

A Fast Algorithm for the Evaluation of Heat Potentials

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ABSTRACT

Numerical methods for solving the heat equation via potential theory have been hampered by the high cost of evaluating heat potentials. When M points are used in the discretization of the boundary and N time steps are computed, an amount of work of the order $O(N^2M^2)$ has traditionally been required. In this paper, we present an algorithm which requires an amount of work of the order $O(NM)$, and we observe speedups of five orders of magnitude for large-scale problems. Thus, the method makes it possible to solve the heat equation by potential theory in practical situations.

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1 Introduction

A classical approach to the solution of the heat equation

$$U_t = \Delta U$$

in a space-time domain $\Omega_T = \prod_{t=0}^T \Omega(t)$ (see Fig. 1) is through the use of heat potentials [3,7]. Given zero initial conditions, one seeks a representation of U as a single layer heat potential

$$S\mu(\mathbf{x}, t) = \int_0^t \int_{\Gamma(t')} K(\mathbf{x}, \mathbf{x}', t - t') \mu(\mathbf{x}', t') d\mathbf{x}' dt' \quad (1)$$

or a double layer heat potential

$$D\mu(\mathbf{x}, t) = \int_0^t \int_{\Gamma(t')} \frac{\partial K}{\partial n'}(\mathbf{x}, \mathbf{x}', t - t') \mu(\mathbf{x}', t') d\mathbf{x}' dt' , \quad (2)$$

where K is a fundamental solution of the heat equation in some region containing Ω , n' denotes the unit outward normal to $\Gamma(t') = \partial\Omega(t')$ at \mathbf{x}' , and μ is a surface density defined on $\Gamma_T = \prod_{t=0}^T \partial\Omega(t)$.

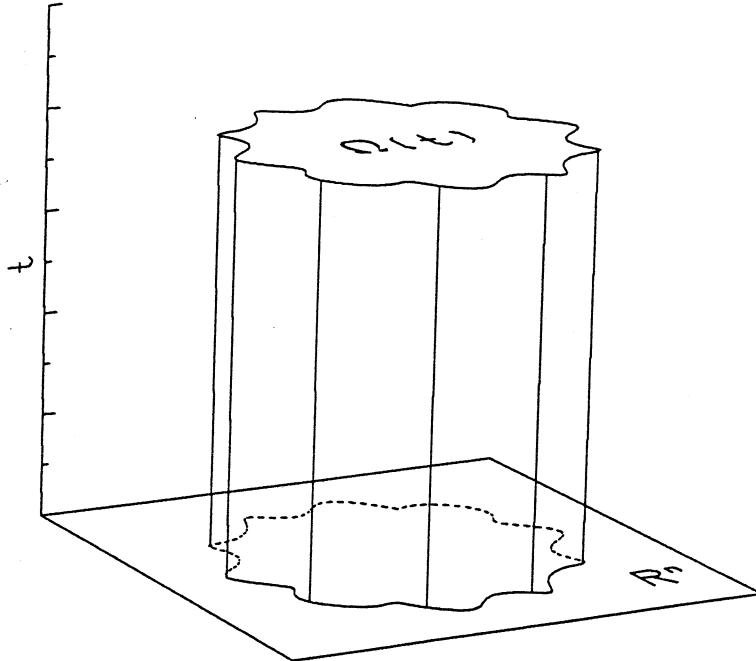


Figure 1

A domain Ω_T contained in space-time $\mathbf{R}^n \times \mathbf{R}$. $\Omega(t)$ is the cross-section of Ω_T at time t . Γ_T is the lateral boundary of Ω_T . Its cross-section at time t is given by $\Gamma(t) = \partial\Omega(t)$.

For example, the initial-Neumann problem where

$$U(x, 0) = 0 \quad \text{in} \quad \Omega(0)$$

$$\frac{\partial U}{\partial n} = g \quad \text{on} \quad \Gamma_T$$

is reduced to the Volterra integral equation of the second kind

$$\frac{1}{2}\mu(x, t) + D\mu(x, t) = g(x, t) \quad \text{on} \quad \Gamma_T$$

by means of the representation $U = S\mu$. Such an approach is used for numerical solution of the heat equation in [4,6].

Other applications of heat potentials include the study of crystal growth and unstable solidification which can be modelled by the integral equation

$$\epsilon C + V + U + SV = 0 ,$$

where the unknown V is the normal velocity of the solid-liquid boundary $\Gamma(t)$, C is the curvature of $\Gamma(t)$, ϵ is a positive constant, and U is a given temperature field incorporating the initial and boundary conditions. Recent numerical methods for unstable solidification have used this formulation [5,8].

However, numerical methods based on heat potentials have been crippled by their history-dependence: both solving the integral equation and evaluating the potential representation require more and more work as time proceeds. Consider, for example, the task of calculating $S\mu$ at a sequence of time levels $t = \Delta t, 2\Delta t, \dots, N\Delta t$. At the n th level, we must sum over n previous levels; therefore, the total work is $O(N^2)$. As for the spatial variables, if we are given M points x_j , $j = 1, 2, \dots, M$ in the discretization of the boundary, the evaluation of $S\mu$ requires $O(M^2)$ work per time step. Thus, solving the heat equation up to a fixed time T by an integral equation method would seem to require at least $O(N^2 M^2)$ work. This high cost has prevented integral equation methods from being used in practice.

In this paper, we develop an algorithm for the rapid evaluation of heat potentials. This algorithm requires only $O(MN)$ work to evaluate $S\mu$ or $D\mu$ at M points on the boundary at each of N time levels. Since there are MN data points and MN values to be computed, this is asymptotically optimal. The basic idea of the algorithm is that the potential can be split into two components, one representing the effects of the source μ over distant time (the history part) and one representing the effects of μ over recent time (the local part). The history part is smooth and can be well approximated by only a few Fourier modes. The local part, on the other hand, can be well approximated by Taylor expansion, using the singularity structure of the fundamental solution.

The outline of the paper is as follows; Section 2 describes the fundamental solution for a box, Section 3 describes the fast algorithm itself, and Section 4 presents some numerical results. We state our conclusions in Section 5.

The algorithm is currently being applied to crystal growth and unstable solidification by Sethian and Strain [9]. In a subsequent paper, we will describe a different local approximation and use the fast algorithm for the numerical solution of the heat equation.

A detailed description of the algorithm is presented only for the single layer potential $S\mu$; the modifications necessary for evaluating $D\mu$ or volume potentials are straightforward. Furthermore, we consider only potentials formed with the “box” kernel defined below; one advantage of the integral equation approach is that the solution in Ω_T does not depend on which kernel is used.

2 The Fundamental Solution in a Box

In this section, we obtain complementary representations for the fundamental solution K of the heat equation in a box $B = [0, 1]^n$ with homogeneous Dirichlet boundary conditions. A Fourier series calculation [2] shows that

$$K(\mathbf{x}, \mathbf{x}', t) = 2^n \sum_{\mathbf{k} \in \mathbf{N}^n} e^{-\pi^2 |\mathbf{k}|^2 t} \prod_{i=1}^n \sin(\pi k_i x_i) \sin(\pi k_i x'_i), \quad (3)$$

where \mathbf{N} denotes the positive integers, $\mathbf{k} = (k_1, \dots, k_n)$ and $x = (x_1, \dots, x_n)$.

On the other hand, the method of images (see [10]) can be used to show that

$$K(\mathbf{x}, \mathbf{x}', t) = (4\pi t)^{-n/2} \sum_{\mathbf{k} \in \mathbf{Z}^n} \sum_{\sigma_1 = \pm 1} \cdots \sum_{\sigma_n = \pm 1} \sigma_1 \sigma_2 \cdots \sigma_n e^{-\|\mathbf{x} - \sigma \cdot \mathbf{x}' - 2\mathbf{k}\|^2 / 4t}, \quad (4)$$

where $\sigma \cdot \mathbf{x}' = (\sigma_1 x'_1, \dots, \sigma_n x'_n)$. This expression can also be derived by the Poisson summation formula [2].

The equality of (3) and (4) is one of the foundations of our algorithm; both sums converge exponentially fast, but in different regions of time. Indeed, the error in using p^n terms of (3) is of the order $O(e^{-p^2 \pi^2 t})$ as $p^2 t \rightarrow \infty$, whereas the error in using $2^n(2p+1)^n$ terms of (4) is of the order $O(e^{-p^2/t})$ as $p^2/t \rightarrow \infty$. Thus, we truncate the Fourier series (3) to evaluate K for large t and the sum of Gaussians (4) to evaluate K for small t .

3 The Fast Algorithm

The fast algorithm will be explained in the simplest context, namely that of evaluating the single layer heat potential

$$S\mu(\mathbf{x}, t) = \int_0^t \int_{\Gamma(t')} K(\mathbf{x}, \mathbf{x}', t - t') \mu(\mathbf{x}', t') d\mathbf{x}' dt' \quad (5)$$

in two space dimensions. Here $\Gamma(t)$ is a family of boundary curves lying in the unit box $B = [0, 1]^2$ and K is the fundamental solution of the heat equation in B with homogeneous

Dirichlet boundary conditions:

$$K(\mathbf{x}, \mathbf{x}', t) = 4 \sum_{\mathbf{k} \in \mathbb{N}^2} e^{-\pi^2 |\mathbf{k}|^2 t} \sin(\pi k_1 x_1) \sin(\pi k_1 x'_1) \sin(\pi k_2 x_2) \sin(\pi k_2 x'_2) \quad (6)$$

$$= \frac{1}{4\pi t} \sum_{\mathbf{k} \in \mathbb{Z}^2} \sum_{\sigma_i = \pm 1} \sigma_1 \sigma_2 e^{-\|\mathbf{x} - \sigma \mathbf{x}' - 2\mathbf{k}\|^2 / 4t} . \quad (7)$$

We begin by splitting the time integral in (5) at time $t - \delta$, with δ a small parameter to be determined later. Thus, we write $S\mu = S_L\mu + S_F\mu$, where

$$S_L\mu(\mathbf{x}, t) = \int_{t-\delta}^t \int_{\Gamma(t')} K(\mathbf{x}, \mathbf{x}', t-t') \mu(\mathbf{x}', t') d\mathbf{x}' dt' , \quad (8)$$

$$S_F\mu(\mathbf{x}, t) = \int_0^{t-\delta} \int_{\Gamma(t')} K(\mathbf{x}, \mathbf{x}', t-t') \mu(\mathbf{x}', t') d\mathbf{x}' dt' . \quad (9)$$

The subscripts L and F refer to the local and Fourier parts, respectively.

3.1 Fast evaluation of $S_F\mu$

First consider the component $S_F\mu$, which contains the history-dependence of the potential. After replacing K with its Fourier expansion (6), $S_F\mu$ becomes a Fourier series

$$S_F\mu(\mathbf{x}, t) = \sum_{k_1=1}^{\infty} \sum_{k_2=1}^{\infty} C_{\mathbf{k}}(t, \delta) \sin(\pi k_1 x_1) \sin(\pi k_2 x_2) , \quad (10)$$

with coefficients

$$C_{\mathbf{k}}(t, \delta) = 4 \int_0^{t-\delta} e^{-\pi^2 |\mathbf{k}|^2 (t-t')} \int_{\Gamma(t')} \sin(\pi k_1 x'_1) \sin(\pi k_2 x'_2) \mu(\mathbf{x}', t') d\mathbf{x}' dt' . \quad (11)$$

This representation, by itself, does not eliminate the problem of history-dependence, because each of the Fourier coefficients $C_{\mathbf{k}}$ at time t is obtained by integrating over all previous history. However, $C_{\mathbf{k}}(t, \delta)$ can be computed from $C_{\mathbf{k}}(t - \Delta t, \delta)$ recursively. That is, by separating the final time interval Δt from the rest, we get

$$C_{\mathbf{k}}(t, \delta) = e^{-\pi^2 |\mathbf{k}|^2 \Delta t} C_{\mathbf{k}}(t - \Delta t, \delta) + 4 \int_{t-\Delta t-\delta}^{t-\delta} e^{-\pi^2 |\mathbf{k}|^2 (t-t')} \int_{\Gamma(t')} \sin(\pi k_1 x'_1) \sin(\pi k_2 x'_2) \mu(\mathbf{x}', t') d\mathbf{x}' dt' . \quad (12)$$

Each coefficient $C_{\mathbf{k}}$ can be updated with constant work per time step, rather than recomputed from $t = 0$; history-dependence is effectively eliminated.

Remark 3.1 This elimination of history actually applies much more generally. Let an operator A generate a semigroup e^{tA} , and consider the problem of evaluating the Duhamel integral

$$F(t) = \int_0^t e^{(t-t')A} f(t') dt'$$

at a sequence of time levels $t = \Delta t, 2\Delta t, \dots, N\Delta t$. Redoing the time integral at each step costs $O(N^2)$ work, but we can compute $F(t + \Delta t)$ recursively from $F(t)$:

$$F(t + \Delta t) = \int_0^{t+\Delta t} e^{(t+\Delta t-t')A} f(t') dt' \quad (13)$$

$$= e^{\Delta t A} \left(F(t) + \int_t^{t+\Delta t} e^{(t-t')A} f(t') dt' \right). \quad (14)$$

This costs only $O(N)$ work up to time $N\Delta t$. In the present paper, A is the Laplacian Δ on the box B with Dirichlet boundary conditions on ∂B , and $f(t')$ is a measure concentrated on $\Gamma(t')$ with density μ .

Another feature of the Fourier series representation (10) for $S_F \mu$ is that it allows us to take advantage of the smoothing effect of the heat operator. Higher modes are damped exponentially, so that the Fourier series representation (10) of the kernel can be truncated after p^2 terms with an exponentially small error.

Lemma 3.1 *Let $t - t' \geq \delta$ and let E_p be the error in truncating the series expansion (6) after p^2 terms*

$$E_p = |K(\mathbf{x}, \mathbf{x}', t - t') - 4 \sum_{k_1=1}^p \sum_{k_2=1}^p e^{-\pi^2 |\mathbf{k}|^2 (t-t')} \prod_{i=1}^2 \sin(\pi k_i x_i) \sin(\pi k_i x'_i)|.$$

Then

$$E_p \leq \frac{e^{-2\pi^2 (p+1)^2 \delta}}{\pi \delta}. \quad (15)$$

Proof:

$$E_p = 4 \left| \sum_{k_1=p+1}^{\infty} \sum_{k_2=p+1}^{\infty} e^{-\pi^2 |\mathbf{k}|^2 (t-t')} \prod_{i=1}^2 \sin(\pi k_i x_i) \sin(\pi k_i x'_i) \right| \quad (16)$$

$$\leq 4 \sum_{k_1=p+1}^{\infty} \sum_{k_2=p+1}^{\infty} e^{-\pi^2 |\mathbf{k}|^2 \delta} = \left(2 \sum_{k_1=p+1}^{\infty} e^{-\pi^2 k_1^2 \delta} \right)^2$$

$$\leq \left(2e^{-\pi^2 (p+1)^2 \delta} \sum_{j=0}^{\infty} e^{-\pi^2 j^2 \delta} \right)^2$$

$$\leq \left(2e^{-\pi^2 (p+1)^2 \delta} \int_0^{\infty} e^{-\pi^2 \delta \cdot x^2} \right)^2$$

$$= \left(2e^{-\pi^2 (p+1)^2 \delta} \cdot \frac{1}{2} \frac{\sqrt{\pi}}{\sqrt{\pi^2 \delta}} \right)^2 = \frac{1}{\pi \delta} e^{-2\pi^2 (p+1)^2 \delta}. \quad (17)$$

An error bound for truncation of the Fourier series representation of $S_F \mu$ now follows immediately.

Lemma 3.2 *Let $E_F(p)$ be the error in truncating the series expansion (10) after p^2 terms*

$$E_F(p) = |S_F\mu(\mathbf{x}, t) - \sum_{k_1=1}^p \sum_{k_2=1}^p C_{\mathbf{k}}(t, \delta) \sin(\pi k_1 x_1) \sin(\pi k_2 x_2)| .$$

Then

$$E_F(p) \leq \frac{|\Gamma_T| |\mu|_\infty}{\pi \delta} e^{-2\pi^2(p+1)^2 \delta} , \quad (18)$$

where $|\Gamma_T|$ is the area of Γ_T and $|\mu|_\infty$ is the maximum of $|\mu|$ over Γ_T .

We now define the updates $U_{\mathbf{k}}(t, \Delta t, \delta)$ by

$$U_{\mathbf{k}}(t, \Delta t, \delta) = 4 \int_{t-\delta-\Delta t}^{t-\delta} e^{-\pi^2 |\mathbf{k}|^2 (t-t')} \int_{\Gamma(t')} \sin(\pi k_1 x'_1) \sin(\pi k_2 x'_2) \mu(\mathbf{x}', t') d\mathbf{x}' dt' . \quad (19)$$

As the calculation of $S\mu$ proceeds in time, the recursion relation (12) provides us with a means for updating the representation of $S_F\mu$ at a total cost which grows only linearly with the number of time steps, rather than quadratically:

$$C_{\mathbf{k}}(n\Delta t, \delta) = e^{-\pi^2 |\mathbf{k}|^2 \Delta t} C_{\mathbf{k}}((n-1)\Delta t, \delta) + U_{\mathbf{k}}(n\Delta t, \Delta t, \delta) . \quad (20)$$

We therefore avoid both the computational cost and excessive storage required by the direct evaluation of the integral $S_F\mu$.

We still need to construct space and time quadratures for evaluating the updates $U_{\mathbf{k}}$ in equation (19). First, consider the calculation of the trigonometric moments of μ

$$\mathcal{M}_{\mathbf{k}}(t', \delta) = \int_{\Gamma(t')} \sin(\pi k_1 x'_1) \sin(\pi k_2 x'_2) \mu(\mathbf{x}', t') d\mathbf{x}' ,$$

assuming μ to be known at M equidistant points on $\Gamma(t')$. The trapezoidal rule for smooth periodic functions converges superalgebraically, so it would be natural to use it to evaluate $\mathcal{M}_{\mathbf{k}}$. Using all M points to integrate each of the first p^2 moments at each time step leads to a nonoptimal method, however, because p must increase as $\delta \rightarrow 0$ and $M \rightarrow \infty$, to ensure that the Fourier series truncation error vanishes (see equation (18) above). But each moment $\mathcal{M}_{\mathbf{k}}(t, \delta)$ involves integration (over a smooth curve) of sine functions with wave numbers $k_i \leq p$. Since accurate integration of such an oscillatory function requires only a fixed number of quadrature points per wavelength, we need only use $O(p)$ of the given points in the integration scheme. (The constant in $O(p)$ will depend, of course, on the smoothness of the boundary Γ and the density μ .) Hence, all of the p^2 coefficients $C_{\mathbf{k}}(n\Delta t, \delta)$ can be updated at a total cost of $O(p^3)$ work. We want $O(M)$ work per time step, so we choose $p = M^{1/3}$. In the error estimate (18), we then have

$$E_F(p) \leq \frac{|\Gamma_T| |\mu|_\infty}{\pi \delta} \cdot e^{-2\pi^2 M^{2/3} \delta} .$$

By choosing $\delta = M^{-\frac{2}{3}+\epsilon}$, $0 < \epsilon < \frac{2}{3}$, we have

$$E_F(p) \leq \frac{M^{\frac{2}{3}-\epsilon} \cdot |\Gamma_T| \|\mu\|_\infty}{\pi} \cdot e^{-2\pi^2 M^\epsilon}, \quad (21)$$

which is decaying superalgebraically with M . For example, with $\epsilon = 4/15$ and $M = 10$, this error bound is already less than 10^{-15} .

Next we must carry out the time integral in the update. Standard approaches like the trapezoidal rule are not uniformly second order accurate as $N, M \rightarrow \infty$ and $\delta \rightarrow 0$, because of the singularity of the heat kernel at $t' = t$, which lies a distance δ away from the endpoint of the interval of integration. However, we can evaluate the integral of an exponential times a polynomial exactly, which suggests the construction of a product integration rule. Thus, we construct weights W_i such that the rule

$$\int_{t-\Delta t-\delta}^{t-\delta} e^{-\pi^2 |\mathbf{k}|^2 (t-t')} g(t') dt' = W_0 g(t - \Delta t - \delta) + W_1 g(t - \delta) \quad (22)$$

is exact whenever g is linear. (Higher order rules are equally easy to construct, but for simplicity, we are seeking a globally second order method.) Some simple algebra gives

$$W_0 = \frac{e^{-z} - 1 + z}{z^2} \Delta t e^{-\pi^2 |\mathbf{k}|^2 \delta} \quad (23)$$

$$W_1 = e^{-z} \frac{e^z - 1 - z}{z^2} \Delta t e^{-\pi^2 |\mathbf{k}|^2 \delta} \quad (24)$$

where $z = \pi^2 |\mathbf{k}|^2 \Delta t$.

By evaluating the updates in the above manner (the trapezoidal rule in space and product integration in time), it is clear that the error incurred in the calculation of the Fourier coefficients $C_{\mathbf{k}}(t, \delta)$ is $O(\Delta t^2)$ plus a term which is decaying superalgebraically with $\Delta s = |\Gamma(t)|/M$. The net work required is $O(M)$ per time step. Now, given the values $C_{\mathbf{k}}(t, \delta)$, it remains only to evaluate the truncated series

$$S_F \mu(x, t) = \sum_{k_1=1}^p \sum_{k_2=1}^p C_{\mathbf{k}}(t, \delta) \sin(\pi k_1 x_1) \sin(\pi k_2 x_2)$$

at the M points x_j given on $\Gamma(t)$. Direct evaluation of the series would require $O(Mp^2)$ work which would preclude optimality. However, $S_F \mu$ contains only information with wave numbers $k_i \leq p$. It suffices, therefore, to evaluate it directly at $O(p)$ of the given points on the one-dimensional set $\Gamma(t)$. The values of $S_F \mu$ can then be reconstructed at the rest of the points by high-order local interpolation along the curve. Using the preceding strategy, the total amount of work required is of the form $O(p^3) + O(M)$ to achieve some fixed interpolation error, say second order in Δs . (However, since the points on the curve are equispaced in arclength, one can actually make the interpolation error

decay superalgebraically, by means of an FFT in arclength. The net computational cost would then be of the form $O(p^3) + O(M \log M)$.

In summary, we can evaluate $S_F \mu$ in $O(M)$ work per time step, with a constant independent of N , and with an error of the form

$$O(\Delta t^2 + \Delta s^2 + M^{2/3-\epsilon} e^{-2\pi^2 M^\epsilon}) ,$$

when $\delta = O(M^{-2/3+\epsilon})$ and second order interpolation is used in arclength. Since the final term is superalgebraic, the error in $S_F \mu$ is second order. Higher order error estimates can be obtained by using higher order product integration and higher order interpolation in arclength.

3.2 Fast evaluation of $S_L \mu$

We must now decide how to evaluate the local part of the potential

$$S_L \mu(\mathbf{x}, t) = \int_{t-\delta}^t \int_{\Gamma(t')} K(\mathbf{x}, \mathbf{x}', t-t') \mu(\mathbf{x}', t') d\mathbf{x}' dt' .$$

Since $t - t' \leq \delta$, the kernel K is sharply peaked at $\mathbf{x}' = \mathbf{x}$. This rapid decay of the heat kernel in space suggests that $S_L \mu(\mathbf{x}, t)$ can be well-approximated by considering only the values of μ in a small space-time neighborhood of $\mathbf{x} \in \Gamma(t)$ as $\delta \rightarrow 0$. To take advantage of this locality, we expand $\Gamma(t')$ and μ in Taylor series, and construct an asymptotic approximation to $S_L \mu$ in powers of δ .

First, assume for simplicity that $\Gamma(t')$ is always a distance $\geq d$ from the boundary of the unit box. Then K can be approximated by the free-space kernel

$$G(\mathbf{x} - \mathbf{x}', t - t') = \frac{e^{-|\mathbf{x} - \mathbf{x}'|^2/4(t-t')}}{4\pi(t-t')}$$

as $t - t' \leq \delta \rightarrow 0$. Indeed, G is the term in

$$K(\mathbf{x}, \mathbf{x}', t - t') = \frac{1}{4\pi(t-t')} \sum_{\mathbf{k} \in \mathbb{Z}^2} \sum_{\sigma_i = \pm 1} \sigma_1 \sigma_2 e^{-\|\mathbf{x} - \sigma \mathbf{x}' - 2\mathbf{k}\|^2/4(t-t')}$$

with $\sigma_i = 1$ and $k = 0$. The remaining terms are decaying exponentially

$$|K(\mathbf{x}, \mathbf{x}', t - t') - G(\mathbf{x} - \mathbf{x}', t - t')| = O\left(\frac{e^{-d^2/\delta}}{\delta}\right)$$

for \mathbf{x}, \mathbf{x}' on $\Gamma(t')$. Thus,

$$S_L \mu(\mathbf{x}, t) = \int_{t-\delta}^t \int_{\Gamma(t')} G(\mathbf{x} - \mathbf{x}', t - t') \mu(\mathbf{x}', t') d\mathbf{x}' dt' + O\left(\frac{e^{-d^2/\delta}}{\delta}\right) \quad (25)$$

as $\delta \rightarrow 0$. This last expression is invariant under Euclidean motions, so that for ease of calculation we may assume that $\mathbf{x} = 0$ and that the tangent line to $\Gamma(t)$ at $\mathbf{x} = 0$ is the x -axis. We also assume that $\Gamma(t')$ extends to infinity, incurring an approximation error which decays like $O(e^{-1/\delta})$ as $\delta \rightarrow 0$. Then $\Gamma(t')$ may be parametrized by

$$x = s, \quad y = y(s, t')$$

where $y(0, t) = y_s(0, t) = 0$, $\kappa = y_{ss}(0, t)$ is the curvature and $v = y_t(0, t)$ is the normal velocity of $\Gamma(t)$ at $s = 0$.

After these notational simplifications, $S_L\mu(0, t)$ assumes the form

$$S_L\mu(0, t) \approx \int_{t-\delta}^t \int_{-\infty}^{\infty} \frac{e^{-s^2/4(t-t')} e^{-y^2(s, t')/4(t-t')}}{4\pi(t-t')} \mu(s, t') \sqrt{1 + y_s^2(s, t')} ds dt',$$

where we have written $\mu(s, t')$ in place of $\mu(\mathbf{x}', t')$ for simplicity. Note that s is equal to the arclength at $s = 0$. The changes of variable $s = \sqrt{4(t-t')} \cdot r$ and $z = \sqrt{4(t-t')}$ give

$$S_L\mu(0, t) \approx \frac{1}{2\pi} \int_0^{2\sqrt{\delta}} \int_{-\infty}^{\infty} e^{-r^2} e^{-y^2(zr, t-z^2/4)/z^2} \mu(zr, t-z^2/4) \sqrt{1 + y_s^2(zr, t-z^2/4)} dr dz.$$

The sharp peak of the Gaussian in r and the short interval of integration in z allow us to compute $S_L\mu$ as an asymptotic series in δ . After Taylor expansion of μ and y about the point $(0, t)$, we obtain to lowest order in δ the result

$$S_L\mu(0, t) = \sqrt{\frac{\delta}{\pi}} \mu(0, t) + O(\delta^{3/2}).$$

Retaining one more order in δ and doing some algebra gives

$$S_L\mu(0, t) = \sqrt{\frac{\delta}{\pi}} \left(\mu(0, t) + \frac{\delta}{12} (\kappa - v)^2 \mu(0, t) - \frac{\delta}{3} (\mu_t - \mu_{ss}) \right) + O(\delta^{5/2}).$$

Since the parameter s is equal to arclength at $s = 0$ and the curvature and normal velocity are invariant under Euclidean motions, the preceding formula holds more generally. We have therefore proven

Lemma 3.3 *Let $\Gamma(t)$ and $\mu(x, t)$ be four times differentiable. Then*

$$S_L\mu(\mathbf{x}(s, t), t) = \sqrt{\frac{\delta}{\pi}} \left[\left(1 + \frac{\delta}{12} (\kappa - v)^2 \right) \mu(s, t) - \frac{\delta}{3} (\mu_t(s, t) - \mu_{ss}(s, t)) \right] + O(\delta^{5/2}), \quad (26)$$

where κ is curvature, v is normal velocity and s is arclength on $\Gamma(t)$.

This calculation can be extended to higher order in δ for sufficiently smooth curves and densities, but we shall carry it no further. The approximation of Lemma 3.3 will suffice for the purposes of this paper: it can clearly be evaluated at M points in $O(M)$ work, completing our derivation of an $O(MN)$ algorithm for evaluating the single layer heat potential $S\mu$.

3.3 Formal Description of the Algorithm

In this section, we describe the fast algorithm in a more procedural form. We first observe that the parameter δ was chosen in subsection 3.1 to be of the order $M^{-2/3+\epsilon}$, independent of the time step Δt . In practice, it is convenient to have δ be equal to an integer number of time steps. We therefore set

$$\delta = \left\lceil \frac{M^{-2/3+\epsilon}}{\Delta t} \right\rceil \cdot \Delta t.$$

Algorithm

Comment [Choose $M, N, \Delta t$ and the small parameter ϵ which defines δ . Set $l = \lceil \frac{M^{-2/3+\epsilon}}{\Delta t} \rceil$ and $\delta = l\Delta t$. Set $p = M^{1/3}$.]

Step 1.

Comment [Use the local approximation $S_L\mu$ to evaluate the single layer heat potential $S\mu$ for the first l time steps.]

```
do  $n = 1, 2, \dots, l$ 
  do  $m = 1, 2, \dots, M$ 
    Evaluate  $S\mu(\mathbf{x}_m, n\Delta t)$  via the approximation for  $S_L\mu(\mathbf{x}_m, n\Delta t)$ 
    given by equation (26), with  $n\Delta t$  in place of  $\delta$  and  $t$ .
  enddo
enddo
```

Step 2.

Comment [Initialize Fourier coefficients.]

```
do  $k_1 = 1, \dots, p$ 
  do  $k_2 = 1, \dots, p$ 
     $\mathbf{k} := (k_1, k_2)$ 
     $C_{\mathbf{k}}(l\Delta t, \delta) := 0$ 
  end do
end do
```

Step 3.

Comment [For all subsequent steps, update the Fourier coefficients and calculate the history part $S_F\mu$ at the points \mathbf{x}_m on the curve. Then add the local approximation $S_L\mu$ at each \mathbf{x}_m to complete the evaluation of the single layer heat potential $S\mu$.]

do $n = l + 1, l + 2, \dots, N$

(A) **do** $k_1 = 1, \dots, p$

do $k_2 = 1, \dots, p$

$\mathbf{k} := (k_1, k_2)$

Evaluate the trigonometric moments $\mathcal{M}_{\mathbf{k}}((n-1)\Delta t, \delta)$ and $\mathcal{M}_{\mathbf{k}}(n\Delta t, \delta)$.

Compute the update $U_{\mathbf{k}}(n\Delta t, \Delta t, \delta)$ of equation (19)

by product integration (equations 22 - 24).

$U_{\mathbf{k}}(n\Delta t, \Delta t, \delta) = W_0 \cdot \mathcal{M}_{\mathbf{k}}((n-1)\Delta t, \delta) + W_1 \cdot \mathcal{M}_{\mathbf{k}}(n\Delta t, \delta)$.

Update the Fourier coefficients by means of equation (20):

$C_{\mathbf{k}}(n\Delta t, \delta) = e^{-\pi^2 |\mathbf{k}|^2 \Delta t} C_{\mathbf{k}}((n-1)\Delta t, \delta) + U_{\mathbf{k}}(n\Delta t, \Delta t, \delta)$

end do

end do

(B) Evaluate Fourier series at p equispaced points on $\Gamma(n\Delta t)$.

Extend values of Fourier series to all M points \mathbf{x}_m by interpolation.

(C) **do** $\mathbf{m} = 1, 2, \dots, M$

Evaluate $S_L \mu(\mathbf{x}_m, n\Delta t)$ by the local approximation (26) and add to $S_F \mu(\mathbf{x}_m, n\Delta t)$.

end do

end do

Remark 3.2. Inspection of the above algorithm shows that the amount of work required is of the order $O(NM)$, assuming fixed degree interpolation in arclength is used. If Fourier interpolation is used in Step 3 (B), the amount of work required is of the order $O(NM \log M)$.

Remark 3.3. As noted previously, the convergence rate of the scheme is dependent on the product integration scheme used, the interpolation scheme used and the order of the local approximation. The scheme described in the text is second order in Δt and of order $\frac{5}{2}$ in δ . We have chosen in our tests to use Fourier interpolation in arclength, which increases the computational complexity by a factor of $\log M$, but effectively removes interpolation as a limiting source of error.

Remark 3.4. In the algorithm outlined above, we end up computing each trigonometric moment $\mathcal{M}_{\mathbf{k}}(n\Delta t, \delta)$ twice, once for the update $U_{\mathbf{k}}(n\Delta t, \Delta t, \delta)$ and once for $U_{\mathbf{k}}((n+1)\Delta t, \Delta t, \delta)$. This is easily avoided by an appropriate modification to the program.

4 Numerical Examples

The algorithm was implemented in FORTRAN and tested on several numerical examples. We evaluated the single layer heat potential of a cosine density $\mu(\theta) = \cos(k\theta)$ of

wavenumber k on a stationary circle

$$\Gamma : (x = R \cos \theta, y = R \sin \theta, 0 \leq \theta \leq 2\pi) .$$

We computed the potential at time $T = 1/2$ with a sequence of numerical parameters in which the number N of time steps and the number M of points on the circle are doubled at each stage, p and the number M_p of points used for integrating over the curve grow like $M^{1/3}$, and δ decreases like $M^{-2/3}$. Thus, the total error should be dominated by the $\delta^{5/2} = M^{-5/3}$ error due to Taylor expansion in the local approximation. The parameters used and corresponding computational times are shown in Table 1.

Case	N	M	δ	p	M_p	Time(Fast)	Time(Direct)
1	10	20	.01	10	20	9	45
2	20	40	.0063	13	40	12	331
3	40	80	.004	16	50	21	4400
4	80	160	.0025	20	63	56	66024
5	160	320	.0016	26	80	213	(1.1 10^6)
6	320	640	.00099	32	102	794	(1.7 10^7)
7	640	1280	.00063	40	128	3074	(2.7 10^8)

Table 1

Table of parameters for Cases 1-7, with CPU times on the Multiflo Trace computer at Yale University.

In cases 1-4, the direct computation times were estimated by evaluating the potential at 20 of the boundary points at each step, using the trapezoidal rule in space and second order composite product integration in time. In cases 5-7, direct CPU times were estimated by extrapolation.

The accuracies of the fast and direct methods are compared in Table 2 for wavenumber $k = 0$. The error reported is the maximum deviation of the computed potential from the exact potential over 20 points on the curve. Finally, Table 3 presents the error produced by the fast algorithm for wavenumbers $k = 0, 1, 2$ and 3.

The following observations can be made from Tables 1-3.

1. The $O(\Delta s^{5/3})$ error displayed by the fast algorithm agrees with the error analysis of section 3.2. The direct algorithm displays $O(\Delta t^2 + \Delta s^2)$ error, but with a larger constant of proportionality, which accounts for its poorer accuracy in the range of parameters tested..
2. The CPU time requirements of the fast algorithm clearly grow only like NM .
3. By the time $N = 640, M = 1280$, the fast algorithm is about 88,000 times faster than the direct method would have been. Case 7 required about 50 min. on the Multiflo Trace. The direct calculation would have taken $8\frac{1}{2}$ years.

Case	fast algorithm	direct algorithm
1	$1.2 \cdot 10^{-4}$	$6.2 \cdot 10^{-3}$
2	$3.1 \cdot 10^{-5}$	$9.0 \cdot 10^{-4}$
3	$9.2 \cdot 10^{-6}$	$1.3 \cdot 10^{-4}$
4	$2.7 \cdot 10^{-6}$	$3.5 \cdot 10^{-5}$
5	$8.9 \cdot 10^{-7}$	$8.5 \cdot 10^{-6}$
6	$2.9 \cdot 10^{-7}$	$2.1 \cdot 10^{-6}$
7	$1.1 \cdot 10^{-7}$	$5.1 \cdot 10^{-7}$

Table 2

Comparison of absolute errors for wavenumber $k = 0$, using fast and direct algorithms.

Case	$k = 0$	$k = 1$	$k = 2$	$k = 3$
1	$1.2 \cdot 10^{-4}$	$1.9 \cdot 10^{-4}$	$1.1 \cdot 10^{-3}$	$7.5 \cdot 10^{-3}$
2	$3.1 \cdot 10^{-5}$	$5.0 \cdot 10^{-5}$	$3.2 \cdot 10^{-4}$	$2.5 \cdot 10^{-3}$
3	$9.2 \cdot 10^{-6}$	$1.5 \cdot 10^{-5}$	$1.0 \cdot 10^{-4}$	$8.3 \cdot 10^{-4}$
4	$2.7 \cdot 10^{-6}$	$4.5 \cdot 10^{-6}$	$3.0 \cdot 10^{-5}$	$2.6 \cdot 10^{-4}$
5	$8.9 \cdot 10^{-7}$	$1.4 \cdot 10^{-6}$	$9.8 \cdot 10^{-6}$	$8.6 \cdot 10^{-5}$
6	$2.9 \cdot 10^{-7}$	$4.2 \cdot 10^{-7}$	$3.0 \cdot 10^{-6}$	$2.6 \cdot 10^{-5}$
7	$1.1 \cdot 10^{-7}$	$1.3 \cdot 10^{-7}$	$9.5 \cdot 10^{-7}$	$8.5 \cdot 10^{-6}$

Table 3

Table of absolute errors produced by the fast algorithm for Cases 1-7, with wavenumbers $k = 0, 1, 2, 3$.

4. Even for as few as 10 time steps and 20 boundary points, the fast algorithm is about five times faster than the direct calculation.

5 Conclusions

In this paper, we have developed a fast algorithm for evaluating heat potentials. A detailed description of the analysis is given only for the single layer potential in two space dimensions, but the outline of the method is the same in one or three space dimensions. The extension to double layer potentials is straightforward.

Our algorithm evaluates a heat potential at MN points, using density values at MN points, in $O(MN)$ work. The direct evaluation requires $O(M^2N^2)$ work, so the fast algorithm achieves a dramatic speedup: with 1280 points on the curve and 640 time steps, the fast algorithm ran 88,000 times faster than the direct calculation would have, and produced an error five times smaller.

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