Comput Visual Sci (2011) 14:39–47
DOI 10.1007/s00791-011-0156-6

Higher-order schemes for the Laplace transformation method for parabolic problems

C. Douglas · I. Kim · H. Lee · D. Sheen

Received: 20 December 2010 / Accepted: 15 June 2011 / Published online: 3 September 2011

Abstract In this paper we solve linear parabolic problems using the three stage noble algorithms. First, the time discretization is approximated using the Laplace transformation method, which is both parallel in time (and can be in space, too) and extremely high order convergent. Second, higher-order compact schemes of order four and six are used for the the spatial discretization. Finally, the discretized linear algebraic systems are solved using multigrid to show the actual convergence rate for numerical examples, which are compared to other numerical solution methods.

Keywords Laplace inversion · Time+space parallel method · Higher-order schemes · Multigrid · Madpack

The research by Prof. Douglas is based on work supported in part by NSF grants CNS-1018072 and CNS-1018079 and Award No. KUS-C1-016-04, made by the King Abdullah University of Science and Technology (KAUST). The research by Prof. Sheen was partially supported by NRF-2008-C00043 and NRF-2009-0080533, 0450-20090014. The research by H. Lee was partially supported by Seoul R & D Program WR080951.

Communicated by: C. W. Oosterlee and A. Borzi.

C. Douglas (✉) · H. Lee
School of Energy Resources and Department of Mathematics, University of Wyoming, Laramie, WY 82072-3036, USA
e-mail: cdougla6@uwyo.edu

Present Address:
H. Lee
Bell Labs Seoul, Alcatel-Lucent, 7fl DMC R&D Center, Digital-Media City, E3-2, Sangam-Dong, Mapo-Gu, Seoul 120-270, Korea

I. Kim · D. Sheen
Department of Mathematics and Interdisciplinary Program in Computational Science & Technology, Seoul National University, Seoul 151-747, Korea

1 Introduction

In the effective and efficient numerical approximation of parabolic problems, there are three major issues to be considered: (1) the discretization in the time variable, (2) the discretization in the spatial variables, and (3) the linear solver at each time step. The first issue is usually resolved using backward Euler, forward Euler, Crank–Nicolson, or Runge–Kutta type time-marching algorithms. The second and third issues are pretty common in many numerical approximation problems, e.g., in obtaining numerical solutions of elliptic problems.

In this paper, based on efficient numerical schemes for the Laplace inversion, we use the Laplace transformation method instead of traditional time-marching algorithms in the discretization in the time axis. This method takes Laplace transforms in time of the parabolic problems, resulting in a set of independent complex-valued elliptic problems on a suitably chosen contour Γ. Each of the independent problems can be solved in parallel. Further, each of the independent problems can also be solved in parallel in the spatial domain, leading to parallel in time-space solvers.

The parareal algorithm [14,23] is another parallel in time-space method. It uses an additional coarse time mesh to solve all of the time steps repeated in parallel on the two sets of time meshes. The convergence of parareal has been shown to be at worst the number of fine time mesh points, i.e., no improvement over serial in time solvers. While parareal converges for some problems in many fewer time steps than the worst case, it is not guaranteed to be computationally beneficial for all problems. The method in this paper uses a predictable number of processors for any given problem based on the number of points on the contour Γ and the number of processors used to solve each spatial domain problem. Thus, it is guaranteed to be computationally useful, similar to standard

parallel parabolic solvers that only parallelize in the spatial domain.

After solving the set of Laplace-transformed problems, the time-domain solutions are obtained by discrete Laplace inversion on the contour Γ. In order to approximate the contour integration fast and accurately, there have been numerous schemes [4,5,26,31,33,35] proposed to approximate mainly the Laplace inversion precisely. More recently, the idea of using the Laplace transformation to solve parabolic problems has been developed actively [27,28], which emphasized the nature of parallelization as well as the deformation of the contour Γ to improve stability and convergence. Analysis and improvements can be found in [15,21,22,24,25,32,34] and the references therein.

Since the time discretization by the Laplace transformation is of arbitrarily high order, it is desirable to employ a high order scheme for the space discretization without unnecessarily deteriorating the sparse structure. Hence, we apply 9-point compact finite difference schemes for the approximation of elliptic operators. Since Young and Dauwalter [36] have developed higher-order compact schemes for general linear elliptic equations in 1965, many researchers have extended the idea in many directions to deal with variable coefficient cases [1,2,17], convection-diffusion problems [16,37,38], Helmholtz equations [29,30], and biharmonic equations [19], and so on. In the present paper we follow the approaches by Singer and Turkel [29,30] to solve Helmholtz-like problems that arise from the Laplace transformation of parabolic problems.

The linear systems obtained by the Laplace transformation in time are complex-symmetric, but non-Hermitian. In the discretization of Helmholtz-type equations several successful numerical solvers have been developed. Among them two fast ones were employed in our simulation: MADPACK, which is a very efficient abstract multigrid solver [8], and QMR [13]. Multigrid can be formulated as an algorithm for an abstract problem that is independent of the partial differential equation, domain, discretization method, and number of processors [6,7]. In such an abstract setting, problems not arising from partial differential equations can be treated also (c.f. aggregation-disaggregation methods) [8,10]. As it is known that there is no CG-type algorithm which is as fast as CG for non-Hermitian linear systems [11], other special techniques are necessary for a fast solver. The QMR algorithm, which is a Krylov subspace method with iterates characterized by a quasi-minimal residual property, performs very well for our problem [20]. We have tested our algorithm with HOADI and parareal schemes.

In Sect. 2, we explain the Laplace transformation method to discretize in the time direction. We use the deformation of the contour introduced in [28], which gives an arbitrary high-order convergence rate with a hyperbolic type deformation. In Sect. 3, fourth-order and sixth-order compact schemes for Dirichlet problems are given. Also, a fourth-order compact scheme for a mixed boundary value problem is given where a Neumann boundary condition is given on a part of boundary and a Dirichlet boundary condition is given on the rest of it. In Sect. 4 numerical examples are presented and compared to the high order ADI scheme [18]. In Sect. 5 we make some conclusions.

2 The Laplace transformation method

Consider a parabolic equation in an abstract setting that allows the proposed scheme to be applied to numerous problems of interest. When u_0 is a given initial function and A is a spatial elliptic operator with its eigenvalues located in the right half plane $\{z \in \mathbb{C} : \Re z > \lambda_0\}$, with some $\lambda_0 > 0$, we want to solve

$$\begin{aligned} &\frac{\partial u}{\partial t} + Au = f, \ t \in (0, T], \\ &\quad u(0) = u_0. \end{aligned} \tag{1}$$

Given some $z \in \mathbb{C}$ and a function $u(\cdot, t)$, the Laplace transform in time is given by

$$\widehat{u}(\cdot, z) := \mathscr{L}[u](z) = \int_0^\infty u(\cdot, t) e^{-zt}\, dt.$$

The Laplace transform of (1) is

$$z\hat{u} + A\hat{u} = u_0 + \hat{f}(\cdot, z), z \in \Gamma. \tag{2}$$

We now have an elliptic problem (2), which we solve using any reasonable elliptic solver. Formally, the solution $\hat{u}(z) = \hat{u}(\cdot, z)$ of (2) for each z is given by

$$\hat{u}(\cdot, z) = (zI + A)^{-1}(u_0(\cdot) + \hat{f}(\cdot, z)). \tag{3}$$

We assume that the real parts of singular points of $u_0(\cdot) + \hat{f}(\cdot, z)$ are bounded above by some positive number.

Let the integral contour Γ be a straight line parallel to the imaginary axis written in the form

$$\begin{aligned} \Gamma := \{&z \in \mathbb{C} : z(\omega) = \alpha + \mathrm{i}\omega, \ \text{where} \\ &\omega \in \mathbb{R} \text{ increases from } -\infty \text{ to } +\infty\}. \end{aligned} \tag{4}$$

The constant $\alpha \in \mathbb{R}$ in the contour is called the Laplace convergence abscissa and α is required to be greater than the real part of any singularity of $\widehat{u}(z)$. Then the *Laplace inversion formula* [3] is

$$u(\cdot, t) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \widehat{u}(\cdot, z) e^{zt}\, dz. \tag{5}$$

2.1 Deformation of contour

Note that as $|z|$ becomes large, if $z \in \Gamma$ has negative real parts, then the discretization error in numerically evaluating the integrand in (5) is significantly reduced for all positive t. Hence, we want to deform the contour to the left half plane while keeping all the singularities to the left of it. This observation led the authors in [28] to propose the smooth contour of hyperbola type by

$$\Gamma = \{z \in \mathbb{C} : z(\omega) = \zeta(\omega) + \mathrm{i}s\omega,\ \omega \in \mathbb{R} \text{ increasing}\},\quad \text{where } \zeta(\omega) = \gamma - \sqrt{\omega^2 + \nu^2}. \tag{6}$$

The shape of a hyperbola contour Γ is determined by the parameters ν, γ, and s. Note that γ and ν must be selected such that $\gamma - \nu$ is larger than the negative of the smallest eigenvalue of A and the real parts of singularities of $\hat{f}(z)$ since the contour cuts the real line at $\gamma - \nu$.

Concrete mathematical analysis requires that we assume that the deformed contour (6) lies in a region that we will now determine. Assume that the spectrum of A, $\sigma(A)$, lies in a sector Σ_δ for some $\delta \in (0, \frac{\pi}{2})$ such that

$$\sigma(A) \subset \Sigma_\delta = \{z \in \mathbb{C} : |\arg z| \le \delta,\ z \neq 0)\}, \tag{7}$$

and that the resolvent $(zI + A)^{-1}$ of $-A$ satisfies

$$\|(zI + A)^{-1}\| \le \frac{M}{1 + |z|} \text{ for } z \in \Sigma_{\pi-\delta} \cup B, \tag{8}$$

where M is a positive constant and B is a small ball about the origin. We assume henceforth that our deformed contour (6) lies in the region $\Sigma_{\pi-\delta} \cup B$. The first restriction (7) avoids the singular points of the integrand in (5) since the solution of Problem (1) can be rewritten as

$$u(t)\,(= u(\cdot, t)) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \big(zI + A\big)^{-1}\big(u_0 + \widehat{f}(z)\big)e^{zt}dz. \tag{9}$$

The integral contour must be kept away from the spectrum of $-A$ and the singular points of $\hat{f}(z)$ when we deform the contour. This restriction is quite natural since all eigenvalues of $-A$ and the singularities of $\hat{f}(z)$ have real parts bounded by a positive number. The second restriction (8) is used in the estimates of stability and errors.

Using the deformed contour (6), the inversion formula (5) can be rewritten using a real variable ø as an infinite integral,

$$u(\cdot, t) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \widehat{u}(\cdot, \zeta(\omega) + \mathrm{i}s\omega)(\zeta'(\omega) + \mathrm{i}s) \cdot e^{(\zeta(\omega)+\mathrm{i}s\omega)t} d\omega.$$

We change the infinite range $(-\infty, \infty)$ of the above integration into a finite region $(-1, 1)$ by the change of variables

$$y(\omega) = \tanh\left(\tfrac{\tau\omega}{2}\right) \text{ and } \omega(y) = \tfrac{2}{\tau}\tanh^{-1}(y) = \tfrac{1}{\tau}\log\tfrac{1+y}{1-y} \tag{10}$$

for a parameter $\tau > 0$. Specifically, this change of variables reduces the integral (10) on an infinite interval to an integral on a finite interval:

$$u(\cdot, t) = \frac{1}{2\pi \mathrm{i}} \int_{-1}^{1} \widehat{u}(\cdot, \zeta(\omega(y)) + \mathrm{i}s\omega(y))(\zeta'(\omega(y)) + \mathrm{i}s) \cdot e^{(\zeta(\omega(y))+\mathrm{i}s\omega(y))t}\omega'(y)dy. \tag{11}$$

2.2 Semi-discrete approximation

Using a quadrature rule, (11) can be discretized in time. For

$$z_j = z(\omega_j),\ \omega_j = \omega(y_j),\ \text{and } y_j = \frac{j}{N_z},\quad \text{for } -N_z < j < N_z, \tag{12}$$

the semi-discrete approximation of $u(\cdot, t)$ is explicitly given by

$$U_{N_z,\tau}(\cdot, t) = \frac{1}{2\pi \mathrm{i} N_z} \sum_{j=-N_z+1}^{N_z-1} \widehat{u}(\cdot, z_j)\frac{dz}{d\omega}(\omega_j)\frac{d\omega}{dy}(y_j)e^{z_j t}. \tag{13}$$

The quadrature scheme (13) was proven in [28] to have an arbitrary high order spectral convergence rate when the source term f has high order regularity. Formally this is stated as follows:

Theorem 1 (Sheen-Sloan-Thomée) *Let $u(t)$ be the solution of (1) and let $U_{N_z,\tau}(t)$ be its approximation defined by (13). Assume that $\widehat{f}(z)$ is analytic to the right of the contour Γ and continuous onto Γ, with $\widehat{f}^{(j)}(z)$ bounded on Γ for $j \le r$ and r an integer ≥ 1. Then for $t > r\tau$,*

$$\|U_{N_z,\tau}(t) - u(t)\| \le \tfrac{C_{r,s}}{N_z^r}\Big(1 + t^r + \tfrac{1}{\tau^r}\Big)\cdot e^{\gamma t}\Big(1 + \log_+ \tfrac{1}{t - r\tau}\Big)\cdot (\|u_0\| + \max_{k\le r} \sup_{z\in\Gamma} \|\widehat{f}^{(k)}(z)\|). \tag{14}$$

2.3 Key features of the proposed algorithm

We summarize with three key features about the method.

Remark 1 The implication of the Theorem 1 is such that the convergence of the proposed scheme is of order $O(N_z^{-r})$ with an arbitrary large $r > 0$ if $\hat{f} \equiv 0$ is analytic. This implies that the discretization errors in the time direction using the Laplace transformation method will be negligible compared to those caused from the spatial discretization part in solving parabolic problems with an analytic inhomogeneous term.

Remark 2 In the summand part of (13) a critical observation is that the

$$\widehat{u}(\cdot, z_j)\frac{dz}{d\omega}(\omega_j)\frac{d\omega}{dy}(y_j), \quad j = 0, \ldots, N_z,$$

are independent of t. Hence, we only have to approximate $\widehat{u}(\cdot, z_j)$ *once* by solving the complex-valued elliptic problem (2) for a set of z_j, $j = 0, 1, \cdots, N_z$, and save the results. Then, if we need the solution at a different time t, the same set of spatial solutions $\widehat{u}(\cdot, z_j)$, $j = 0, 1, \cdots, N_z$, can be reused in the evaluation of the summation (13). The only change are the factors $e^{z_j t}$ for the new time t.

Remark 3 Notice that each elliptic problem (2) for a z_j from the set of z_j, $j = 0, 1, \cdots, N_z$, is independent of other elliptic problems for the remaining z_j's, which suggests an embarrassingly parallel solution method. Communication times are minimized in solving the elliptic problems (2) in parallel by assigning each processor an independent elliptic problem to solve without communicating with other processors while solving its assigned problem. Unlike many other higher-order schemes (e.g., [18]), ours is embarrassingly parallel and scales well as $N_z \to \infty$.

3 High order accurate schemes

We now restrict to the case of $A = -a\Delta$ in two dimensions with $f \equiv 0$ and $\emptyset = (0, 1)^2$. Let the domain $\emptyset$ be discretized into $N_{\mathbf{x}} \times N_{\mathbf{x}}$ uniform rectangles with sides $h = \frac{1}{N_{\mathbf{x}}}$ and mesh points $(x_j, y_k) = (jh, kh)$ for $j = 0, \cdots, N_{\mathbf{x}}$, $k = 0, \cdots, N_{\mathbf{x}}$. Then (2) is of Helmholtz-type, for which fourth and sixth order finite difference schemes have been derived by Singer-Turkel [29,30]. So,

$$z\widehat{u} - a(\widehat{u}_{xx} + \widehat{u}_{yy}) = u_0, \tag{15}$$

where $z \in \Gamma \subset \mathbb{C}$. Let $\widehat{u}_{j,k}$ be a numerical approximation to $\widehat{u}(x_i, y_j)$ and $(u_0)_{j,k} = u_0(x_i, y_j)$ the approximate initial value. A 9-point compact finite difference scheme is written in the form

$$\begin{aligned} &A_0\widehat{u}_{j,k} + A_s\sigma_s + A_c\sigma_c = B_0(u_0)_{j,k} + B_s\psi_s + B_c\psi_c,\\ &\quad j, k = 1, \cdots, N_{\mathbf{x}} - 1,\\ &\widehat{u}_{j,k} = 0 \quad \text{if} \quad jk(j - N_{\mathbf{x}})(k - N_{\mathbf{x}}) = 0, \end{aligned} \tag{16}$$

where

$$\begin{aligned} \sigma_s &= \widehat{u}_{j,k+1} + \widehat{u}_{j+1,k} + \widehat{u}_{j,k-1} + \widehat{u}_{j-1,k},\\ \sigma_c &= \widehat{u}_{j+1,k+1} + \widehat{u}_{j+1,k-1} + \widehat{u}_{j-1,k-1} + \widehat{u}_{j-1,k+1},\\ \psi_s &= (u_0)_{j,k+1} + (u_0)_{j+1,k} + (u_0)_{j,k-1} + (u_0)_{j-1,k},\\ \psi_c &= (u_0)_{j+1,k+1} + (u_0)_{j+1,k-1}\\ &\quad + (u_0)_{j-1,k-1} + (u_0)_{j-1,k+1}. \end{aligned}$$

With the following coefficients in (16),

$$\begin{aligned} &A_0 = \tfrac{10a}{3} + h^2 z(1 + \tfrac{h^2 z}{12a}),\ A_s = -\tfrac{2a}{3},\ A_c = -\tfrac{a}{6},\\ &B_0 = h^2(\tfrac{2}{3} + \tfrac{h^2 z}{12a}),\ \text{and}\ B_s = \tfrac{h^2}{12}, \end{aligned}$$

(16) with $B_c = 0$ becomes a 4th-order approximation scheme for the the homogeneous Dirichlet problem [30]. Instead of Dirichlet boundary conditions imposed on all boundary parts, let us consider a special case such that only the boundary condition at the left-side boundary is replaced by the Neumann boundary condition $\frac{\partial \widehat{u}}{\partial v}(0, y) = \widehat{g}(y)$, $0 < y < 1$. In addition to (16) again with $B_c = 0$, the following approximation for $j = 0$ is added

$$\begin{aligned} &A_0\widehat{u}_{0,k} + A_s(\widehat{u}_{0,k-1} + 2\widehat{u}_{1,k} + \widehat{u}_{0,k+1}) + 2A_\sigma(\widehat{u}_{1,k-1} + \widehat{u}_{1,k+1})\\ &\quad = B_0(u_0)_{0,k} + B_s\psi_s\\ &\qquad + a\Big(1 - \frac{h^2 z}{6a}\Big)^{-1}\Big(2h\widehat{g}_k + \frac{h^3}{3a}(u_{0x})_{0,k}\Big). \end{aligned} \tag{17}$$

This scheme is still of 4th order, and furthermore the replacement u_{0x} with second-order discretization in (17) still preserves the convergence [29].

Concerning a 6th-order convergent scheme for spatial approximation, we have the following formula for the homogeneous Dirichlet problem:

$$\begin{aligned} &A_0 = \tfrac{10a}{3} + h^2\Big(\tfrac{46z}{45} + \tfrac{h^2}{12}\tfrac{z^2}{a} + \tfrac{h^4}{360}\tfrac{z^3}{a^2}\Big),\\ &A_s = -\Big(\tfrac{2a}{3} + \tfrac{h^2}{90}z\Big),\ A_c = -\Big(\tfrac{a}{6} - \tfrac{h^2}{180}z\Big),\ \text{and}\\ &B_0 = h^2\Big(1 + \tfrac{h^2}{12}\tfrac{z}{a} + \tfrac{h^4}{360}\tfrac{z^2}{a^2}\Big). \end{aligned} \tag{18}$$

Then, a compact 6th-order scheme is given [30] by (16) with the right hand side replaced by

$$\begin{aligned} &B_0(u_0)_{j,k} + \Big(\frac{h^4}{12} + \frac{h^6}{360}\frac{z}{a}\Big)(u_{0xx} + u_{0yy})\\ &\quad + \frac{h^6}{360}(4u_{0xxyy} + u_{0xxxx} + u_{0yyyy}). \end{aligned}$$

Observe that the 4th-order schemes can be regarded as shifted linear forms for which the special algorithm [12] can be applied, while the 6th-order scheme is not a shifted linear form since the coefficients A_s and A_c in the left hand side depend on z. The linear systems for both cases, however, are non-Hermitian and thus the usual CG algorithm are not applicable. Instead, we can apply a multigrid or a QMR algorithm for solving these non-Hermitian linear systems of the form $\mathbf{Ax} = \mathbf{b}$.

4 Numerical examples

In this section, we consider two examples to demonstrate that we have a high order convergence in both time and space.

We solve the elliptic problems using MADPACK [8–10], which implements abstract multilevel algorithms. QMR [13]

Table 1 Convergence of the 4th-order scheme using MADPACK for Example 1

z	ϵ_{10}	ϵ_{20}	ρ_{20}	ϵ_{40}	ρ_{40}	ϵ_{80}	ρ_{80}
(10.57, 0.00)	0.170E-03	0.143E-04	3.57	0.960E-06	3.90	0.611E-07	3.97
(10.34, 3.21)	0.168E-03	0.141E-04	3.57	0.947E-06	3.90	0.603E-07	3.97
(9.62, 6.49)	0.162E-03	0.136E-04	3.57	0.909E-06	3.90	0.578E-07	3.98
(8.36, 9.90)	0.152E-03	0.127E-04	3.58	0.845E-06	3.91	0.536E-07	3.98
(6.47, 13.56)	0.138E-03	0.115E-04	3.58	0.759E-06	3.93	0.480E-07	3.98
(3.75, 17.58)	0.120E-03	0.101E-04	3.57	0.658E-06	3.95	0.414E-07	3.99
(−0.13, 22.18)	0.100E-03	0.864E-05	3.53	0.550E-06	3.97	0.344E-07	4.00
(−5.82, 27.75)	0.776E-04	0.714E-05	3.44	0.442E-06	4.01	0.273E-07	4.01
(−14.87, 35.16)	0.527E-04	0.570E-05	3.21	0.338E-06	4.08	0.206E-07	4.04
(−32.36, 47.11)	0.265E-04	0.425E-05	2.64	0.236E-06	4.17	0.139E-07	4.09
(−63.75, 65.24)	0.103E-04	0.289E-05	1.84	0.159E-06	4.18	0.884E-08	4.17

was also investigated as the linear equation solver. Since QMR's convergence rates were almost the same as those for using multigrid, we leave these tables out of this paper and refer the interested reader to [20].

Multigrid methods are well known to provide very fast, including sometimes linear in time and space, solutions to elliptic problems. It is natural to try such a solver. MADPACK works either on a single processing core or many using MPI to communicate with other cores.

Example 1 Consider the set of complex-valued elliptic problems:

$$z\widehat{u} - \frac{1}{5\pi^2}(\widehat{u}_{xx} + \widehat{u}_{yy}) = e\,\sin(2\pi x)\sin(\pi y) \text{ in } [0,1]^2,$$
$$u = 0 \text{ on } \partial[0,1]^2. \tag{19}$$

This example comes from the Laplace transformation of

$$u_t - \frac{1}{5\pi^2}(u_{xx} + u_{yy}) = 0, \text{ and } u(x,y,0) = e\,\sin(2\pi x)\sin(\pi y),$$

whose exact solution is given by

$$u(x,y,t) = e^{1-t}\sin(2\pi x)\sin(\pi y).$$

We adopt the contour representation in the form of (11). Let

$$\Gamma = \{z \in \mathbb{C} : z(\omega) = \zeta(\omega) + \mathrm{i}s\omega, \omega \in \mathbb{R}, \ \omega \text{ increasing}\},$$
$$\omega(y) = \frac{2}{\tau}\tanh^{-1}(y) = \frac{1}{\tau}\log\frac{1+y}{1-y}, \text{ and}$$
$$\zeta(\omega) = \gamma - \sqrt{\omega^2 + \nu^2}.$$

The error $\|U_{N_z,\tau}(t) - u(t)\|$ in (14) can be understood as the summation of discretization error and the truncation error. In [34], the authors suggest a way to find an optimal set of parameters by balancing the discretization and truncation errors. In our approach, we first transform the infinite interval $(-\infty, \infty)$ to a finite interval $(-1, 1)$ with parameter τ and choose the number N_z with which $(-1, 1)$ is uniformly partitioned into $2N_z - 1$ subintervals. Therefore, the discretization and truncation parts are simultaneously affected by the choice of τ and N_z. Although the optimal choice of parameters in [34] does not fit quite to our case, we adopt heuristically this approach. Recalling the formula in [34],

$$\alpha = 1.1721,\ a(\alpha) = \cosh^{-1}\left(\frac{2\alpha}{(4\alpha - \pi)\sin\alpha}\right),$$
$$\gamma = \frac{4\pi\alpha - \pi^2}{a(\alpha)}\frac{N_z}{t},\ \nu = \gamma\sin(\alpha),\ s = \cot(\alpha), \text{ and}$$
$$\tau = \frac{\log(2N_z - 1)}{\gamma\sin(\alpha)\sinh\left(a(\alpha)\frac{N_z - 1}{N_z}\right)}, \tag{20}$$

the parameters are chosen as $\gamma = 134.8$, $\nu = 124.2$, $s = 0.4213$ and $\tau = 0.02633$. Tables 1–2 demonstrate clearly that the spatial errors decay asymptotically at the rate of 4 and 6 orders for the chosen contour points z_j's. Notice that the set of eigenvalues of $-\frac{1}{5\pi^2}(\partial_x^2 + \partial_y^2)$ is $\{\frac{k^2+l^2}{5} : k, l = 1, 2, \cdots\} = \{\frac{2}{5}, 1, \frac{8}{5}, \cdots\}$. Thus, instead of choosing the parameters as above, any other reasonable contour Γ of the form (6) which cuts the real axis at $\gamma - \nu > 0$ will be sufficient to be adopted for solving Problem (19).

We applied the 4th and 6th-order schemes for different z's and used these approximations for Laplace inversion at time $t = 1$. For inversion we used $N_z = 30$ for the number of points on the contour with $N_{\mathbf{x}} \in \{10, 20, 40, 80\}$ for the number points in the spatial mesh discretization. We compared the approximate solutions computed using our method with the exact solution $u(t, x, y) = e^{1-t}\sin(2\pi x)\sin(\pi y)$. For reference, the 30 contour points are depicted in Fig. 1.

We compare our method with the high order ADI method (HOADI) in [18], a very fast time-marching scheme of second order in time and fourth order in space. We used Karaa's code with our example in our comparisons. We discretize the time interval [0, 1] by 1,000, 500, and 100 steps and the space by meshes of size 10×10, 20×20, 40×40, and 80×80. The L^2-errors and reduction rates at $t = 1$ are

Table 2 Convergence of the 6th-order scheme using MADPACK for Example 1

z	ϵ_{10}	ϵ_{20}	ρ_{20}	ϵ_{40}	ρ_{40}	ϵ_{80}	ρ_{80}
(10.57, 0.00)	0.138E-05	0.304E-07	5.50	0.513E-09	5.89	0.817E-11	5.97
(10.34, 3.21)	0.136E-05	0.299E-07	5.51	0.503E-09	5.89	0.801E-11	5.97
(9.62, 6.49)	0.131E-05	0.284E-07	5.53	0.475E-09	5.90	0.755E-11	5.98
(8.36, 9.90)	0.123E-05	0.260E-07	5.56	0.433E-09	5.91	0.686E-11	5.98
(6.47, 13.56)	0.113E-05	0.232E-07	5.61	0.380E-09	5.93	0.601E-11	5.98
(3.75, 17.58)	0.103E-05	0.201E-07	5.68	0.323E-09	5.96	0.509E-11	5.99
(−0.13, 22.18)	0.937E-06	0.171E-07	5.78	0.267E-09	6.00	0.416E-11	6.00
(−5.82, 27.75)	0.860E-06	0.142E-07	5.92	0.213E-09	6.06	0.328E-11	6.02
(−14.87, 35.16)	0.758E-06	0.116E-07	6.03	0.162E-09	6.16	0.246E-11	6.04
(−32.36, 47.11)	0.345E-06	0.941E-08	5.20	0.113E-09	6.38	0.167E-11	6.08
(−63.75, 65.24)	0.719E-07	0.909E-08	2.98	0.769E-10	6.89	0.110E-11	6.12

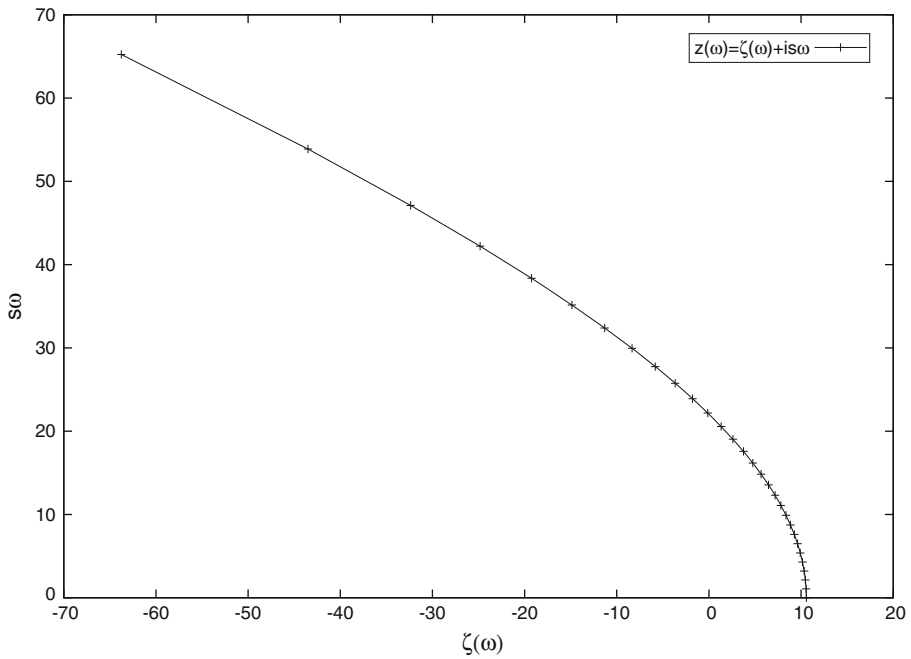

Fig. 1 Contour and z-points used in Laplace inversion for Example 1

reported in Table 4. Comparing these errors and reduction rates for 1,000 and 500 time steps in Table 4 with those for 4th order scheme in Table 3, the results are similar. However, we emphasize that only 30 elliptic solves are required for our method while 500 to 1,000 elliptic solves are required for the high order ADI method. If we reduce the time steps to 100, we see that the time errors dominate in the high order ADI scheme as shown in the last row of Table 4. Instead, our method uses an arbitrarily high order scheme in time discretization so that we can guarantee that the time error does not dominate.

As we stressed in Sect. 2, each elliptic problem for z_j, $j = 0, 1, \cdots, N_z$ is independent of each of the elliptic problems for the remainining z_j's. This property naturally results in a parallelization method that assigns each elliptic problem to a different processor (or core), which can be enhanced with spatial parallelization.

Example 2 Consider the following parabolic problem with the mixed boundary condition:

$$
\begin{aligned}
&u_t - \frac{1}{\pi^2 - 1}\left(u_{xx} + u_{yy}\right) = 0 \\
&\quad \text{for} \quad (\mathbf{x}, t) \in (0, 1)^2 \times (0, T], \\
&u_x = \frac{\pi}{z+1}\cos(\pi x)\cosh(y) \\
&\quad \text{for} \quad (\mathbf{x}, t) \in \{0\} \times (0, 1) \times (0, T], \\
&u = \frac{1}{z+1}\sin(\pi x)\cosh(y) \\
&\quad \text{for} \quad (\mathbf{x}, t) \in \partial(0, 1)^2 \setminus [\{0\} \times (0, 1)] \times (0, T], \\
&u(\mathbf{x}, 0) = \sin(\pi x)\cosh(y) \ \text{ for } \ (\mathbf{x}, t) \in (0, 1)^2.
\end{aligned}
\tag{21}
$$

Table 3 Full convergence of Laplace transformation method using MADPACK for Example 1

Type	ϵ_{10}	ϵ_{20}	ρ_{20}	ϵ_{40}	ρ_{40}	ϵ_{80}	ρ_{80}
4th order	0.304E-03	0.170E-04	4.16	0.102E-05	4.06	0.630E-07	4.01
6th order	0.122E-04	0.191E-06	6.00	0.295E-08	6.02	0.486E-10	5.92

Table 4 Full convergence of higher order ADI method in [18] for Example 1

Type	ϵ_{10}	ϵ_{20}	ρ_{20}	ϵ_{40}	ρ_{40}	ϵ_{80}	ρ_{80}
HOADI (1000 time steps)	0.268E-03	0.165E-04	4.02	0.101E-05	4.03	0.428E-07	4.56
HOADI (500 time steps)	0.268E-03	0.165E-04	4.02	0.945E-06	4.12	0.222E-07	5.41
HOADI (100 time steps)	0.266E-03	0.144E-04	4.21	0.114E-05	3.65	0.210E-05	−0.544

Table 5 Convergence of the 4th-order scheme using MADPACK for Example 2

z	ϵ_{10}	ϵ_{20}	ρ_{20}	ϵ_{40}	ρ_{40}	ϵ_{80}	ρ_{80}
(10.57, 0.00)	0.596E-04	0.373E-05	4.00	0.234E-06	4.00	0.146E-07	4.00
(10.34, 3.21)	0.593E-04	0.372E-05	3.99	0.233E-06	3.99	0.146E-07	4.00
(9.62, 6.49)	0.582E-04	0.368E-05	3.99	0.231E-06	3.99	0.145E-07	4.00
(8.36, 9.90)	0.564E-04	0.361E-05	3.97	0.226E-06	3.99	0.142E-07	4.00
(6.47, 13.56)	0.535E-04	0.349E-05	3.94	0.219E-06	3.99	0.137E-07	4.00
(3.75, 17.58)	0.496E-04	0.331E-05	3.91	0.209E-06	3.98	0.131E-07	4.00
(−0.13, 22.18)	0.448E-04	0.311E-05	3.85	0.197E-06	3.98	0.123E-07	4.00
(−5.82, 27.75)	0.393E-04	0.286E-05	3.78	0.181E-06	3.98	0.114E-07	3.99
(−14.87, 35.16)	0.341E-04	0.253E-05	3.75	0.163E-06	3.96	0.102E-07	3.99
(−32.36, 47.11)	0.303E-04	0.218E-05	3.80	0.140E-06	3.96	0.878E-08	3.99
(−63.75, 65.24)	0.262E-04	0.163E-05	4.01	0.115E-06	3.82	0.728E-08	3.99

The Neumann and Dirichlet boundary condition are imposed on the boundary portion $\{0\} \times (0, 1)$ and the rest of the boundary $\partial(0, 1)^2 \setminus [\{0\} \times (0, 1)]$, respectively. The exact solution is given by

$$u(x, y, t) = e^{-t} \sin(\pi x) \cosh(y).$$

By applying the Laplace transformation to (21), we have the following:

$$z\widehat{u} - \frac{1}{\pi^2 - 1}(\widehat{u}_{xx} + \widehat{u}_{yy}) = \sin(\pi x) \cosh(y)$$

$$\text{for } \mathbf{x} \in (0, 1)^2,$$

$$\widehat{u}_x = \frac{\pi}{z + 1} \cos(\pi x) \cosh(y) \quad \text{for} \quad \mathbf{x} \in \{0\} \times (0, 1),$$

$$\widehat{u} = \frac{1}{z + 1} \sin(\pi x) \cosh(y)$$

$$\text{for} \quad \mathbf{x} \in \partial(0, 1)^2 \setminus [\{0\} \times (0, 1)]\,. \tag{22}$$

We calculate the approximate solution of (22) using a 4th order convergence scheme with Neumann boundary condition as in (17). MADPACK is used as the linear solver and the solution is used in the Laplace inversion formula with the same coefficients as in Example 1 for generating the contour. The results are shown in Tables 5–6.

Example 3 We consider the parallel performance of our algorithm for Problem (19). We have used the same parameters as in Example 1 except $N_Z = 32$ and $N_x \times N_x = 160 \times 160$ in the spatial mesh. Computations were performed on a cluster with 44 Intel Xeon Quad Core processors each of which has 2 Gbytes of RAM. Message Passing was done with the MPI interface using 1 GHz Ethernet. We have tested the parallel runs with 1, 2, 4, 8, 16, 32 number of processors. The comparison of parallel performances between the Laplace transformation method and the parareal method are shown in Table 7. In Table 7, one can observe that the parallel Laplace transformation method is much better than the parareal method in their parallel performance. Indeed, our algorithm computes one spatial elliptic problem of size $N_x \times N_y$ only once per each of required processors, while the parareal algorithm computes spatial elliptic problems of the same size iteratively several times until convergence to and from the fine grid and coarse grid with respect to time.

Table 6 Full convergence of Laplace transformation method using MADPACK for Example 2

Solver	ϵ_{10}	ϵ_{20}	ρ_{20}	ϵ_{40}	ρ_{40}	ϵ_{80}	ρ_{80}
MADPACK	0.373E-04	0.241E-05	3.95	0.151E-06	3.99	0.944E-08	4.00

Table 7 Comparison of parallel performance between Laplace transformation method (LTM) and parareal method for Example 1

np	LTM		Parareal method	
	Time	Speedup	Time	Speedup
1	17.501	1	17.815	1
2	9.363	1.87	11.360	1.56
4	5.741	3.05	7.701	2.31
8	3.405	5.15	4.983	3.58
16	1.709	10.29	3.322	5.36
32	0.862	20.34	2.552	6.98

5 Conclusions

In this paper we applied the Laplace transform and the inverse Laplace transform to a class of parabolic problems. The advantages include the following key points:

- The convergence rate associated with the time derivative can be made arbitrarily high order, which actually appears in numerical examples that we gave in Sect. 4.
- We can vary the order of the spatial discretization so that we can balance the time and space errors.
- The solution method becomes embarrassingly parallel, so that time stepping is far faster than conventional methods such as high order ADI solvers.
- Comparing to higher order ADI schemes or parareal algorithms, our method solves spatial problems only once per each contour points while others solve spatial problems iteratively several times until convergence with respect to time.
- The number of processing cores can be optimized by picking an ideal number of points N_z on the contour Γ. Each of the N_z elliptic problems can be solved independently of the other problems. Additionally, all N_z problems can be solved in parallel themselves using parallel methods for the elliptic problems (e.g., parallel multigrid or a domain decomposition method).
- The method clearly extends to three dimensional spatial problems in a clean way that is still embarrassingly parallel for the time stepping.

Acknowledgments We thank Prof. Karaa for providing the high order ADI code used in [18].

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