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A Naturally Parallelizable Computational Method for Inhomogeneous Parabolic Problems

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Abstract: A parallel numerical algorithm is introduced and analyzed for solving inhomogeneous initial-boundary value parabolic problems. The scheme is based on the method recently introduced in Sheen, Sloan, and Thomée (2000) for homogeneous problems. We give a method based on a suitable choice of multiple parameters. Our scheme allows one to compute solutions in a wide range of time. Instead of using a standard time-marching method, which is not easily parallelizable, we take the Laplace transform in time of the parabolic problems. The resulting elliptic problems can be solved in parallel. Solutions are then computed by a discrete inverse Laplace transformation. The parallelization of the algorithm is natural in the sense that it requires no data communication among processors while solving the time-independent elliptic problems. Numerical results are also presented.

Subject Classification: 65M12, 65M15, 65M99.

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1 Introduction

In this work we are interested in describing and analyzing a parallelizable method to solve linear inhomogeneous parabolic problems of the form

$$\begin{aligned} u_t + \mathcal{A}u &= f(x,t), \qquad (x,t) \in \Omega \times (0,T], \\ u(x,0) &= u_0(x), \qquad x \in \Omega, \end{aligned} \tag{1.1}$$

where $\Omega \in \mathbf{R}^d$ is a bounded domain with a smooth boundary $\partial\Omega$, $T > 0$ and $\mathcal{A}$ is a symmetric, strongly elliptic, invertible operator defined on a dense subset $D(\mathcal{A})$ of $L^2(\Omega)$. The inhomogeneous term $f \in C^1([0,T];L^2(\Omega))$, and the initial data $u_0 \in L^2(\Omega)$ are given and we assume the homogeneous Dirichlet boundary condition. (Our approach could be extended, with appropriate technical details, for other types of linear homogeneous boundary conditions.)

Instead of solving the above initial-boundary value problem based on the traditional time-marching approach, which is not easily parallelizable in the time axis, we employ an alternative approach by using the Laplace transformation in the time variable.

The solution of (1.1) can be written as Pazy (1983) (p. 105)

$$u(\cdot,t) = S(t)u_0(\cdot) + \int_0^t S(s)f(\cdot,t-s)\,ds, \qquad 0 < t \le T, \tag{1.2}$$

where, for $t > 0$, $S(t) : L^2(\Omega) \to D(\mathcal{A})$ is the analytic semigroup generated by the operator $-\mathcal{A}$ Pazy (1983) (Theorems 7.2.7 and 2.6.13). In particular, for $t > 0$ and $v_0 \in L^2(\Omega)$, $S(t)v_0 := v(t)$, where v is the solution of the linear initial-boundary value problem

$$v_t + \mathcal{A}v = 0, \qquad v(\cdot,0) = v_0(\cdot), \qquad 0 < t \le T, \tag{1.3}$$

with the zero boundary condition. Thus, in (1.2) $S(t)u_0$ can be computed if we solve (1.3) with $v_0(\cdot) = u_0(\cdot)$. Further, for each $0 < s \le t \le T$, $S(s)f(\cdot,t-s)$ can be computed by solving (1.3) with $v_0(\cdot) = f(\cdot,t-s)$. In our parallel computational scheme to follow, we compute the most expensive part of solving the homogeneous problem (1.3) only once by a non-time stepping scheme, and handle several initial data by relatively inexpensive matrix vector multiplications.

For notational convenience, throughout the paper, for any $v \in C([0,T];L^2(\Omega))$, we do not distinguish between $v(t)$ and $v(\cdot,t)$, $t \in [0,T]$.

In order to solve (1.3) for several initial data $v_0 \in L^2(\Omega)$, we adopt the method given in Sheen, Sloan, and Thomée

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(2000). First we apply the Laplace transform

$$\widehat{v}(z) = \int_0^\infty e^{-zt} v(t)\, dt \quad \text{for } \mathrm{Re}\, z \geq -\gamma.$$

to (1.3) and obtain the complex-valued elliptic problems

$$z\widehat{v} + \mathcal{A}\widehat{v} = v_0 \qquad \text{for } \mathrm{Re}\, z \geq -\gamma. \tag{1.4}$$

Here, γ is a suitably chosen real number less than the smallest positive eigenvalue λ_0 of $\mathcal{A}$. The solution of (1.4) is $\widehat{v}(z) = R(z; -\mathcal{A})v_0$, where $R(z; -\mathcal{A}) = (zI + \mathcal{A})^{-1}$ is the resolvent of $-\mathcal{A}$. Since all the eigenvalues of $-\mathcal{A}$ are real and bounded above by $-\lambda_0$, the resolvent exists for all $z \in \mathbf{C} \setminus (-\infty, -\lambda_0]$. This enables one to retrieve the solution $v(t) = S(t)v_0$ of (1.3) by using the inverse Laplace transform defined through a contour integral Pazy (1983) (Theorem 1.7.7):

$$\begin{aligned} v(t) = S(t)v_0 &= \frac{1}{2\pi \mathrm{i}} \int_\Gamma e^{zt} R(z;\mathcal{A}) v_0\, dz \\ &= \frac{1}{\pi} \mathrm{Im} \int_{\Gamma^+} e^{zt} \widehat{v}(z)\, dz, \quad 0 < t \leq T, \end{aligned} \tag{1.5}$$

where the contour Γ in the complex plane is chosen as $\Gamma = \Gamma_\gamma = \{z = -\gamma - \sigma \pm \mathrm{i}\sigma; \sigma \geq 0\}$, with $\mathrm{Im}\, z$ increasing from $-\infty$ to ∞, and Γ^+ the portion of Γ lying in the second quadrant of the complex plane Sheen, Sloan, and Thomée (2000). The last equality (1.5) is obtained by using $\widehat{v}(\overline{z}) = \overline{\widehat{v}(z)}$. Hence, by using the properties of the deformed contour Γ_γ in (1.5), we get

$$\begin{aligned} v(t) &= \frac{e^{-\gamma t}}{\pi} \mathrm{Im}\, \nu \int_0^\infty e^{\nu\sigma t} \widehat{v}(-\gamma + \nu\sigma)\, d\sigma, \\ &\nu = -1 + i. \end{aligned} \tag{1.6}$$

The above Laplace transform approach enables a natural parallelization as the set of elliptic problems (1.4) can be solved independently for all z. The choice of Γ_γ (a deformation of the vertical line $\{-\gamma \pm \mathrm{i}\sigma; \sigma \geq 0\}$) is an essential ingredient in obtaining a robust *discrete* Laplace transform based approach (with analysis) in Sheen, Sloan, and Thomée (2000). Due to the choice of Γ_γ, the algorithm in Sheen, Sloan, and Thomée (2000) for solving *homogeneous* parabolic initial-value problems cannot be directly applied to (1.1). In this work using semigroup theory and a multiparameter variant of the method in Sheen, Sloan, and Thomée (2000), we propose a non-time stepping algorithm (with analysis) for the *inhomogeneous* equation (1.1).

A different non-time stepping approach to tackle inhomogeneous parabolic and hyperbolic problems with zero initial data based on the Fourier transformation has been discussed in detail in Douglas, Jr., Santos, Sheen, and Bennethum (1993), Douglas, Jr., Santos, and Sheen (1994), Lee, Lee, Sheen, and Yeom (1999). These earlier results and the recent work Sheen, Sloan, and Thomée (2000) and Chaplain, Ganesh, and Graham (2001) are the main motivations for this paper.

In fact, this paper is a first step towards a future project to tackle a *tumour growth* mathematical model on general domains described by semi-linear reaction-diffusion systems with parameters from the Turing space, see Chaplain, Ganesh, and Graham (2001) and references therein. In Chaplain, Ganesh, and Graham (2001), simulation of the model was considered on simple spherical surfaces using a spectral method of lines approach with time-stepping. The *long time* simulation process for the model on general domains naturally requires as a first step a non-time stepping method to tackle linear parabolic problems of the form (1.1) (arising by an appropriate linearization of the model). For time-stepping methods for parabolic problems, we refer to the book Thomée (1997) and references therein.

In the next section the algorithm introduced in Sheen, Sloan, and Thomée (2000) is reviewed briefly for solving homogeneous parabolic problems, and motivations for its variant are introduced. Then in Section 3 we present our algorithm for solving inhomogeneous problems with a convergence analysis. Numerical results are given in Section 4.

2 Linear homogeneous problems

2.1 The algorithm

In this section we describe in a compact algorithmic fashion the method introduced in a recent work Sheen, Sloan, and Thomée (2000) to solve general linear homogeneous problems of the form (1.3). This will form a basis to introduce our approach to solve the inhomogeneous linear problem (1.1).

Algorithm Lin-Hom:

1. Choose a quadrature rule (of degree of precision $q \geq 2$) on $[0, 1]$.

2. Convert the half-line integral in (1.6) into an equivalent integral on $[0,1]$.
3. Apply the quadrature rule to discretize the resulting integral on $[0,1]$.
4. For each quadrature point, obtain the unknowns $\widehat{v}$ by solving (1.4).

In Step 1, we choose either the composite trapezoidal or Simpson rule on $[0,1]$, i.e. $q=2$ or 4 respectively.

In Step 2, we use the change of variables $\sigma = \frac{q}{\tau}\ln\frac{1}{y}$ to convert the integral in (1.6) in the σ variable to an integral on $[0,1]$ in the y variable where $\tau > 0$ is a crucial parameter independent of the time variable t. A precise choice of τ will be explained later.

For a positive integer N, let the quadrature points be $y_n = n/N \in [0,1]$ and the weights be $\beta_n, n = 0,\cdots,N$. The discrete approximation to (1.6) is given by

$$\begin{aligned} v_N(t) &:= S_N(t;\tau)v_0 \\ &:= \frac{qe^{-\gamma t}}{\tau\pi}\operatorname{Im}\nu\sum_{n=1}^{N-1}\beta_n y_n^{(-\frac{qt}{\tau}\nu-1)}\widehat{v}(z_n(\tau)), \end{aligned} \tag{2.1}$$

where the end point singularities are ignored as in Sheen, Sloan, and Thomée (2000); Davis and Rabinowitz (1975) and $z_n(\tau)$ is defined by

$$z_n(\tau) = -\gamma + \nu\frac{q}{\tau}\ln\frac{N}{n}, \qquad n = 1,\cdots,N-1. \tag{2.2}$$

Thus to compute $v_N(t)$ in (2.1), we need to solve (1.4) only for $z = z_n(\tau), n = 1,\cdots,N-1$. It is clear that $z_n(\tau)$ is independent of t. Hence, the elliptic problem (1.4) for each $z_n(\tau), n = 1,\cdots,N-1$, can be solved *in parallel*, by using for example finite element approximation (with spatial mesh size h). Let $\widehat{v}_N^h$ be the resulting approximation. Hence our fully-discrete approximation to $S(t)v_0$ is given by

$$\begin{aligned} v_N^h(t) &:= S_N^h(t;\tau)v_0 \\ &:= \frac{qe^{-\gamma t}}{\tau\pi}\operatorname{Im}\nu\sum_{n=1}^{N-1}\beta_n y_n^{(-\frac{qt}{\tau}\nu-1)}\widehat{v}_N^h(z_n(\tau)), \end{aligned} \tag{2.3}$$

For each $n = 1,\cdots,N-1$, we need to solve finite-dimensional systems of linear algebraic equations of the form

$$(z_n(\tau)I_h + \mathcal{A}_h)\widehat{\mathbf{v}}_{\mathbf{N}}^{\mathbf{h}} = \mathbf{v}_{\mathbf{0}}^{\mathbf{h}}. \tag{2.4}$$

The approximate solutions v_N^h can then be obtained by multiplying the matrices $(z_n(\tau)I_h + \mathcal{A}_h)^{-1}$ with $\mathbf{v}_{\mathbf{0}}^{\mathbf{h}}$. Throughout the paper, by *multiplying an inverse matrix with a vector* we mean computing a sparse LU-decomposition of the matrix and then applying forward elimination and backward substitution with the vector. The expensive part of the computation in the above algorithm is the computation of the LU-decomposition of the matrix $(z_n(\tau)I_h + \mathcal{A}_h)$ for $n = 1,\cdots,N-1$. This can solved *in parallel*, independent of the time-variable for each $z_n(\tau)I_h$, $n = 1,\cdots,N-1$. Then $S_N^h(t;\tau)v_0$ can be evaluated for each $t \in (0,T]$ by using the formula (2.3).

An error analysis of the above method for linear homogeneous problem (1.3) is carried out in detail in Sheen, Sloan, and Thomée (2000); for convenience, we quote the main result below.

Theorem 2.1. *There exists a constant $C = C(\lambda_0 - \gamma) > 0$, such that for $N \geq 3$,*

$$\|S_N(t;\tau)v_0 - S(t)v_0\| \leq \\ C\|v_0\|e^{-\gamma t}\begin{cases} \frac{1}{N^q}\left(\frac{1+t^q}{\tau^q(1+t-\tau)} + \frac{t^q}{\tau^q}\ln_+\frac{1}{t-\tau}\right), & t > \tau, \\ \frac{1}{N^q}\left(\ln_+\ln N + \frac{1}{\tau^q} + \ln_+\frac{1}{\tau}\right), & t = \tau, \\ \frac{1}{N^{qt/\tau}}\left(\frac{1+\tau^q}{\tau^q} + \ln_+\frac{1}{\tau-t} + \ln_+\frac{1}{t}\right), & 0 < t < \tau, \end{cases}$$

where $\ln_+$ *denotes the usual nonnegative part of the natural logarithm* $\ln$.

(Here, and in what follows $\|\cdot\|$ will denote the usual $L^2(\Omega)$ norm.)

Remark 2.1. Based on the above theorem and observations in Sheen, Sloan, and Thomée (2000), we list some important factors that are to be considered for implementation of **Algorithm Lin-Hom** and motivate the need to consider a variant of the algorithm with multiple parameters.

1. For a single choice of the parameter τ, for optimal convergence it is recommended that $v_N(t)$ is to be computed only for $t > \tau$. Further, the term $(\frac{t}{\tau})^q$ in the error estimate of Theorem 2.1 forces the restriction that $t \in (\tau, b\tau]$ for some appropriate constant b. Based on empirical results computed using the trapezoidal rule (i.e. $q = 2$), it is recommended in Sheen, Sloan, and Thomée (2000) that $b = 2$. For simplicity, we take $b = q$.
2. Consequently, if we are interested in computing an approximation solution $v_N(t)$ for all $t \in (0,T]$, we

need to use a parameter, say $\tau_1 = T/q$ for $t \in (\tau_1, T]$, another parameter $\tau_2 = T/q^2$ for $t \in (\tau_2, q\tau_2]$ and so on. Thus we need to divide (0,T] into parameter based subintervals in geometric way by choosing multiple parameters $\tau_1, \cdots, \tau_L$ for some finite number L so that $\tau_L = T/q^L$.

3. To compute $v_N(t)$, for small time t, we need to choose τ_L also small. In this case the error estimate in Theorem 2.1 involves the term $\frac{1}{(N\tau_L)^q}$. So an arbitrary choice of N (independent of τ_L) would not yield convergence. This entails N and L to be dependent on each other.

In our algorithm to follow, we proceed by first choosing several values of the parameter τ (with re-ordering of the indices, for convenience). Let

$$\tau_l = T/q^{L-l+1} \qquad \text{for } l = 1, \cdots, L, \tag{2.5}$$

where the number of parameters L (depending on N) is chosen later in (3.1) based on convergence analysis.

3 Linear inhomogeneous problems

3.1 The algorithm

Now we are in a position to describe an algorithm to obtain an approximation to the solution $u(t), 0 < t \leq T$, given by (1.2) of the inhomogeneous problem (1.1). This involves solving the linear homogeneous problem (1.3) with several initial data $u_0(\cdot)$ and $f(\cdot, t-s)$ for $0 < s \leq t \leq T$ based on **Algorithm Lin-Hom** with $N \geq 2q$. As motivated in the last section, our first step consists of choosing several parameters $\tau_l, l = 1, \cdots, L$, as in (2.5). We choose $L \geq 1$ in the formula (2.5) to be

$$\begin{aligned} L &= L(N) \\ &= \begin{cases} \left[\log_q N\right] & \text{if } f(\cdot,t) \notin D(\mathcal{A}) \\ & \quad \text{for some } t \in (0,T], \\ \left[\frac{q}{q+1}\log_q N\right] & \text{if } f(\cdot,t) \in D(\mathcal{A}) \\ & \quad \text{for all } t \in (0,T], \end{cases} \end{aligned} \tag{3.1}$$

where $[\cdot]$ denotes the usual integer part function. For example, in the case of Simpson's rule ($q = 4$) and $N = 100$ or 400, we have $L = 3$ or 4 respectively, if $f(\cdot,t) \notin D(\mathcal{A})$ for some $t \in (0,T]$ and $L = 2$ or 3 otherwise. The above choice of L is required to obtain convergence properties, as we shall see in Theorem 3.1.

It is easy to show that (2.5) and (3.1) imply the following relations:

$$\begin{cases} \frac{T}{N} \leq \tau_1 < \frac{qT}{N} & \text{if } f(\cdot,t) \notin D(\mathcal{A}) \\ & \quad \text{for some } t \in (0,T], \\ \frac{T}{N^{q/(q+1)}} \leq \tau_1 < \frac{qT}{N^{q/(q+1)}} & \text{if } f(\cdot,t) \in D(\mathcal{A}) \\ & \quad \text{for all } t \in (0,T]. \end{cases} \tag{3.2}$$

For time-discretization on $[\tau_1, T]$ based on a quadrature rule of degree of precision $p \geq 2$, first we choose an integer $M > 0$:

$$M = \begin{cases} 1 & \text{if } f(\cdot,t) \notin D(\mathcal{A}) \\ & \quad \text{for some } t \in (0,T], \\ \left[N^{q/(p(q+1))} + 1\right] & \text{if } f(\cdot,t) \in D(\mathcal{A}) \\ & \quad \text{for all } t \in (0,T]. \end{cases} \tag{3.3}$$

(For $p = q = 4$, for instance, if $N = 100$ or 400, it would suffice to choose $M = 3$ or 4 respectively.) Next we subdivide $[\tau_1, \tau_2]$ into M equal subintervals of width Δt. This implies using (2.5),

$$\Delta t = \frac{\tau_2 - \tau_1}{M} = \frac{T(q-1)}{Mq^L} = \frac{(q-1)}{M}\tau_1. \tag{3.4}$$

Further for each $l = 1, \cdots, L$, since $\tau_{l+1} - \tau_l = q^{l-1}(\tau_2 - \tau_1)$, we subdivide $[\tau_l, \tau_{l+1}]$ into $M_l (= Mq^{l-1})$ equal subintervals of width Δt. Consequently, we have a uniform partition of $[\tau_1, T]$ with $M_T (= \sum_{l=1}^{L} M_l)$ subintervals of width Δt. Let

$$s_k = \tau_1 + k\Delta t, \qquad k = 0, \cdots, M_T \tag{3.5}$$

be the equally spaced grid points in $[\tau_1, T]$.

For any $t \in [\tau_1, T]$ fixed with $t = s_j$, for some $j = 2, \cdots, M_T$, we write the solution $u(t)$ in (1.2) as

$$\begin{aligned} u(t) &= S(t)u_0 + \int_0^{\tau_1} S(s)f(t-s)\, ds \\ &\quad + \int_{\tau_1}^{t} S(s)f(t-s)\, ds. \end{aligned} \tag{3.6}$$

To discretize the second integral in (3.6), we choose a quadrature rule on $[\tau_1, t]$ of degree of precision p with equally spaced quadrature points s_m as in (3.5) and some weights w_m, $m = 0, \cdots, j$. Since the semigroup operator $S(s)$ is not smooth for s close to 0, we discretize the integral on $[0, \tau_1]$ in (3.6) using the two point trapezoidal rule.

Then we get the first discrete approximation $\widetilde{u}_N(t)$ to the solution $u(t)$ (with $t = s_j$):

$$\widetilde{u}_N(t) = S(t)u_0 + \frac{\tau_1}{2}\left[S(\tau_1)f(t-\tau_1) + S(0)f(t)\right] + \sum_{m=0}^{j} w_m S(s_m) f(t-s_m). \tag{3.7}$$

We discretize the semigroup operators $S(s_m)$, $m = 0,\cdots,j$, using **Algorithm Lin-Hom** with parameter $\tau(m)$, where

$$\tau(m) = \begin{cases} \tau_1 & \text{if } \tau_1 \le s_m \le \tau_2 \\ \tau_l & \text{if } \tau_l < s_m \le \tau_{l+1}, \\ & \quad \text{for some } l = 2,\cdots L, \end{cases} \tag{3.8}$$

(with $\tau_{L+1} = T$). More precisely, for a fixed time $t = s_j$, and for a given initial data v_0, we approximate $S(s_m)v_0$, $m = 0,\cdots,j$, by $S_N(s_m;\tau(m))v_0$, where $S_N(\cdot;\tau(m))v_0$ is as defined in (2.1) with $\tau = \tau(m)$. Using (3.5), we have

$$\tau(m) = \begin{cases} \tau_1 & \text{if } 0 \le m \le M_1 \\ \tau_l & \text{if } 1+\cdots+M_{l-1} < m \le 1+\cdots+M_l, \\ & \quad \text{for some } l = 2,\cdots L. \end{cases} \tag{3.9}$$

Thus, for a fixed time $t = s_j$, $j = 2,\cdots,M_T$, our computable approximation $u_N(t)$ to the solution $u(t)$ of the inhomogeneous problem (1.1) is given by

$$u_N(t) = S_N(t;\tau(j))u_0 + \frac{\tau_1}{2}\left[S_N(\tau_1;\tau_1)f(t-\tau_1) + f(t)\right] + \sum_{m=0}^{j} w_m S_N(s_m;\tau(m)) f(t-s_m). \tag{3.10}$$

Equivalently, for $t = s_j$, $j = 2,\cdots,M_T$,

$$u_N(t) = S_N(s_j;\tau(j))u_0 + \frac{\tau_1}{2}\left[S_N(\tau_1;\tau_1)f(j\Delta t) + f(s_j)\right] + \sum_{m=0}^{j} w_m S_N(s_m;\tau(m)) f((j-m)\Delta t). \tag{3.11}$$

Finally, using finite-element/difference or spectral approximation for elliptic problems (1.4) for each $z = z_n(\tau(m)), n = 1,\cdots,N-1$, $m = 0,\cdots,j$, we obtain the fully-discrete approximation to the solution of (1.1):

$$u_N^h(t) = S_N^h(s_j;\tau(j))u_0 + \frac{\tau_1}{2}\left[S_N^h(\tau_1;\tau_1)f(j\Delta t) + f(s_j)\right] + \sum_{m=0}^{j} w_m S_N^h(s_m;\tau(m)) f((j-m)\Delta t). \tag{3.12}$$

The involved terms $S_N^h(s_m;\tau(m))f((j-m)\Delta t)$'s in (3.12) can be computed by solving finite dimensional systems of the form (2.4) *in parallel*. Then for each $z_n(\tau(m)), n = 1,\cdots,N-1$, $m = 0,\cdots,j$, given by (2.2) with $\tau = \tau(m)$, the spatial approximation of (1.4) with mesh size h gives the inverse $[z_n(\tau(m))I_h + \mathcal{A}_h]^{-1}$. Multiply these inverse matrices by vectors $\mathbf{u_0^h}$ and $\mathbf{f}(\cdot,(j-m)\Delta t)^h$, in order to obtain the fully-discretized approximation $u_N^h(t)$.

We summarize our method for solving inhomogeneous problems as follows:

Algorithm Lin-Inhom:

1. Fix N and choose parameters τ_l, $l = 1,\cdots,L$, as in (2.5) and (3.1).
2. Subdivide $[\tau_1, T]$ by choosing equally spaced grid points given by (3.5).
3. For any $t = s_j \in [\tau_1, T]$, $j = 2,\cdots,M_T$, and for each $m = 0,\cdots,j$, use the algorithm **Lin-Hom** to get the approximate inverse $[z_n(\tau(m))I_h + \mathcal{A}_h]^{-1}$, $n = 1,\cdots,N-1$.
4. For $n = 1,\cdots,N-1, m = 0,\cdots,j$, multiply $[z_n(\tau(m))I_h + \mathcal{A}_h]^{-1}$ by the vectors $\mathbf{u_0^h}$ and $\mathbf{f}(\cdot,(j-m)\Delta t)^h$ and obtain $u_N^h(t)$ using (3.12).

It is important to note that in the above Algorithm **Lin-Inhom** we compute the inverse (more precisely, compute a sparse LU-decomposition) of $[\mathcal{A}_h + z_n(\tau_l)I_h]$, $n = 1,\cdots,N-1$, $l = 1,\cdots,L$, only once. The computation of such inverse matrices is the most expensive part in solving parabolic problems. So compared to solving a linear homogeneous parabolic problem, our algorithm for solving inhomogeneous problems involves only a few additional relatively inexpensive matrix vector multiplications, and this can also be done *in parallel*.

We described the discrete approximation $u_N(t)$ to the solution $u(t)$ given by (1.2) only for $t = s_j$ for $j = 2,\cdots M_T$. For $j = 0,1$ the above procedure holds with natural modifications. If $j = 0$, *i.e.* $t = \tau_1$, the third term on the RHS of (3.6) vanishes and hence we ignore the last term in our approximation $u_N(t)$ given by (3.10). If $j = 1$, *i.e.* $t = \tau_1 + \Delta t$, we use the Simpson's rule with three quadrature points $0, \tau_1, \tau_1 + \Delta t$ (possibly not equally spaced) and get the corresponding approximation $u_N(t)$. For N

sufficiently large, carrying out the computation only for $t = s_j, \ j = 0, \cdots M_T$ is sufficient for most practical cases. In case $u_N(t)$ is required at a non-nodal point, it can be obtained by the usual interpolation technique.

It is important to choose equally spaced points s_j given by (3.5) on $[\tau_1, T]$ to get only maximum $O(N)$ matrix vector multiplications in Step 4 of **Algorithm lin-inhom**. However, we may choose τ_1 smaller than Δt to grade appropriately to tackle the non-smooth behaviour of the semigroup operator $S(s)$ for s sufficiently close to 0. Our choice of L, M gives such a grading from the point of view of optimal computational cost and from our next subsection analysis of rate of convergence .

Clearly, choosing non-equally spaced points in $[\tau_1, T]$ increases the computational cost substantially due to the terms $S(s)f(t-s)$. Hence we need to avoid Gauss type quadrature rules for time discretization.

3.2 Convergence Analysis

In this section we will derive an error analysis of **Lin-Inhom.** We use the following notation: $\|\cdot\|_\infty$ denotes the norm in $C([0,T]; L^2(\Omega))$ (i.e. supremum norm in the time-variable and $L^2(\Omega)$ norm in the space variable); $\|\cdot\|_{k,\infty}$ denotes the norm in $C^k([0,T]; L^2(\Omega))$, for $k = 1, \cdots, p$; for $g \in C([0,T]; L^2(\Omega))$ and for a fixed $s \in [0,T]$, $\|g(s)\|$ denotes the usual norm in $L^2(\Omega)$.

Throughout the paper, for $a, b \in \mathbf{R}$, by $a \lesssim b$ we denote $a \leq Cb$ for some generic constant C independent of the number of degrees of freedom N. It is useful to note that in practice $N \leq 1000$ and hence $L \leq 4$.

Theorem 3.1. *Assume that in* (1.1)*, the inhomogeneous term $f \in C^p([0,T]; L^2(\Omega))$, $p \geq 2$. Let N be given. Let L, M and the equally spaced quadrature points be respectively given by* (3.1), (3.3) *and* (3.5)*. Let k be the smallest integer such that $(k-1)q \geq L$. Then for any $t = s_j > \tau_k$, $M < j \leq M_T$, the approximate solution $u_N(t)$ given by* (3.10) *and the solution $u(t)$ of* (1.1) *satisfy*

$$\|u(t) - u_N(t)\| \lesssim \begin{cases} \frac{\ln N}{N}(\|u_0\| + \|f\|_\infty) & \textit{if } f(\cdot,t) \notin D(\mathcal{A}) \\ & \textit{for some } t \in (0,T], \\ \frac{\ln N}{N^{2q/(q+1)}}(\|u_0\| + \|f\|_\infty \\ \quad + \|\mathcal{A}f\|_\infty) & \textit{if } f(\cdot,t) \in D(\mathcal{A}) \\ & \textit{for all } t \in (0,T]. \end{cases} \tag{3.13}$$

Proof. We have

$$u(t) - u_N(t) = [u(t) - \widetilde{u}_N(t)] + [\widetilde{u}_N(t) - u_N(t)], \tag{3.14}$$

where $\widetilde{u}_N(t)$ is given by (3.7). Since $t = s_j > \tau_k$, using (3.8), we have $\tau(j) = \tau_l$ for some $l = 2, \cdots L$ with $(l-1)q \geq (k-1)q \geq L$. We write

$$u(t) - \widetilde{u}_N(t) = J_1 + J_2 \tag{3.15}$$

where

$$J_1 = \int_0^{\tau_1} S(s)f(t-s)\,ds - \frac{\tau_1}{2}[S(\tau_1)f(t-\tau_1) + S(0)f(t)], \tag{3.16}$$

$$J_2 = \int_{\tau_1}^{t} S(s)f(t-s)\,ds - \sum_{m=0}^{j} w_m S(s_m) f(t-s_m) \tag{3.17}$$

Further

$$J_1 = \int_0^{\tau_1} [S(s) - S(0)]f(t-s)\,ds + \int_0^{\tau_1} S(0)f(t-s)\,ds - \frac{\tau_1}{2}[S(0)f(t) + S(0)f(t-\tau_1)] + \frac{\tau_1}{2}[S(0)f(t-\tau_1) - S(\tau_1)f(t-\tau_1)]. \tag{3.18}$$

Since $f \in C^2([0,T]; L^2(\Omega))$, using the standard error estimate for the trapezoidal rule, we have

$$\|J_1\| \lesssim \int_0^{\tau_1} \|S(s)f(t-s) - S(0)f(t-s)\|\,ds + {\tau_1}^3\|f''\|_\infty + \tau_1\|S(0)f(t-\tau_1) - S(\tau_1)f(t-\tau_1)\| \tag{3.19}$$

For the case of $f(\cdot,t) \in D(\mathcal{A})$ for all $t \in (0,T]$, using the Lipschitz continuity of the analytic semigroup $S(\cdot)$ Pazy (1983)(Theorem 2.6.13), from (3.19) we get

$$\|J_1\| \lesssim \|\mathcal{A}f\|_\infty \int_0^{\tau_1} s\,ds + {\tau_1}^3\|f''\|_\infty + \tau_1^2\|\mathcal{A}f\|_\infty \lesssim \tau_1^2\left\{\|\mathcal{A}f\|_\infty + \|f''\|_\infty\right\}. \tag{3.20}$$

If, instead, $f(\cdot,t) \notin D(\mathcal{A})$ for some $t \in (0,T]$, by the continuity of the semigroup $S(\cdot)$ it follows from (3.19) that

$$\|J_1\| \lesssim \tau_1\|f''\|_\infty. \tag{3.21}$$

To estimate J_2 in (3.15), since $S(\cdot)$ is the analytic semigroup generated by $-\mathcal{A}$, we have Pazy (1983)(Lemma 2.4.5)

$$\frac{d^p}{ds^p}S(s) = \left(S'(\frac{s}{p})\right)^p$$

and Pazy (1983)(Theorem 2.5.2)

$$\left\|S'(s)\right\| = \|\mathcal{A}S(s)\| \lesssim \frac{1}{s} \qquad \text{for } s > 0,$$

so that

$$\left\|\frac{d^p}{ds^p}S(s)\right\| \lesssim \frac{1}{s^p} \qquad \text{for } s > 0. \tag{3.22}$$

Hence, using the fact that the time-quadrature rule has the degree of precision $p \geq 2$ and $f \in C^p([0,T];L^2(\Omega))$, it follows from (3.17), (3.22) and (3.4), that

$$\begin{aligned}
\|J_2\| &\lesssim \Delta t^p \int_{\tau_1}^t \left\|\frac{d^p}{ds^p}\{S(s)f(\cdot,t-s)\}\right\| ds \\
&\lesssim \Delta t^p \|f\|_{p,\infty} \int_{\tau_1}^t \frac{1}{s^p} ds \\
&\lesssim \Delta t^p \|f\|_{p,\infty} \left[t^{-p+1} + \tau_1^{-p+1}\right] \\
&\lesssim \Delta t^p \|f\|_{p,\infty} \tau_1^{-p+1} \\
&\lesssim \left(\frac{\tau_1}{M}\right)^p \|f\|_{p,\infty} \tau_1^{-p+1} \\
&\lesssim \frac{\tau_1}{M^p} \|f\|_{p,\infty}.
\end{aligned} \tag{3.23}$$

Hence, from (3.15), (3.20), (3.21), and (3.23), (3.3) and (3.2), we get

$$\|u(t) - \widetilde{u}_N(t)\| \lesssim \begin{cases} \tau_1 \|f\|_{p,\infty} & \text{if } f(\cdot,t) \notin D(\mathcal{A}) \\ & \text{for some } t \in (0,T], \\ \tau_1^2 [\|\mathcal{A}f\|_\infty + \|f\|_{p,\infty}] & \text{if } f(\cdot,t) \in D(\mathcal{A}) \\ & \text{for all } t \in (0,T]. \end{cases} \tag{3.24}$$

Using (3.2) in (3.24),

$$\|u(t) - \widetilde{u}_N(t)\| \lesssim \begin{cases} \frac{1}{N} \|f\|_{p,\infty} & \text{if } f(\cdot,t) \notin D(\mathcal{A}) \\ & \text{for some } t \in (0,T], \\ \frac{1}{N^{2q/(q+1)}} [\|\mathcal{A}f\|_\infty + \|f\|_{p,\infty}] & \text{if } f(\cdot,t) \in D(\mathcal{A}) \\ & \text{for all } t \in (0,T]. \end{cases} \tag{3.25}$$

We turn to estimate the second term in (3.14) by decomposing it as follows:

$$\widetilde{u}_N(t) - u_N(t) = I_1 + I_2 + I_3, \tag{3.26}$$

where,

$$\begin{aligned}
I_1 &= [S(t) - S_N(t;\tau(j))]u_0, \\
I_2 &= \frac{\tau_1}{2}[S(\tau_1) - S_N(\tau_1;\tau_1)]f(t-\tau_1), \\
I_3 &= \sum_{m=0}^{j} w_m [S(s_m) - S_N(s_m;\tau(m))] f(t-s_m)
\end{aligned}$$

Using $t > \tau_l$, Theorem 2.1, (3.3) and (2.5),

$$\begin{aligned}
\|I_1\| &\lesssim \|u_0\| e^{-\gamma t} \frac{1}{N^q}\Big(\frac{1+t^q}{\tau_l^q(1+t-\tau_l)} + \frac{t^q}{\tau_l^q}\ln_+ \frac{1}{t-\tau_l}\Big) \\
&\lesssim \|u_0\| e^{-\gamma t} \frac{1}{N^q}\Big(\frac{1}{\tau_l^q} + \frac{t^q}{\tau_l^q}\ln_+ \frac{1}{t-\tau_l}\Big) \\
&\lesssim \|u_0\| e^{-\gamma t} \frac{1}{(N\tau_l)^q}\Big(1 + \ln \frac{1}{\Delta t}\Big) \\
&\lesssim \|u_0\| e^{-\gamma t} \frac{1}{(N\tau_l)^q}\Big(1 + \ln \frac{M}{\tau_1}\Big) \\
&\lesssim \|u_0\| e^{-\gamma t} \frac{1}{(N\tau_l)^q} \ln N \\
&\lesssim \|u_0\| \frac{1}{(N\tau_1)^q} \left[\frac{\tau_1}{\tau_l}\right]^q \ln N \\
&\lesssim \|u_0\| \frac{1}{(N\tau_1)^q} q^{(1-l)q} \ln N,
\end{aligned} \tag{3.27}$$

where we have used $M = O(N^\alpha), \tau_1 = O(N^{-\beta})$ for some $\alpha, \beta > 0$. Since $(l-1)q \geq L$, we have $q^{(1-l)q} \lesssim q^{-L} \lesssim \tau_1$. Thus, using (2.5) and (3.2) in (3.27),

$$\begin{aligned}
\|I_1\| &\lesssim \frac{1}{N^q \tau_1^{q-1}} \|u_0\| \\
&\lesssim \begin{cases} \frac{\ln N}{N} \|u_0\| & \text{if } f(\cdot,t) \notin D(\mathcal{A}) \\ & \text{for some } t \in (0,T], \\ \frac{\ln N}{N^q N^{-q(q-1)/(q+1)}} \|u_0\| & \text{if } f(\cdot,t) \in D(\mathcal{A}) \\ & \text{for all } t \in (0,T]. \end{cases} \\
&\lesssim \begin{cases} \frac{\ln N}{N} \|u_0\| & \text{if } f(\cdot,t) \notin D(\mathcal{A}) \\ & \text{for some } t \in (0,T], \\ \frac{\ln N}{N^{2q/(q+1)}} \|u_0\| & \text{if } f(\cdot,t) \in D(\mathcal{A}) \\ & \text{for all } t \in (0,T]. \end{cases}
\end{aligned} \tag{3.28}$$

Further by Theorem 2.1

$$\|I_2\| \lesssim \tau_1 \|f\|_\infty e^{-\gamma \tau_1} \frac{1}{N^q}\Big(\ln_+ \ln N + \frac{1}{\tau_1^q} + \ln_+ \frac{1}{\tau_1}\Big).$$

Following the arguments used to derive (3.28), we have

$$\|I_2\| \lesssim \frac{\ln N}{N^q \tau_1^{q-1}} \|f\|_\infty \lesssim \begin{cases} \frac{\ln N}{N}\|f\|_\infty & \text{if } f(\cdot,t) \notin D(\mathcal{A}) \\ & \text{for some } t \in (0,T], \\ \frac{\ln N}{N^{2q/(q+1)}}\|f\|_\infty & \text{if } f(\cdot,t) \in D(\mathcal{A}) \\ & \text{for all } t \in (0,T]. \end{cases} \tag{3.29}$$

Using (3.9), we have

$$\begin{aligned} \|I_3\| &\le w_0 \|[S(\tau_1) - S_N(\tau_1;\tau_1)]\, f(t-\tau_1)\| \\ &\quad + \sum_{m=1}^{M_T} w_m \|[S(s_m) - S_N(s_m;\tau(m))]\, f(t-s_m)\| \\ &= w_0 \|[S(\tau_1) - S_N(\tau_1;\tau_1)]\, f(t-\tau_1)\| + \sum_{i=1}^{L} \\ &\quad \sum_{m=(1+\cdots+M_{i-1})+1}^{1+\cdots+M_i} \|[S(s_m) - S_N(s_m;\tau(m))]\, f(t-s_m)\|, \end{aligned} \tag{3.30}$$

where we have used the notation $1+\cdots+M_{i-1}=0$, for $i=1$. Now, applying Theorem 2.1, (3.8) and following arguments used for estimates I_1 and I_2, we get

$$\|I_3\| \lesssim \|f\|_\infty w_0 \frac{\ln N}{N^q \tau_1^q} + \|f\|_\infty \frac{\ln N}{N^q} \sum_{i=1}^{L} \sum_{m=(1+\cdots+M_{i-1})+1}^{M_1+\cdots+M_i} w_m \frac{1}{\tau_i^q}.$$

Since $[\tau_1, T] = \cup_{i=1}^{L} [\tau_i, \tau_{i+1}]$ and the time quadrature rule has degree of precision $p \ge 2$, using (2.5),

$$\begin{aligned} \|I_3\| &\lesssim \|f\|_\infty \frac{\ln N}{N^q} \sum_{i=1}^{L} \frac{\tau_{i+1}-\tau_i}{\tau_i^q} \\ &\lesssim \|f\|_\infty \frac{\ln N}{N^q} \sum_{i=1}^{L} \frac{1}{\tau_i^{q-1}} \\ &\lesssim \|f\|_\infty \frac{\ln N}{N^q \tau_1^{q-1}} \sum_{i=1}^{L} q^{(1-i)(q-1)} \\ &\lesssim \|f\|_\infty \frac{\ln N}{N^q \tau_1^{q-1}}. \end{aligned} \tag{3.31}$$

As in (3.29) it follows from (3.31) that

$$\|I_3\| \lesssim \begin{cases} \frac{\ln N}{N}\|f\|_\infty & \text{if } f(\cdot,t) \notin D(\mathcal{A}) \text{ for some } t \in (0,T], \\ \frac{\ln N}{N^{2q/(q+1)}}\|f\|_\infty & \text{if } f(\cdot,t) \in D(\mathcal{A}) \text{ for all } t \in (0,T]. \end{cases} \tag{3.32}$$

Combining the estimates (3.28), (3.29), and (3.32) in (3.26), we get

$$\|\widetilde{u}_N(t) - u_N(t)\| \lesssim \begin{cases} \frac{\ln N}{N}(\|u_0\| + \|f\|_\infty) & \text{if } f(\cdot,t) \notin D(\mathcal{A}) \\ & \quad \text{for some } t \in (0,T], \\ \frac{\ln N}{N^{2q/(q+1)}}(\|u_0\| + \|f\|_\infty) & \text{if } f(\cdot,t) \in D(\mathcal{A}) \\ & \quad \text{for all } t \in (0,T]. \end{cases} \tag{3.33}$$

The theorem now follows by using (3.24) and (3.33) in (3.14).

□

Remark 3.1. Since in practice $L \le 4$ (i.e. $N \le 1000$), if we use Simpson's rule ($q=4$) in our approximation, Theorem 3.1 holds for all $t = s_j \in (\tau_2, T]$. Accordingly, in addition to tackling general inhomogeneous problems, our approach generalizes the method in Sheen, Sloan, and Thomée (2000) for homogeneous problems for small time.

Remark 3.2. According to Theorem 3.1 the rate of convergence of our numerical scheme with N degrees of freedom (and without spatial discretization of the resulting elliptic problems) is $O(N^{-\alpha})$, where nonumber

$$\alpha = \begin{cases} 1-\varepsilon & \text{if } f(\cdot,t) \notin D(\mathcal{A}) \\ & \quad \text{for some } t \in (0,T], \\ \frac{2q}{q+1} - \varepsilon & \text{if } f(\cdot,t) \in D(\mathcal{A}) \\ & \quad \text{for all } t \in (0,T]. \end{cases} \tag{3.34}$$

In (3.34), $0 < \varepsilon < 1$ is a sufficiently small number occurring due to $\ln N$ term in Theorem 3.1 (and certain overestimates in our proof). The sub-optimal convergence rate is due to the approximation of non-smooth integrands (a common feature in quadrature schemes). However, we can obtain optimal $O(N^{-q})$ convergence if the inhomogeneous term is sufficiently smooth as we shall see in the next subsection.

If the spatial discretization (using for example, continuous piecewise linear functions) with mesh size h is used to solve the resulting elliptic problems, then the error involved in the computable fully discrete approximation u_N^h in (3.12) is given by

$$u_N^h(t) - u(t) = \left[u_N^h(t) - u^h(t)\right] + \left[u^h(t) - u(t)\right]. \quad (3.35)$$

As above the error in the first term of (3.35) is $O(N^{-\alpha})$, while for smooth initial data the second term in (3.35) is $O(h^2)$. Hence following Remark 3.1 for all $t = s_j \in (\tau_2, T]$, we have

$$\|u_N^h(t) - u(t)\| = O(N^{-\alpha} + h^2). \quad (3.36)$$

3.3 Higher order convergence

Throughout this subsection, we assume that $f(\cdot,t) \in D(\mathcal{A}^q)$, for all $t \in (0,T]$ and for simplicity let f be smooth. Since $D(A^q) \subset D(A^j)$, $j = 1,\cdots q-1$ (see Pazy (1983),Theorem 2.6.8), using Pazy (1983)(Theorem 2.6.13) we have for all $s > 0$,

$$\frac{d^j}{ds^j} S(s) f(\cdot,t) = S(s) A^j f(\cdot,t), \qquad j = 1,\cdots q. \quad (3.37)$$

Due to this smoothness property we do not split the integral on $[0,t]$ in (1.2). For simplicity, in this subsection we let $p = q$.

For approximation we proceed as follows: Firstly, we choose L, M as in $f(.,t) \in D(\mathcal{A})$ case. With $s_k,\ k = 0,\cdots M_T$ defined in (3.5) and $s_{-1} = 0$, and for $t = s_j$ fixed we choose a quadrature rule on [0,t] of degree of precision p with quadrature points $s_k,\ k = -1,\cdots M_T$ and weights $w_k,\ k = -1,\cdots M_T$. Our approximation to the solution u of (1.2) is

$$\begin{aligned} u_N(t) &= S_N(s_j;\tau(j))\, u_0 \\ &\quad + \sum_{m=-1}^{j} w_m S_N(s_m;\tau(m))\, f((j-m)\Delta t). \end{aligned} \quad (3.38)$$

The main reason for expecting higher order convergence is that, if we let

$$\begin{aligned} E_1 &= \int_0^t S(s) f(t-s)\, ds \\ &\quad - \sum_{m=-1}^{j} w_m S(s_m) f(t-s_m) \end{aligned} \quad (3.39)$$

then using (3.37), continuity of the semigroup and the fact that the quadrature rule has degree of precision $p = q$, we get

$$\begin{aligned} \|E_1\| &\lesssim \Delta t^p \int_{0^+}^t \left\| \frac{d^p}{ds^p} \{S(s) f(\cdot, t-s)\} \right\| ds \\ &\lesssim \Delta t^p \lesssim \left(\frac{\tau_1}{M}\right)^p \lesssim \frac{1}{N^q}. \end{aligned} \quad (3.40)$$

Accordingly, based on the ideas in the last subsection and following the results in Sheen, Sloan, and Thomée (2000), we conjecture that for t not small, for example $t > 1$

$$\|u(t) - u_N(t)\| = O(N^{-\alpha}) \quad (3.41)$$

where (with $0 < \varepsilon < 1$ is a sufficiently small)

$$\alpha = q - \varepsilon \quad \text{if } f(\cdot,t) \in D(\mathcal{A}^q) \quad \text{for all } t \in (0,T]. \quad (3.42)$$

This brief subsection was in fact motivated by our computational results in the next section.

4 Numerical Results

We demonstrate the applicability of our algorithm for an inhomogeneous heat equation. The parallelization of our scheme is essentially based on the parallel approach involved in **Algorithm Lin-Hom** of Sheen, Sloan, and Thomée (2000) for homogeneous problems. The parallel nature of **Algorithm Lin-Hom** is substantiated in Sheen, Sloan, and Thomée (2000)(p. 193-194) and hence we skip the parallel demonstration in this work.

We substantiate the theory in Section 3 in detail below for a test example with inhomogeneous terms f chosen so that one of the following criteria

- $f(\cdot,t) \in D(\mathcal{A})$ for all $t \in (0,T]$, but $f(\cdot,t) \notin D(\mathcal{A}^2)$ for some $t \in (0,T]$;
- $f(\cdot,t) \notin D(\mathcal{A})$ for some $t \in (0,T]$;
- $f(\cdot,t) \in D(\mathcal{A}^q)$, for all $t \in (0,T]$,

is satisfied and that exact solutions for the corresponding examples are known.

Example Consider the linear inhomogeneous parabolic problem

$$\begin{aligned} u_t - u_{xx} &= f(x,t), \quad (x,t) \in (0,\pi) \times (0,4], && (4.1) \\ u(0,t) = 0 &= u(\pi,t), \quad t \in (0,4], && (4.2) \\ u(x,0) &= u_0(x), \quad x \in (0,\pi). && (4.3) \end{aligned}$$

Here $\mathcal{A}u = -u_{xx}$ with domain

$$D(\mathcal{A}) = \left\{ v \in H^2(0,\pi) : v(0) = v(\pi) = 0 \right\}.$$

We choose appropriate smooth functions $f(x,t)$ and $u_0(x)$ so that an exact solution of (4.1)–(4.3) is of the form

$$u(x,t) = ae^{-c^2 t} \sin dx + bx^r (\pi - x)^s \tag{4.4}$$

for some parameters a, b, c, d, r, s to be specified below. In fact if we take

$$f(x,t) = ae^{-c^2 t}(d^2 - c^2)\sin dx + bx^{r-2}(\pi - x)^{s-2} \times \\ \left\{ (r - r^2)(\pi - x)^2 + 2rsx(\pi - x) + (s - s^2)x^2 \right\} \tag{4.5}$$

and

$$u_0(x) = a \sin dx + bx^r (\pi - x)^s \tag{4.6}$$

it is easy to check that u defined by (4.4) is a solution (4.1)–(4.3). In (4.5), if we choose $b = 0$, then clearly $f(x,t)$ and all its even derivatives w.r.t. x vanish at the boundary $x = 0, \pi$. Further it is easy to show the following:

- **Case 1**: $b \neq 0, r = s = 3$. Then $f(\cdot,t) \in D(\mathcal{A})$, but $f(\cdot,t) \notin D(\mathcal{A}^2)$ for all $t \in (0,T]$;
- **Case 2**: $b \neq 0, r = s = 2$. Then $f(\cdot,t) \notin D(\mathcal{A})$ for all $t \in (0,T]$;
- **Case 3**: $b = 0$. Then $f(\cdot,t) \in D(\mathcal{A}^4)$, for all $t \in (0,T]$.

For numerical experiments, for all **Case 1,2** and **3**, we took $a = 0.1, c = 2, d = 1$ and for **Case 1,2** we chose $b = 0.01$.

We implemented our **Algorithm Lin-Inhom** for the above test example for all the three cases using Simpson's rule ($q = 4$) for discretization of the spectral integral in (1.6). Further we chose a quadrature rule of degree of precision $p = 4$ (described in Cox (1975)) with equally spaced quadrature points s_k to discretize the time integral on $[\tau_1, t]$ (on $[0,t]$ for **Case 3**). The weights w_m of the quadrature are used to compute u_N^h in (3.12) (and in (3.38)).

The quadrature rule in Cox (1975) was obtained by cubic spline approximation of the integrand (with not-a-knot condition). Since the rule allows both even and odd number of quadrature points, we chose the quadrature rule in Cox (1975) and its implementation in a NAG subroutine (EO2BDF) for time-discretization (instead of Simpson's rule) to handle several values of $t = s_j$.

In all our numerical experiments for spatial discretization we used continuous piecewise linear finite element approximations on uniform meshes with $h = \pi/K$. To check the $O(N^{-\alpha})$ convergence of our algorithm, with α given by (3.34) and (3.42), we chose K in such a way that the error is dominated by the time discretization part. In fact, we increased K according to the increment in N so that the order of convergence in the *spatial discretization* is higher: precisely, $h^2 < N^{-\beta}$, where for **Case 1** $\beta = 2q/(q+1) = 1.6$, for **Case 2** $\beta = 1$ and for **Case 3** $\beta = 4$. Due to this choice and using (3.36), (3.34) and (3.42), we expect in our numerical experiments for all $t = s_j \in (\tau_2, 4]$

$$\mathcal{E}_{N,K} := \|u_N^h(t) - u(t)\| = O(N^{-EOC}), \tag{4.7}$$

where the *expected order of convergence EOC* is approximately 1.6, 1 and 4 for **Case 1,2** and **3** respectively. We chose γ in (2.2) to be zero.

In our computation we chose the number L of τ parameters first and then N according to the formula (3.1). The computed numerical results for **Case 1,2** and **3** given respectively in Table 1,2 and 3 substantiate our theoretical results. Results in Table 1,2 and 3 are given for certain selected comparable time values $t = s_j \in (1,4]$. (Note that for $L = 2$, from (2.5) we get $\tau_2 = 1$.)

Table 1 : Error for **Case 1**

t	$L=2$ $\mathcal{E}_{32,5}$	$L=3$ $\mathcal{E}_{180,25}$	EOC	$L=4$ $\mathcal{E}_{1024,125}$	EOC
1.5	.10E-1	.67E-3	1.58	.45E-4	1.56
2.0	.10E-1	.67E-3	1.58	.45E-4	1.56
2.5	.10E-1	.68E-3	1.58	.45E-4	1.56
3.0	.10E-1	.68E-3	1.58	.45E-4	1.56
3.5	.10E-1	.68E-3	1.58	.45E-4	1.56
4.0	.10E-1	.68E-3	1.58	.45E-4	1.56

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Table 2 : Error for **Case 2**

t	$L=2$ $\mathcal{E}_{32,5}$	$L=3$ $\mathcal{E}_{180,25}$	EOC	$L=4$ $\mathcal{E}_{1024,125}$	EOC
1.75	.74E-2	.20E-2	0.92	.60E-3	0.90
2.50	.73E-2	.21E-2	0.90	.60E-3	0.90
3.25	.69E-2	.21E-2	0.90	.60E-3	0.90
4.00	.67E-2	.21E-2	0.83	.60E-3	0.90

Table 3 : Error for **Case 3**

t	$L=2,\mathcal{E}_{32,5}$	$L=3,\mathcal{E}_{180,160}$	EOC
1.5	0.565E-03	0.108E-05	3.62
2.0	0.232E-03	0.302E-06	3.85
2.5	0.123E-03	0.136E-06	3.94
3.0	0.714E-04	0.763E-06	3.96
3.5	0.425E-04	0.456E-07	3.96
4.0	0.255E-04	0.278E-07	3.95

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