on Matrix Analysis and Applications*, 19(3):755–771, 1998.
- [10] N. Dunford and J.T. Schwartz. *Linear Operators Part II: Spectral Theory. Self Adjoint Operators in Hilbert Space*. Interscience Publishers, 1963.
- [11] L. Eldén. Numerical solution of the sideways heat equation by difference approximation in time. *Inverse Problems*, 11:913–923, 1995.
- [12] L. Eldén and F. Berntsson. Spectral and wavelet methods for solving an inverse heat conduction problem. In *International Symposium on Inverse Problems in Engineering Mechanics*, Nagano, Japan, 1998.
- [13] L. Eldén, F. Berntsson, and T. Regińska. Wavelet and Fourier methods for solving the sideways heat equation. *SIAM J. Sci. Comput.*, 21(6):2187–2205, 2000.
- [14] H. Engl, M. Hanke, and A. Neubauer. *Regularization of Inverse Problems*. Kluwer Academic Publishers, Dordrecht, the Netherlands, 1996.
- [15] L. C. Evans. *Partial Differential Equations*. American Mathematical Society, 1998.
- [16] E. Gallopoulos and Y. Saad. Efficient solution of parabolic equations by Krylov approximation methods. *SIAM J. Scient. Stat. Comput.*, 13(5):1236–1264, 1992.
- [17] M. S. Gockenbach. *Understanding and Implementing the Finite Element Method*. Soc. Industr. Appl. Math., 2006.
- [18] P. C. Hansen. *Rank-Deficient and Discrete Ill-Posed Problems. Numerical Aspects of Linear Inversion*. Society for Industrial and Applied Mathematics, Philadelphia, 1997.
- [19] M. Hochbruck and C. Lubich. Exponential integrators for quantum-classical molecular dynamics. *BIT, Numerical Mathematics*, 39(1):620–645, 1999.
- [20] M. Hochbruck, C. Lubich, and H. Selhofer. Exponential integrators for large systems of differential equations. *SIAM J. Scient. Comput.*, 19(5):1552–1574, 1998.
- [21] M. Hochbruck and A. Ostermann. Exponential Runge-Kutta methods for parabolic problems. *Applied Numer. Math.*, 53:323–339, 2005.
- [22] M. Hochbruck and J. van den Eshof. Preconditioning Lanczos approximations to the matrix exponential. *SIAM J. Scient. Comput.*, 27(4):1438–1457, 2006.
- [23] V. Maz’ya and T. Shaposhnikova. *Jacques Hadamard, A Universal Mathematician*. American Mathematical Society, 1998.
- [24] I. Moret and P. Novati. RD-rational approximations of the matrix exponential. *BIT, Numerical Mathematics*, 44(3):595–615, 2004.
- [25] F. Natterer and F. Wübbeling. A propagation-backpropagation method for ultrasound tomography. *Inverse Problems*, 11:1225–1232, 1995.
- [26] F. Natterer and F. Wübbeling. Marching schemes for inverse acoustic scattering problems. *Numerische Mathematik*, 100:697–710, 2005.
- [27] D. P. O’Leary and J. A. Simmons. A bidiagonalization-regularization procedure for large scale discretizations of ill-posed problems. *SIAM Journal on Scientific and Statistical Computing*, 2(4):474–489, 1981.
- [28] B. N. Parlett. *The symmetric eigenvalue problem*. SIAM, Philadelphia, 1998.
- [29] M. Papolizio and V. Simoncini. Acceleration techniques for approximating the matrix exponential operator. *SIAM J. Matrix Anal. Appl.*, 30:657–683, 2008.
- [30] Z. Qian and C.-L. Fu. Regularization strategies for a two-dimensional inverse heat conduction problem. *Inverse Problems*, 23:1053–1068, 2007.
- [31] T. Regińska. Sideways heat equation and wavelets. *J. Comput. Appl. Math.*, 63:209–214, 1995.
- [32] T. Regińska and L. Eldén. Solving the sideways heat equation by a wavelet-Galerkin method. *Inverse Problems*, 13:1093–1106, 1997.
- [33] T. Regińska and L. Eldén. Stability and convergence of a wavelet-Galerkin method for the sideways heat equation. *J. Inverse Ill-Posed Problems*, 8:31–49, 2000.
- [34] H. Tal-Ezer. Spectral methods in time for parabolic problems. *SIAM J. Numer. Anal.*, 26:1–11,

1989.

- [35] J. van den Eshof, A. Frommer, Th. Lippert, K. Schilling, and H.A. van der Vorst. Numerical methods for the QCD overlap operator. I: Sign-function and error bounds. *Comput. Phys. Commun.*, 146(2):203–224, 2002.
- [36] P. L. Woodfield, M. Monde, and Y. Mitsutake. Implementation of an analytical two-dimensional inverse heat conduction technique to practical problems. *Int. J. Heat Mass Transfer*, 49:187–197, 2006.