

LAPLACE TRANSFORM METHOD FOR PARABOLIC PROBLEMS WITH TIME-DEPENDENT COEFFICIENTS*

HYOSEOP LEE[†], JINWOO LEE[‡], AND DONGWOO SHEEN[§]

Abstract. The Laplace transform method has proven to be very efficient for dealing with parabolic problems whose coefficients are time independent, and it is easily parallelizable. However, the method has not been proven to be applicable to linear problems whose coefficients are time dependent. The reason is that the Laplace transform of two time-dependent functions leads to a convolution of the Laplace transformed functions in the dual variable. In this paper, we propose a Laplace transform method to linear parabolic problems with time-dependent coefficients, which is as efficient as the method for parabolic problems with time-independent coefficients. Several numerical results are provided, which support the efficiency of the proposed scheme.

Key words. Laplace transform, time dependent, evolution equation, parallel method

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1. Introduction. Recently there has been increasing attention given to applying the Laplace transform method to solving evolution problems [10, 15, 17, 18, 20, 21, 22, 23, 24, 27], including integro-differential equations [11, 19] and backward parabolic problems [12, 13], to mention a few. Additional relevant references can be found in numerical analysis journals. Although the Laplace transform schemes have proven to be very efficient, and some of them are of spectral convergence rate in time discretization [4, 5, 7, 8, 9, 25], a serious drawback is that this kind of linear transform method is not easily applicable to time-dependent coefficient problems. The aim of this paper is to tackle this difficulty.

Let us consider the following evolution equation with time-dependent coefficients:

$$(1.1a) \quad \frac{\partial u}{\partial t}(t) + A(t)u(t) = 0, \quad t \in (0, T_*],$$

$$(1.1b) \quad u(0) = u_0,$$

where $A(t)$ is a time-dependent elliptic operator in a Banach space H with its domain $D(A(t))$ dense in H for all $t < T_*$. Denote the Laplace transform of $v(t)$ by

$$\widehat{v}(z) = \int_0^\infty v(t)e^{-zt} dt.$$

Then, if the Laplace transform of $A(t)u(t)$ was regarded as a separable form

$$\widehat{B}(z)\widehat{u}(z),$$

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[†]Bell Labs Seoul, R&D Center, Digital Media City E3-2, Sangam-dong, Mapo-gu, Seoul 120-270, Korea (hs.lee@alcatel-lucent.com). This author was supported by Seoul Metropolitan Government work program grant WR080951.

[‡]Department of Mathematics, Kwangwoon University, Seoul 139-701, Korea (jinwoolee@kw.ac.kr). This author was supported by Kwangwoon University in 2010.

[§]Department of Mathematics and Interdisciplinary Program in Computational Science and Technology, Seoul National University, Seoul 151-747, Korea (sheen@snu.ac.kr).

with a suitable operator of $\widehat{B}(z)$, one might be able to apply the Laplace transform method. However, the fundamental nature of the linear integral transform (e.g., Laplace transform) of the product $A(t)u(t)$ is of convolution type, and thus time-dependent coefficient problems and nonlinear problems are not tractable with the usual Laplace transform method.

In this paper we propose a new method in which we can apply the Laplace transform method to time-dependent coefficient problems.

Gavrilyuk and Makarov [6] proposed an iteration scheme to solve (1.1), and López-Fernández [14] combined a multistep time-stepping method with the Laplace transform method to compute solutions at each time step. Here, we briefly review the method given in [6] and compare it to our method. Let $0 = t_0 < t_1 < \cdots < t_n = 1$ be nodes and let $\tau_k = t_k - t_{k-1}$, where t_1, \dots, t_{n-1} may be chosen as Chebyshev nodes as in [6]. Then the time-dependent problem (1.1) can be written as a set of time-independent problems with inhomogeneous terms,

$$(1.2a) \quad \frac{\partial u}{\partial t}(t) + A(t_k)u(t) = (A(t_k) - A(t))u(t), \quad t \in (t_{k-1}, t_k],$$

$$(1.2b) \quad u(t_{k-1}) = u_{k-1},$$

where $u_k = u(t_k)$ for $k = 1, \dots, n$. The solution of (1.2) can be written as

$$(1.3) \quad u(t) = e^{-(t-t_{k-1})A(t_k)}u_{k-1} + \int_{t_{k-1}}^t e^{-(t-\eta)A(t_k)}(A(t_k) - A(\eta))u(\eta) d\eta$$

for $t \in [t_{k-1}, t_k]$. Let $L_{p,n-1}(\eta)$, $p = 1, \dots, n$, be the Lagrange interpolation basis polynomials of degree $n-1$ associated with the nodes t_1, \dots, t_n , such that $L_{p,n-1}(t_k) = \delta_{pk}$, the Kronecker delta. Then the system (1.3) is equivalently written as in the following system of linear equations with respect to the unknown function values u_k , $k = 1, \dots, n$:

$$(1.4) \quad u_k = e^{-\tau_k A_k} u_{k-1} + \sum_{p=1}^n \alpha_{kp} u_p, \quad k = 1, \dots, n,$$

where

$$\alpha_{kp} = \int_{t_{k-1}}^{t_k} e^{-(t_k-\eta)A(t_k)}[A(t_k) - A(\eta)]L_{p,n-1}(\eta) d\eta.$$

Notice that (1.4) is a system of linear equations for u_k , $k = 1, \dots, n$, with given data u_0 . Let $\mathbf{u} = (u_1, \dots, u_n)^t \in H^n$, and let $\boldsymbol{\alpha}$ be the $n \times n$ operator matrix with its k th component α_{kp} . Then, (1.4) is equivalent to

$$(\mathbf{S} - \boldsymbol{\alpha})\mathbf{u} = \mathbf{u}_0, \quad \mathbf{u}_0 = (e^{-\tau_1 A_1} u_0, 0, \dots, 0)^t \in H^n,$$

where

$$\mathbf{S} = \begin{pmatrix} I & 0 & \cdots & 0 & 0 \\ -e^{-\tau_1 A_1} & I & \cdots & 0 & 0 \\ 0 & e^{-\tau_2 A_2} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & I & 0 \\ 0 & 0 & \cdots & -e^{-\tau_{n-1} A_{n-1}} & I \end{pmatrix}.$$

The problem can be solved by a reasonable iterative scheme, for instance,

$$\mathbf{u}^{(k+1)} = \mathbf{S}^{-1}(\boldsymbol{\alpha}\mathbf{u}^{(k)} + \mathbf{u}_0), \quad k = 0, 1, \dots, \quad \mathbf{u}^{(0)} \text{ arbitrary.}$$

Observe that each multiplication $e^{-\tau_k A_k} u_j^{(k)}$ amounts to a Laplace inversion procedure by solving partial differential equations of the form

$$\begin{aligned} \frac{\partial u}{\partial t}(t) + A(t_k)u(t) &= 0, \quad t \in (t_{k-1}, t_k], \\ u(t_{k-1}) &= u_j^{(k)}. \end{aligned}$$

The whole procedure is a bit costly.

In this work we will look at the problem (1.1) from a fundamentally different viewpoint. We reformulate the problem into a time-independent one that provides an identical solution at any given time. Then we apply the Laplace transform method to the reformulated problem. The computational cost of our scheme is essentially the same as the time-independent one. We will discuss this kind of method for nonlinear problems in a forthcoming paper.

2. The Laplace transform method. Before presenting a new method for the time-dependent coefficient problem, let us briefly review the Laplace transform method for the time-independent case. Consider the following evolution equation:

$$(2.1a) \quad \frac{\partial u}{\partial t}(t) + Au(t) = 0, \quad t \in (0, T_*],$$

$$(2.1b) \quad u(0) = u_0,$$

where u_0 is a given initial data in a Banach space H , and $A : H \rightarrow H$ is an elliptic operator, which is, for the moment, assumed to be independent of t .

Let Σ be a sector in the complex plane that is contained in the resolvent set $\rho(-A)$ of $-A$, where $\rho(-A) = \{\lambda \in \mathbb{C} \mid \lambda I + A \text{ is invertible}\}$. With an appropriate contour Γ in the sector Σ , we take the Laplace transform with respect to the time variable to get the following set of complex-valued elliptic problems:

$$(2.2) \quad (zI + A)\hat{u}(z) = u_0, \quad z \in \Gamma.$$

The problems (2.2) can be approximated by using any space discretization method such as finite element, finite difference, or finite volume methods. Denote by $zI_h + A_h$ the spatial approximation of $zI + A$ and denote by $u_{h,0}$ the spatial approximation of u_0 . Then the spatial approximate solution $\hat{u}_h(z)$ is represented by $(zI_h + A_h)^{-1}u_{0,h}$. Then, the time-domain solution $u_h(t) = u_h(\cdot, t)$ is recovered via the Laplace inversion formula:

$$(2.3) \quad u_h(\cdot, t) = \frac{1}{2\pi i} \int_{\Gamma} (zI_h + A_h)^{-1} u_{0,h} e^{tz} dz.$$

A careful choice of a finite number of points $z_k, k = -N_z, \dots, N_z$, on the contour Γ with suitable weights approximates the integral (2.3) exponentially. Several numerical schemes for Laplace inversion have been analyzed in the recent monographs [2, 9].

If the spatial operator A in (2.1) is time dependent, i.e., $A = A(t)$, and one takes the Laplace transform of the equation, a convolution-type equation is obtained:

$$(2.4) \quad z\hat{u}(z) + (\hat{a} * \hat{u})(z) = u_0.$$

Certainly it is not desirable to solve the problem (2.4) since it requires saving and using all of the other values of $\hat{u}(z_k)$'s for $z_k \neq z_j$ when one wants to solve for $\hat{u}(z_j)$. We thus try to attack the problem from a different direction.

3. Avoiding convolution. Here we make some observations that might lead to a new formulation. If $A(t) = a(t)A_0$ for a positive scalar function $a(t)$ and a time-independent spatial operator A_0 , we take the following change of variables:

$$(3.1) \quad T(t) = \int_0^t a(\tau) \, d\tau, \quad U(T) = u(t),$$

so that $\frac{\partial u}{\partial t} = \frac{\partial U}{\partial T}a(t)$. Then, the problem (1.1) can be rewritten in the form

$$(3.2a) \quad \frac{\partial U}{\partial T} + A_0 U(T) = 0, \quad T \in (0, \tilde{T}_*],$$

$$(3.2b) \quad U(0) = u_0,$$

where $\tilde{T}_* = T(T_*)$. Observe that the solution of the reformulated problem (3.2) at the later time T is identical to the solution $u(t)$ of the original problem (2.1), due to (3.1). We stress that the spatial operator A_0 in (3.2) is independent of time.

One can then apply the Laplace transform method mentioned in sections 1 and 2 to solve (3.2) easily since its coefficient is independent of time. Thus, with an appropriate choice of a contour Γ contained in Σ , the solution can be written as follows:

$$(3.3) \quad u(t) = U(T) = \frac{1}{2\pi i} \int_{\Gamma} [\zeta I + A_0]^{-1} u_0 e^{\zeta T} \, d\zeta.$$

If there is an additional reaction term so that $\frac{\partial u}{\partial t} + a(t)A_0 u + b(t)u = 0$, the term can be eliminated in a simple way. For example, by multiplying by an integrating factor $\mu(t) := e^{\int_0^t b(\tau) \, d\tau}$ to the equation, we obtain $\frac{d}{dt} [\mu(t)u] + a(t)A_0 [\mu(t)u] = 0$. Then the idea of (3.1)–(3.3) can be applied to find $\mu(t)u(t)$. We note that $\mu(t)$ is a scalar function. However, the idea of using integrating factors is not always applicable. For example, if there is an additional convection term, it is not immediately clear how to apply the method.

To generalize the above time-independent formulation, we start with (3.3). Recall that if $f \in \mathcal{F}(A)$ is analytic in a domain containing the closure of an open set U containing $\sigma(A)$, the Dunford–Cauchy integral formula [3] is given by

$$(3.4) \quad f(A) = \frac{1}{2\pi i} \int_{\partial U} f(z)(zI - A)^{-1} \, dz;$$

i.e., the integral is identical to the value of f at the pole of the integrand. This leads us to write $u(t)$ in (3.3) formally as follows:

$$\begin{aligned} u(t) &= \frac{1}{2\pi i} \int_{\Gamma} [\zeta I + T A_0]^{-1} u_0 e^{\zeta} \, d\zeta \\ &= \frac{1}{2\pi i} \int_{\Gamma} \left[\zeta I + \int_0^t A(\tau) \, d\tau \right]^{-1} u_0 e^{\zeta} \, d\zeta \\ (3.5) \quad &= \frac{1}{2\pi i} \int_{\Gamma} \left[\zeta I + \frac{1}{t} \int_0^t A(\tau) \, d\tau \right]^{-1} u_0 e^{\zeta t} \, d\zeta. \end{aligned}$$

Fixing t in the bracket of (3.5) at s , we designate the right-hand side as $v(t)$. That is,

$$(3.6) \quad v(t) = \frac{1}{2\pi i} \int_{\Gamma} \left[\zeta I + \frac{1}{s} \int_0^s A(\tau) \, d\tau \right]^{-1} u_0 e^{\zeta t} \, d\zeta.$$

Notice that $u(s) = v(s)$. Denoting $\tilde{A}_s = \frac{1}{s} \int_0^s A(\tau) \, d\tau$, we see that $v(t)$ is the solution to the following evolution problem:

$$(3.7) \quad v_t + \tilde{A}_s v = 0, \quad v(0) = u_0.$$

We highlight that (3.7) has a coefficient independent of time t , and the solution v at $t = s$ is identical to that of the original problem (1.1). Thus we finally arrive at a new idea for solving (1.1) at any specific time s by introducing the new operator \tilde{A}_s independent of time t . Let us call this operator a *frozen coefficient operator* and call the new method a *frozen coefficient method* that will be analyzed in the next section.

4. The frozen coefficient method.

4.1. Assumptions. We make the following assumptions throughout the paper:

1. The operator $A(t)$ is integrable on $[0, T_*]$ so that $\int_s^t A(\tau) \, d\tau$ exists for $s, t \in [0, T_*]$. Denote by $\tilde{A}_{t_0}(x)$ the frozen coefficient operator of $A(x, t)$ over $[0, t_0]$ such that

$$\tilde{A}_{t_0}(x) = \frac{1}{t_0} \int_0^{t_0} A(x, \tau) \, d\tau.$$

2. $A(t) = A(\cdot, t)$ is a second-order uniformly elliptic operator in a spatial domain Ω with homogeneous Dirichlet boundary conditions such that for given $t_0 > 0$ there exist two positive constants $c_* = c_*(t_0)$ and $c^* = c^*(t_0)$, which are independent of x , and

$$(4.1) \quad 0 < c_* |\xi|^2 \leq \xi^t \tilde{A}_{t_0}(x) \xi < c^* |\xi|^2 \quad \text{for all nonzero } \xi \in \mathbb{R}^n.$$

3. The spectrum $\sigma(\tilde{A}_{t_0})$ of \tilde{A}_{t_0} should be contained in a sector in the right half-plane,

$$(4.2) \quad \sigma(\tilde{A}_{t_0}) \subset \Sigma_\delta = \{z \in \mathbb{C} : |\arg z| \leq \delta, z \neq 0\} \text{ with } \delta \in (0, \pi/2),$$

and the resolvent operator $(zI + \tilde{A}_{t_0})^{-1}$ of $-\tilde{A}_{t_0}$ satisfies

$$(4.3) \quad \|(zI + \tilde{A}_{t_0})^{-1}\| \leq \frac{M}{1 + |z|} \quad \text{for } z \in \Sigma_{\pi-\delta} \cup B,$$

where B is a neighborhood of the origin and M is independent of z but possibly dependent on t_0 .

4. In order to use the frozen coefficient method, we need the following commutativity assumption:

$$(4.4) \quad A(t) \left(t\tilde{A}_t - s\tilde{A}_s \right) = \left(t\tilde{A}_t - s\tilde{A}_s \right) A(t) \quad \text{for } 0 \leq s \leq t \leq T_*.$$

4.2. Systematic derivation. We prove that the solution $u(t)$ of (1.1) can be represented using a frozen coefficient operator as stated in the following theorem.

THEOREM 4.1. *Under the assumptions made in section 4.1, if a solution of (1.1) exists, then it takes the form*

$$(4.5) \quad u(t) = e^{-t\tilde{A}_t} u_0, \quad \text{for } t \in (0, T_*].$$

Proof. Let u be any solution of (1.1) for a fixed time $t \in (0, T_*]$. We introduce the auxiliary function

$$(4.6) \quad w(s) := e^{-\int_s^t A(\tau) d\tau} u(s) \quad \text{for } s \in [0, t].$$

Differentiating (4.6) with respect to s and recalling (1.1), we get

$$(4.7) \quad \begin{aligned} w'(s) &= A(s) e^{-\int_s^t A(\tau) d\tau} u(s) + e^{-\int_s^t A(\tau) d\tau} u'(s) \\ &= A(s) e^{-\int_s^t A(\tau) d\tau} u(s) - e^{-\int_s^t A(\tau) d\tau} A(s) u(s) \\ &= \left(A(s) e^{-\int_s^t A(\tau) d\tau} - e^{-\int_s^t A(\tau) d\tau} A(s) \right) u(s) = 0, \end{aligned}$$

where the commutative rule (4.4) is used in the last equality. Consequently,

$$(4.8) \quad u(t) = w(t) = w(0) = e^{-\int_0^t A(\tau) d\tau} u_0,$$

which completes the proof. \square

Remark 4.2. Notice that the commutative assumption (4.4) is crucial in the proof of Theorem 4.1 and is fulfilled by the class of operators

$$(4.9) \quad A(t, x) = \left(\sum_{j=1}^J a_j(t) A_j \right),$$

where the $a_j(t)$'s are scalar functions and the A_j 's are time-independent spatial operators that are commutative, i.e., $A_j A_k = A_k A_j$. In particular, the class contains the operators with coefficients depending only on a time variable of the form $A(x, t) = \sum_{j,k=1}^d c_{jk}(t) \frac{\partial^2}{\partial x_j \partial x_k} + \sum_{j=1}^d c_j(t) \frac{\partial}{\partial x_j} + c_0(t)$, where d denotes the dimension of the space.

Now we show that the solution $u(t)$ in (1.1) can be obtained by solving a problem with a time-independent coefficient. Given $t_0 \in (0, T_*]$, we reformulate the problem (1.1) as follows:

$$(4.10) \quad \frac{\partial v}{\partial t} + \tilde{A}_{t_0} v = 0, \quad v(0) = u_0.$$

Since \tilde{A}_{t_0} is independent of time (dependent only on t_0), it can be solved by the Laplace transform method without introducing convolution. With an appropriate contour $\tilde{\Gamma}$ that will be specified in Theorem 4.3, one has the solution in the following form:

$$(4.11) \quad v(t) = \frac{1}{2\pi i} \int_{\tilde{\Gamma}} \left[zI + \tilde{A}_{t_0} \right]^{-1} u_0 e^{zt} dz.$$

THEOREM 4.3. *Under the assumptions made in section 4.1, the solution $u(t)$ of (1.1) at time t_0 is identical to the solution $v(t)$ of (4.10) at time t_0 .*

Proof. By Theorem 4.1, the Dunford–Cauchy integration formula (3.4) with $f(z) = u_0 e^z$, and the change of variables $\lambda = t_0 z$, we have

$$(4.12) \quad \begin{aligned} u(t_0) &= e^{-t_0 \tilde{A}_{t_0}} u_0 = \frac{1}{2\pi i} \int_{\Gamma} \left[\lambda I + t_0 \tilde{A}_{t_0} \right]^{-1} u_0 e^{\lambda} d\lambda \\ &= \frac{1}{2\pi i} \int_{\tilde{\Gamma}} \left[zI + \tilde{A}_{t_0} \right]^{-1} u_0 e^{t_0 z} dz \\ &= v(t_0), \end{aligned}$$

where the integral contour $\tilde{\Gamma}$ is the transform of Γ under the change of variables $\lambda = t_0 z$. \square

Since t_0 is arbitrary, we can use the following formula for the solution $u(t)$ of (1.1):

$$(4.13) \quad u(t) = \frac{1}{2\pi i} \int_{\tilde{\Gamma}} [zI + \tilde{A}_t]^{-1} u_0 e^{zt} dz.$$

In the next subsection, we will focus on the operators of type (4.9) and show how to apply the frozen coefficient method more effectively when we are interested in solutions at multiple times.

4.3. Solutions at multiple times. One often needs to obtain the solution to (1.1) at several times $t = t_1, t_2, \dots, t_\ell$. Since the formula (4.13) depends on each t_k , one has to evaluate

$$(4.14) \quad \hat{u}(z_j) := [z_j I + \tilde{A}_{t_k}]^{-1} u_0$$

for all t_k, z_j for $k = 1, \dots, \ell, j = -N_z, \dots, N_z$, which corresponds to solving the elliptic problems

$$(4.15) \quad (z_j I + \tilde{A}_{t_k}) \hat{u} = u_0, \quad \hat{u} \text{ fulfilling boundary conditions,}$$

$\ell \times (2N_z + 1)$ times. We seek a better way that reduces the number of times for solving (4.15) to only $(2N_z + 1)$.

Let us start from the case of $A(t) = a(t)A_0$, with A_0 being independent of the t variable. Let $\alpha(t) = \frac{1}{t} \int_0^t a(\tau) d\tau$, and use the Dunford–Cauchy integral formula (3.4) again. Then (4.13) can be rewritten as follows:

$$(4.16a) \quad u(t) = \frac{1}{2\pi i} \int_{\tilde{\Gamma}} [zI + \alpha(t)A_0]^{-1} u_0 e^{zt} dz$$

$$(4.16b) \quad = \frac{1}{2\pi i} \int_{\tilde{\Gamma}} [zI + A_0]^{-1} u_0 e^{zt\alpha(t)} dz.$$

Notice that the time-dependency of the term in the bracket of (4.16a) is removed in that of (4.16b). Instead, the role of the time specification is transferred to the exponent of the scalar function. Thus if we want to get the solutions at multiple times $t_j, j = 1, \dots, \ell$, we evaluate $[zI + A_0]^{-1} u_0$ for $z = z_j, j = -N_z, \dots, N_z$ only once and use them repeatedly to evaluate (4.16b) for all $t = t_1, \dots, t_\ell$.

4.4. Decomposition of the operator. Let us extend the previous formulation to the following class of problems:

$$(4.17) \quad \frac{\partial u}{\partial t} + \left(\sum_{j=1}^J a_j(t) A_j \right) u = 0, \quad u(0) = u_0,$$

where the A_j 's are time-independent spatial operators that are commutative, i.e., $A_j A_k = A_k A_j$. Set $\tilde{\alpha}_{t,j} = \frac{1}{t} \int_0^t a_j(\tau) d\tau$ for $j = 1, \dots, J$. Due to the commutativity of the A_j 's, one has, for all j, k ,

$$(a_j(t)A_j + a_k(t)A_k)(\tilde{\alpha}_{t,j}A_j + \tilde{\alpha}_{t,k}A_k) = (\tilde{\alpha}_{t,j}A_j + \tilde{\alpha}_{t,k}A_k)(a_j(t)A_j + a_k(t)A_k).$$

Owing to Theorem 4.1, the solution of (4.17) can be represented by

$$(4.18) \quad u(t) = \exp \left(-t \sum_{j=1}^J \tilde{\alpha}_{t,j} A_j \right) u_0.$$

Using (4.16), we have the following:

$$(4.19) \quad \begin{aligned} u(t) &= \prod_{j=1}^J \exp \left(-t \tilde{\alpha}_{t,j} A_j \right) u_0 = \exp \left(-t \tilde{\alpha}_{t,1} A_1 \right) \prod_{j=2}^J \exp \left(-t \tilde{\alpha}_{t,j} A_j \right) u_0 \\ &= \frac{1}{2\pi i} \int_{\Gamma} \left[z_1 I + A_1 \right]^{-1} \prod_{j=2}^J \exp \left(-t \tilde{\alpha}_{t,j} A_j \right) u_0 e^{z_1 t \tilde{\alpha}_{t,1}} dz_1 \\ &= \left(\frac{1}{2\pi i} \right)^J \prod_{j=1}^J \left(\int_{\Gamma} \left[z_j I + A_j \right]^{-1} e^{z_j t \tilde{\alpha}_{t,j}} dz_j \right) u_0. \end{aligned}$$

Remark 4.4. One can select different contours for each operator A_j to get an optimal convergence instead of employing a single Γ in (4.19).

Remark 4.5. If the operators A_j are to be discretized, the commutative condition for the discretized operators should be preserved in order to apply (4.19).

5. Discretization of the method. In this section we describe how to evaluate the indefinite integral (4.13) or (4.16). The integral contour Γ in these forms can be chosen appropriately in the complex plane either parallel to the imaginary axis or deformed to the left of the complex plane as long as all the singularities are located to the left of the contour [1]. For the sake of numerical efficiency, we prefer to use a deformed contour in a sector $\Sigma_{\pi-\delta}$ with $0 < \delta < \frac{\pi}{2}$ so that $\operatorname{Re}(z) \rightarrow -\infty$ as $\operatorname{Im} z \rightarrow \pm\infty$, forcing the factor e^{zt} to decay exponentially toward both ends of the deformed contour for any positive t .

Three types of contours, such as parabola, hyperbola, and Talbot shapes, have been widely used [5, 9, 16, 24, 26, 28, 30]. We employ the hyperbolic contour in this paper. Following the notation used by Weideman and Trefethen in [30], the contour can be parameterized with a parameter w ,

$$(5.1) \quad z = \mu(1 + \sin(iw - \beta)), \quad -\infty < w < \infty.$$

The parameters μ and β set the width and the asymptotic angle of the hyperbolic contour, respectively.

Substituting the contour into the integral (4.13), it becomes

$$u(x, t) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} [z(w)I + \tilde{A}_t]^{-1} u_0(x) e^{z(w)t} z'(w) dw.$$

The trapezoidal rule with uniform node spacing Δw for w yields the approximation $u_{\Delta w, N_z}(x, t)$ of $u(x, t)$, where

$$(5.2) \quad u_{\Delta w, N_z}(x, t) = \frac{\Delta w}{2\pi i} \sum_{k=-N_z}^{N_z} [z(w_k)I + \tilde{A}_t]^{-1} u_0(x) e^{z(w_k)t} z'(w_k), \quad w_k = k\Delta w.$$

In this formula there are three free parameters, μ , Δw , and β . Since the frozen coefficient method solves the reformulated problem with time-independent coefficients,

error analyses done for the Laplace transform method are still valid. There is much literature that describes how to choose the parameters for optimal convergence. We adopt the optimal parameters proposed in [30], which are applicable where the spectrum lies on the negative real axis. They are explicitly given by

$$(5.3) \quad \beta_* = 1.1721, \quad \Delta w_* = \frac{1.0818}{N_z}, \quad \text{and} \quad \mu_* = 4.4921 \frac{N_z}{t},$$

provided t and N_z are fixed. With this choice, the convergence of $u_{\Delta w, N_z}$ is calculated asymptotically as

$$(5.4) \quad |u_{\Delta w, N_z}(x, t) - u(x, t)| = O(e^{-2.32N_z}) \approx O(10^{-N_z}) \quad \text{as } N_z \rightarrow \infty.$$

To compute solutions at multiple times, one can utilize (4.16) with the following discretization form:

$$(5.5) \quad u_{\Delta w, N_z}(x, t) = \frac{\Delta w}{2\pi i} \sum_{k=-N_z}^{N_z} [z(w_k)I + A_0]^{-1} u_0(x) e^{z(w_k)t\alpha(t)} z'(w_k),$$

with $w_k = k\Delta w$. This time, we use a fixed contour for different times. Thus we do not make use of the optimal parameters given in (5.3). In order to find a new optimal set of parameters, suppose instead that we seek solutions at $t \in [t_0, t_1]$. Set

$$\Lambda = \frac{\max_{t \in [t_0, t_1]} t\alpha(t)}{\min_{t \in [t_0, t_1]} t\alpha(t)},$$

where $t_0 > 0$ and $\alpha(t) \geq \alpha_0$ for some positive constant α_0 . Among the three parameters, β , Δw , and μ , the two parameters should be chosen as

$$(5.6) \quad \Delta w = \frac{A(\beta)}{N_z}, \quad \mu = \frac{4\pi\beta - \pi^2}{A(\beta)} \frac{N_z}{\max_{t \in [t_0, t_1]} t\alpha(t)},$$

where $A(\beta)$ is defined by

$$A(\beta) = \cosh^{-1} \left(\frac{(\pi - 2\beta)\Lambda + 4\beta - \pi}{(4\beta - \pi) \sin \beta} \right).$$

In this case, the convergence rate is estimated as $O(e^{-B(\beta)N_z})$, where

$$(5.7) \quad B(\beta) = \frac{\pi^2 - 2\pi\beta}{A(\beta)}.$$

Maximizing numerically $B(\beta)$ in (5.7), we determine β and use the value in the calculation of Δw and μ in (5.6).

Remark 5.1. Instead of the optimal parameters (5.3), one can use those given by López-Fernández, Palencia, and Schädle in [16].

Remark 5.2. If N_z is too large, then the roundoff error of the discretization becomes problematic. This problem can be resolved by controlling the roundoff errors as in [16, 29].

Remark 5.3. The parameters are valid only when the spectrum of operators A_t is located on the negative real axis.

6. Numerical examples. In this section we investigate numerical examples to show the performance of the proposed scheme and confirm the predicted convergence ratio. To see the time discretization errors without contaminant from space discretization, we deal with an ordinary differential equation in Example 6.1. Then, the method is applied to parabolic-type partial differential equations being incorporated with the finite element method in Examples 6.2 and 6.3. We took the hyperbolic contours for the numerical inversion of the Laplace transform, even though the other types of contours could be chosen.

In the tables to follow, ϵ_{N_z} denotes the absolute error of the numerical solution where N_z quadrature points on the contour are used, and B_{N_z} is the rate of convergence defined as follows:

$$B_{N_z} = \frac{1}{3} \log \frac{\epsilon_{N_z-3}}{\epsilon_{N_z}}.$$

Example 6.1. We consider an ordinary differential equation of the form

$$(6.1) \quad u' - (t+1)(t-1)u = 0 \quad \text{for } 0 < t < 1, \quad \text{with } u(0) = 1.$$

The analytic solution is $u(t) = e^{t^3/3-t}$.

We applied the discretization (5.2) using the frozen coefficient method with $\tilde{A}_t = -(\frac{t^2}{3} - 1)$ and the hyperbolic contour (5.1). Optimal parameters for the contour are employed as given in (5.3). The errors in Table 1 exhibit almost the same exponential convergence behavior as that of the Laplace transform method applied to time-independent problems. It almost matches the convergence order $O(e^{-2.32N_z})$ as predicted in (5.4).

Example 6.2. We consider the one-dimensional heat equation having a time-dependent coefficient of the form

$$(6.2a) \quad \frac{\partial u}{\partial t} - tu_{xx} = 0 \quad \text{for } 0 < x < \pi, \quad t > 0,$$

$$(6.2b) \quad u(0, t) = u(1, t) = 0, \quad t > 0, \quad u(x, 0) = \sin(x) + \sin(2x) + \sin(3x).$$

The exact solution is given as $u(x, t) = e^{-1/2t^2} \sin(x) + e^{-2t^2} \sin(2x) + e^{-9/2t^2} \sin(3x)$.

We carry out two experiments with this example. First, we apply the discretization (5.2) for the frozen coefficient method with $\tilde{A}_t = -\frac{t}{2} \frac{\partial^2}{\partial x^2}$. In this case, we can use

TABLE 1
Numerical errors of Example 6.1 with $N_z = 3, 6, 9$, and 12.

t	ϵ_3	ϵ_6	B_6	ϵ_9	B_9	ϵ_{12}	B_{12}
0.10	0.17E-04	0.15E-07	2.35	0.89E-11	2.47	0.29E-13	1.90
0.20	0.13E-04	0.29E-08	2.82	0.13E-10	1.81	0.14E-13	2.26
0.30	0.22E-05	0.13E-07	1.71	0.11E-10	2.36	0.24E-13	2.04
0.40	0.57E-05	0.12E-07	2.07	0.63E-13	4.04	0.35E-13	0.20
0.50	0.91E-05	0.54E-08	2.47	0.75E-11	2.20	0.31E-13	1.83
0.60	0.94E-05	0.49E-09	3.29	0.95E-11	1.31	0.33E-13	1.88
0.70	0.82E-05	0.44E-08	2.51	0.82E-11	2.10	0.19E-13	2.02
0.80	0.67E-05	0.65E-08	2.31	0.60E-11	2.33	0.19E-13	1.93
0.90	0.56E-05	0.74E-08	2.21	0.43E-11	2.48	0.22E-13	1.77
1.00	0.52E-05	0.76E-08	2.18	0.37E-11	2.54	0.15E-13	1.84

different optimal parameters for each time t as given in (5.3) that guarantee the convergence order $O(e^{-2.32N_z})$. The trade-off is that $\hat{u}(z)$ in (4.14) should be calculated for each t_k .

In the second experiment we apply the discretization (5.5) with $A_0 = \frac{\partial^2}{\partial x^2}$ and $\alpha(t) = -t/2$. In this case, we calculate a set of $(zI + A_0)^{-1}u_0$ once and obtain the solutions at multiple times simultaneously. The trade-off is that the convergence ratio is given as (5.7).

For both cases to approximate $\hat{u}(z)$, we use the standard C^0 -piecewise linear finite elements. The number of uniform spatial division N_x is fixed as 32,000. The rather large number of spatial points is chosen to make the errors in the results reflect the errors of the time-integration method and not the errors in the space discretization.

Table 2 shows the errors for the first experiment. The number of quadrature points on the contour is increased by 3 at each step starting from 3. Roughly, the values of B_{N_z} are near 2.32, as predicted, except in the last column of the table. The sudden decrease of B_{N_z} at $N_z = 12$ is due to the error arising from the spatial discretization.

Table 3 shows the errors for the second experiment. The number of quadrature points on the contour is increased by 3 at each step starting from 18. The contour is chosen with parameters $\Lambda = 100$, $\beta = 0.9171$. The experiment shows the convergence ratio $O(e^{-0.6N_z})$ on average, as expected in (5.7).

TABLE 2

Numerical errors of Example 6.2 with $N_x = 32,000$ and $N_z = 3, 6, 9$, and 12 on a time-dependent contour.

t	ϵ_3	ϵ_6	B_6	ϵ_9	B_9	ϵ_{12}	B_{12}
0.10	0.244E-02	0.202E-05	2.36	0.198E-08	2.31	0.318E-09	0.61
0.20	0.252E-02	0.250E-05	2.30	0.249E-08	2.30	0.133E-08	0.21
0.30	0.217E-02	0.222E-05	2.30	0.367E-08	2.13	0.210E-08	0.19
0.40	0.190E-02	0.227E-05	2.24	0.464E-08	2.06	0.566E-08	-0.07
0.50	0.168E-02	0.254E-05	2.16	0.492E-08	2.08	0.508E-08	-0.01
0.60	0.222E-02	0.143E-05	2.45	0.342E-08	2.01	0.239E-08	0.12
0.70	0.211E-02	0.103E-05	2.54	0.141E-08	2.20	0.107E-07	-0.68
0.80	0.148E-02	0.976E-06	2.44	0.539E-08	1.73	0.410E-08	0.09
0.90	0.852E-03	0.139E-05	2.14	0.187E-08	2.20	0.562E-08	-0.37
1.00	0.393E-03	0.115E-05	1.94	0.550E-08	1.78	0.176E-08	0.38

TABLE 3

Numerical errors of Example 6.2 with $N_x = 32,000$ and $N_z = 18, 21, 24, 27$, and 30 on a time-independent contour.

t	ϵ_{18}	ϵ_{21}	B_{21}	ϵ_{24}	B_{24}	ϵ_{27}	B_{27}	ϵ_{30}	B_{30}
0.10	0.31E-04	0.47E-05	0.63	0.75E-06	0.61	0.12E-06	0.60	0.82E-08	0.90
0.20	0.28E-04	0.43E-05	0.63	0.73E-06	0.59	0.11E-06	0.62	0.82E-08	0.88
0.30	0.25E-04	0.38E-05	0.63	0.69E-06	0.57	0.10E-06	0.64	0.81E-08	0.84
0.40	0.21E-04	0.33E-05	0.62	0.64E-06	0.55	0.90E-07	0.65	0.78E-08	0.82
0.50	0.17E-04	0.29E-05	0.59	0.59E-06	0.54	0.79E-07	0.67	0.71E-08	0.80
0.60	0.14E-04	0.26E-05	0.56	0.53E-06	0.53	0.70E-07	0.68	0.62E-08	0.81
0.70	0.11E-04	0.24E-05	0.50	0.48E-06	0.53	0.63E-07	0.68	0.53E-08	0.83
0.80	0.84E-05	0.22E-05	0.45	0.44E-06	0.53	0.56E-07	0.69	0.44E-08	0.84
0.90	0.80E-05	0.19E-05	0.47	0.39E-06	0.54	0.51E-07	0.68	0.37E-08	0.87
1.00	0.26E-05	0.22E-05	0.06	0.32E-06	0.64	0.50E-07	0.62	0.30E-08	0.94

Example 6.3. We consider the one-dimensional convection-diffusion problem with time-dependent coefficients of the form

$$(6.3a) \quad \frac{\partial u}{\partial t} - \frac{2}{1+t^2}u_{xx} + \frac{1}{1+t^2}u_x + \left(1 - \frac{1+\pi^2}{1+t^2}\right)u = 0 \quad \text{for } 0 < x < 1, \quad t > 0,$$

$$(6.3b) \quad u(0, t) = 0, u(1, t) = 0, \quad t > 0, \quad u(x, 0) = \sin(\pi x) e^x, \quad 0 < x < 1.$$

The exact solution is given as $u(x, t) = \sin(\pi x) e^{x-t}$.

In this example we investigate the solution method (4.19) that can utilize $\hat{u}_h(z_j)$ at multiple time t_k 's. We begin with decomposing the spatial operator into

$$A_1 = \left(-2\frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x} - \pi^2 I\right), \quad \alpha_1(t) = \frac{1}{1+t^2}, \quad \text{and} \quad A_2 = I, \quad \alpha_2(t) = \left(1 - \frac{1}{1+t^2}\right).$$

The problem (6.3) has three time-dependent coefficients that do not have a common factor. The idea of decomposition is that each subproblem contains only one time-dependent coefficient $\alpha_j(t)$. As explained in section 4.3, we sequentially solve the subproblems with initial data that is the solution of the previous step. That is, the solution $u(x, t_0) = u_2(x, t_0)$ is approximated by the sequential relation

$$\frac{\partial u_j}{\partial t} + \alpha_j(t)A_j u_j = 0, \quad u_j(x, 0) = u_{j-1}(x, t_0) \quad \text{for } j = 1, 2,$$

where $u_0(x, t_0)$ is defined as $u(x, 0)$. Each subproblem can be solved on a single contour regardless of time t_k .

As in the previous example, the same finite element method with the number of the spatial division $N_x = 32,000$ is used. For each subproblem the parameters are given as $\Lambda_1 = 7.880$ and $\beta_1 = 1.042$, and $\Lambda_2 = 647.66$ and $\beta_2 = 0.882$, respectively. Numerical results are shown in Table 4. Due to the larger value Λ_2 , the rate of convergence is dominated by A_2 with $B_{N_z} \sim 0.5$, as we expect from (5.7).

TABLE 4

Numerical errors of Example 6.3 with $N_x = 32,000$ and $N_z = 18, 21, 24, 27$, and 30 on a time-independent contour.

t	ϵ_{18}	ϵ_{21}	B_{21}	ϵ_{24}	B_{24}	ϵ_{27}	B_{27}	ϵ_{30}	B_{30}
0.1	0.16E-03	0.55E-04	0.36	0.14E-04	0.46	0.31E-05	0.51	0.57E-06	0.56
0.2	0.15E-03	0.50E-04	0.37	0.13E-04	0.45	0.28E-05	0.51	0.51E-06	0.57
0.3	0.13E-03	0.45E-04	0.36	0.12E-04	0.46	0.25E-05	0.51	0.45E-06	0.57
0.4	0.12E-03	0.41E-04	0.37	0.10E-04	0.46	0.22E-05	0.51	0.40E-06	0.57
0.5	0.11E-03	0.37E-04	0.36	0.94E-05	0.45	0.20E-05	0.51	0.37E-06	0.57
0.6	0.96E-04	0.33E-04	0.36	0.85E-05	0.45	0.18E-05	0.51	0.34E-06	0.56
0.7	0.89E-04	0.29E-04	0.37	0.78E-05	0.44	0.17E-05	0.51	0.31E-06	0.56
0.8	0.88E-04	0.27E-04	0.40	0.70E-05	0.45	0.15E-05	0.51	0.29E-06	0.56
0.9	0.66E-04	0.26E-04	0.31	0.60E-05	0.49	0.14E-05	0.48	0.27E-06	0.56
1.0	0.78E-04	0.21E-04	0.44	0.60E-05	0.41	0.12E-05	0.53	0.26E-06	0.51

Remark 6.4. In these examples, we calculated the time integral of the frozen coefficient exactly. If a time-dependent coefficient cannot be computed exactly, it should be approximated by some quadrature method. Since the integral is taken with respect to the time variable, and the partial derivatives are taken with respect to the space, the integral approximation of the \tilde{A}_{t_0} applies only to the time-dependent scalar coefficient functions. If we have to consider both the space and time discretization

of \tilde{A}_{t_0} , it can also be implemented easily. For example, let us consider $A(x, t) = \sum_{j,k=1}^d c_{jk}(t) \frac{\partial^2}{\partial x_j \partial x_k} + \sum_{j=1}^d c_j(t) \frac{\partial}{\partial x_j} + c_0(t)$. Then $\tilde{A}_{t_0} = \frac{1}{t_0} \int_0^{t_0} (\sum_{j,k=1}^d c_{jk}(t) \frac{\partial^2}{\partial x_j \partial x_k} + \sum_{j=1}^d c_j(t) \frac{\partial}{\partial x_j} + c_0(t)) dt = \frac{1}{t_0} (\sum_{j,k=1}^d \int_0^{t_0} c_{jk}(t) dt \frac{\partial^2}{\partial x_j \partial x_k} + \sum_{j=1}^d \int_0^{t_0} c_j(t) dt \frac{\partial}{\partial x_j} + \int_0^{t_0} c_0(t) dt)$. We first approximate the integral terms using a quadrature method and apply the spatial discretization to the differential operators. Thus, even in the case of full discretization of the frozen operator, the computational cost of getting the solution is essentially the same as that of the time-independent case; i.e., the most time consuming part is the N_z number of solving complex-valued elliptic problems. An error analysis for the discretization of \tilde{A}_{t_0} with respect to time from a different viewpoint is carried out by Yoon [31].

Remark 6.5. We tested the examples with other types of contours, and the results are very similar to those presented above and thus are not reported here.

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