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EXPLICIT UNCONDITIONALLY STABLE METHODS FOR THE HEAT EQUATION VIA POTENTIAL THEORY

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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. 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 $\mathcal{O}(\Delta x^2)$, where Δx is the finest spatial grid spacing. In contrast, for the Dirichlet and Neumann problems on the unit ball in all dimensions $d \geq 1$, we show that the simplest Volterra marching scheme, i.e., the forward Euler scheme, is *unconditionally stable*. Our proof is based on an explicit spectral radius bound of the marching matrix, leading to an estimate that an L^2-norm of the solution to the integral equation is bounded by $c_d T^{d/2}$ times the norm of the right-hand side. For the Robin problem on the half-space in any dimension, with constant Robin (heat transfer) coefficient κ, we exhibit a constant C such that the forward Euler scheme is stable if $\Delta t < C/\kappa^2$, independent of any spatial discretization. This relies on new lower bounds on the spectrum of real symmetric Toeplitz matrices defined by convex sequences. Finally, we show that the forward Euler scheme is unconditionally stable for the Dirichlet problem on any smooth *convex* domain in any dimension, in the L^∞-norm.

1. Introduction

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

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

for $0 \leq t \leq T$, subject to suitable boundary conditions, in a smooth domain $D \subset \mathbb{R}^d$. Without loss of generality, we will assume that the diffusion coefficient (thermal conductivity) α is 1 in most of our discussion. We consider three standard boundary conditions: the Dirichlet boundary condition

$$u(\boldsymbol{x}, t) = f(\boldsymbol{x}, t)|_{\boldsymbol{x}\in\Gamma, t>0}, \quad \boldsymbol{x} \in \Gamma = \partial D, \tag{2}$$

the Neumann boundary condition

$$\frac{\partial u(\boldsymbol{x}, t)}{\partial \boldsymbol{\nu}_{\boldsymbol{x}}} = g(\boldsymbol{x}, t)|_{\boldsymbol{x}\in\Gamma,\ t>0}, \quad \boldsymbol{x} \in \Gamma, \tag{3}$$

and the Robin boundary condition

$$\frac{\partial u(\boldsymbol{x}, t)}{\partial \boldsymbol{\nu}_{\boldsymbol{x}}} + \kappa u(\boldsymbol{x}, t) = h(\boldsymbol{x}, t)|_{\boldsymbol{x}\in\Gamma, t>0}, \quad \boldsymbol{x} \in \Gamma. \tag{4}$$

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Here, $\kappa > 0$ is the *heat transfer coefficient*, and (4) models heat transfer via Newton's law of cooling [Crank 1956]. For all three boundary conditions, we assume that proper compatibility conditions are satisfied between the initial and boundary data.

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:

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

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 $\Delta t < 1/(2d)\Delta x^2$ for the case of the standard second-order finite-difference Laplacian stencil on a uniform spatial grid with step size Δx in each direction; see, for example, [Thomas 1995, p. 158]. The constraint changes when using less standard stencils. For nonuniform grids, the time-step restriction is more complicated to analyze, but generally requires that $\Delta t = \mathcal{O}(h_{\min}^2)$, where $h_{\min}$ is the finest mesh spacing in the discretization.

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. [Peaceman and Rachford 1955].

When finite-difference methods are used to solve general initial-boundary value problems, GKSO (Gustafsson–Kreiss–Sundström–Osher) theory plays a critical role [Gustafsson et al. 1995; 1972; Osher 1969; Strikwerda 1989; Trefethen 1983] 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 [Kress 1989; Pogorzelski 1966]. The Green's function for the heat equation is

$$G(\boldsymbol{x}, t) = \frac{1}{(4\pi t)^{d/2}} e^{-|\boldsymbol{x}|^2/(4t)}, \qquad \boldsymbol{x} \in \mathbb{R}^d. \tag{5}$$

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

$$\mathcal{S}[\sigma](\boldsymbol{x}, t) = \int_0^t \int_\Gamma G(\boldsymbol{x} - \boldsymbol{y}, t - \tau)\sigma(\boldsymbol{y}, \tau)\, ds(\boldsymbol{y})\, d\tau \tag{6}$$

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

$$\mathcal{D}[\sigma](\boldsymbol{x},t)=\int_0^t\int_\Gamma \frac{\partial G(\boldsymbol{x}-\boldsymbol{y},t-\tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})}\sigma(\boldsymbol{y},\tau)\,ds(\boldsymbol{y})\,d\tau, \tag{7}$$

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

$$\mathcal{I}[u_0](\boldsymbol{x},t)=\int_D G(\boldsymbol{x}-\boldsymbol{y},t-\tau)u_0(\boldsymbol{y})\,d\boldsymbol{y} \tag{8}$$

and the volume potential is defined by

$$\mathcal{V}[F](\boldsymbol{x},t)=\int_0^t\int_D G(\boldsymbol{x}-\boldsymbol{y},t-\tau)F(\boldsymbol{y},\tau)\,d\boldsymbol{y}\,d\tau. \tag{9}$$

By the linearity of the problem, we may decompose the solution into

$$u(\boldsymbol{x},t)=u^{(F)}(\boldsymbol{x},t)+u^{(B)}(\boldsymbol{x},t), \tag{10}$$

where all initial and volume data is captured by the free-space volume forced term

$$u^{(F)}(\boldsymbol{x},t)=\mathcal{I}[u_0](\boldsymbol{x},t)+\mathcal{V}[F](\boldsymbol{x},t), \tag{11}$$

while $u^{(B)}$ is the solution to a pure boundary value problem with zero initial data, zero volume forcing, and modified boundary data. Note that $u^{(F)}$ needs only *evaluation* of initial and volume potentials; it requires no linear solve. Thus, there is no stability issue with $u^{(F)}$, and its error is simply the quadrature error in evaluating the integrals that appear in (8) and (9). In other words, unlike finite-difference or finite-element methods, the volume part is completely decoupled from the boundary part in integral equation methods from the perspective of stability analysis.

For the Dirichlet problem, we proceed by representing $u^{(B)}(\boldsymbol{x},t)$ as a double-layer potential with unknown density σ. The jump relation (see Section 2) then leads to the second-kind Volterra equation

$$\left(-\tfrac{1}{2}+\mathcal{D}\right)[\sigma](\boldsymbol{x},t)=\tilde{f}(\boldsymbol{x},t),\quad (\boldsymbol{x},t)\in\Gamma\times[0,T], \tag{12}$$

where $\mathcal{D}$ is interpreted in a principal-value sense, and the corrected data is

$$\tilde{f}(\boldsymbol{x},t):=f(\boldsymbol{x},t)-u^{(F)}(\boldsymbol{x},t),\quad \boldsymbol{x}\in\Gamma.$$

The main objective of this paper is to demonstrate certain advantages of integral equation methods by giving, for several combinations of archetypal geometries and boundary conditions, rigorous stability bounds for the simplest explicit time-marching scheme, namely the forward Euler scheme. This scheme is derived by assuming $\sigma(\boldsymbol{y},t)$ is piecewise constant over each time interval $[j\Delta t,(j+1)\Delta t)$, taking on the value $\sigma(\boldsymbol{y},j\Delta t)$. For (12), this leads to a marching scheme of the form

$$\sigma(\boldsymbol{x},n\Delta t)=2\sum_{j=0}^{n-1}\int_{j\Delta t}^{(j+1)\Delta t}\int_\Gamma \frac{\partial G(\boldsymbol{x}-\boldsymbol{y},n\Delta t-\tau)}{\partial\boldsymbol{\nu}(\boldsymbol{y})}\sigma(\boldsymbol{y},j\Delta t)\,ds(\boldsymbol{y})\,d\tau-2\tilde{f}(\boldsymbol{x},n\Delta t), \tag{13}$$

where $n=1,2,\dots$. This falls into the class of collocation schemes [Kress 1989, §13.3], as well as convolution quadrature schemes [Lubich 1986]. It is explicit, since $\sigma(\boldsymbol{x},n\Delta t)$ does not appear on the right-hand side. It is also first-order accurate (e.g., see Section 5.1). For the Neumann and Robin problems, second-kind Volterra equations are obtained by representing $u^{(B)}(\boldsymbol{x},t)$ instead as a single-layer potential; other than a change of kernel, the forward Euler scheme remains the same.

The principal reason that integral equation methods have received relatively little attention for solving the heat equation has been that direct evaluation of layer (or volume) potentials requires 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 [Greengard and Strain 1990; 1991; Greengard and Sun 1998; Ibáñez and Power 2002; Lubich and Ostermann 1993; Lubich and Schneider 1992; Strain 1994; Tausch 2007; Wang 2017; Wang and Greengard 2018; Wang et al. ≥ 2019] for further discussion.

We now summarize the results in this paper. Perhaps the simplest geometry is the half-space $D = \mathbb{R}^d_+ := \{\boldsymbol{x} = (x_1, x_2, \dots, x_d) \in \mathbb{R}^d \mid x_d \ge 0\}$, with $\Gamma = \partial D = \mathbb{R}^{d-1}$. It is easy to check that the integral kernel of $\mathcal{D}$ is identically zero on Γ, so (12) reduces to

$$\sigma(\boldsymbol{x},t) = -2\tilde{f}(\boldsymbol{x},t). \tag{14}$$

This is an analytic solution, so that stability follows trivially. A similar trivial analytic solution arises when the single-layer potential is used to solve the Neumann problem on the half-space. Thus, we consider the Dirichlet and Neumann problems on possibly the next-simplest domain, the unit ball $B^d \subset \mathbb{R}^d$ (i.e., Γ is the unit sphere S^{d-1}). For both these latter cases, we show that the forward Euler scheme is unconditionally stable in all dimensions $d \ge 1$. Specifically, we show that for $T \ge 1$,

$$\|\sigma\|_2 \le c_d T^{d/2} \|\tilde{f}\|_2 \tag{15}$$

for all N and Δt such that $N\Delta t \le T$. Here N is the total number of time steps, Δt is the time-step size, $\|\cdot\|_2$ denotes a space-time L^2-norm,[1] and c_d is a positive constant depending on d. The estimate (15) is obtained by a Gershgorin spectral radius bound of the marching matrix; we show that this is no longer tight for the Dirichlet problem if a fairly mild condition is imposed on Δt. Indeed, we are able to show the improved estimate in two dimensions,

$$\|\sigma\|_2 \le 7\|\tilde{f}\|_2 \tag{16}$$

for $\Delta t \le 1$ and any N.

Returning to the d-dimensional half-space, the simplest boundary condition for which the integral equation is nontrivial is the Robin condition. We show that here the forward Euler scheme has a time-step restriction determined by the physical parameter κ, namely $\Delta t < \pi/(c^2\kappa^2)$ with $c = 3 - \sqrt{2}$. Finally, considering more general domains, we prove that the forward Euler scheme for the Dirichlet problem is unconditionally stable for smooth convex domains in all dimensions, in the L^∞-norm.

Firstly, in Section 2 we summarize the necessary properties of layer potentials. Then in Section 3 we present a lower bound for the spectrum of a Toeplitz operator defined by a convex sequence; this will be needed later to handle cases where the sequences are not summable and thus Gershgorin is inapplicable.

[1] Explicitly, $\|\sigma\|_2^2 := \sum_{j=0}^{N} \int_\Gamma \sigma(\boldsymbol{x}, j\Delta t)^2\, ds(\boldsymbol{y})$; i.e., the norm is l^2 in time $[0,T]$ but L^2 over the surface Γ.

The Dirichlet and Neumann problems on the unit ball are then treated in Section 4, the Robin problem on the half-space in Section 5, and the Dirichlet problem on C^1 convex domains in Section 6. We conclude in Section 7. Finally, the Appendix covers estimates on special functions used in the body of the paper.

2. Properties of heat potentials

By construction, the single and double-layer heat potentials (6) and (7) satisfy the heat equation. They also satisfy certain well-known jump conditions when the target point $\boldsymbol{x}$ approaches the boundary from either side [Kress 1989; Pogorzelski 1966]. In particular, for $\boldsymbol{x}_0 \in \Gamma$, the normal derivative of the single-layer potential $\mathcal{S}[\sigma]$ satisfies the relation

$$\lim_{\epsilon\to 0+} \frac{\partial \mathcal{S}[\sigma](\boldsymbol{x}_0 \pm \epsilon \boldsymbol{\nu}(\boldsymbol{x}_0), t)}{\partial \boldsymbol{\nu}(\boldsymbol{x}_0)} = \mp\tfrac{1}{2}\sigma(\boldsymbol{x}_0, t) + \mathcal{S}_{\boldsymbol{\nu}}[\sigma](\boldsymbol{x}_0, t), \tag{17}$$

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

$$\lim_{\epsilon\to 0+} \mathcal{D}[\sigma](\boldsymbol{x}_0 \pm \epsilon \boldsymbol{\nu}(\boldsymbol{x}_0), t) = \pm\tfrac{1}{2}\sigma(\boldsymbol{x}_0, t) + \mathcal{D}[\sigma](\boldsymbol{x}_0, t), \tag{18}$$

where both $\mathcal{S}_{\boldsymbol{\nu}}[\sigma](\boldsymbol{x}_0, t)$ and $\mathcal{D}[\sigma](\boldsymbol{x}_0, t)$ are interpreted in the Cauchy principal value sense. If we represent the solution to the heat equation (1) via a double-layer potential $u(\boldsymbol{x}, t) = \mathcal{D}[\sigma](\boldsymbol{x}, t)$, then the integral equation (12) follows immediately from the jump relation (18).

The kernel of the double-layer potential is given explicitly by

$$\frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, t-\tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} = \frac{(\boldsymbol{x}-\boldsymbol{y})\cdot \boldsymbol{\nu}(\boldsymbol{y})}{2^{d+1}\pi^{d/2}(t-\tau)^{1+d/2}} e^{-|\boldsymbol{x}-\boldsymbol{y}|^2/(4(t-\tau))} \tag{19}$$

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

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

Finally, the initial potential (8) is well known to satisfy the homogeneous heat equation with initial data $u_0(\boldsymbol{x})$, while the volume potential (9) satisfies the inhomogeneous heat equation

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

with zero initial data.

Remark 1. Using these properties, it is straightforward to see that representing the solution to the Dirichlet problem in the form

$$u(\boldsymbol{x}, t) = \mathcal{D}[\sigma](\boldsymbol{x}, t) + \mathcal{I}[u_0](\boldsymbol{x}, t) + \mathcal{V}[F](\boldsymbol{x}, t)$$

leads to the integral equation (12), with the only unknown corresponding to the double-layer density σ.

Remark 2. On the unit sphere S^{d-1}, $\boldsymbol{\nu}(\boldsymbol{y}) = \boldsymbol{y}$ and $|\boldsymbol{x}| = |\boldsymbol{y}| = 1$. Thus, $(\boldsymbol{x}-\boldsymbol{y})\cdot\boldsymbol{\nu}(\boldsymbol{y}) = -(1-\boldsymbol{x}\cdot\boldsymbol{y})$, $|\boldsymbol{x}-\boldsymbol{y}|^2 = 2(1-\boldsymbol{x}\cdot\boldsymbol{y})$, and (19) reduces to

$$\frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, t-\tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} = -\frac{1-\boldsymbol{x}\cdot\boldsymbol{y}}{2^{d+1}\pi^{d/2}(t-\tau)^{1+d/2}} e^{-(1-\boldsymbol{x}\cdot\boldsymbol{y})/(2(t-\tau))}. \tag{20}$$

3. Spectral bounds for real symmetric Toeplitz operators

Although for many of the later results we can use simple Gershgorin spectral bounds for matrices, for the tight bound for the zeroth mode of the $d = 2$ Dirichlet disc (Section 4.2.2), and the Robin case in the half-space (Section 5), a more delicate spectral bound on Toeplitz matrices is needed.

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 in the Hilbert space $L^2(S^1)$, we write

$$f(\theta) = \sum_{n=-\infty}^{\infty} f_n e^{in\theta}, \tag{21}$$

in terms of the orthogonal basis $\{e^{in\theta}\}_{n\in\mathbb{Z}}$, where f_n $(n \in \mathbb{Z})$ is the n-th 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

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

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 $(T_f(u))_n$ denotes the n-th Fourier coefficient of $T_f(u)$, then

$$(T_f(u))_n = \begin{cases} \sum_{m=0}^{\infty} f_{n-m} u_m, & n \ge 0, \\ 0, & n < 0, \end{cases}$$

where u_m is the m-th Fourier coefficient of u.

Definition 3. A sequence $\{a_n\}_{n\in\mathbb{Z}_+}$ is said to be convex if $\delta^2 a_n \ge 0$ 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

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

The following theorem can be found in [Katznelson 1968, Chapter I, Theorem 4.1].

Theorem 4. *If $a_n \to 0$ and the sequence $\{a_n\}_{n\in\mathbb{Z}_+}$ is convex, then the series*

$$v(\theta) = \sum_{n=1}^{\infty} n(\delta^2 a_n) F_{n-1}(\theta) \tag{22}$$

converges in $L^1([-\pi, \pi])$ to a nonnegative 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

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

[Katznelson 1968, Chapter I, (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

$$\lim_{\theta\to 0} \theta v(\theta) = 0. \tag{23}$$

Bounds on the spectrum of finite Toeplitz matrices are of interest in many applications [Dembo 1988; Hertz 1992; Laudadio et al. 2008; Melman 1999]. When a real symmetric Toeplitz operator (or matrix) is generated by a positive sequence, the Gershgorin circle theorem [Thomas 1995, §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 the operator it defines is unbounded.

Theorem 5. *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 nonnegative function defined by the sequence* $\{v_n\}_{n\in\mathbb{Z}_+}$ *as in Theorem 4. 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*

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

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

$$u(\theta) = \sum_{n=0}^{N} u_n e^{in\theta}. \tag{24}$$

Theorem 4 implies

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

Remark 6. 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 7. 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 $(c, v_1 + a_1, v_2 + a_2, \dots)$ is a convex sequence. If T_a is a bounded operator, then the previous theorem implies a lower bound on the spectrum of V:

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

Remark 8. If the function $v(\theta)$ defined in (22) is unbounded, then the Toeplitz operator T_v that it defines is not a bounded operator and is not defined on all of H^2. The discussion above easily applies to show that this operator is defined on a dense subset, and its closure is self-adjoint: (23) 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

$$\left(\frac{1-e^{i\theta}}{r-e^{i\theta}}\right)u \in H^2 \quad \text{and} \quad \lim_{r\to 1^+}\left\|\left(\frac{1-e^{i\theta}}{r-e^{i\theta}}\right)u - u\right\|_2 = 0.$$

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

4. The Dirichlet and Neumann problems on the unit ball B^d

We consider first the forward Euler scheme (13) for the Dirichlet problem (12). For general $d \geq 1$, our approximation of the unknown density σ is piecewise constant in time,

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

where $t_j = j\Delta t$. We restate (13) in the form

$$-\tfrac{1}{2}\sigma_j(\boldsymbol{x}) + \sum_{k=0}^{j-1} V_{j-k}[\sigma_k](\boldsymbol{x}) = f_j(\boldsymbol{x}) := f(\boldsymbol{x}, j\Delta t) \tag{25}$$

for $j = 0, 1, 2, \ldots$, where the tilde has been dropped from f, and where the action of each spatial integral operator $V_{j-k} : C(\Gamma) \to C(\Gamma)$ is defined by

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

Here the operator kernel is itself the integral of the heat kernel over one time-step,

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

Due to time-shift invariance, a simpler way to write the spatial kernel is

$$\mathcal{V}_l(\boldsymbol{x}, \boldsymbol{y}) = \int_0^{\Delta t} \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, l\Delta t - \tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})}\, d\tau, \qquad l \geq 1,$$

and $\mathcal{V}_0(\boldsymbol{x}, \boldsymbol{y})$ is set identically to 0. For initialization of time-stepping we set $\sigma_0 \equiv f_0 \equiv 0$.

4.1. ***The Dirichlet problem in one dimension.*** The boundary Γ of the unit ball in one dimension consists of only two points $\boldsymbol{x} = \pm 1$. Let the time-stepped density at these two points be $\boldsymbol{\sigma}^\pm = \{\sigma_j^\pm\}_{j=0}^N$ and the data $\boldsymbol{f}^\pm = \{f_j^\pm\}_{j=0}^N$. We will stack each pair into a single column, e.g., $[\boldsymbol{\sigma}^-, \boldsymbol{\sigma}^+]^T$. Recalling (14), the density at each boundary point is trivially coupled to the data at that same point; however, the coupling to the other boundary point will involve the double-layer kernel acting at a distance of 2. Thus, (25) becomes a 2×2 system with trivial diagonal blocks and Toeplitz off-diagonal blocks. Namely, after N time-steps the stacked vectors are related by

$$\begin{bmatrix} -\frac{1}{2}I & V \\ V & -\frac{1}{2}I \end{bmatrix} \begin{bmatrix} \boldsymbol{\sigma}^- \\ \boldsymbol{\sigma}^+ \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}^- \\ \boldsymbol{f}^+ \end{bmatrix}, \tag{26}$$

where I is the size-$(N+1)$ identity matrix. Here the action of the lower-triangular Toeplitz matrix $V \in \mathbb{R}^{(N+1)\times(N+1)}$ is given by

$$[V\boldsymbol{\sigma}^\pm]_j = \sum_{k=0}^{j-1} v_{j-k}\sigma_k^\pm \quad \text{for } j = 1, \ldots, N,$$

with the convolution coefficients $\{v_l\}$ given by

$$v_l = -\int_0^{\Delta t} \gamma(l\Delta t - \tau)\, d\tau, \quad l \ge 1, \quad \text{and} \quad v_0 = 0. \tag{27}$$

Here the underlying kernel is the double-layer acting at a distance of 2,

$$\gamma(t) := \frac{1}{2\sqrt{\pi}} t^{-3/2} e^{-1/t}, \quad t > 0. \tag{28}$$

We denote the symmetric part of V by W and make its dependence on N and Δt explicit; thus

$$W(N;\Delta t) := \tfrac{1}{2}(V + V^T). \tag{29}$$

We have the following lemma.

Lemma 9. *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*

$$\rho(N;\Delta t) \le C_1(T), \tag{30}$$

where

$$C_1(T) := \int_0^T \gamma(T-\tau)\, d\tau = \frac{1}{2\sqrt{\pi}} \int_{1/T}^\infty \frac{1}{\sqrt{u}} e^{-u}\, du < \frac{1}{2}. \tag{31}$$

Proof. Using the Gershgorin circle theorem [Thomas 1995, §3.3] and the fact that the diagonal entries of W are all zero, we have

$$\rho(N;\Delta t) \le \max_i \sum_{j=1}^{N+1} |w_{ij}| \le 2\sum_{l=1}^{N} \tfrac{1}{2}|v_l| \le \sum_{l=1}^{N} |v_l|. \tag{32}$$

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 (31) 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 (31) follows from the change of variables $u = 1/(T - \tau)$. A further change of variables $x = \sqrt{u}$ leads to

$$C_1(T) = \frac{1}{\sqrt{\pi}} \int_{1/\sqrt{T}}^{\infty} e^{-x^2}\, dx < \frac{1}{\sqrt{\pi}} \int_0^{\infty} e^{-x^2}\, dx = \frac{1}{2} \quad \text{for all } T > 0. \tag{33}$$

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

It is clear from (26) that to get a stability bound we need to control the gap between $C_1(T)$ and $\frac{1}{2}$. For $T \ge 1$, this turns out to shrink only polynomially in T:

$$\frac{1}{2} - C_1(T) = \frac{1}{2\sqrt{\pi}} \int_0^{1/T} \frac{1}{\sqrt{u}} e^{-u}\, du > \frac{1}{2e\sqrt{\pi}} \int_0^{1/T} \frac{1}{\sqrt{u}}\, du = \frac{1}{e\sqrt{\pi T}}. \tag{34}$$

This very easily allows us to prove the following.

Theorem 10. *Suppose that $T \ge 1$. Then, using $\|\cdot\|$ for the l^2-norm in $\mathbb{R}^{2(N+1)}$,*

$$\|[\boldsymbol{\sigma}^-, \boldsymbol{\sigma}^+]\| \le e\sqrt{\pi T}\, \|[\boldsymbol{f}^+, \boldsymbol{f}^-]\| \tag{35}$$

for all N and Δt such that $N\Delta t \le T$. That is, for the $d = 1$ unit ball where $\Gamma = \{-1, 1\}$, the forward Euler scheme for solving the second-kind Volterra integral equation (12) is unconditionally stable on any finite time interval $[0, T]$.

Proof. We use a technique that will recur throughout this paper: we take the inner product of (26) with $-[\boldsymbol{\sigma}^-, \boldsymbol{\sigma}^+]^T$, giving

$$\tfrac{1}{2}\|[\boldsymbol{\sigma}^+, \boldsymbol{\sigma}^-]\|^2 - 2\langle W\boldsymbol{\sigma}^+, \boldsymbol{\sigma}^-\rangle = -(\langle \boldsymbol{f}^+, \boldsymbol{\sigma}^+\rangle + \langle \boldsymbol{f}^-, \boldsymbol{\sigma}^-\rangle). \tag{36}$$

Applying the Cauchy–Schwarz inequality and (30) to the second term on the left side, and Cauchy–Schwarz to the right-hand side, we obtain

$$\tfrac{1}{2}\|[\boldsymbol{\sigma}^+, \boldsymbol{\sigma}^-]\|^2 - 2C_1(T)\|\boldsymbol{\sigma}^+\| \cdot \|\boldsymbol{\sigma}^-\| \le \|[\boldsymbol{\sigma}^+, \boldsymbol{\sigma}^-]\| \cdot \|[\boldsymbol{f}^+, \boldsymbol{f}^-]\|.$$

Using the arithmetic-geometric mean inequality on the left-hand side of this estimate gives

$$\big(\tfrac{1}{2} - C_1(T)\big)\|[\boldsymbol{\sigma}^+, \boldsymbol{\sigma}^-]\|^2 \le \|[\boldsymbol{\sigma}^+, \boldsymbol{\sigma}^-]\| \cdot \|[\boldsymbol{f}^+, \boldsymbol{f}^-]\|.$$

Finally dividing by $\big(\tfrac{1}{2} - C_1(T)\big)\|[\boldsymbol{\sigma}^+, \boldsymbol{\sigma}^-]\|$ and applying (34) gives

$$\|[\boldsymbol{\sigma}^-, \boldsymbol{\sigma}^+]\| \le \frac{1}{\frac{1}{2} - C_1(T)} \|[\boldsymbol{f}^+, \boldsymbol{f}^-]\| \le e\sqrt{\pi T}\, \|[\boldsymbol{f}^+, \boldsymbol{f}^-]\|,$$

which completes the proof. □

4.2. ***The Dirichlet problem in two dimensions.*** We now consider (25) when Γ is the unit circle S^1. We decompose both $\sigma_j(\boldsymbol{y})$ and $f_j(\boldsymbol{x})$ into Fourier series:

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

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

From (20), writing $s = \theta - \phi$, the n-th Fourier mode of the kernel is

$$\begin{aligned} \int_{S^1} \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, t-\tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} e^{in\phi}\, d\phi &= \int_0^{2\pi} -\frac{1-\cos(\theta-\phi)}{8\pi(t-\tau)^2} e^{-(1-\cos(\theta-\phi))/(2(t-\tau))} e^{in\phi}\, d\phi \\ &= -\gamma_n(t-\tau) e^{in\theta}, \end{aligned} \tag{37}$$

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

$$\gamma_n(t) := \frac{1}{8\pi t^2} \int_0^{2\pi} (1-\cos(s)) e^{-(1-\cos(s))/(2t)} \cos(ns)\, ds, \quad t > 0. \tag{38}$$

Since $\{e^{in\theta}\}$ are orthonormal, each Fourier mode evolves independently. The marching scheme (or recurrence) (25) for the n-th mode is then

$$-\tfrac{1}{2}\sigma_j^n - \sum_{k=0}^{j-1} v_{j-k}^n \sigma_k^n = f_j^n, \quad j = 0, 1, 2, \ldots, \tag{39}$$

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

$$v_l^n = \int_0^{\Delta t} \gamma_n(l\Delta t - \tau)\, d\tau, \quad l \geq 1, \tag{40}$$

and we set $v_0^n = 0$. The system (39) for $j = 0, 1, \ldots, N$ can be written in matrix-vector form

$$\left(-\tfrac{1}{2} I - V^n\right) \boldsymbol{\sigma}^n = \boldsymbol{f}^n, \tag{41}$$

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

$$W^n(N; \Delta t) := \frac{V^n + (V^n)^T}{2} = \frac{1}{2} \begin{bmatrix} 0 & v_1^n & v_2^n & \cdots & v_N^n \\ v_1^n & 0 & v_1^n & \cdots & v_{N-1}^n \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ v_N^n & v_{N-1}^n & \cdots & v_1^n & 0 \end{bmatrix}. \tag{42}$$

4.2.1. *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 13). The second is that, when $\Delta t < 1$, we have the stronger result that the L^2-norm of the solution is bounded by a constant multiple of the L^2-norm of f. We require the following lemma.

Lemma 11. *Fix $T > 0$. Then, for any N and Δt with $N\Delta t \le T$, 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*

$$\rho_n(N; \Delta t) \le C_2(T), \tag{43}$$

where, in terms of the definition (38),

$$C_2(T) := \int_0^T \gamma_0(T-\tau)\, d\tau = \frac{1}{4\pi}\int_0^{2\pi} e^{-(1-\cos(s))/(2T)}\, ds < \frac{1}{2}. \tag{44}$$

Proof. Let $n \in \mathbb{Z}$. Since the integrand in (38), excluding the $\cos ns$ factor, is nonnegative, 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 theorem, and the fact that the diagonal entries of W^n are all zero, we have

$$\rho_n(N; \Delta t) \le \max_i \sum_{j=1}^{N+1} |w_{ij}^n| \le 2\sum_{l=1}^{N} \tfrac{1}{2}|v_l^n| \le \sum_{l=1}^{N} v_l^0. \tag{45}$$

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 (44) 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 (44) we insert (38), interchange the order of integration and apply the change of variables $\lambda = (1-\cos(s))/(2(T-\tau))$; thus

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

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

Analogous to before, it is clear from (41) that to get a stability bound we need to bound from below the gap between $C_2(T)$ and $\frac{1}{2}$. This motivates the following.

Proposition 12.

$$C_2(T) = \frac{1}{2}e^{-1/(2T)} I_0\Big(\frac{1}{2T}\Big), \tag{46}$$

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

$$\frac{1}{2} - C_2(T) \ge \frac{1}{10T}. \tag{47}$$

Proof. Equation (46) follows from the integral representation of $I_0(x)$ in (102), and (47) follows from the facts that $I_0(x) \le 1 + \frac{1}{2}x^2$ [Olver et al. 2010, §10.25.2] and $e^{-x} \le 1 - \frac{1}{2}x$ for $x \le 1$. □

Theorem 13. *Suppose that $T \geq 1$. Then for all $n \in \mathbb{Z}$,*

$$\|\boldsymbol{\sigma}^n\| \leq 10T\|\boldsymbol{f}^n\| \tag{48}$$

for all N and Δt such that $N\Delta t \leq T$. That is, when Γ is the unit circle S^1, the forward Euler scheme for solving the second-kind Volterra integral equation (12) 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 (41) into two independent real systems

$$\begin{aligned}\left(-\tfrac{1}{2}I - V^n\right)\boldsymbol{\sigma}_r^n &= \boldsymbol{f}_r^n,\\ \left(-\tfrac{1}{2}I - V^n\right)\boldsymbol{\sigma}_i^n &= \boldsymbol{f}_i^n,\end{aligned} \tag{49}$$

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 (49) by $-(\boldsymbol{\sigma}_r^n)^T$, we have

$$\tfrac{1}{2}\|\boldsymbol{\sigma}_r^n\|^2 + (\boldsymbol{\sigma}_r^n)^T V^n \boldsymbol{\sigma}_r^n = \tfrac{1}{2}\|\boldsymbol{\sigma}_r^n\|^2 + (\boldsymbol{\sigma}_r^n)^T W^n \boldsymbol{\sigma}_r^n = -(\boldsymbol{\sigma}_r^n)^T \boldsymbol{f}_r^n. \tag{50}$$

Applying (43) on the left side (50) and the Cauchy–Schwartz inequality on the right side, we obtain

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

That is, finally applying Proposition 12,

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

A similar result holds for $\|\boldsymbol{\sigma}_i^n\|$. As $\|\boldsymbol{\sigma}^n\| = \sqrt{\|\boldsymbol{\sigma}_r^n\|^2 + \|\boldsymbol{\sigma}_i^n\|^2}$, these two inequalities give (48). □

4.2.2. *Tighter bounds.* We now show that the dependence on T in (48) can be removed when the time step satisfies $\Delta t \leq 1$. This is a physically reasonable requirement since we have assumed that the diffusion coefficient is 1, and the domain has area of order 1. We first provide a bound on $\rho_n(N; \Delta t)$ for $n \neq 0$ that is independent of the total time $N\Delta t$.

Lemma 14. *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 (42). Then for all $n \neq 0$,*

$$\rho_n(N; \Delta t) \leq \frac{1}{2|n| + 1}. \tag{51}$$

Proof. Clearly, it is sufficient to prove (51) for $n > 0$. For this, let us note that substituting (38) into (40), exchanging the order of integration, and making the change of variables $\lambda = (1 - \cos(s))/(2(l\Delta t - \tau))$, we obtain

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

By the integral representation (102) of I_n, we have

$$v_l^n = \begin{cases} \frac{1}{2} e^{-1/(2\Delta t)} I_{|n|}\Big(\frac{1}{2\Delta t}\Big), & l = 1, \\ \frac{1}{2}\Big(e^{-1/(2l\Delta t)} I_{|n|}\Big(\frac{1}{2l\Delta t}\Big) - e^{-1/(2(l-1)\Delta t)} I_{|n|}\Big(\frac{1}{2(l-1)\Delta t}\Big)\Big), & l > 1. \end{cases} \tag{52}$$

From (52), defining $i_n(x) := e^{-x} I_n(x)$ and $x_l = 1/(2l\Delta t)$, we consider the sum

$$S_n = 2\sum_{l=1}^{N} |v_l^n| = i_n(x_1) + \sum_{l=2}^{N} |i_n(x_l) - i_n(x_{l-1})|. \tag{53}$$

By Lemma 33 (see the Appendix), the function $i_n(x)$ assumes its unique maximum at $r_n > 0$; it increases monotonically on $[0, r_n]$ and decreases monotonically on $[r_n, +\infty)$. We now consider (53) on a case-by-case basis.

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

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

where the last inequality follows from (106).

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

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

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

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

By (45) 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 15. *For all $n \neq 0$,*

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

Thus, all nonzero modes are unconditionally stable. The zeroth Fourier mode is a bit more subtle, and requires the convex sequence results of Section 3. It brings in a weak restriction on Δt, as follows.

Lemma 16. *Suppose that* $a = 0.05$ *and* $\Delta t \le 1$. *Then* $c_2 I + W^0 + aW^1$ *is a positive definite matrix if*

$$c_2 = \tfrac{1}{2}e^{-1/2} I_0\big(\tfrac{1}{2}\big) + \tfrac{1}{6}a \approx 0.33085\ldots. \tag{54}$$

Proof. Define the sequence $y_j = \frac{1}{2}(v_j^0 + a v_j^1)$ for $j \ge 1$ and $y_0 = c_2$. Theorem 5 then shows that a sufficient condition for the positive semidefiniteness of $c_2 I + W^0 + aW^1$ is that the sequence $\{y_j\}_{j\in\mathbb{Z}_+}$ is convex. But $y_1 = \frac{1}{4} f(x_1)$ and $y_j = \frac{1}{4}(f(x_j) - f(x_{j-1}))$ $(j > 1)$, where f is the function defined in Lemma 39, 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 nonnegativity of the third order difference of f, which follows from the fact that $f'''(x) > 0$ for all $x > 0$ as proved in Lemma 39. For $j = 0$, the convexity of the sequence requires that one choose c_2 such that

$$c_2 + y_2 = y_0 + y_2 \ge 2y_1. \tag{55}$$

By the integral representation (102) of I_0, it is easy to see that $e^{-x} I_0(x)$ is strictly decreasing. Thus, we have $e^{-1/2} I_0\big(\frac{1}{2}\big) \ge e^{-1/(2\Delta t)} I_0(1/(2\Delta t))$ for $\Delta t \le 1$. Furthermore,

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

by (106). Hence, (55) is achieved by choosing

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

for $\Delta t \le 1$. □

Corollary 17. *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 16, the smallest eigenvalue of W^0 is bounded by

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

Thus a simple bound using the value of c_2 from Lemma 16 is

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

completing the proof. □

4.3. ***The Dirichlet problem in 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 [Morimoto 1998]:

$$\sigma(\boldsymbol{y},\tau) = \sum_{n=0}^{\infty}\sum_{m=1}^{a_{n,d}} \sigma^{nm}(\tau) Y_n^m(\boldsymbol{y}), \qquad \boldsymbol{y} \in S^{d-1} \subset \mathbb{R}^d,\ \tau \ge 0$$

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 harmonic polynomials of degree n on $\mathbb{R}^d$, whose restrictions to the unit sphere are spanned by $\{Y_n^m\}$, the 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 [Olver et al. 2010, §18.3] of degree n and order m.

The spherical harmonics admit the integral representation [Morimoto 1998]

$$Y_n^m(\boldsymbol{x})=\frac{a_{n,d}}{\omega_d}\int_{S^{d-1}}P_{n,d-1}(\boldsymbol{x}\cdot\boldsymbol{y})Y_n^m(\boldsymbol{y})\,dS(\boldsymbol{y}), \tag{56}$$

where ω_d is the area of S^{d-1} defined in (87), and the $P_{n,d-1}$ are Gegenbauer polynomials [loc. cit., Chapter 2] (also called ultraspherical polynomials), defined by the Rodrigues formula

$$P_{n,d-1}(t)=\frac{(-1)^n}{2^n}\frac{\Gamma\big(\frac{1}{2}(d-1)\big)}{\Gamma\big(n+\frac{1}{2}(d-1)\big)}\frac{1}{(1-t^2)^{(d-3)/2}}\frac{d^n}{dt^n}(1-t^2)^{n+(d-3)/2}. \tag{57}$$

The Funk–Hecke formula [loc. cit., Theorem 2.39] states that

$$\int_{S^{d-1}}f(\boldsymbol{x}\cdot\boldsymbol{z})P_{n,d-1}(\boldsymbol{y}\cdot\boldsymbol{z})\,dS(\boldsymbol{z})=\beta_{n,d-1}P_{n,d-1}(\boldsymbol{x}\cdot\boldsymbol{y}), \tag{58}$$

where

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

and f is any measurable function such that

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

In $d=3$ this reduces to $f\in L^1[-1,1]$.

We compute the double-layer heat potential nm-th Fourier mode,

$$\begin{aligned}\int_{S^{d-1}}\frac{\partial G(\boldsymbol{x}-\boldsymbol{y},t-\tau)}{\partial\boldsymbol{\nu}(\boldsymbol{y})}Y_n^m(\boldsymbol{y})\,dS(\boldsymbol{y})&=-\int_{S^{d-1}}\frac{1-\boldsymbol{x}\cdot\boldsymbol{y}}{2^{d+1}\pi^{d/2}(t-\tau)^{1+d/2}}e^{-(1-\boldsymbol{x}\cdot\boldsymbol{y})/(2(t-\tau))}Y_n^m(\boldsymbol{y})\,dS(\boldsymbol{y})\\&=-\frac{a_{n,d}}{\omega_d}\int_{S^{d-1}}\gamma_{n,d}(t-\tau)P_{n,d-1}(\boldsymbol{x}\cdot\boldsymbol{z})Y_n^m(\boldsymbol{z})\,dS(\boldsymbol{z})\\&=-\gamma_{n,d}(t-\tau)Y_n^m(\boldsymbol{x}),\end{aligned} \tag{59}$$

where, by analogy with (38),

$$\gamma_{n,d}(t):=\frac{\omega_{d-1}}{2^{d+1}\pi^{d/2}t^{(d+2)/2}}\int_{-1}^{1}(1-x)e^{-(1-x)/(2t)}P_{n,d-1}(x)(1-x^2)^{(d-3)/2}\,dx. \tag{60}$$

The third equality makes use of (56), (58), and exchanging the order of integration. The last step follows again from (56). 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 (59) 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 $\sigma(\boldsymbol{x}, t)$ takes the constant value $\sigma_j(\boldsymbol{x}) = \sigma(\boldsymbol{x}, j\Delta t)$ 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. A straightforward calculation leads to the following recurrence for the nm-th spherical harmonic mode, analogous to (39):

$$-\tfrac{1}{2}\mu_j - \sum_{k=0}^{j-1} v_{j-k}^n \mu_k = g_j, \qquad j = 0, 1, 2, \ldots, \tag{61}$$

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

$$v_l^n = \int_0^{\Delta t} \gamma_{n,d}(l\Delta t - \tau)\, d\tau, \qquad l > 0, \tag{62}$$

involve the kernel modes (60), and, as before, $v_0^n = 0$.

4.3.1. *Stability analysis.* The normalization in (57) leads to [Morimoto 1980; Müller 1966]

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

As the other terms in (60) are nonnegative, we have

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

An almost identical proof to that of Lemma 11 leads to the following lemma.

Lemma 18. *Fix $T > 0$. Then, for any N and Δt with $N\Delta t \le T$, 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 (42), with v_l^n given by (62), has the bound*

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

where

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

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 $\lambda = (1-x)/(2(T-\tau))$, giving

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

and

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

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

$$
\begin{aligned}
\tfrac{1}{2} - C_d(T) &\geq \frac{1}{2^{d/2}\sqrt{\pi}\,\Gamma\big(\frac{1}{2}(d-1)\big)} \int_{-1}^{1} \frac{(1+x)^{(d-3)/2}}{\sqrt{1-x}} \left(\frac{1}{e} \int_0^{(1-x)/(2T)} \lambda^{d/2}\, d\lambda \right) dx \\
&= \frac{1}{ed2^{d-1}\sqrt{\pi}\,\Gamma\big(\frac{1}{2}(d-1)\big)T^{d/2}} \int_{-1}^{1} (1-x^2)^{(d-3)/2}(1-x)\, dx \\
&= \frac{2}{ed2^{d-1}\sqrt{\pi}\,\Gamma\big(\frac{1}{2}(d-1)\big)T^{d/2}} \int_{0}^{1} (1-x^2)^{(d-3)/2}\, dx \\
&= \frac{2}{ed2^{d-1}\sqrt{\pi}\,\Gamma\big(\frac{1}{2}(d-1)\big)T^{d/2}} \int_{0}^{\pi/2} \cos^{d-2}(\theta)\, d\theta \\
&= \frac{1}{ed2^{d-1}\Gamma\big(\frac{1}{2}d\big)T^{d/2}},
\end{aligned} \tag{63}
$$

where the last equality follows from an integral identity in [Gradshteyn and Ryzhik 2014, §3.62].

Armed with this polynomial control of the gap, and following the same reasoning as used to show (48), we obtain the following theorem regarding the stability of the forward Euler scheme in higher dimensions.

Theorem 19. *Fix $d > 2$ and $T \geq 1$. For all $n = 0, 1, \ldots$ and $m = 1, \ldots, a_{n,d}$,*

$$
\|\boldsymbol{\sigma}^{nm}\| \leq \frac{1}{\frac{1}{2} - C_d(T)} \|\boldsymbol{f}^{nm}\| \leq ed2^{d-1}\Gamma\big(\tfrac{1}{2}d\big)T^{d/2}\|\boldsymbol{f}^{nm}\| \tag{64}
$$

for all N and 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 (12) is unconditionally stable on any finite time interval $[0, T]$.

Remark 20. When $d = 2$, H_n is spanned by $e^{in\theta}$ and $e^{-in\theta}$. The decomposition of $L^2(S^1)$ into spherical harmonics is the usual Fourier series expansion. And if we identify $P_{n,1}(x)$ with the Chebyshev polynomials $T_n(x)$, then all calculations in this subsection are valid for $d = 2$. We instead presented the analysis in two dimensions using the usual Fourier series for the reader's convenience.

Remark 21. It is easy to see that the bound (64) actually also includes the cases of $d = 1$ and $d = 2$ proved earlier, and thus holds for all $d \geq 1$.

4.4. ***The Neumann problem on the unit ball.*** For the Neumann condition (3), we represent $u^{(B)}$ as the single-layer potential $\mathcal{S}[\sigma]$. The jump relation (17) leads to the second-kind Volterra integral equation

$$
\big(\tfrac{1}{2} + \mathcal{S}_{\boldsymbol{\nu}}\big)[\sigma](\boldsymbol{x}, t) = \tilde{g}(\boldsymbol{x}, t), \quad (\boldsymbol{x}, t) \in \Gamma \times [0, T], \tag{65}
$$

where $\mathcal{S}_{\boldsymbol{\nu}}$ indicates the normal derivative of the single-layer with respect to the target point, restricted to Γ, interpreted in a principal value sense, as in Section 2. In (65) the right-hand side is the corrected data

$$
\tilde{g}(\boldsymbol{x}, t) := g(\boldsymbol{x}, t) - \frac{\partial u^{(F)}(\boldsymbol{x}, t)}{\partial \boldsymbol{\nu}}, \quad \boldsymbol{x} \in \Gamma.
$$

On the unit sphere S^{d-1}, straightforward calculation shows that the kernel of the double-layer potential $\mathcal{D}$ is exactly the same as that of $\mathcal{S}_{\boldsymbol{\nu}}$. Thus, the forward Euler scheme for (65) leads to the identical marching matrix except a sign change in diagonal entries. Since we prove the bound (64) by bounding the spectral radius of the marching matrix excluding the diagonal part, we observe that (64) holds as well for (65) with f replaced by $\tilde{g}$. This leads to the unconditional stability of the forward Euler scheme for the Neumann problem on the unit ball, for all $d \geq 1$.

5. The Robin problem on the half-space

For the Robin boundary condition (4), we also represent $u^{(B)}$ via a single-layer potential $\mathcal{S}[\sigma]$. The jump relation (17) leads to the second-kind Volterra equation

$$\left(\tfrac{1}{2} + \mathcal{S}_{\boldsymbol{\nu}} + \kappa \mathcal{S}\right)[\sigma](\boldsymbol{x}, t) = \tilde{h}(\boldsymbol{x}, t), \quad (\boldsymbol{x}, t) \in \Gamma \times [0, T], \tag{66}$$

with corrected Robin data

$$\tilde{h}(\boldsymbol{x}, t) := h(\boldsymbol{x}, t) - \frac{\partial u^{(F)}(\boldsymbol{x}, t)}{\partial \boldsymbol{\nu}} - \kappa u^{(F)}(\boldsymbol{x}, t). \tag{67}$$

When $D = \mathbb{R}^d_+$, where Γ is naturally identified as $\mathbb{R}^{d-1} \subset \mathbb{R}^d$, the kernel of $\mathcal{S}_{\boldsymbol{\nu}}$ is identically zero due to the fact that $(\boldsymbol{x} - \boldsymbol{y}) \cdot \boldsymbol{\nu}_{\boldsymbol{x}} = 0$. Thus, (66) reduces to

$$\left(\tfrac{1}{2} + \kappa \mathcal{S}\right)[\sigma](\boldsymbol{x}, t) = \tilde{h}(\boldsymbol{x}, t), \quad (\boldsymbol{x}, t) \in \mathbb{R}^{d-1} \times [0, T]. \tag{68}$$

Here we assume that $\tilde{h}$ is sufficiently smooth and decays sufficiently fast at infinity so that the problem is well-posed.

5.1. ***The Robin problem in one dimension.*** In one dimension, the boundary Γ of the half-line consists of a single point $x = 0$. The integral equation (68) reduces to the Abel integral equation (multiplying both sides by 2, and denoting the right-hand side by f instead):

$$\sigma(t) + \frac{\kappa}{\sqrt{\pi}} \int_0^t \frac{\sigma(\tau)}{\sqrt{t-\tau}}\, d\tau = 2 f(t). \tag{69}$$

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

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

where $\Gamma(\alpha)$ is the gamma function (88). Thus, the integral operator on the left side of (69) is simply $\left(\Gamma\left(\tfrac{1}{2}\right)\kappa/\sqrt{\pi}\right)\mathcal{R}_{1/2} = \kappa \mathcal{R}_{1/2}$. For all real functions g, the operator $\mathcal{R}_\alpha$ satisfies the positivity property [Mustapha and Schötzau 2014, Lemma 3.1]

$$\int_0^T g(t) \mathcal{R}_\alpha[g](t)\, dt \geq 0. \tag{70}$$

Taking the inner product of (69) with σ over a fixed interval $[0, T]$, and using (70), gives

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

where Cauchy–Schwartz was used in the last step. So on any finite interval $[0, T]$ this gives the continuous version of the L^2 stability bound

$$\|\sigma\| \le 2\|f\|.$$

We now proceed to discretization. Recall that the forward Euler scheme uses a piecewise constant approximation $\sigma(t) \approx \sigma_m := \sigma(t_m)$ on $[t_m, t_{m+1})$ on the uniform grid $t_m = m\Delta t$. Then performing the integrals exactly in (69) gives the explicit marching rule

$$\sigma_n = 2f_n - \sum_{m=0}^{n-1} v_{n-m}\sigma_m, \quad n = 1, \dots, N, \tag{71}$$

with the lower-triangular Toeplitz matrix weights

$$v_j = 2\sqrt{h}(\sqrt{j} - \sqrt{j-1}) = \frac{2\sqrt{h}}{\sqrt{j} + \sqrt{j-1}}, \quad j = 1, 2, \dots, \tag{72}$$

and where $f_n := f(t_n)$ and $h := \kappa^2\Delta t/\pi$. For smooth solutions $\sigma \in C^1([0, T])$, this rule can be proved to be first-order accurate by combining compactness of the integral operator, Céa's lemma, and noting that the piecewise constant approximant has error $\mathcal{O}(\Delta t)$; see [Kress 1989, §13.1–3].

For initialization, as before we set $\sigma_0 = f_0 = 0$, and 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, (71) takes the form of the lower-triangular Toeplitz linear system

$$(I + V)\boldsymbol{\sigma} = 2\boldsymbol{f}, \tag{73}$$

where $V \in \mathbb{R}^{(N+1)\times(N+1)}$ has elements $v_{n,m} = v_{n-m}$ for $n > m$, and $v_{n,m} = 0$ otherwise. Here, v_n is defined in (72) 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 [Baker 2000; Jones and McKee 1985; Brunner 2004]. 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 [Jones and McKee 1985; Messina and Vecchio 2017]. In [Lubich 1983a], a more relevant stability result is obtained for systems of the form (73), but assuming that the sequence $\{v_j\}$ 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 [Eggermont 1984; Lubich 1983b; 1985; Vögeli et al. 2018]. These papers, however, are mostly concerned with implicit marching schemes. An exception is [Lubich 1986], 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 22 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.

Theorem 22. *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* (73) *obeys*

$$\|\boldsymbol{\sigma}\| \le \frac{2}{1 - c\sqrt{h}} \|\boldsymbol{f}\|, \tag{74}$$

where $\|\cdot\|$ *denotes the* l^2*-norm. That is, the marching scheme* (71) *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

$$\boldsymbol{\sigma}^T V \boldsymbol{\sigma} \ge -c\sqrt{h}\|\boldsymbol{\sigma}\|^2 \quad \text{for any } \boldsymbol{\sigma} \in \mathbb{R}^{N+1}, \tag{75}$$

i.e., that the smallest eigenvalue of V is bounded from below. Writing $\sqrt{h} W_{N+1} := \frac{1}{2}(V + V^T)$ as the scaled symmetric part of V, note that $\boldsymbol{\sigma}^T V \boldsymbol{\sigma} = \sqrt{h} \boldsymbol{\sigma}^T W_{N+1} \boldsymbol{\sigma}$, and that W_{N+1} is independent of the time step. Note that W_{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

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

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 5 and Remark 6, we have

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

That is, (75) holds if $c = 2v_1 - v_2 = 3 - \sqrt{2}$. To complete the proof, take the inner product of (73) with $\boldsymbol{\sigma}$ to get

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

Applying (75) to the left-hand side and the Cauchy–Schwarz inequality to the right-hand side, we have

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

from which (74) follows for any $\boldsymbol{\sigma} \ne \mathbf{0}$. It holds trivially when $\boldsymbol{\sigma} = \mathbf{0}$. □

Remark 23. 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 24. 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, in practice the only spatial discretization needed would be quadrature to evaluate (11) to get $f(t)$, as in (67). With $f(t)$ computed, there is no spatial variable left to discretize.)

5.2. *The Robin problem in higher dimensions.* In higher dimensions $d \geq 2$, the boundary Γ of the half-space $\mathbb{R}^d_+$ can be identified as $\mathbb{R}^{d-1}$ by natural embedding. The integral equation (68) is rewritten as

$$\sigma(\boldsymbol{x},t) + \frac{\kappa}{\sqrt{\pi}} \int_0^t \frac{1}{\sqrt{t-\tau}} \int_{\mathbb{R}^{d-1}} \frac{1}{(4\pi(t-\tau))^{(d-1)/2}} e^{-|\boldsymbol{x}-\boldsymbol{y}|^2/(4(t-\tau))} \sigma(\boldsymbol{y},\tau)\, d\boldsymbol{y}\, d\tau = 2f(\boldsymbol{x},t), \tag{76}$$

where $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^{d-1}$. Again we have multiplied both sides by 2 and denote the right-hand side by f. We observe that the kernel inside the spatial integral on the left side of (76) is exactly the heat kernel in $\mathbb{R}^{d-1}$. It is well known that the Fourier transform of the heat kernel $G(\boldsymbol{x},t)$ in $\mathbb{R}^{d-1}$ is simply $e^{-|\boldsymbol{\xi}|^2 t}$, in terms of the Fourier variable $\boldsymbol{\xi} \in \mathbb{R}^{d-1}$. Using this fact and that the convolution in physical space becomes pointwise multiplication in frequency, and taking the Fourier transform in $\mathbb{R}^{d-1}$ of both sides of (76), we obtain

$$\hat{\sigma}(\boldsymbol{\xi},t) + \frac{\kappa}{\sqrt{\pi}} \int_0^t \frac{e^{-|\boldsymbol{\xi}|^2(t-\tau)}}{\sqrt{t-\tau}} \hat{\sigma}(\boldsymbol{\xi},\tau)\, d\tau = 2\hat{f}(\boldsymbol{\xi},t), \quad \boldsymbol{\xi} \in \mathbb{R}^{d-1}. \tag{77}$$

Note that in the special case $\boldsymbol{\xi} = 0$ this recovers (69).

Fixing $\boldsymbol{\xi}$, we proceed much as in the one-dimensional case. That is, we approximate $\hat{\sigma}(\boldsymbol{\xi},t)$ by a constant $\hat{\sigma}_m(\boldsymbol{\xi}) := \hat{\sigma}_m(\boldsymbol{\xi},t_m)$ on $[t_m, t_{m+1})$ with $t_m = m\Delta t$, and perform the integrals exactly. Let us define the vectors $\hat{\boldsymbol{\sigma}}(\boldsymbol{\xi})$ and $\hat{\boldsymbol{f}}(\boldsymbol{\xi})$ by $\{\hat{\sigma}_n(\boldsymbol{\xi})\}_{n=0}^N$, $\{\hat{f}_n(\boldsymbol{\xi})\}_{n=0}^N \in \mathbb{R}^{N+1}$, respectively. Using this notation, the forward Euler scheme for (77) takes the form of the lower-triangular Toeplitz linear system

$$(I + \widehat{V}(\boldsymbol{\xi}))\hat{\boldsymbol{\sigma}}(\boldsymbol{\xi}) = 2\hat{\boldsymbol{f}}(\boldsymbol{\xi}), \tag{78}$$

where $\widehat{V}(\boldsymbol{\xi}) \in \mathbb{R}^{(N+1)\times(N+1)}$ has elements $v_{n,m}(\boldsymbol{\xi}) = v_{n-m}(\boldsymbol{\xi})$ for $n > m$, and $v_{n,m} = 0$ otherwise. Here, v_n is defined by

$$v_n(\boldsymbol{\xi}) = 2\sqrt{h}\frac{1}{2\sqrt{\Delta t}} \int_0^{\Delta t} \frac{e^{-|\boldsymbol{\xi}|^2(n\Delta t-\tau)}}{\sqrt{n\Delta t-\tau}}\, d\tau, \tag{79}$$

with, as before, $h = \kappa^2 \Delta t/\pi$.

Lemma 25. *For any $\Delta t > 0$ and any fixed $\boldsymbol{\xi}$, the sequence $\{v_n(\boldsymbol{\xi})\}_{n\in\mathbb{N}}$ is convex.*

Proof. Let $x = |\boldsymbol{\xi}|^2 \Delta t$. Applying the change of variables $u = n - \tau/\Delta t$ on the integral in (79) leads to

$$v_n(\boldsymbol{\xi}) = \sqrt{h} \int_{n-1}^n \frac{e^{-xu}}{\sqrt{u}}\, du. \tag{80}$$

Thus, in order to show that $\{v_n(\boldsymbol{\xi})\}_{n\in\mathbb{N}}$ is a convex sequence, we only need to show that the function

$$g(t) = \int_{t-1}^t \frac{e^{-xu}}{\sqrt{u}}\, du$$

is convex for $t \geq 1$. Here $x \geq 0$ is a fixed parameter. Differentiating $g(t)$ twice leads to

$$g''(t) = p'(t) - p'(t-1),$$

with

$$p(t) = \frac{e^{-xt}}{\sqrt{t}}.$$

Now

$$p''(t) = \frac{3e^{-tx}}{4t^{5/2}} + \frac{xe^{-tx}}{t^{3/2}} + \frac{x^2e^{-tx}}{\sqrt{t}},$$

which is positive for any $x \geq 0$ and $t > 0$. This shows that $p'(t)$ is monotonically increasing for $t > 0$. Thus, $p'(t) > p'(t-1)$ for $t \geq 1$, and $g''(t) > 0$ for $t \geq 1$, completing the proof. □

Lemma 26. *For any* $\boldsymbol{\xi} \in \mathbb{R}^{d-1}$,

$$v_2(\boldsymbol{\xi}) - 2v_1(\boldsymbol{\xi}) \geq v_2(0) - 2v_1(0) = -2(3-\sqrt{2})\sqrt{h}. \tag{81}$$

Proof. Using the expression (80), we only need to show that

$$f(x) := \int_1^2 \frac{e^{-xu}}{\sqrt{u}}\,du - 2\int_0^1 \frac{e^{-xu}}{\sqrt{u}}\,du \geq f(0)$$

for $x \geq 0$. For this, we calculate

$$\begin{aligned} f'(x) &= 2\int_0^1 \sqrt{u}e^{-xu}\,du - \int_1^2 \sqrt{u}e^{-xu}\,du \\ &= 3\int_0^1 \sqrt{u}e^{-xu}\,du - \int_0^2 \sqrt{u}e^{-xu}\,du \\ &= 3\int_0^1 \sqrt{u}e^{-xu}\,du - 2\sqrt{2}\int_0^1 \sqrt{u}e^{-2xu}\,du \\ &> 2\sqrt{2}\int_0^1 \sqrt{u}e^{-xu}(1-e^{-xu})\,du \geq 0 \quad \text{for } x \geq 0. \end{aligned}$$

That is, f is monotonically increasing for $x \geq 0$, completing the proof. □

Lemma 25 together with Theorem 5 and Remark 6 leads to

$$\hat{\boldsymbol{\sigma}}(\boldsymbol{\xi})^T \widehat{V}(\boldsymbol{\xi})\hat{\boldsymbol{\sigma}}(\boldsymbol{\xi}) \geq \tfrac{1}{2}(v_2(\boldsymbol{\xi}) - 2v_1(\boldsymbol{\xi}))\|\hat{\boldsymbol{\sigma}}(\boldsymbol{\xi})\|^2 \quad \text{for any } \boldsymbol{\xi} \in \mathbb{R}^{d-1}. \tag{82}$$

Combining the above estimate with (81), we obtain

$$\hat{\boldsymbol{\sigma}}(\boldsymbol{\xi})^T \widehat{V}(\boldsymbol{\xi})\hat{\boldsymbol{\sigma}}(\boldsymbol{\xi}) \geq -c\sqrt{h}\|\hat{\boldsymbol{\sigma}}(\boldsymbol{\xi})\|^2 \quad \text{for any } \boldsymbol{\xi} \in \mathbb{R}^{d-1}, \tag{83}$$

where

$$c = 3 - \sqrt{2}. \tag{84}$$

An argument similar to that in the proof of Theorem 13 then gives

$$\|\hat{\boldsymbol{\sigma}}(\boldsymbol{\xi})\| \leq \frac{2}{1-c\sqrt{h}}\|\hat{\boldsymbol{f}}(\boldsymbol{\xi})\| \quad \text{for any } \boldsymbol{\xi} \in \mathbb{R}^{d-1}. \tag{85}$$

Taking the L^2-norm in Fourier space and then applying the Plancherel theorem, we have

$$\|\boldsymbol{\sigma}\| \le \frac{2}{1-c\sqrt{h}}\|\boldsymbol{f}\|. \tag{86}$$

That is, we obtain exactly the same bound (74) as in one dimension, which shows that the forward Euler scheme is stable for (76) if $\Delta t < \pi/(c^2\kappa^2)$, where κ is the heat transfer coefficient.

Remark 27. 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 integral equation (68) yields the analytic solution $\sigma(\boldsymbol{x}, t) = 2\tilde{h}(\boldsymbol{x}, t)$.

6. The Dirichlet problem on an arbitrary smooth convex domain

We now study the stability property of the forward Euler scheme (13) for the Dirichlet problem on an arbitrary C^1 convex domain, i.e., the boundary integral equation (12).

We first establish a connection between the heat kernel and the Laplace kernel. The Green's function for the Laplace equation in $\mathbb{R}^d$ is

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

where

$$\omega_d = \frac{2\pi^{d/2}}{\Gamma\left(\frac{1}{2}d\right)} \tag{87}$$

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

$$\Gamma(z) = \int_0^\infty x^{z-1}e^{-x}\,dx. \tag{88}$$

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

$$\frac{\partial G_{\mathrm{L}}(\boldsymbol{x}-\boldsymbol{y})}{\partial \boldsymbol{\nu}(\boldsymbol{y})} = \frac{\Gamma\left(\frac{1}{2}d\right)}{2\pi^{d/2}}\frac{(\boldsymbol{x}-\boldsymbol{y})\cdot\boldsymbol{\nu}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|^d}. \tag{89}$$

It is well known to satisfy Gauss' lemma [Kress 1989]:

$$\int_\Gamma \frac{\partial G_{\mathrm{L}}(\boldsymbol{x}-\boldsymbol{y})}{\partial \boldsymbol{\nu}(\boldsymbol{y})}\,dS(\boldsymbol{y}) = -\tfrac{1}{2}, \quad \boldsymbol{x}\in\Gamma. \tag{90}$$

Lemma 28.
$$\lim_{t\to\infty}\int_0^t \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, t-\tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})}\,d\tau = \frac{\partial G_{\mathrm{L}}(\boldsymbol{x}-\boldsymbol{y})}{\partial \boldsymbol{\nu}(\boldsymbol{y})}. \tag{91}$$

Proof. By (19), we have

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

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

$$\int_0^t \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, t-\tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})}\, d\tau = \frac{(\boldsymbol{x}-\boldsymbol{y})\cdot \boldsymbol{\nu}(\boldsymbol{y})}{2\pi^{d/2}|\boldsymbol{x}-\boldsymbol{y}|^d} \int_{|\boldsymbol{x}-\boldsymbol{y}|^2/(4t)}^{\infty} \lambda^{d/2-1} e^{-\lambda}\, d\lambda. \tag{92}$$

Taking the limit $t \to \infty$ and using the definition of the gamma function (88), we obtain (91). □

The following provides the key ingredient for the stability of the forward Euler scheme in an arbitrary smooth convex domain.

Lemma 29. *Suppose that $D \subset \mathbb{R}^d$ is a C^1 convex domain and Γ is its boundary. Then*

$$\frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, t-\tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} \le 0, \qquad \frac{\partial G_{\mathrm{L}}(\boldsymbol{x}-\boldsymbol{y})}{\partial \boldsymbol{\nu}(\boldsymbol{y})} \le 0, \qquad \boldsymbol{x}, \boldsymbol{y} \in \Gamma, \tag{93}$$

and

$$\lim_{t\to\infty} \int_0^t \int_\Gamma \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, t-\tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})}\, dS(\boldsymbol{y})\, d\tau = -\tfrac{1}{2}, \qquad \boldsymbol{x} \in \Gamma. \tag{94}$$

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

$$C_d(t) = \left\| \int_0^t \int_\Gamma \left| \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, t-\tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} \right| dS(\boldsymbol{y})\, d\tau \right\|_\infty. \tag{95}$$

Then $C_d(t)$ is a monotonic increasing function of t and

$$C_d(t) < \tfrac{1}{2}. \tag{96}$$

Proof. Equation (93) follows from the expressions (19) and (89) and the fact that $\boldsymbol{x}\cdot\boldsymbol{y} \le 0$ for $\boldsymbol{x}, \boldsymbol{y} \in \Gamma$ when D is convex due to the convex separation theorem [Boyd and Vandenberghe 2004]; (94) follows from (90) and (91). The monotonic increasing property of $C_d(t)$ follows from (92) and the fact that the integrand is of the same sign everywhere by (93). Finally, (96) is a simple consequence of (93) and (94). □

Recall that the forward Euler scheme (13) for the Dirichlet problem is

$$\tfrac{1}{2}\sigma(\boldsymbol{x}, n\Delta t) = \sum_{j=0}^{n-1} \int_{j\Delta t}^{(j+1)\Delta t} \int_\Gamma \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, n\Delta t-\tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} \sigma(\boldsymbol{y}, j\Delta t)\, ds(\boldsymbol{y})\, d\tau - f(\boldsymbol{x}, n\Delta t). \tag{97}$$

Here we have dropped the tilde from f again.

Theorem 30. *Let $D \subset \mathbb{R}^d$ be a bounded, convex domain with C^1-boundary. Fix $T > 0$. The solution σ to (97) satisfies*

$$\|\sigma\|_\infty \le \frac{1}{\frac{1}{2} - C_d(T)} \|f\|_\infty \tag{98}$$

for any N and Δt such that $N\Delta t \le T$. Here $C_d(T)$ is defined in (95), $\|\cdot\|_\infty$ denotes the L^∞-norm in space and the l^∞-norm in the discrete temporal variable. In other words, the forward scheme (13) is unconditionally stable on $[0, T]$ for any $T > 0$.

Proof. Taking the absolute value on both sides of (97), we have

$$
\begin{aligned}
\tfrac{1}{2}|\sigma(\boldsymbol{x}, n\Delta t)| &\le \sum_{j=0}^{n-1} \int_{j\Delta t}^{(j+1)\Delta t} \int_\Gamma \left| \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, n\Delta t - \tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} \sigma(\boldsymbol{y}, j\Delta t) \right| ds(\boldsymbol{y})\, d\tau + |f(\boldsymbol{x}, n\Delta t)| \\
&\le \sum_{j=0}^{n-1} \int_{j\Delta t}^{(j+1)\Delta t} \|\sigma(\cdot, j\Delta t)\|_\infty \int_\Gamma \left| \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, n\Delta t - \tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} \right| ds(\boldsymbol{y})\, d\tau + \|f(\cdot, n\Delta t)\|_\infty \\
&\le \|\sigma\|_\infty \sum_{j=0}^{n-1} \int_{j\Delta t}^{(j+1)\Delta t} \int_\Gamma \left| \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, n\Delta t - \tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} \right| ds(\boldsymbol{y})\, d\tau + \|f\|_\infty \\
&= \|\sigma\|_\infty \int_0^{(n-1)\Delta t} \int_\Gamma \left| \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, n\Delta t - \tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} \right| ds(\boldsymbol{y})\, d\tau + \|f\|_\infty, \qquad (99)
\end{aligned}
$$

where the first inequality follows from the triangle inequality, the second one follows from taking the L^∞-norm in the spatial variable for both σ and f, and the third one follows from taking the maximum norm in the discrete temporal variable. We continue our calculation

$$
\begin{aligned}
\tfrac{1}{2}|\sigma(\boldsymbol{x}, n\Delta t)| &\le \|\sigma\|_\infty \int_0^{n\Delta t} \int_\Gamma \left| \frac{\partial G(\boldsymbol{x}-\boldsymbol{y}, n\Delta t - \tau)}{\partial \boldsymbol{\nu}(\boldsymbol{y})} \right| ds(\boldsymbol{y})\, d\tau + \|f\|_\infty \\
&\le C_d(T)\|\sigma\|_\infty + \|f\|_\infty. \qquad (100)
\end{aligned}
$$

Since the inequality above is valid for any $\boldsymbol{x} \in \Gamma$ and any n such that $n\Delta t \le T$, its left-hand side can be replaced by $\frac{1}{2}\|\sigma\|_\infty$, completing the proof. □

Remark 31. It is clear that the L^∞ bound (96) for the Dirichlet problem on a convex domain is less informative than the L^2 bound (64) for the unit ball since (64) bounds $1/\big(\frac{1}{2} - C_d(T)\big)$ explicitly by $ed2^{d-1}\Gamma\big(\frac{1}{2}d\big)T^{d/2}$. The L^2-bounds also allow for potentially unbounded data, with a finite square norm.

7. Conclusions and further remarks

We have analyzed the stability of the forward Euler scheme for solving the Dirichlet and Neumann problems 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 time-domain boundary integral equations. While finite-difference methods require that the Courant number $\Delta t/(\Delta x)^2$ be $\mathcal{O}(1)$, we have shown that integral equation methods can be both explicit and unconditionally stable for any fixed final time T.

We have also studied the Robin problem on the half-space in all dimensions and shown that stability of the forward Euler scheme follows if $\Delta t < \pi/(c^2\kappa^2)$, where $c = 3 - \sqrt{2}$ and κ is the heat transfer coefficient. As pointed out in Remark 23, this bound is very close to the optimal bound where $c \approx 1.52041925043874$.

A critical element in the proof of unconditional stability of the forward Euler scheme is the pointwise nonpositivity of the double-layer heat kernel on the unit sphere S^{d-1}, a property which extends to any convex domain. Combining this with the elementary fact that a unit double-layer density generates a surface potential approaching $-\frac{1}{2}$ enabled us to extend this stability result to arbitrary smooth convex domains, in the Dirichlet case and the L^∞-norm, albeit with a less informative bound on the norm of the solution.

A key ingredient in the Robin proofs was a bound on the smallest eigenvalue of real symmetric Toeplitz matrices via the convexity of the associated sequence. This may be of independent interest in signal processing applications. Another ingredient for the proofs was 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. A detailed analysis combining these ingredients showed that in the Dirichlet disc ($d = 2$), the density is bounded in norm by the data, uniformly in time, so long as $\Delta t \le 1$.

While this paper is purely analytic, we note that the numerical experiments in [Wang 2017] are consistent with the theory presented here. More detailed experiments will be reported in a forthcoming paper [Wang et al. $\geq$ 2019] that considers the full initial-boundary value problem including forcing terms.

Some other questions arise naturally from our study. First, for the Dirichlet problem on the unit ball in higher dimensions, one may ask whether the scheme is stable for all time given some mild constraint on Δt. Second, one may ask about the stability analysis of the Robin problem on the unit ball in all dimensions. Third, it is natural to inquire about the stability of other explicit time-marching schemes such as Adams–Bashforth multistep methods or explicit Runge–Kutta methods. Fourth, it would be interesting to see if the convexity assumption could be relaxed, and stability proved for arbitrary, sufficiently smooth domains. Integral equation methods become difficult to analyze when the boundary of the domain is not at least C^1. We are currently investigating these issues and will report our findings in the future.

8. Appendix: 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 [Olver et al. 2010, Chapter 10]

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

It satisfies the recurrence relations [loc. cit., §10.29.2]

$$I_\nu'(z) = I_{\nu-1}(z) - \frac{\nu}{z} I_\nu(z), \qquad I_\nu'(z) = I_{\nu+1}(z) + \frac{\nu}{z} I_\nu(z). \tag{101}$$

When ν is fixed and $x \to \infty$ [loc. cit., §10.30.4],

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

When ν is an integer n, the function I_n admits the integral representation [loc. cit., §10.32.3]

$$I_n(z) = \frac{1}{\pi} \int_0^\pi e^{z\cos\theta} \cos(n\theta)\, d\theta. \tag{102}$$

The following results can be found in [Yang and Zheng 2017].

Lemma 32. *Let* $W_\nu(x) = x I_\nu(x)/(I_{\nu+1}(x))$ *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* $\nu > \frac{1}{2}$,

$$\nu - \tfrac{1}{2} + \sqrt{x^2 + \nu^2 - \tfrac{1}{4}} \le W_{\nu-1}(x) \le \nu - \tfrac{1}{2} + \sqrt{x^2 + \left(\nu + \tfrac{1}{2}\right)^2}, \tag{103}$$

and

$$\nu - 1 + \sqrt{x^2 + (\nu+1)^2} \le W_{\nu-1}(x) \tag{104}$$

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

Lemma 33. *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*,

$$\max\bigl(n^2 - \tfrac{1}{2}, \tfrac{1}{2}n^2 + n\bigr) \le r_n \le n^2 + n. \tag{105}$$

(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*

$$\max_{[0,+\infty)} e^{-x} I_n(x) < \frac{1}{2n+1}. \tag{106}$$

Proof. (a) Using the recurrence (101), 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 $I_n'(x)/I_n(x) = 1$, we have $S_{n,n-1} = -n^2$. 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 (103) and (104) with $I_n'(r_n)/I_n(r_n) = 1$ and simplifying the resulting expressions, we obtain (105).

(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 (103), it follows that $I_n'(x)/I_n(x) > 1$ for $x < n^2 - \frac{1}{2}$ and $I_n'(x)/I_n(x) < 1$ for $x > n^2 + n$. Combining these facts with (a), we have $I_n'(x)/I_n(x) > 1$ for $x < r_n$ and $I_n'(x)/I_n(x) < 1$ for $x > r_n$. That is,

$$\frac{d}{dx}(e^{-x} I_n(x)) > 0 \quad \text{for } x < r_n,$$
$$\frac{d}{dx}(e^{-x} I_n(x)) < 0 \quad \text{for } x > r_n,$$

which completes the proof of (b).

(c) By the identity §10.35.5 in [Olver et al. 2010], we have

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

Section 10.37 of [loc. cit.] states that for fixed $x > 0$, the function $I_\nu(x)$ 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 [Hartman 1964, Chapter III, §4].

Lemma 34 [Petrovitch 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*

$$\begin{aligned} u'(t) \geq f(u(t),t), \quad & t \in (t_0, t_0+\delta)(\delta > 0) \\ u(t_0) \geq y(t_0).& \end{aligned} \tag{107}$$

Then

$$u(t) \geq y(t), \quad t \in [t_0, t_0+\delta]. \tag{108}$$

The inequality in (108) is reversed if both inequalities in (107) are reversed.

(b) *(decreasing t) Suppose that u satisfies the inequalities*

$$\begin{aligned} u'(t) \leq f(u(t),t), \quad & t \in (t_0-\delta, t_0)(\delta > 0) \\ u(t_0) \geq y(t_0).& \end{aligned} \tag{109}$$

Then

$$u(t) \geq y(t), \quad t \in [t_0-\delta, t_0]. \tag{110}$$

The inequality in (110) is reversed if both inequalities in (109) are reversed.

Lemma 35. *Let*

$$g_0(x) = (4x-3)I_0(x) - (4x-1)I_1(x). \tag{111}$$

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

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

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

From Section 10.37 of [Olver et al. 2010], 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, $\lim_{x\to 3/4^+} l_0(x) = +\infty$ 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

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

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

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

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

By the recurrence relations (101), r_ν satisfies the 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

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

By Lemma 34, we have

$$l_0(x) \le u_0(x), \quad x \ge x^*; \qquad l_0(x) \ge r_0(x), \quad x \in \left(\tfrac{3}{4}, x^*\right).$$

Equivalently,

$$g_0(x) \ge 0, \quad x \ge x^*; \qquad g_0(x) < 0, \quad x \in \left[\tfrac{3}{4}, x^*\right),$$

completing the proof. □

Remark 36. Numerical computation shows that $x^* \approxeq 1.452165365078841\ldots$.

Corollary 37. *Let*

$$h_0(x) = (x-2)g_0(x) = (x-2)[(4x-3)I_0(x) - (4x-1)I_1(x)], \tag{112}$$

where $g_0(x)$ is defined in (111). Then $h_0(x) \ge 0$ on $\left[\frac{3}{4}, x^*\right]$ and $[2, \infty)$, *and $h_0(x) \le 0$ on* $[x^*, 2)$.

Lemma 38. *Let*

$$h_1(x) = (4x^2 - 7x)I_1(x) - (4x^2 - 9x + 3)I_0(x). \tag{113}$$

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

Proof. Let $x_1^* = \frac{1}{8}(\sqrt{33} + 9) = 1.843\ldots$ 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 $x \in \left[\frac{3}{4}, x_1^*\right)$. We break $\left[\frac{3}{4}, \infty\right)$ 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

$$u_0'(x) - \left(1 + \frac{1}{x}u_0(x) - u_0^2(x)\right) = \frac{3(x-3)}{(4x^2 - 9x + 3)^2}, \tag{114}$$

which is greater than zero if $x > 3$ and less than zero if $x < 3$. At $x = 3$, we have $u_0(3) = \frac{5}{4} = 1.25$ and $r_0(3) = 1.23459\ldots < 1.25 = u_0(3)$. Thus, using Lemma 34 in the increasing direction we have $r_0(x) < u_0(x)$ on $[3, \infty)$; and using Lemma 34 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) $x \in \left[\frac{7}{4}, x_1^*\right]$. 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) $x \in \left[\frac{3}{4}, \frac{7}{4}\right]$. By (114), we have $u_0'(x) - (1 + (1/x)u_0(x) - u_0^2(x)) \leq 0$ on $\left[\frac{3}{4}, \frac{7}{4}\right]$. Also, $u_0\left(\frac{3}{4}\right) = 2 < r_0\left(\frac{3}{4}\right) = 2.8\ldots$. Using Lemma 34, we have $r_0(x) > u_0(x)$, or equivalently $h_1(x) > 0$ on $\left[\frac{3}{4}, \frac{7}{4}\right]$. □

Lemma 39. *Let* $f_0(x) = e^{-1/x} I_0(1/x)$, $f_1(x) = e^{-1/x} I_1(1/x)$, *and* $f(x) = f_0(x) + af_1(x)$ *with* $a = 0.05$. *Then* $f'''(x) > 0$ *on* $(0, \infty)$.

Proof. Using the recurrence relation (101), we obtain

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

where $h_0(x)$ is defined in (112). Similarly,

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

where $h_1(x)$ is defined in (113). 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) $x \in \left[0, \frac{1}{4}\right]$. On this interval, $3 - 4x \geq 2$, $0 \leq 1 - 4x \leq 1$, and $2 - x \geq 1.75$; thus

$$h_0(x) \geq 1.75(2I_0(x) - I_1(x)) > 1.75 I_0(x).$$

Also $4x^2 - 7x \geq -1.5$, $4x^2 - 9x + 3 \leq 3$; thus $h_1(x) \geq -1.5 I_1(x) - 3I_0(x) > -4.5 I_0(x)$. Combining these results, we have

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

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

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

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

$$h_0(x) + a h_1(x) > (0.6 - 0.05 \times 3) I_1(x) > 0.$$

(d) $x \in \left[\frac{3}{4}, x^*\right] \cup [2, \infty)$. On these two subintervals, both $h_0(x)$ and $h_1(x)$ are positive by Corollary 37 and Lemma 38. Thus $h_0(x) + a h_1(x) > 0$.

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

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

where $g_0(x)$ is defined in (111). By Lemma 35, $g_0(x) > 0$ 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,

$$h_0(x) + a h_1(x) \ge \min_{x \in (x^*, 2)} h_0(x) + 0.05 \times h_1(2) > 0. \qquad \square$$

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