Explicit unconditionally stable methods for the heat equation via potential theory

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Abstract

In this paper, we study the stability properties of explicit marching schemes for second-kind Volterra integral equations that arise when solving boundary value problems for the heat equation by means of potential theory. We show that, for the Dirichlet problem on the unit ball in all dimensions $d \geq 2$, the simplest marching scheme is *unconditionally stable*. By contrast, it is well known that explicit finite difference or finite element schemes for the heat equation are stable only if the time step Δt is of the order $O(\Delta x^2)$, where Δx is the finest spatial grid spacing. We also consider Robin boundary conditions for $d = 1$, and show that there is a constant C depending only on the Robin (heat transfer) coefficient κ such that the simplest first-order accurate scheme is stable if $\Delta t < C(\kappa)$, independent of the spatial discretization. Our estimates involve new bounds for ratios of modified Bessel functions, and for the smallest eigenvalues of real symmetric Toeplitz matrices, which may be of analytic interest in other applications.

Keywords: heat equation, Abel equation, forward Euler scheme, Volterra integral equation, stability analysis, Toeplitz matrix, modified Bessel function of the first kind

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1. Introduction

In this paper, we study the stability of integral equation methods for the heat equation

$$\begin{aligned} \frac{\partial u}{\partial t}(\mathbf{x}, t) - \Delta u(\mathbf{x}, t) &= F(\mathbf{x}, t) \\ u(\mathbf{x}, 0) &= u_0(\mathbf{x}) \end{aligned} \tag{1}$$

for $0 \leq t \leq T$, subject to suitable boundary conditions in a smooth, bounded domain D. For the sake of simplicity, we have assumed that the diffusion coefficient (thermal conductivity) is one. In dimensions $d > 1$, we assume Dirichlet boundary conditions are imposed on $\Gamma = \partial D$:

$$u(\mathbf{x}, t) = f(\mathbf{x}, t)|_{\mathbf{x} \in \Gamma,\ t > 0}.$$

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We assume that the initial and boundary data are compatible, namely that $f(\mathbf{x},0) = u_0(\mathbf{x})$ for $\mathbf{x} \in \Gamma$. In the one-dimensional setting, we consider both Dirichlet boundary conditions on a half line $x \geq 0$ (so that the boundary consists of a single point), and Robin boundary conditions of the form

$$-u_x(0,t) + \kappa u(0,t) = f(t) \ . \tag{2}$$

Here, $\kappa > 0$ is the *heat transfer coefficient*, and (2) models boundary coupling to an exterior reservoir of given temperature $\kappa f(t)$, either via a thin conductive layer, or via convection with Newton's law of cooling [4]. The Neumann case $\kappa = 0$ instead imposes boundary flux $f(t)$.

Before turning to the integral equation framework, we briefly review the finite difference approach. For this, we assume we are given a spatial mesh discretizing the domain D with grid points x_n and seek to approximate the solution $u_m^n \approx u(x_n, t_m)$ at time steps $t_0, t_1, \ldots, t_N$ with $t_m = m\Delta t$. Two of the simplest schemes for solving (1) are the forward and backward Euler methods:

$$\frac{u_n^{m+1} - u_n^m}{\Delta t} = \Delta_h[u]_n^m + F(x_n, t_m)$$

and

$$\frac{u_n^{m+1} - u_n^m}{\Delta t} = \Delta_h[u]_n^{m+1} + F(x_n, t_m) \ ,$$

respectively. Here $\Delta_h[u]_n^m$ denotes the finite difference approximation of the Laplacian evaluated at the grid point x_n at time t_m. It is well known that the backward Euler scheme is unconditionally stable, while, in d dimensions, the forward Euler scheme requires that the time step satisfy the condition that $\Delta t < \frac{1}{2d}\Delta x^2$, assuming a uniform spatial grid with step size Δx in each direction (see, for example, [40, p. 158]). For nonuniform grids, the time step restriction is more complicated to analyze, but generally requires that $\Delta t = O(h_{min}^2)$ where h_{min} is the finest mesh spacing in the discretization.

Unfortunately, the backward Euler scheme, is *implicit* and requires the solution of a large sparse linear system at each time step t_m. The forward Euler scheme, on the other hand, is *explicit* and inexpensive. The stability restriction, however, forces extremely small time steps to be taken, making long-time simulations impractical. This has spurred the development of a variety of alternative approaches, including locally one-dimensional schemes, alternating direction implicit methods, etc. [34].

When finite difference methods are used to solve general initial-boundary value problems, GKSO theory plays a critical role [11, 12, 33, 38, 41], and requires that the interior marching scheme be Cauchy stable (that is, beyond the stability condition above, the discrete boundary conditions must satisfy additional criteria). In short, stability imposes rather intricate constraints on the coupling between the interior marching scheme and the boundary conditions themselves. Similar considerations are involved when using finite element methods.

An alternative to direct discretization of the governing PDE is to recast the problem as a boundary integral equation using heat potentials [36, 18]. In dimension $d = 1$, the solution to the heat equation (1) on the half-line $x \geq 0$ with Dirichlet boundary data

$$u(0,t) = f(t) \tag{3}$$

is given analytically by the representation

$$u(x,t) = \int_0^t \frac{\partial G}{\partial x}(x,t-\tau)\mu(\tau)\,d\tau \;+\; v(x,t)\ , \tag{4}$$

where $G(x,t) = \frac{e^{-x^2/4t}}{\sqrt{4\pi t}}$ is the Green's function for the heat equation in free space, and v is the following explicit solution to (1) comprising the initial potential plus the volume potential:

$$v(x,t) := \int_0^\infty G(x-y,t)u_0(y)\,dy + \int_0^t \int_0^\infty G(x-y,t-\tau)F(y,\tau)\,dy\,d\tau\ . \tag{5}$$

The first term in (4) is a *double layer heat potential* living on the single boundary point. Since v does not in general satisfy the boundary condition, enforcing (3) using the standard jump relation (section 3, noting that the $\mathcal{D}$ term is zero), the double layer density is simply

$$\mu(t) = -2\tilde{f}(t)\ , \tag{6}$$

for the "corrected" Dirichlet data $\tilde{f}(t) := f(t) - v(0,t)$. This is an exact solution, so that stability follows trivially. The error is simply that made in evaluating the integrals that appear in (4) and (5).

The Robin boundary condition (2) leads to a more interesting model in the one-dimensional case. Representing $u(x,t)$ now in the form of a *single layer heat potential*

$$u(x,t) = \int_0^t G(x,t-\tau)\sigma(\tau)\,d\tau \;+\; v(x,t) \tag{7}$$

with v as in (5), a similar application of the jump relations (section 3) leads to a weakly singular Abel-type Volterra integral equation of the second kind for σ:

$$\tfrac{1}{2}\sigma(t) + \frac{\kappa}{\sqrt{4\pi}}\int_0^t \frac{\sigma(\tau)}{\sqrt{t-\tau}}d\tau \;=\; \tilde{f}(t)\ , \qquad t>0\ , \tag{8}$$

with corrected Robin data

$$\tilde{f}(t) := f(t) - v_x(0,t) + \kappa v(0,t)\ .$$

A simple numerical solver for (8) is to sample $\sigma_m := \sigma(t_m)$ on the uniform grid $t_m = m\Delta t$, use the piecewise constant approximation $\sigma(t) \approx \sigma_m$ on $[t_m, t_{m+1}]$, and perform the integrals exactly, to give

$$\sigma_n = 2\tilde{f}_n - \sum_{m=0}^{n-1} w_{n-m}\sigma_m, \qquad n = 1,\ldots,N \tag{9}$$

with the lower-triangular Toeplitz matrix weights

$$w_j = 2\sqrt{h}(\sqrt{j} - \sqrt{j-1}) = \frac{2\sqrt{h}}{\sqrt{j}+\sqrt{j-1}}\ , \qquad j = 1,2,\ldots\ , \tag{10}$$

$\tilde{f}_n := \tilde{f}(t_n)$, and $h = \kappa^2\,\Delta t/\pi$. We will refer to this scheme as the *forward Euler* method for the Volterra equation (8); it is a simple collocation scheme [18, Sec. 13.3] as well as a convolution quadrature scheme [23]. The scheme is explicit, since σ_n does not appear on the right-hand side. For smooth solutions $\sigma \in C^1([0,T])$ it is also first-order accurate, as can be shown by combining compactness of the integral operator, Céa's lemma, and noting that the piecewise constant approximant has error $\mathcal{O}(\Delta t)$ (see [18, Sec. 13.1–3]).

In dimension $d > 1$, the Green's function for the heat equation is

$$G(\mathbf{x}, t) = \frac{1}{(4\pi t)^{d/2}} e^{-\frac{|\mathbf{x}|^2}{4t}}, \quad \mathbf{x} \in \mathbb{R}^d \ . \tag{11}$$

We assume that the boundary Γ of D is at least C^2, and let σ be a square integrable function on $\Gamma \times [0, T]$. Then the single layer heat potential $\mathcal{S}$ is defined by the formula

$$\mathcal{S}[\sigma](\mathbf{x}, t) = \int_0^t \int_\Gamma G(\mathbf{x} - \mathbf{y}, t - \tau) \sigma(\mathbf{y}, \tau) ds(\mathbf{y}) d\tau \tag{12}$$

and the double layer heat potential $\mathcal{D}$ is defined by

$$\mathcal{D}[\sigma](\mathbf{x}, t) = \int_0^t \int_\Gamma \frac{\partial G(\mathbf{x} - \mathbf{y}, t - \tau)}{\partial \boldsymbol{\nu}(\mathbf{y})} \sigma(\mathbf{y}, \tau) ds(\mathbf{y}) d\tau, \tag{13}$$

where $\boldsymbol{\nu}(\mathbf{y})$ is the unit outward normal vector at $\mathbf{y} \in \Gamma$. The initial potential is defined by

$$\mathcal{U}[u_0](\mathbf{x}, t) = \int_D G(\mathbf{x} - \mathbf{y}, t - \tau) u_0(\mathbf{y}) d\mathbf{y} \tag{14}$$

and the volume potential is defined by

$$\mathcal{W}[F](\mathbf{x}, t) = \int_0^t \int_D G(\mathbf{x} - \mathbf{y}, t - \tau) F(\mathbf{y}, \tau) d\mathbf{y} d\tau. \tag{15}$$

The solution to the Dirichlet problem for (1) can be obtained (see section 3) by solving the second kind Volterra equation

$$\left(-\tfrac{1}{2} + \mathcal{D}\right)[\sigma](\mathbf{x}, t) = \tilde{f}(\mathbf{x}, t), \quad (\mathbf{x}, t) \in \Gamma \times [0, T], \tag{16}$$

where $\mathcal{D}$ is interpreted in a principal value sense, and, analogously to the $d = 1$ case, the corrected data is

$$\tilde{f}(\mathbf{x}, t) := f(\mathbf{x}, t) - v(\mathbf{x}, t) \ , \quad \text{where } \ v(\mathbf{x}, t) := \mathcal{U}[u_0](\mathbf{x}, t) + \mathcal{W}[F](\mathbf{x}, t) \ , \mathbf{x} \in \Gamma \ .$$

By the forward Euler method for (16), we mean a marching scheme of the form

$$\begin{aligned} \sigma(\mathbf{x}, n\Delta t) \ &= \ 2 \sum_{j=0}^{n-1} \int_{j\Delta t}^{(j+1)\Delta t} \int_\Gamma \frac{\partial G(\mathbf{x} - \mathbf{y}, n\Delta t - \tau)}{\partial \boldsymbol{\nu}(\mathbf{y})} \sigma(\mathbf{y}, j\Delta t) ds(\mathbf{y}) d\tau \\ &- \ 2\tilde{f}(\mathbf{x}, n\Delta t). \end{aligned} \tag{17}$$

That is, we assume $\sigma(\mathbf{y}, t)$ is piecewise constant over each time interval $[j\Delta t, (j+1)\Delta t]$, taking on the value $\sigma(\mathbf{y}, j\Delta t)$. This is an explicit, first order accurate formula for the value of the unknown at the nth time step.

The goals of this work are to show that the $d = 1$ marching scheme (9) has a time step restriction determined by the physical parameter κ, namely $\Delta t < \frac{\pi}{c^2\kappa^2}$ with $c \approx 1.5$, and that the marching scheme (17) is unconditionally stable in all dimensions $d \geq 2$.

The principal reasons that integral equation methods have received relatively little attention for solving the heat equation has been that direct evaluation of layer (or volume) potentials require quadratic work in the total number of unknowns as well as the design of suitable quadrature rules. Recent advances in fast algorithms for heat potentials, however, have removed this obstacle. We refer the reader to the papers [8, 9, 10, 15, 25, 24, 37, 39, 43, 44, 45] and the references therein for further discussion.

The mathematical tools needed to prove our stability results involve spectral bounds for Toeplitz operators. We provide these in section 2. In section 3, we summarize the necessary properties of layer potentials. The one-dimensional problem is then treated in section 4, the two-dimensional problem in section 5, and higher-dimensional problems in section 6.

2. Spectral bounds for real symmetric Toeplitz operators

Let S^1 be the unit circle in the complex plane, parametrized by polar angle θ with normalized arc length measure $d\lambda = \frac{1}{2\pi} d\theta$.

For any f, g in the Hilbert space $L^2(S^1)$, we write

$$f(\theta) = \sum_{n=-\infty}^{\infty} f_n e^{in\theta}, \qquad g(\theta) = \sum_{n=-\infty}^{\infty} g_n e^{in\theta}, \tag{18}$$

in terms of the orthogonal basis $\{e^{in\theta}\}_{n\in\mathbb{Z}}$, where f_n $(n \in \mathbb{Z})$ is the nth Fourier coefficient of f defined by

$$f_n = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) e^{-in\theta} d\theta.$$

The Hardy space H^2 is defined by

$$H^2 = \{f \in L^2(S^1) \,|\, f_n = 0, n < 0\},$$

and we let P denote the orthogonal projection of $L^2(S^1)$ onto H^2. The Toeplitz operator $T^f : H^2 \to H^2$ with symbol $f \in L^\infty(S^1)$, is defined by

$$T^f(u) = P(fu) \ .$$

The operator T^f is closely related to an infinite-dimensional Toeplitz matrix with entries t_{ij}, $i, j \in \mathbb{N}$ that satisfy $t_{ij} = t_{i+1,j+1}$ for all i, j. That is, the matrix is constant along diagonals and determined by a two-sided sequence $(t_n)_{n\in\mathbb{Z}}$ with $t_{ij} = t_{i-j}$. The Fourier transform maps T^f onto the class of Toeplitz matrices on $l^2(\mathbb{Z}_+)$; that is, if $\left(T^f(u)\right)_n$ denotes the nth Fourier coefficient of $T^f(u)$, then

$$\left(T^f(u)\right)_n = \begin{cases} \sum_{m=0}^{\infty} f_{n-m} u_m \ , & n \geq 0 \\ 0 \ , & n < 0 \end{cases}$$

where u_m is the mth Fourier coefficient of u.

Definition 1. A sequence $\{a_n\}_{n\in\mathbb{Z}_+}$ is said to be convex if $\delta^2 a_n \geq 0$ for every $n > 0$, where $\delta^2 a_n := a_{n-1} - 2a_n + a_{n+1}$ is the central second difference.

Recall that for $n \in \mathbb{Z}_+$ the Fejér kernel $F_n(x)$ is defined to be

$$F_n(\theta) = \sum_{j=-n}^{n} \left(1 - \frac{|j|}{n+1}\right) e^{ij\theta} = \frac{1}{n+1} \left[\frac{\sin\left(\frac{n+1}{2}\theta\right)}{\sin\left(\frac{\theta}{2}\right)}\right]^2 .$$

The following theorem can be found in [17, Chapter 1, Theorem 4.1].

Theorem 1. *If $a_n \to 0$ and the sequence $\{a_n\}_{n\in\mathbb{Z}_+}$ is convex, then the series*

$$v(\theta) = \sum_{n=1}^{\infty} n\,(\delta^2 a_n)\, F_{n-1}(\theta) \tag{19}$$

converges in $L^1([-\pi,\pi])$ to a non-negative function, which is continuous except at 0*, such that* $v_n = a_n$.

It is often the case that the function $v(\theta)$ blows up as $\theta \to 0$. Using the elementary estimate on the Fejér kernel

$$F_n(\theta) \leq \min\left\{(n+1), \frac{\pi^2}{(n+1)\theta^2}\right\},$$

[17, Chapter 1, formula 3.10] and the fact that, for a convex sequence tending to zero, we have $\lim_{n\to\infty} n(a_n - a_{n+1}) = 0$, one can show that

$$\lim_{\theta\to 0} \theta v(\theta) = 0\ . \tag{20}$$

Bounds on the spectrum of finite Toeplitz matrices are of interest in many applications [5, 14, 19, 26]. When a real symmetric Toeplitz operator (or matrix) is generated by a positive sequence, the Gerschgorin circle theorem [40, §3.3] often gives a satisfactory upper bound on its spectral radius or the largest eigenvalue. Curiously, satisfactory lower bounds on the smallest eigenvalue do not seem to be available. The following theorem leads to a tight lower bound on the smallest eigenvalue of a real symmetric Toeplitz matrix, defined by a convex sequence, even when v is unbounded.

Theorem 2. *Suppose that $\{v_n\}_{n\in\mathbb{N}}$ is a convex sequence and* $\lim_{n\to\infty} v_n = 0$*. Set* $v_0 = 2v_1 - v_2$*, and let $v(\theta)$ be the non-negative function defined by the sequence $\{v_n\}_{n\in\mathbb{Z}_+}$ as in Theorem 1. Suppose that V is the self-adjoint Toeplitz matrix defined by $V_{ii} = 0$ and $V_{ij} = v_{|i-j|}$. Then, for any $\boldsymbol{u} \in \mathbb{C}^N$, we have the lower bound*

$$\langle V\boldsymbol{u}, \boldsymbol{u}\rangle \geq (v_2 - 2v_1)\|\boldsymbol{u}\|^2.$$

Proof. For a finite length vector $\boldsymbol{u} = (u_0, \ldots, u_N, 0, 0, \ldots)_{n\in\mathbb{Z}_+}$, define the function

$$u(\theta) = \sum_{n=0}^{N} u_n e^{in\theta}. \tag{21}$$

Theorem 1 implies that

$$
\begin{aligned}
0 \le \frac{1}{2\pi}\int_0^{2\pi} v(\theta)|u(\theta)|^2 d\theta &= \frac{1}{2\pi}\int_0^{2\pi} v(\theta)\sum_{0\le j,k\le N} u_j \bar{u}_k e^{i(j-k)\theta} d\theta \\
&= \sum_{0\le j,k\le N} v_{k-j} u_j \bar{u}_k \\
&= \langle V\boldsymbol{u}, \boldsymbol{u}\rangle + (2v_1 - v_2)\|\boldsymbol{u}\|^2.
\end{aligned}
$$

□

Remark 1. If V_N is the upper left $N \times N$ principal submatrix of V, then, by an application of the Rayleigh-Ritz theorem, its spectrum is bounded below by $(v_2 - 2v_1)$.

Remark 2. For certain applications the sequence, $\{v_n\}_{n\in\mathbb{N}}$, generating T^v is not convex. In this case, one may consider an operator of the form, $cI + T^v + T^a$ with c and $\{a_n\}_{n\in\mathbb{N}}$ chosen so that $(c, v_1 + a_1, v_2 + a_2, \ldots)$ is a convex sequence. If T^a is a bounded operator, then the previous theorem implies a lower bound on the spectrum of V

$$\langle V\boldsymbol{u}, \boldsymbol{u}\rangle \ge -(c + \|T_a\|)\|\boldsymbol{u}\|^2 \text{ for } \boldsymbol{u} \in \mathbb{C}^N.$$

Remark 3. If v is unbounded, then the Toeplitz operator it determines is not defined on all of H^2. Equation (20) implies that if $u \in H^2$, then $v(1 - e^{i\theta})u \in L^2$. Thus $T^v w = P(vw) \in H^2$, for w in the subspace $(1 - e^{i\theta})H^2$. It is not difficult to see that this subspace is dense. If $u \in H^2$ and $r > 1$, then

$$\left(\frac{1 - e^{i\theta}}{r - e^{i\theta}}\right) u \in H^2$$

and

$$\lim_{r\to 1^+} \left\| \left(\frac{1 - e^{i\theta}}{r - e^{i\theta}}\right) u - u \right\|_2 = 0.$$

Since $\langle T^v w, w\rangle \ge 0$, for w in this domain, the Friedrichs extension of T^v is a closed self-adjoint, non-negative operator defined on a dense subspace $D_v \subset H^2$.

3. Properties of heat potentials

By construction, the single and double layer heat potentials (12) and (13) satisfy the heat equation. They also satisfy certain well-known jump conditions when the target point $\mathbf{x}$ approaches the boundary from either side [18, 36]. In particular, for $\mathbf{x}_0 \in \Gamma$, the normal derivative of the single layer potential $\mathcal{S}[\sigma]$ satisfies the relation

$$\lim_{\epsilon\to 0+} \frac{\partial \mathcal{S}[\sigma](\mathbf{x}_0 \pm \epsilon\boldsymbol{\nu}(\mathbf{x}_0), t)}{\partial \boldsymbol{\nu}(\mathbf{x}_0)} = \mp\tfrac{1}{2}\sigma(\mathbf{x}_0, t) + \mathcal{S}_{\boldsymbol{\nu}}[\sigma](\mathbf{x}_0, t),$$

and the double layer potential $\mathcal{D}[\sigma]$ satisfies the relation

$$\lim_{\epsilon\to 0+} \mathcal{D}[\sigma](\mathbf{x}_0 \pm \epsilon\boldsymbol{\nu}(\mathbf{x}_0), t) = \pm\tfrac{1}{2}\sigma(\mathbf{x}_0, t) + \mathcal{D}[\sigma](\mathbf{x}_0, t), \tag{22}$$

where both $\mathcal{S}_{\boldsymbol{\nu}}[\sigma](\mathbf{x}_0,t)$ and $\mathcal{D}[\sigma](\mathbf{x}_0,t)$ are interpreted in the Cauchy principal value sense. If we represent the solution to the heat equation (1) via a double layer potential $u(\mathbf{x},t) = \mathcal{D}[\sigma](\mathbf{x},t)$, then the integral equation (16) follows immediately from the jump relation (22).

The kernel of the double layer potential is given explicitly by

$$\frac{\partial G(\mathbf{x}-\mathbf{y},t-\tau)}{\partial \boldsymbol{\nu}(\mathbf{y})} = \frac{(\mathbf{x}-\mathbf{y})\cdot\boldsymbol{\nu}(\mathbf{y})}{2^{d+1}\pi^{d/2}(t-\tau)^{1+d/2}} e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4(t-\tau)}} \tag{23}$$

and the kernel of $\mathcal{S}_{\boldsymbol{\nu}}$ is given by

$$\frac{\partial G(\mathbf{x}-\mathbf{y},t-\tau)}{\partial \boldsymbol{\nu}(\mathbf{x})} = -\frac{(\mathbf{x}-\mathbf{y})\cdot\boldsymbol{\nu}(\mathbf{x})}{2^{d+1}\pi^{d/2}(t-\tau)^{1+d/2}} e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4(t-\tau)}}$$

and $\boldsymbol{\nu}(\mathbf{y})$ replaced with $\boldsymbol{\nu}(\mathbf{x})$. In one dimension, both kernels vanish at the single boundary point $y = x_0 = 0$.

Finally, the initial potential (14) is well known to satisfy the homogeneous heat equation with initial data $u_0(\mathbf{x})$, while the volume potential (15) satisfies the inhomogeneous heat equation

$$\frac{\partial u}{\partial t}(\mathbf{x},t) - \Delta u(\mathbf{x},t) = F(\mathbf{x},t)$$

with zero initial data.

Remark 4. Using these properties, it is straightforward to see that representing the solution to the Dirichlet problem in the form

$$u(\mathbf{x},t) = \mathcal{D}[\sigma](\mathbf{x},t) + \mathcal{U}[u_0](\mathbf{x},t) + \mathcal{W}[F](\mathbf{x},t)$$

leads to the integral equation (16), with the only unknown corresponding to the double layer density σ.

Remark 5. On the unit sphere S^{d-1}, $\boldsymbol{\nu}(\mathbf{y}) = \mathbf{y}$ and $|\mathbf{x}| = |\mathbf{y}| = 1$. Thus, $(\mathbf{x}-\mathbf{y})\cdot\boldsymbol{\nu}(\mathbf{y}) = -(1-\mathbf{x}\cdot\mathbf{y})$, $|\mathbf{x}-\mathbf{y}| = 2(1-\mathbf{x}\cdot\mathbf{y})$, and (23) reduces to

$$\frac{\partial G(\mathbf{x}-\mathbf{y},t-\tau)}{\partial \boldsymbol{\nu}(\mathbf{y})} = -\frac{1-\mathbf{x}\cdot\mathbf{y}}{2^{d+1}\pi^{d/2}(t-\tau)^{1+d/2}} e^{-\frac{1-\mathbf{x}\cdot\mathbf{y}}{2(t-\tau)}}. \tag{24}$$

3.1. Connection with the Laplace kernel

The Green's function for the Laplace equation in $\mathbb{R}^d$ is

$$G_{\mathrm{L}}(\mathbf{x},\mathbf{y}) = \begin{cases} -\frac{1}{2\pi}\ln|\mathbf{x}-\mathbf{y}|, & d=2, \\ \frac{1}{(d-2)\omega_d}\frac{1}{|\mathbf{x}-\mathbf{y}|^{d-2}}, & d\ge 3, \end{cases}$$

where

$$\omega_d = \frac{2\pi^{d/2}}{\Gamma(d/2)} \tag{25}$$

is the area of the unit sphere $S^{d-1} \subset \mathbb{R}^d$. Here Γ is the gamma function defined by the formula

$$\Gamma(z) = \int_0^\infty x^{z-1}e^{-x}dx. \tag{26}$$

The kernel of the Laplace double layer potential operator is given by

$$\frac{\partial G_{\mathrm{L}}(\mathbf{x}-\mathbf{y})}{\partial \boldsymbol{\nu}(\mathbf{y})} = \frac{\Gamma(d/2)}{2\pi^{d/2}} \frac{(\mathbf{x}-\mathbf{y})\cdot\boldsymbol{\nu}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^d}. \tag{27}$$

It is well known to satisfy Gauss' Lemma [18]:

$$\int_\Gamma \frac{\partial G_{\mathrm{L}}(\mathbf{x}-\mathbf{y})}{\partial \boldsymbol{\nu}(\mathbf{y})} dS(\mathbf{y}) = -\tfrac{1}{2}\ , \quad \mathbf{x}\in\Gamma. \tag{28}$$

Some connections between heat potentials and harmonic potentials (those satisfying the Laplace equation) are given by the following two lemmas.

Lemma 1.

$$\lim_{t\to\infty}\int_0^t \frac{\partial G(\mathbf{x}-\mathbf{y}, t-\tau)}{\partial \boldsymbol{\nu}(\mathbf{y})} d\tau = \frac{\partial G_{\mathrm{L}}(\mathbf{x}-\mathbf{y})}{\partial \boldsymbol{\nu}(\mathbf{y})}. \tag{29}$$

Proof. By (23), we have

$$\int_0^t \frac{\partial G(\mathbf{x}-\mathbf{y}, t-\tau)}{\partial \boldsymbol{\nu}(\mathbf{y})} d\tau = \frac{(\mathbf{x}-\mathbf{y})\cdot\boldsymbol{\nu}(\mathbf{y})}{2^{d+1}\pi^{d/2}} \int_0^t \frac{1}{(t-\tau)^{1+d/2}} e^{-\frac{|\mathbf{x}-\mathbf{y}|^2}{4(t-\tau)}} d\tau.$$

The change of variables $\lambda = \frac{|\mathbf{x}-\mathbf{y}|^2}{4(t-\tau)}$ leads to

$$\int_0^t \frac{\partial G(\mathbf{x}-\mathbf{y}, t-\tau)}{\partial \boldsymbol{\nu}(\mathbf{y})} d\tau = \frac{(\mathbf{x}-\mathbf{y})\cdot\boldsymbol{\nu}(\mathbf{y})}{2\pi^{d/2}|\mathbf{x}-\mathbf{y}|^d} \int_{\frac{|\mathbf{x}-\mathbf{y}|^2}{4t}}^\infty \lambda^{\frac{d}{2}-1} e^{-\lambda} d\lambda.$$

Taking the limit $t\to\infty$ and using the definition of the gamma function (26), we obtain (29). □

Lemma 2. *Suppose that D is a C^1 convex domain. Then*

$$\frac{\partial G(\mathbf{x}-\mathbf{y}, t-\tau)}{\partial \boldsymbol{\nu}(\mathbf{y})} \le 0, \quad \frac{\partial G_{\mathrm{L}}(\mathbf{x}-\mathbf{y})}{\partial \boldsymbol{\nu}(\mathbf{y})} \le 0, \quad \mathbf{x},\mathbf{y}\in\Gamma, \tag{30}$$

and

$$\lim_{t\to\infty}\int_0^t \int_\Gamma \frac{\partial G(\mathbf{x}-\mathbf{y}, t-\tau)}{\partial \boldsymbol{\nu}(\mathbf{y})} dS(\mathbf{y}) d\tau = -\frac{1}{2}, \quad \mathbf{x}\in\Gamma. \tag{31}$$

For $t\in(0,\infty)$,

$$\int_0^t \int_\Gamma \left|\frac{\partial G(\mathbf{x}-\mathbf{y}, t-\tau)}{\partial \boldsymbol{\nu}(\mathbf{y})}\right| dS(\mathbf{y}) d\tau < \frac{1}{2}, \quad \mathbf{x}\in\Gamma. \tag{32}$$

Proof. (30) follows from the expressions (23) and (27) and the fact that $\mathbf{x}\cdot\mathbf{y}\le 0$ for $\mathbf{x},\mathbf{y}\in\Gamma$ when D is convex due to the convex separation theorem [2]. (31) follows from (28) and (29), and (32) is a simple consequence of (30) and (31). □

4. The one-dimensional case

4.1. The Dirichlet problem

We consider first the forward Euler scheme (17) for the Dirichlet problem (16). Given a piecewise constant approximation of the unknown density σ

$$\sigma(\mathbf{y},\tau)=\sigma(\mathbf{y},t_j)=\sigma_j(\mathbf{y}),\quad \tau\in[t_j,t_{j+1})\quad \text{for } j=0,1,\ldots.$$

with $t_j=j\Delta t$, we restate (17) in the form

$$-\tfrac{1}{2}\sigma_j(\mathbf{x})+\sum_{k=0}^{j-1}V_{j-k}[\sigma_k](\mathbf{x})=f_j(\mathbf{x}):=f(\mathbf{x},j\Delta t), \tag{33}$$

for $j=0,1,2,\ldots$, where (as before) the tilde has been dropped from f, and where

$$V_{j-k}[\sigma_k](\mathbf{x})=\int_\Gamma \mathcal{V}_{j-k}(\mathbf{x},\mathbf{y})\sigma_k(\mathbf{y})ds(\mathbf{y})$$

and

$$\mathcal{V}_{j-k}(\mathbf{x},\mathbf{y})=\int_{k\Delta t}^{(k+1)\Delta t}\frac{\partial G(\mathbf{x}-\mathbf{y},j\Delta t-\tau)}{\partial\boldsymbol{\nu}(\mathbf{y})}d\tau.$$

Note that

$$V_l(\mathbf{x},\mathbf{y})=\int_0^{\Delta t}\frac{\partial G(\mathbf{x}-\mathbf{y},l\Delta t-\tau)}{\partial\boldsymbol{\nu}(\mathbf{y})}d\tau,\quad l\geq 1.$$

$V_0(\mathbf{x},\mathbf{y})$ is set to 0.

The boundary Γ of the unit ball in one dimension consists of only two points $x=\pm1$. And (33) becomes a 2×2 system on the vector $[\sigma_j(-1)\ \ \sigma_j(+1)]^T$. Diagonalization of this 2×2 system leads to the following scalar equation for each eigenmode

$$-\frac{1}{2}\sigma_j^{\pm}\mp\sum_{k=0}^{j-1}v_{j-k}\sigma_k^{\pm}=f_j^{\pm},\qquad j=0,1,2,\ldots, \tag{34}$$

where the convolution coefficient v_l is given by the formula

$$v_l=\frac{1}{2\sqrt{\pi}}\int_0^{\Delta t}(l\Delta t-\tau)^{-3/2}e^{-\frac{1}{(l\Delta t-\tau)}}d\tau,\quad l\geq 1 \tag{35}$$

with

$$\gamma(t)\ :=\ \frac{1}{2\sqrt{\pi}}t^{-3/2}e^{-\frac{1}{t}},\qquad t>0\ , \tag{36}$$

and we set $v_0=0$.

The system (34) for $j=0,1,\cdots,N$ can be written in matrix-vector form

$$\left(-\tfrac{1}{2}I\mp V\right)\boldsymbol{\sigma}^{\pm}=\boldsymbol{f}^{\pm}, \tag{37}$$

where I is the $(N+1)\times(N+1)$ identity matrix, $V \in \mathbb{R}^{(N+1)\times(N+1)}$ with entries $v_{j,k} = v_{j-k}$, $\boldsymbol{\sigma}^{\pm} = \{\sigma_j^{\pm}\}_{j=0}^{N}$, $\boldsymbol{f}^{\pm} = \{f_j^{\pm}\}_{j=0}^{N}$. we denote the symmetric part of V by W with its dependence on N and Δt written out explicitly, thus

$$W(N;\Delta t) \;:=\; \frac{V+V^T}{2}. \tag{38}$$

We have the following lemma.

Lemma 3. *Fix $T>0$. Then, for any N and Δt with $N\Delta t \le T$, the spectral radius $\rho(N;\Delta t)$ of the matrix $W(N;\Delta t)$ has the bound*

$$\rho(N;\Delta t) \;\le\; C_1(T)\;, \tag{39}$$

where

$$C_1(T) \;:=\; \int_0^T \gamma(T-\tau)d\tau \;=\; \frac{1}{2\sqrt{\pi}}\int_{\frac{1}{T}}^{\infty}\frac{1}{\sqrt{u}}e^{-u}du \;<\; \frac{1}{2}\;. \tag{40}$$

Proof. Using the Gershgorin circle theorem [40, §3.3], and the fact that the diagonal entries of W^n are all zero, we have

$$\rho(N;\Delta t) \;\le\; \max_i \sum_{j=1}^{N+1}|w_{ij}| \le 2\sum_{l=1}^{N}\tfrac{1}{2}|v_l| \le \sum_{l=1}^{N} v_l\;. \tag{41}$$

Now setting $t = N\Delta t$, we may collapse this sum into a single integral

$$\begin{aligned}\sum_{l=1}^{N} v_l = \sum_{l=1}^{N}\int_0^{\Delta t}\gamma(l\Delta t-\tau)d\tau &= \sum_{k=1}^{N}\int_0^{\Delta t}\gamma(N\Delta t-(k-1)\Delta t-\tau)d\tau \\ = \sum_{k=1}^{N}\int_{(k-1)\Delta t}^{k\Delta t}\gamma(N\Delta t-\tau)d\tau &= \int_0^{N\Delta t}\gamma(N\Delta t-\tau)d\tau = C_1(N\Delta t)\end{aligned}$$

according to the definition (40) of the function C_1. Combining the last two results we have $\rho(N;\Delta t) \le C_1(N\Delta t)$. The expression in (40) follows from the change of variables $u = \frac{1}{T-\tau}$. A further change of variables $x = \sqrt{u}$ leads to

$$C_1(T) = \frac{1}{\sqrt{\pi}}\int_{\frac{1}{\sqrt{T}}}^{\infty} e^{-x^2}dx < \frac{1}{\sqrt{\pi}}\int_0^{\infty} e^{-x^2}dx = \frac{1}{2}\;, \qquad \text{for all } T>0\;. \tag{42}$$

Finally, the above expression shows that $C_1(T)$ is a monotonically non-decreasing function of T, so that $\rho(N;\Delta t) \le C_1(N\Delta t) \le C_1(T)$. □

It is clear from (37) that to get a stability bound we will need to control the gap between $C_1(T)$ and $\frac{1}{2}$. For $T \ge 1$, we have

$$\frac{1}{2} - C_1(T) = \frac{1}{2\sqrt{\pi}}\int_0^{\frac{1}{T}}\frac{1}{\sqrt{u}}e^{-u}du > \frac{1}{2e\sqrt{\pi}}\int_0^{\frac{1}{T}}\frac{1}{\sqrt{u}}du = \frac{1}{e\sqrt{\pi T}}. \tag{43}$$

Theorem 3. *Suppose that $T \geq 1$. Then*

$$\|\boldsymbol{\sigma}^{\pm}\| \;\leq\; e\sqrt{\pi T}\|\boldsymbol{f}^{\pm}\| \tag{44}$$

for all N, Δt such that $N\Delta t \leq T$. That is, when Γ is the unit circle S^0, the forward Euler scheme for solving the second kind Volterra integral equation (16) *is unconditionally stable on any finite time interval* $[0, T]$.

Proof. Multiplying both sides of (37) by $-(\boldsymbol{\sigma}^{\pm})^T$, we have

$$\tfrac{1}{2}\|\boldsymbol{\sigma}^{\pm}\|^2 \pm (\boldsymbol{\sigma}^{\pm})^T V\boldsymbol{\sigma}^{\pm} = \tfrac{1}{2}\|\boldsymbol{\sigma}^{\pm}\|^2 \pm (\boldsymbol{\sigma}^{\pm})^T W\boldsymbol{\sigma}^{\pm} = -(\boldsymbol{\sigma}^{\pm})^T\boldsymbol{f}^{\pm} \ . \tag{45}$$

Applying (39) on the left side (45) and the Cauchy–Schwartz inequality on the right side, we obtain

$$\left(\tfrac{1}{2} - C_1(T)\right)\|\boldsymbol{\sigma}^{\pm}\|^2 \leq \tfrac{1}{2}\|\boldsymbol{\sigma}^{\pm}\|^2 \pm (\boldsymbol{\sigma}^{\pm})^T W\boldsymbol{\sigma}^{\pm} = -(\boldsymbol{\sigma}^{\pm})^T\boldsymbol{f}^{\pm} \leq \|\boldsymbol{\sigma}^{\pm}\|\|\boldsymbol{f}^{\pm}\| \ .$$

That is, finally applying (43),

$$\|\boldsymbol{\sigma}^{\pm}\| \leq \frac{1}{\frac{1}{2} - C_1(T)}\|\boldsymbol{f}^{\pm}\| \leq e\sqrt{\pi T}\|\boldsymbol{f}^{\pm}\| \ ,$$

which completes the proof. □

4.2. The Robin problem

We now analyze the Robin problem, recast as the Abel integral equation (8), repeated here for convenience (multiplying both sides by two, and from now on dropping the tilde on the right-hand side f):

$$\sigma(t) + \frac{\kappa}{\sqrt{\pi}}\int_0^t \frac{\sigma(\tau)}{\sqrt{t-\tau}}d\tau \;=\; 2f(t). \tag{46}$$

Firstly we show stability of the continuous problem for $\kappa > 0$. The Riemann–Liouville fractional integral operator $\mathcal{R}_\alpha$ is defined by the formula

$$\mathcal{R}_\alpha[g](t) = \frac{1}{\Gamma(\alpha)}\int_0^t \frac{g(\tau)}{(t-\tau)^{1-\alpha}}d\tau, \qquad \alpha \in (0, 1),$$

where $\Gamma(\alpha)$ is the gamma function (26). Thus, the integral operator on the left side of (8) is simply $\frac{\Gamma(1/2)\kappa}{\sqrt{\pi}}\mathcal{R}_{1/2} = \kappa\mathcal{R}_{1/2}$. For all real functions g, $\mathcal{R}_\alpha$ satisfies the non-negative property [31, Eq. (2.1)]

$$\int_0^T g(t)\mathcal{R}_\alpha[g](t)dt \geq 0 \ . \tag{47}$$

Taking the inner product of (46) with σ over a fixed interval $[0, T]$, and using (47), gives

$$\|\sigma\|^2_{L^2([0,T])} \leq 2(\sigma, f) \leq 2\|\sigma\|_{L^2([0,T])}\|f\|_{L^2([0,T])}$$

where Cauchy–Schwartz was used in the last step. Thus on any finite interval $[0, T]$ we have the L^2 stability bound

$$\|\sigma\| \leq 2\|f\| \ .$$

The above proof ingredient will recur several times in the discrete setting.

Recall from the introduction that the forward Euler scheme for (46) uses a piecewise constant approximation of the density σ and the explicit formula (9). For initialization, we set $\sigma_0 = f_0 = 0$. Let us define the vectors $\boldsymbol{\sigma}$ and $\boldsymbol{f}$ by $\{\sigma_n\}_{n=0}^N, \{f_n\}_{n=0}^N \in \mathbb{R}^{N+1}$, respectively. Using this notation, (9) takes the form of the lower-triangular Toeplitz linear system

$$(I + W)\boldsymbol{\sigma} = 2\boldsymbol{f} \ , \tag{48}$$

where $W \in \mathbb{R}^{(N+1)\times(N+1)}$ has elements $w_{n,m} = w_{n-m}$ for $n > m$, and $w_{n,m} = 0$ otherwise. Here, w_n is defined in (10) with $h = \kappa^2\,\Delta t/\pi$.

There is a substantial literature on the numerical analysis and stability of Volterra equations in the one-dimensional setting. For a discussion of convergence theory and step-size control, see [1, 16] and the monograph [3]. Much work on stability has been devoted to an analysis of the model problem

$$y(t) + \int_0^t [\lambda_0 + \lambda_1(t-\tau)]y(\tau)\,d\tau = f(t),$$

or to problems with a continuous kernel [16, 27]. In [20], a more relevant stability result is obtained for systems of the form (48), but assuming that the sequence $\{w_j\}$ is in l^1, which is not the case here.

For previous work on Abel-type equations with singular kernels, we refer the reader to [6, 21, 22, 42]. These papers, however, are mostly concerned with implicit marching schemes. An exception is Lubich's 1986 paper [23], which does a careful stability analysis for a variety of schemes and makes clear the connection between completely monotonic sequences and stability. An interesting result from that paper is Corollary 2.2, which states that "the stability region of an explicit convolution quadrature ... is bounded." Theorem 4 below, which is consistent with Lubich's result, gives a precise value for the time step restriction. It also guarantees that σ decays once the right-hand side f has switched off.

Before turning to that theorem, however, it is worth noting that this time-step restriction does *not* apply to the equation (16) in higher dimensions. We will show below that explicit methods for the Dirichlet problem can be unconditionally stable.

Theorem 4. *There is a constant $0 < c < 3 - \sqrt{2}$ such that, for any N and any $\boldsymbol{f} \in \mathbb{R}^{N+1}$, the solution to (48) obeys*

$$\|\boldsymbol{\sigma}\| \leq \frac{2}{1 - c\sqrt{h}}\|\boldsymbol{f}\| \ , \tag{49}$$

where $\|.\|$ denotes the l^2-norm. That is, the marching scheme (9) is stable for $h < 0.39 < (1/c)^2$ or $\Delta t < \pi/(c^2\kappa^2)$ where κ is the heat transfer coefficient.

Proof. We first show that there exists a constant $c > 0$ such that

$$\boldsymbol{\sigma}^T W \boldsymbol{\sigma} \geq -c\sqrt{h}\|\boldsymbol{\sigma}\|^2 \qquad \text{for any} \quad \boldsymbol{\sigma} \in \mathbb{R}^{N+1}, \tag{50}$$

i.e. that the smallest eigenvalue of W is bounded from below. Writing $\sqrt{h}T_{N+1} := \frac{1}{2}(W+W^T)$ as the symmetric part of W, note that $\boldsymbol{\sigma}^T W \boldsymbol{\sigma} = \sqrt{h}\boldsymbol{\sigma}^T T_{N+1}\boldsymbol{\sigma}$, and that T_{N+1} is independent of the time-step. Note that T_{N+1} is the $(N+1)\times(N+1)$ upper left principal submatrix of the infinite symmetric Toeplitz matrix T_v, defined by the sequence $0, v_1, v_2, \ldots$ with

$$v_j = \frac{1}{\sqrt{j}+\sqrt{j-1}} = \sqrt{j}-\sqrt{j-1}, \qquad j \in \mathbb{N}.$$

It is straightforward to check that the sequence $\{v_j\}_{j\in\mathbb{N}}$ is convex and that $\lim_{j\to\infty} v_j = 0$. By Theorem 2 and Remark 1, we have

$$\boldsymbol{\sigma}^T T_{N+1}\boldsymbol{\sigma} \geq (v_2 - 2v_1)\|\boldsymbol{\sigma}\|^2.$$

That is, (50) holds if $c = 2v_1 - v_2 = 3-\sqrt{2}$. To complete the proof, take the inner product of (48) with $\boldsymbol{\sigma}$ to get

$$\|\boldsymbol{\sigma}\|^2 + \boldsymbol{\sigma}^T W\boldsymbol{\sigma} = 2\boldsymbol{\sigma}^T \boldsymbol{f}\,.$$

Applying (50) to the left-hand side and the Cauchy–Schwartz inequality to the right-hand side, we have

$$(1-c\sqrt{h})\|\boldsymbol{\sigma}\|^2 \leq 2\|\boldsymbol{\sigma}\|\|\boldsymbol{f}\|\,,$$

from which (49) follows for any $\boldsymbol{\sigma} \neq \mathbf{0}$. It holds trivially when $\boldsymbol{\sigma} = \mathbf{0}$. □

Remark 6. The above proof gives $c = 3-\sqrt{2} \approx 1.5858$. By numerically computing the smallest eigenvalue of successively larger Toeplitz matrices V, or, better, by evaluating $v(\pi) = 2\sum_{j>0}(-1)^{j-1}v_j$, one can obtain an optimal estimate of $c \approx 1.52041925043874$. We omit the details of this computation and mention it only to illustrate that the explicit bound is within about 4% of the optimal one.

Remark 7. With unit diffusion constant, the transfer coefficient κ has units $(\text{length})^{-1}$. Thus our time-step condition $\Delta t < \pi/(c\kappa)^2$ is proportional to the square of the physical length $1/\kappa$. Although reminiscent of the explicit finite-difference stability condition $\Delta t < c\Delta x^2$, our stability condition is, by contrast, independent of any spatial discretization. (Indeed, once $f(t)$ is available, there is no need for spatial discretization.)

Remark 8. In the limit $\kappa \to 0$, the scheme is unconditionally stable. This is to be expected, since when $\kappa = 0$, the Robin boundary condition becomes a Neumann condition and the representation (7) yields the analytic solution $\sigma(t) = 2f(t)$.

5. The Dirichlet problem in two dimensions

We now consider (33) when Γ is the unit circle S^1. We decompose both $\sigma_j(\mathbf{y})$ and $f_j(\mathbf{x})$ into Fourier series:

$$\sigma_j(\mathbf{y}) = \sum_{n=-\infty}^{+\infty} \sigma_j^n e^{in\phi}, \quad \mathbf{y} = (\cos\phi, \sin\phi),$$

$$f_j(\mathbf{x}) = \sum_{n=-\infty}^{+\infty} f_j^n e^{in\theta}, \quad \mathbf{x} = (\cos\theta, \sin\theta).$$

From (24), writing $s=\theta-\phi$, the nth Fourier mode of the kernel is

$$\begin{aligned}\int_{S^1} \frac{\partial G(\mathbf{x}-\mathbf{y},t-\tau)}{\partial \boldsymbol{\nu}(\mathbf{y})} e^{in\phi} d\phi &= \int_0^{2\pi} -\frac{1-\cos(\theta-\phi)}{8\pi(t-\tau)^2} e^{-\frac{1-\cos(\theta-\phi)}{2(t-\tau)}} e^{in\phi} d\phi \\ &= -\gamma_n(t-\tau) e^{in\theta}, \end{aligned} \tag{51}$$

where, noting that the imaginary part of e^{-ins} cancels by symmetry, we have

$$\gamma_n(t) := \frac{1}{8\pi t^2} \int_0^{2\pi} (1-\cos(s)) e^{-\frac{1-\cos(s)}{2t}} \cos(ns) ds , \qquad t>0 . \tag{52}$$

Since $\{e^{in\theta}\}$ are orthonormal, each Fourier mode evolves independently. The marching scheme (or recurrence) (33) for the nth mode is then

$$-\tfrac{1}{2}\sigma_j^n - \sum_{k=0}^{j-1} v_{j-k}^n \sigma_k^n = f_j^n, \qquad j=0,1,2,\ldots, \tag{53}$$

where the convolution coefficient v_l^n is given by the formula

$$v_l^n = \int_0^{\Delta t} \gamma_n(l\Delta t-\tau) d\tau, \quad l \geq 1, \tag{54}$$

and we set $v_0^n=0$. The system (53) for $j=0,1,\cdots,N$ can be written in matrix-vector form

$$\left(-\tfrac{1}{2}I - V^n\right) \boldsymbol{\sigma}^n = \boldsymbol{f}^n, \tag{55}$$

where I is the $(N+1)\times(N+1)$ identity matrix, $V^n \in \mathbb{R}^{(N+1)\times(N+1)}$ with entries $v_{j,k}^n = v_{j-k}^n$, $\boldsymbol{\sigma}^n = \{\sigma_j^n\}_{j=0}^N$, $\boldsymbol{f}^n = \{f_j^n\}_{j=0}^N$. The symmetric part of V^n we denote by W^n, and often make its dependence on N and Δt explicit, thus

$$W^n(N;\Delta t) := \frac{V^n+(V^n)^T}{2} = \frac{1}{2} \begin{bmatrix} 0 & v_1^n & v_2^n & \cdots & v_N^n \\ v_1^n & 0 & v_1^n & \cdots & v_{N-1}^n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ v_N^n & v_{N-1}^n & \cdots & v_1^n & 0 \end{bmatrix}. \tag{56}$$

5.1. Stability analysis

We now prove two key results. The first is that the forward Euler scheme is unconditionally stable for any fixed time interval $[0,T]$ (Theorem 5). More precisely, this theorem permits the solution to grow linearly in time. The second is that for $\Delta t<1$, the L^2 norm of the solution is bounded independently of T. We will require the following lemma.

Lemma 4. *Fix $T>0$. Then, for any N and Δt with $N\Delta t \leq T$, and all $n\in\mathbb{Z}$, the spectral radius $\rho_n(N;\Delta t)$ of the matrix $W^n(N;\Delta t)$ has the bound*

$$\rho_n(N;\Delta t) \leq C_2(T) , \tag{57}$$

where, in terms of the definition (52),

$$C_2(T) := \int_0^T \gamma_0(T-\tau) d\tau = \frac{1}{4\pi} \int_0^{2\pi} e^{-\frac{1-\cos(s)}{2T}} ds < \tfrac{1}{2} . \tag{58}$$

Proof. Let $n \in \mathbb{Z}$. Since the integrand in (52), excluding the $\cos ns$ factor, is non-negative, we observe that $|\gamma_n(t)| \le \gamma_0(t)$, so $|v_l^n| \le v_l^0$ for all $l \ge 1$. Using this, the Gershgorin circle theorem [40, §3.3], and using the fact that the diagonal entries of W^n are all zero, we have

$$\rho_n(N; \Delta t) \ \le\ \max_i \sum_{j=1}^{N+1} |w_{ij}^n| \le 2 \sum_{l=1}^{N} \tfrac{1}{2} |v_l^n| \le \sum_{l=1}^{N} v_l^0 \ . \tag{59}$$

Now setting $t = N\Delta t$, we may collapse this sum into a single integral

$$\begin{aligned} \sum_{l=1}^{N} v_l^0 &= \sum_{l=1}^{N} \int_0^{\Delta t} \gamma_0(l\Delta t - \tau) d\tau = \sum_{k=1}^{N} \int_0^{\Delta t} \gamma_0(N\Delta t - (k-1)\Delta t - \tau) d\tau \\ &= \sum_{k=1}^{N} \int_{(k-1)\Delta t}^{k\Delta t} \gamma_0(N\Delta t - \tau) d\tau = \int_0^{N\Delta t} \gamma_0(N\Delta t - \tau) d\tau = C_2(N\Delta t) \end{aligned}$$

according to the definition (58) of the function C_2. Combining the last two results we have $\rho_n(N; \Delta t) \le C_2(N\Delta t)$. To prove the expression in (58) we insert (52), interchange the order of integration and apply the change of variables $\lambda = \frac{1-\cos(s)}{2(T-\tau)}$, thus

$$\begin{aligned} C_2(T) &:= \int_0^T \gamma_0(T-\tau) d\tau = \int_0^T \frac{1}{8\pi (T-\tau)^2} \int_0^{2\pi} (1-\cos(s)) e^{-\frac{1-\cos(s)}{2(T-\tau)}} ds d\tau \\ &= \frac{1}{4\pi} \int_0^{2\pi} e^{-\frac{1-\cos(s)}{2T}} ds < \tfrac{1}{2} \ , \qquad \text{for all } T > 0 \ . \end{aligned}$$

Finally, the above expression shows that $C_2(T)$ is a monotonically non-decreasing function of T, so that $\rho_n(N; \Delta t) \le C_2(N\Delta t) \le C_2(T)$. □

It is clear from (55) that to get a stability bound we will need to control the gap between $C_2(T)$ and $\frac{1}{2}$. This motivates the following.

Proposition 1.

$$C_2(T) \ = \ \tfrac{1}{2} e^{-\frac{1}{2T}} I_0\left(\frac{1}{2T}\right) \ , \tag{60}$$

where $I_n(\cdot)$ is the modified regular Bessel function of order n (see Appendix). For $T \ge 1$,

$$\tfrac{1}{2} - C_2(T) \ \ge \ \frac{1}{10T} \ . \tag{61}$$

Proof. (60) follows from the integral representation of $I_0(x)$ (A.2). (61) follows from the facts that $I_0(x) \le 1 + \frac{x^2}{2}$ [32, §10.25.2] and $e^{-x} \le 1 - \frac{x}{2}$ for $T \ge 1$. □

Theorem 5. *Suppose that $T \ge 1$. Then for all $n \in \mathbb{Z}$,*

$$\|\boldsymbol{\sigma}^n\| \ \le \ 10T \|\boldsymbol{f}^n\| \tag{62}$$

for all N, Δt such that $N\Delta t \le T$. That is, when Γ is the unit circle S^1, the forward Euler scheme for solving the second kind Volterra integral equation (16) *is unconditionally stable on any finite time interval* $[0, T]$.

Proof. Since we are working in the Fourier domain, $\boldsymbol{\sigma}^n$ and $\boldsymbol{f}^n$ are complex-valued. Thus, we split (55) into two independent real systems

$$\begin{aligned} \left(-\tfrac{1}{2}I - V^n\right)\boldsymbol{\sigma}_r^n &= \boldsymbol{f}_r^n, \\ \left(-\tfrac{1}{2}I - V^n\right)\boldsymbol{\sigma}_i^n &= \boldsymbol{f}_i^n, \end{aligned} \tag{63}$$

where $\boldsymbol{\sigma}_r^n$ and $\boldsymbol{\sigma}_i^n$ are the real and imaginary part of $\boldsymbol{\sigma}^n$, respectively.

Multiplying both sides of the first equation in (63) by $-(\boldsymbol{\sigma}_r^n)^T$, we have

$$\tfrac{1}{2}\|\boldsymbol{\sigma}_r^n\|^2 + (\boldsymbol{\sigma}_r^n)^T V^n \boldsymbol{\sigma}_r^n = \tfrac{1}{2}\|\boldsymbol{\sigma}_r^n\|^2 + (\boldsymbol{\sigma}_r^n)^T W^n \boldsymbol{\sigma}_r^n = -(\boldsymbol{\sigma}_r^n)^T \boldsymbol{f}_r^n \ . \tag{64}$$

Applying (57) on the left side (64) and the Cauchy–Schwartz inequality on the right side, we obtain

$$\left(\tfrac{1}{2} - C_2(T)\right)\|\boldsymbol{\sigma}_r^n\|^2 \le \tfrac{1}{2}\|\boldsymbol{\sigma}_r^n\|^2 + (\boldsymbol{\sigma}_r^n)^T W^n \boldsymbol{\sigma}_r^n = -(\boldsymbol{\sigma}_r^n)^T \boldsymbol{f}_r^n \le \|\boldsymbol{\sigma}_r^n\|\|\boldsymbol{f}_r^n\| \ .$$

That is, finally applying Proposition 1,

$$\|\boldsymbol{\sigma}_r^n\| \le \frac{1}{\frac{1}{2} - C_2(T)}\|\boldsymbol{f}_r^n\| \le 10T\|\boldsymbol{f}_r^n\| \ .$$

Similar result holds for $\|\boldsymbol{\sigma}_i^n\|$. Combining the two inequalities gives (62). □

We now show that the dependence on T in (62) can be removed when the time step satisfies $\Delta t \le 1$. This is a physically reasonable requirement since we have assumed that the diffusion coefficient is one, and the domain has of order unit area. We first provide a bound on $\rho_n(N;\Delta t)$ for $n \neq 0$ that is independent of $N\Delta t$.

Lemma 5. *Let N and $\Delta t > 0$ be arbitrary, and let $\rho_n(N;\Delta t)$ be the spectral radius of $W^n(N;\Delta t)$ defined in (56). Then for all $n \neq 0$,*

$$\rho_n(N;\Delta t) \ \le \ \frac{1}{2|n|+1} \ . \tag{65}$$

Proof. Clearly, it is sufficient to prove (65) for $n > 0$. For this, let us note that substituting (52) into (54), exchanging the order of integration, and making the change of variables $\lambda = \frac{1-\cos(s)}{2(l\Delta t - \tau)}$, we obtain

$$v_l^n = \begin{cases} \frac{1}{4\pi}\int_0^{2\pi} e^{-\frac{1-\cos(s)}{2\Delta t}}\cos(ns)ds, & l = 1, \\ \frac{1}{4\pi}\int_0^{2\pi}\left(e^{-\frac{1-\cos(s)}{2l\Delta t}} - e^{-\frac{1-\cos(s)}{2(l-1)\Delta t}}\right)\cos(ns)ds, & l > 1. \end{cases}$$

By the integral representation (A.2) of I_n, we have

$$v_l^n = \begin{cases} \frac{1}{2}e^{-\frac{1}{2\Delta t}} I_{|n|}(\frac{1}{2\Delta t}), & l = 1, \\ \frac{1}{2}\left(e^{-\frac{1}{2l\Delta t}} I_{|n|}(\frac{1}{2l\Delta t}) - e^{-\frac{1}{2(l-1)\Delta t}} I_{|n|}(\frac{1}{2(l-1)\Delta t})\right), & l > 1. \end{cases} \tag{66}$$

From (66), defining $f(x) := e^{-x}I_n(x)$ and $x_l = 1/(2l\Delta t)$, we consider the sum

$$S_n = 2\sum_{l=1}^{N}|v_l^n| = f(x_1) + \sum_{l=2}^{N}|f(x_l) - f(x_{l-1})| \ . \tag{67}$$

By Lemma 9 (see Appendix), $f(x)$ increases monotonically on $[0, r_n]$ and decreases monotonically on $[r_n, +\infty)$, with r_n the unique maximum. We now consider (67) on a case-by-case basis.

(a) All x_l lie on $[0, r_n]$: Since $x_l < x_{l-1}$ and $f(x)$ increases on $[0, r_n]$, we have

$$\begin{aligned} S_n &\le f(x_1) - \sum_{l=2}^{N} (f(x_l) - f(x_{l-1})) = 2f(x_1) - f(x_N) \\ &\le 2f(x_1) < \frac{2}{2n+1}. \end{aligned}$$

where the last inequality follows from (A.6).

(b) All x_l lie on $[r_n, \infty)$: In this case, we have

$$S_n \le f(x_1) + \sum_{l=2}^{N} (f(x_l) - f(x_{l-1})) = f(x_N) < \frac{1}{2n+1}.$$

(c) $x_1 > \cdots > x_m \ge r_n > x_{m+1} > \cdots > x_N$: In this case, we have

$$\begin{aligned} S_n &\le f(x_1) + \sum_{l=2}^{m} (f(x_l) - f(x_{l-1})) \\ &\quad + |f(x_m) - f(x_{m+1})| - \sum_{l=m+2}^{N} (f(x_l) - f(x_{l-1})) \\ &= f(x_m) + |f(x_m) - f(x_{m+1})| + f(x_{m+1}) - f(x_N) \\ &\quad < f(x_m) + |f(x_m) - f(x_{m+1})| + f(x_{m+1}) \\ &= 2\max(f(x_m), f(x_{m+1})) \\ &\quad < \frac{2}{2n+1}. \end{aligned}$$

By (59) we have

$$\rho_n(N; \Delta t) \le \sum_{l=1}^{N} |v_l^n| = \tfrac{1}{2} S_n < \frac{1}{2n+1},$$

completing the proof. □

Corollary 1. *For all $n \neq 0$,*

$$\|\boldsymbol{\sigma}^n\| \le \frac{1}{\frac{1}{2} - \frac{1}{2|n|+1}} \|\boldsymbol{f}^n\| \le 6\|\boldsymbol{f}^n\|.$$

Thus all non-zero modes are unconditionally stable. The zeroth Fourier mode is a bit more subtle, and brings in a weak restriction on Δt, as follows.

Lemma 6. *Suppose that $a = 0.05$ and $\Delta t \le 1$. Then $c_2 I + W^0 + aW^1$ is positive definite if*

$$c_2 = \tfrac{1}{2}e^{-1/2} I_0\left(\tfrac{1}{2}\right) + \tfrac{1}{6}a \;\approx\; 0.33085\ldots \tag{68}$$

Proof. Define the sequence $y_j = w_j^0 + aw_j^1 = \frac{1}{2}(v_j^0 + av_j^1)$ for $j \ge 1$ and $y_0 = c_2$. Theorem 2 then shows that a sufficient condition for the positive semi-definiteness of $c_2 I + W^0 + aW^1$ is that the sequence $\{y_j\}_{j\in\mathbb{Z}_+}$ is convex. But $y_1 = \frac{1}{4}f(x_1)$, $y_j = \frac{1}{4}(f(x_j) - f(x_{j-1}))$ $(j > 1)$, where f is the function defined in Lemma 13, and $x_j = 2j\Delta t$. That is, y_j is the first order difference of f. Furthermore, the convexity of $\{y_j\}_{j\in\mathbb{N}}$ is equivalent to the non-negativity of the third order difference of f, which follows from the fact that $f'''(x) > 0$ for all $x > 0$ as proved in Lemma 13. For $j = 0$, the convexity of the sequence requires that one choose c_2 such that

$$c_2 + y_2 = y_0 + y_2 \ge 2y_1. \tag{69}$$

By the integral representation (A.2) of I_0, it is easy to see that $e^{-x}I_0(x)$ is strictly decreasing. Thus, we have $e^{-1/2}I_0\left(\frac{1}{2}\right) \ge e^{-\frac{1}{2\Delta t}} I_0\left(\frac{1}{2\Delta t}\right)$ for $\Delta t \le 1$. Furthermore,

$$\max_{[0,\infty)} e^{-x} I_1(x) < \tfrac{1}{3}$$

by (A.6). Hence, (69) is achieved by choosing

$$c_2 = \tfrac{1}{2}e^{-1/2}I_0\left(\tfrac{1}{2}\right) + \tfrac{1}{6}a > 2y_1 = \tfrac{1}{2}e^{-\frac{1}{2\Delta t}}\left(I_0\left(\frac{1}{2\Delta t}\right) + I_1\left(\frac{1}{2\Delta t}\right)\right)$$

for $\Delta t \le 1$. □

Corollary 2. *Suppose that $\Delta t \le 1$. Then, for arbitrary N,*

$$\|\boldsymbol{\sigma}^0\| \;\le\; 7\|\boldsymbol{f}^0\|.$$

Proof. Set $a = 0.05$. By Lemma 6, the smallest eigenvalue of W^0 is bounded by

$$\lambda^0_{\min} \ge -c_2 - a\lambda^1_{\max} \ge -c_2 - a\rho_1 \ge -c_2 - \frac{1}{3}a.$$

Thus a simple bound using the value of c_2 from Lemma 6 is

$$\begin{aligned} 7\|\boldsymbol{\sigma}^0\|^2 &\le \left(\tfrac{1}{2} - c_2 - \frac{1}{3}a\right)\|\boldsymbol{\sigma}^0\|^2 \le \tfrac{1}{2}\|\boldsymbol{\sigma}^0\|^2 + (\boldsymbol{\sigma}^0)^T W^0 \boldsymbol{\sigma}^0 = -(\boldsymbol{\sigma}^0)^T \boldsymbol{f}^0 \\ &\le \|\boldsymbol{\sigma}^0\|\|\boldsymbol{f}^0\|, \end{aligned}$$

completing the proof. □

6. Higher dimensions

In dimensions $d > 2$, we consider the Dirichlet problem on the unit ball, with data specified on the unit sphere S^{d-1}. The unknown density σ is decomposed using the corresponding spherical harmonics [29]

$$\sigma(\mathbf{y}, \tau) = \sum_{n=0}^{\infty}\sum_{m=1}^{a_{n,d}} \sigma^{nm}(\tau) Y_n^m(\mathbf{y}),$$

where

$$a_{n,d} = (2n + d - 2)\frac{(n + d - 3)!}{n!(d - 2)!}.$$

Here, $a_{n,d}$ is the dimension of $H_n(S^{d-1})$, the space of homogeneous polynomials of degree n on $\mathbb{R}^d$ restricted to S^{d-1}, while Y_n^m are spherical harmonics of degree n. When $d = 3$, $a_{n,d} = 2n+1$, the inner summation is usually written as $\sum_{m=-n}^{n}$, and the spherical harmonics $Y_n^m(\theta, \phi)$ are defined by

$$Y_n^m(\theta, \phi) = \sqrt{\frac{2n + 1}{4\pi}}\sqrt{\frac{(n - |m|)!}{(n + |m|)!}}P_n^{|m|}(\cos\theta)e^{im\phi},$$

where $P_n^m(\cos\theta)$ is the associated Legendre polynomial [32, §18.3] of degree n and order m.

The spherical harmonics admit the following integral representation [29]

$$Y_n^m(\mathbf{x}) = \frac{a_{n,d}}{\omega_d}\int_{S^{d-1}} P_{n,d-1}(\mathbf{x}\cdot\mathbf{y})Y_n^m(\mathbf{y})dS(\mathbf{y}), \tag{70}$$

where ω_d is the area of S^{d-1} defined in (25), and the $P_{n,d-1}$ are Gegenbauer polynomials [29, Chapter 2] (also called ultraspherical polynomials), defined by the Rodrigues formula

$$P_{n,d-1}(t) = \frac{(-1)^n}{2^n}\frac{\Gamma\left(\frac{d-1}{2}\right)}{\Gamma\left(n + \frac{d-1}{2}\right)}\frac{1}{(1 - t^2)^{\frac{d-3}{2}}}\frac{d^n}{dt^n}(1 - t^2)^{n+\frac{d-3}{2}}. \tag{71}$$

The Funk–Hecke formula [29, Chapter 2, Theorem 2.39] states that

$$\int_{S^{d-1}} f(\mathbf{x}\cdot\mathbf{z})P_{n,d-1}(\mathbf{y}\cdot\mathbf{z})dS(\mathbf{z}) = \beta_{n,d-1}P_{n,d-1}(\mathbf{x}\cdot\mathbf{y}), \tag{72}$$

where

$$\beta_{n,d-1} = \omega_{d-1}\int_{-1}^{1} P_{n,d-1}(t)f(t)(1 - t^2)^{\frac{d-3}{2}}dt$$

and f is any measurable function such that

$$\int_{-1}^{1} |f(t)|(1 - t^2)^{\frac{d-3}{2}}dt \ < \ \infty \ .$$

In $\mathbb{R}^3$, this reduces to $f \in L^1[-1, 1]$.

We compute the double layer heat potential nmth Fourier mode,

$$\begin{aligned}
&\int_{S^{d-1}} \frac{\partial G(\mathbf{x} - \mathbf{y}, t - \tau)}{\partial\boldsymbol{\nu}(\mathbf{y})}Y_n^m(\mathbf{y})dS(\mathbf{y}) \\
&= -\int_{S^{d-1}} \frac{1 - \mathbf{x}\cdot\mathbf{y}}{2^{d+1}\pi^{d/2}(t - \tau)^{1+d/2}}e^{-\frac{1-\mathbf{x}\cdot\mathbf{y}}{2(t-\tau)}}Y_n^m(\mathbf{y})dS(\mathbf{y}) \\
&= -\frac{a_{n,d}}{\omega_d}\int_{S^{d-1}} \gamma_{n,d}(t - \tau)P_{n,d-1}(\mathbf{x}\cdot\mathbf{z})Y_n^m(\mathbf{z})dS(\mathbf{z}) \\
&= -\gamma_{n,d}(t - \tau)Y_n^m(\mathbf{x}) \ ,
\end{aligned} \tag{73}$$

where, by analogy with (52),

$$\gamma_{n,d}(t) := \frac{\omega_{d-1}}{2^{d+1}\pi^{d/2}t^{(d+2)/2}} \int_{-1}^{1} (1-x)e^{-\frac{1-x}{2t}} P_{n,d-1}(x)(1-x^2)^{(d-3)/2} dx \ . \tag{74}$$

The third equality makes use of (70), (72), and exchanging the order of integration. The last step follows again from (70). Notice that $\gamma_{n,d}$ does not depend on the order m.

Since the $\{Y_n^m\}$ form an orthonormal basis for functions in $L^2(S^{d-1})$ and (73) shows that each spherical harmonic evolves independently under the action of the double layer heat potential operator, we may consider the time evolution for each mode nm separately.

For the forward Euler scheme, we again assume that $\sigma(\mathbf{x}, t)$ takes the constant value $\sigma_j(\mathbf{x}) = \sigma(\mathbf{x}, j\Delta t)$ over each interval $[j\Delta t, (j+1)\Delta t]$, $j = 0, 1, \ldots$. Equivalently, each spherical harmonic mode $\sigma^{nm}(t)$ takes the constant value $\sigma_j^{nm} = \sigma^{nm}(j\Delta t)$ over the interval $[j\Delta t, (j+1)\Delta t]$, $j = 0, 1, \ldots$. A straightforward calculation leads to the following recurrence for the nmth spherical harmonic mode, analogous to (53):

$$-\tfrac{1}{2}\mu_j - \sum_{k=0}^{j-1} v_{j-k}^n \mu_k = g_j, \qquad j = 0, 1, 2, \ldots, \tag{75}$$

where we use the abbreviations $\mu_j := \sigma_j^{nm}$, $g_j = f_j^{nm}$, and the matrix elements

$$v_l^n = \int_0^{\Delta t} \gamma_{n,d}(l\Delta t - \tau) d\tau, \qquad l > 0, \tag{76}$$

and, as before, $v_0^n = 0$.

6.1. Stability analysis

The normalization in (71) leads to [28, 30]

$$|P_{n,d-1}(x)| \leq 1 = P_{0,d-1}(x), \quad x \in [-1, 1].$$

As the other terms in (74) are non-negative, we have

$$|\gamma_{n,d}(t-\tau)| \leq \gamma_{0,d}(t-\tau) \ , \qquad t - \tau > 0 \ .$$

An almost identical proof as in Lemma 4 leads to the following lemma.

Lemma 7. *Fix $T > 0$. Then, for any N and Δt with $N\Delta t \leq T$, and all $n \in \mathbb{Z}_+$, the spectral radius $\rho_{n,d}(N; \Delta t)$, of the symmetric Toeplitz matrix $W^n(N; \Delta t)$ as defined by* (56) *with v_l^n given by* (76)*, has the bound*

$$\rho_{n,d}(N; \Delta t) \ \leq \ C_d(T) \ ,$$

where

$$C_d(T) := \int_0^T \frac{\omega_{d-1}}{2^{d+1}\pi^{d/2}(T-\tau)^{(d+2)/2}} \int_{-1}^{1} \frac{(1-x)}{e^{\frac{1-x}{2(T-\tau)}}} (1-x^2)^{(d-3)/2} dx d\tau < \tfrac{1}{2} \ .$$

As before, we are also able to bound from below the gap between $C_d(T)$ and $\frac{1}{2}$, given a weak condition on T. For this, we interchange the order of integration and apply the change of variable $\lambda = \frac{1-x}{2(T-\tau)}$, giving

$$C_d(T) = \int_{-1}^{1} \frac{\omega_{d-1}}{2^{d+1}\pi^{d/2}} \frac{(1+x)^{(d-3)/2}}{\sqrt{1-x}} \left(2^{d/2} \int_{\frac{1-x}{2T}}^{\infty} \lambda^{d/2} e^{-\lambda} d\lambda \right) dx$$

and

$$\tfrac{1}{2} - C_d(T) = \frac{1}{2^{d/2}\sqrt{\pi}\Gamma\left(\frac{d-1}{2}\right)} \int_{-1}^{1} \frac{(1+x)^{(d-3)/2}}{\sqrt{1-x}} \left(\int_0^{\frac{1-x}{2T}} \lambda^{d/2} e^{-\lambda} d\lambda \right) dx.$$

Assume now $T \geq 1$. Then for $x \in [-1, 1]$, $\frac{1-x}{2T} \leq 1$. Thus, $e^{-\lambda} \geq e^{-1}$ for $\lambda \in [0, \frac{1-x}{2T}]$ and

$$\begin{aligned}
\tfrac{1}{2} - C_d(T) &\geq \frac{1}{2^{d/2}\sqrt{\pi}\Gamma\left(\frac{d-1}{2}\right)} \int_{-1}^{1} \frac{(1+x)^{(d-3)/2}}{\sqrt{1-x}} \left(\frac{1}{e} \int_0^{\frac{1-x}{2T}} \lambda^{d/2} d\lambda \right) dx \\
&= \frac{1}{ed2^{d-1}\sqrt{\pi}\Gamma\left(\frac{d-1}{2}\right) T^{\frac{d}{2}}} \int_{-1}^{1} (1-x^2)^{(d-3)/2}(1-x) dx \\
&= \frac{2}{ed2^{d-1}\sqrt{\pi}\Gamma\left(\frac{d-1}{2}\right) T^{\frac{d}{2}}} \int_{0}^{1} (1-x^2)^{(d-3)/2} dx \\
&= \frac{2}{ed2^{d-1}\sqrt{\pi}\Gamma\left(\frac{d-1}{2}\right) T^{\frac{d}{2}}} \int_{0}^{\frac{\pi}{2}} \cos^{d-2}(\theta) d\theta \\
&= \frac{1}{ed2^{d-1}\Gamma\left(\frac{d}{2}\right) T^{\frac{d}{2}}},
\end{aligned}$$

where the last equality follows from an integral identity in [7, §3.62].

Armed with this polynomial control of the gap, and following the same reasoning as used to show (62), we obtain the following theorem regarding the stability of the forward Euler scheme in higher dimensions.

Theorem 6. *Fix $d > 2$, and $T \geq 1$. For all $n = 0, 1, \ldots$ and $m = 1, \ldots, a_{n,d}$,*

$$\|\boldsymbol{\sigma}^{nm}\| \leq \frac{1}{\frac{1}{2} - C_d(T)} \|\boldsymbol{f}^{nm}\| \leq ed2^{d-1}\Gamma\left(\frac{d}{2}\right) T^{\frac{d}{2}} \|\boldsymbol{f}^{nm}\|$$

for all N, Δt such that $N\Delta t \leq T$. That is, when Γ is the unit sphere S^{d-1}, the forward Euler scheme for solving the second kind Volterra integral equation (16) *is unconditionally stable on any finite time interval* $[0, T]$.

7. Conclusions and further remarks

We have analyzed the stability of the simplest explicit, first-order accurate time marching scheme for solving the Dirichlet problem for the heat equation in the unit ball, with data specified on the unit sphere $S^{d-1} \subset \mathbb{R}^d$, using second-kind Volterra boundary integral equations. While finite difference methods require that the Courant number $\Delta t/(\Delta x)^2$ be bounded by

$\frac{1}{2d}$, we have shown that, for the Dirichlet problem, integral equation methods can be both explicit and unconditionally stable for any fixed final time T.

We have also shown that, when solving the heat equation on the unit disk in two dimensions with unit diffusion constant, the scheme is stable for all time, so long as $\Delta t \le 1$. Finally, for Robin boundary conditions in one dimension, we have shown that stability follows if $\Delta t < 0.39\pi/\kappa^2$, where κ is the heat transfer coefficient. We conjecture that similar results hold in higher dimensions as well.

One of the key ingredients in our proof is a tight rational function bound for the ratio of modified Bessel functions of the first kind with large positive real argument, which may be of interest in its own right for other physical applications. A second ingredient in our proofs is a bound on the smallest eigenvalue of real symmetric Toeplitz matrices via the convexity of the associate Fourier series sequence. This may be of interest in some signal processing applications. It is worth observing that a critical element in our proof is the pointwise non-positivity of the double layer heat kernel on the unit sphere S^{d-1}. This property holds for any convex domain. In fact, using the results in section 3.1, it is straightforward to extend our stability proof in the L^∞ norm on an arbitrary convex domain.

While this paper is purely analytic, we note that the numerical experiments in [43] are consistent with the theory presented here. More detailed experiments will be reported in a forthcoming paper [45] that considers the full initial-boundary value problem including forcing terms.

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Appendix A. Properties of the modified Bessel functions of the first kind

The modified Bessel function of the first kind $I_\nu(x)$ is defined by the formula [32, Chapter 10]

$$I_\nu(z) = \left(\tfrac{1}{2}z\right)^\nu \sum_{k=0}^{\infty} \frac{\left(\frac{1}{2}z\right)^{2k}}{k!\Gamma(\nu+k+1)}.$$

It satisfies the recurrence relations [32, §10.29.2]

$$I'_\nu(z) = I_{\nu-1}(z) - \frac{\nu}{z} I_\nu(z), \quad I'_\nu(z) = I_{\nu+1}(z) + \frac{\nu}{z} I_\nu(z). \tag{A.1}$$

When ν is fixed and $x \to \infty$ [32, §10.30.4],

$$I_\nu(x) \sim \frac{e^x}{\sqrt{2\pi x}}, \quad x \in \mathbb{R}.$$

When ν is an integer n, I_n admits the integral representation [32, §10.32.3]

$$I_n(z) = \frac{1}{\pi}\int_0^\pi e^{z\cos\theta}\cos(n\theta)d\theta. \tag{A.2}$$

The following results can be found in [46].

Lemma 8. *Let* $W_\nu(x) = \frac{xI_\nu(x)}{I_{\nu+1}(x)}$ *and* $S_{p,\nu} = W_\nu^2(x) - 2pW_\nu(x) - x^2$. *Then* $S_{\nu,\nu-1}(x)$ *is monotonically decreasing from* 0 *to* $-\infty$ *on* $(0,\infty)$ *for* $\nu > 1/2$,

$$\nu - \tfrac{1}{2} + \sqrt{x^2 + \nu^2 - \frac{1}{4}} \leq W_{\nu-1}(x) \leq \nu - \tfrac{1}{2} + \sqrt{x^2 + \left(\nu + \tfrac{1}{2}\right)^2}, \tag{A.3}$$

and

$$\nu - 1 + \sqrt{x^2 + (\nu+1)^2} \leq W_{\nu-1}(x) \tag{A.4}$$

for $\nu \geq \frac{1}{2}$, *with* $x \in (0,\infty)$.

Lemma 9. *Let* n *be a positive integer. Then*

(a) *There is only one zero* r_n *for the equation*

$$\frac{I_n'(x)}{I_n(x)} = 1$$

on $(0,+\infty)$. *Furthermore,*

$$\max(n^2 - \tfrac{1}{2}, \frac{n^2}{2} + n) \leq r_n \leq n^2 + n. \tag{A.5}$$

(b) *The function* $e^{-x}I_n(x)$ *increases monotonically on* $[0, r_n]$ *and decreases monotonically on* $[r_n, +\infty)$.

(c) *The maximum value of* $e^{-x}I_n(x)$ *on* $[0,\infty)$ *satisfies*

$$\max_{[0,+\infty)} e^{-x}I_n(x) < \frac{1}{2n+1}. \tag{A.6}$$

Proof. (a) Using the recurrence (A.1), we have

$$W_{n-1}(x) = x\frac{I_n'(x)}{I_n(x)} + n.$$

Thus,

$$S_{n,n-1}(x) = x^2\left(\frac{I_n'(x)}{I_n(x)}\right)^2 - x^2 - n^2.$$

When $\frac{I_n'(x)}{I_n(x)} = 1$, $S_{n,n-1} = -n^2$. By the monotonicity and the range of $S_{n,n-1}(x)$, $S_{n,n-1}$ takes the value $-n^2$ at only one point and we denote that point by r_n.

Substituting $x = r_n$ into (A.3) and (A.4) with $\frac{I_n'(r_n)}{I_n(r_n)} = 1$ and simplifying the resulting expressions, we obtain (A.5).

(b) We have

$$\frac{d}{dx}(e^{-x}I_n(x)) = e^{-x}I_n(x)\left(\frac{I_n'(x)}{I_n(x)} - 1\right).$$

Using (A.3), it follows that $\frac{I_n'(x)}{I_n(x)} > 1$ for $x < n^2 - \frac{1}{2}$ and $\frac{I_n'(x)}{I_n(x)} < 1$ for $x > n^2 + n$. Combing these facts with (a), we have $\frac{I_n'(x)}{I_n(x)} > 1$ for $x < r_n$ and $\frac{I_n'(x)}{I_n(x)} < 1$ for $x > r_n$. That is, $\frac{d}{dx}(e^{-x}I_n(x)) > 0$ for $x < r_n$ and $\frac{d}{dx}(e^{-x}I_n(x)) < 0$ for $x > r_n$, which completes the proof of (b).

(c) By the identity §10.35.5 in [32], we have

$$1 = e^{-x}\left(I_0(x) + 2\sum_{k=1}^{\infty} I_k(x)\right).$$

Section 10.37 of [32] states that for fixed $x > 0$, $I_\nu(x)$ is positive and decreasing for $0 < \nu < \infty$. Hence,

$$1 > e^{-x}\left(I_n(x) + 2\sum_{k=1}^{n} I_n(x)\right) = (2n+1)e^{-x}I_n(x),$$

which completes the proof.

□

The following lemma about differential inequalities can be found in [13, Chapter III, §4]. See also [35].

Lemma 10 (Petrovitsch 1901)**.** *Suppose that $f(y,t)$ is continuous in an open domain D. Suppose further that y is the solution to the Cauchy problem*

$$y'(t) = f(y(t),t), \quad y(t_0) = y_0, \quad (y_0, t_0) \in D.$$

(a) (Increasing t). Suppose that u satisfies the inequalities

$$\begin{aligned} &u'(t) \geq f(u(t),t), \quad t \in (t_0, t_0+\delta)\,(\delta > 0) \\ &u(t_0) \geq y(t_0). \end{aligned} \tag{A.7}$$

Then

$$u(t) \geq y(t), \quad t \in [t_0, t_0+\delta]. \tag{A.8}$$

The inequality in (A.8) *is reversed if both inequalities in* (A.7) *are reversed.*

(b) (Decreasing t). Suppose that u satisfies the inequalities

$$\begin{aligned} &u'(t) \leq f(u(t),t), \quad t \in (t_0-\delta, t_0)\,(\delta > 0) \\ &u(t_0) \geq y(t_0). \end{aligned} \tag{A.9}$$

Then

$$u(t) \geq y(t), \quad t \in [t_0-\delta, t_0]. \tag{A.10}$$

The inequality in (A.10) *is reversed if both inequalities in* (A.9) *are reversed.*

Lemma 11. *Let*

$$g_0(x) = (4x-3)I_0(x) - (4x-1)I_1(x). \tag{A.11}$$

Then $g_0(x)$ has a unique zero, denoted as x^*, on $(\frac{3}{4}, \infty)$. Furthermore, $g_0(x) < 0$ on $[\frac{3}{4}, x^*)$ and $g_0(x) > 0$ on (x^*, ∞).

Proof. Let $r_\nu(x) = \frac{I_\nu(x)}{I_{\nu+1}(x)}$. In particular,

$$r_0(x) = \frac{I_0(x)}{I_1(x)}.$$

From §10.37 of [32], we know that $I_\nu(x)$ is positive and increasing on $(0, \infty)$ for fixed $\nu(\geq 0)$ and $I_\nu(x)$ is decreasing on $0 < \nu < \infty$ for fixed x. Thus, $r_\nu(x) > 1$ on $(0, \infty)$ for $\nu \geq 0$. Let

$$l_0(x) = \frac{4x-1}{4x-3}.$$

Then it is clear that the sign of $g_0(x)$ is determined by comparing $r_0(x)$ with $l_0(x)$. First, $\lim_{x \to \frac{3}{4}^+} l_0(x) = +\infty$ and thus $l_0(x) > r_0(x)$ as $x \to \frac{3}{4}^+$. Second, the series expansion of $l_0(x)$ and the asymptotic expansion of $r_0(x)$ are as follows:

$$l_0(x) = 1 + \frac{1}{2\,x} + \frac{3}{8\,x^2} + \frac{9}{32\,x^3} + \frac{27}{128\,x^4} + \frac{81}{512\,x^5} + O\left(\frac{1}{x^6}\right),$$

$$r_0(x) = 1 + \frac{1}{2\,x} + \frac{3}{8\,x^2} + \frac{3}{8\,x^3} + \frac{63}{128\,x^4} + \frac{27}{32\,x^5} + O\left(\frac{1}{x^6}\right).$$

Hence, $r_0(x) > l_0(x)$ as $x \to \infty$. Combining these two facts, there is at least one point $x^* \in (\frac{3}{4}, \infty)$ where $r_0(x^*) = l_0(x^*)$. Or equivalently,

$$g_0(x^*) = 0.$$

By the recurrence relations (A.1), r_ν satisfies the following Riccati equation

$$r_\nu'(x) = 1 + \frac{2\nu+1}{x} r_\nu(x) - r_\nu^2(x).$$

In particular, for $\nu = 0$,

$$r_0'(x) = 1 + \frac{1}{x} r_0(x) - r_0^2(x).$$

We now calculate

$$l_0'(x) - (1 + \frac{1}{x} l_0(x) - l_0^2(x)) = -\frac{3}{x(4x-3)^2} < 0 \quad x \in (\frac{3}{4}, \infty).$$

By Lemma 10, we have

$$l_0(x) \leq u_0(x), \quad x \geq x^*; \qquad l_0(x) \geq r_0(x), \quad x \in (\frac{3}{4}, x^*).$$

Equivalently,

$$g_0(x) \geq 0, \quad x \geq x^*; \qquad g_0(x) < 0, \quad x \in [\frac{3}{4}, x^*),$$

completing the proof. □

Remark 9. Numerical computation shows that $x^* \approxeq 1.452165365078841\ldots$.

Corollary 3. *Let*

$$h_0(x) = (x-2)g_0(x) = (x-2)[(4x-3)I_0(x) - (4x-1)I_1(x)], \tag{A.12}$$

where $g_0(x)$ is defined in (A.11). *Then $h_0(x) \geq 0$ on $[\frac{3}{4}, x^*]$ and $[2, \infty)$; $h_0(x) \leq 0$ on $[x^*, 2)$.*

Lemma 12. *Let*

$$h_1(x) = (4x^2 - 7x)I_1(x) - (4x^2 - 9x + 3)I_0(x). \tag{A.13}$$

Then $h_1(x) > 0$ on $[\frac{3}{4}, \infty)$.

Proof. Let $x_1^* = \frac{\sqrt{33}+9}{8} = 1.843\ldots$ be the larger root of $4x^2 - 9x + 3$. Then $4x^2 - 9x + 3 > 0$ for $x > x_1^*$ and $4x^2 - 9x + 3 < 0$ for $x \in [\frac{3}{4}, x_1^*)$. We break $[\frac{3}{4}, \infty)$ into several subintervals and show the positivity of $h_1(x)$ on each subinterval.

(a) $x \in [x_1^*, \infty)$. Let

$$u_0(x) = \frac{4x^2 - 7x}{4x^2 - 9x + 3}.$$

Then

$$u_0'(x) - (1 + \frac{1}{x}u_0(x) - u_0^2(x)) = \frac{3\,(x-3)}{(4\,x^2 - 9\,x + 3)^2}, \tag{A.14}$$

which is greater than zero if $x > 3$ and less than zero if $x < 3$. At $x = 3$, $u_0(3) = \frac{5}{4} = 1.25$ and $r_0(3) = 1.23459\ldots < 1.25 = u_0(3)$. Thus, Using Lemma 10 in the increasing direction we have $r_0(x) < u_0(x)$ on $[3, \infty)$; and using Lemma 10 in the decreasing direction, we still have $r_0(x) < u_0(x)$ on $[x_1^*, 3)$. Equivalently, $h_1(x) > 0$ on $[x_1^*, \infty)$.

(b) $x \in [\frac{7}{4}, x_1^*]$. On this subinterval, we have $4x^2 - 7x \geq 0$ and $-4x^2 + 9x - 3 \geq 0$. Hence, $h_1(x) > 0$, since $I_1(x)$ and $I_0(x)$ are always positive on $[0, \infty)$.

(c) $x \in [\frac{3}{4}, \frac{7}{4}]$. By (A.14), we have $u_0'(x) - (1 + \frac{1}{x}u_0(x) - u_0^2(x)) \leq 0$ on $[\frac{3}{4}, \frac{7}{4}]$. Also, $u_0(\frac{3}{4}) = 2 < r_0(\frac{3}{4}) = 2.8\ldots$. Using Lemma 10, we have $r_0(x) > u_0(x)$, or equivalently $h_1(x) > 0$ on $[\frac{3}{4}, \frac{7}{4}]$.

□

Lemma 13. *Let $f_0(x) = e^{-\frac{1}{x}}I_0(\frac{1}{x})$, $f_1(x) = e^{-\frac{1}{x}}I_1(\frac{1}{x})$, $f(x) = f_0(x) + af_1(x)$ with $a = 0.05$. Then $f'''(x) > 0$ on $(0, \infty)$.*

Proof. Using the recurrence relation (A.1), we obtain

$$f_0'''(x) = \frac{1}{x^4}e^{-\frac{1}{x}}h_0\left(\frac{1}{x}\right),$$

where $h_0(x)$ is defined in (A.12). Similarly,

$$f_1'''(x) = \frac{1}{x^4}e^{-\frac{1}{x}}h_1\left(\frac{1}{x}\right),$$

where $h_1(x)$ is defined in (A.13). Thus, in order to show that $f'''(x) > 0$ on $(0, \infty)$, we only need to show that $h_0(x) + ah_1(x) > 0$ on $(0, \infty)$.

We break it into several steps.

(a) $x \in [0, 1/4]$. On this interval, $3 - 4x \geq 2$, $0 \leq 1 - 4x \leq 1$, $2 - x \geq 1.75$, thus $h_0(x) \geq 1.75(2I_0(x) - I_1(x)) > 1.75I_0(x)$. And $4x^2 - 7x \geq -1.5$, $4x^2 - 9x + 3 \leq 3$, thus $h_1(x) \geq -1.5I_1(x) - 3I_0(x) > -4.5I_0(x)$. Combinging these results, we have

$$h_0(x) + ah_1(x) > (1.75 + 0.05 \times (-4.5))I_0(x) > 0.$$

(b) $\frac{1}{4} \leq x \leq \frac{9-\sqrt{33}}{8} < 0.5$. On this interval, $3 - 4x > 1$, $4x - 1 \geq 0$, $2 - x > 1.5$, thus $h_0(x) > 1.5I_0(x)$. And $4x^2 - 7x > -2.5$, $0 \leq 4x^2 - 9x + 3 \leq 1$, thus $h_1(x) > -2.5I_1(x) - I_0(x) > -3.5I_0(x)$. Combining these results, we have

$$h_0(x) + ah_1(x) > (1.5 + 0.05 \times (-3.5))I_0(x) > 0.$$

(c) $\frac{9-\sqrt{33}}{8} \leq x \leq 3/4$. On this interval, $3 - 4x \geq 0$, $4x - 1 > 0.6$, $2 - x > 1$, thus $h_0(x) > 0.6I_1(x)$. And $4x^2 - 7x \geq -3$, $-(4x^2 - 9x + 3) \geq 0$, thus $h_1(x) \geq -3I_1(x)$. Combining these results, we have

$$h_0(x) + ah_1(x) > (0.6 - 0.05 \times 3)I_1(x) > 0.$$

(d) $x \in [\frac{3}{4}, x^*] \cup [2, \infty)$. On these two subintervals, both $h_0(x)$ and $h_1(x)$ are positive by Corollary 3 and Lemma 12. Thus $h_0(x) + ah_1(x) > 0$.

(e) $x \in (x^*, 2)$. We calculate

$$h_1'(x) = (x - 3)g_0(x),$$

where $g_0(x)$ is defined in (A.11). By Lemma 11, $g_0(x) > 0$ on (x^*, ∞). Thus, $h_1'(x) < 0$ on $(x^*, 2)$. This shows that $h_1(x) > h_1(2) \approx 0.901688$ on $(x^*, 2)$. On the other hand, it is straightforward to show that $g_0'(x) > 0$ and $g_0''(x) < 0$ on $(x^*, 2)$. Hence, $h_0''(x) = g_0''(x)(x - 2) + 2g_0'(x) > 0$ on $(x^*, 2)$, indicating that $h_0(x)$ achieves its minimum at exactly one point. Numerical calculation shows that

$$\min_{x \in (x^*, 2)} h_0(x) \approx -0.043\ldots > -0.044.$$

Hence,

$$h_0(x) + ah_1(x) \geq \min_{x \in (x^*, 2)} h_0(x) + 0.05 \times h_1(2) > 0.$$

□

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