26 A Spectral Method for the Fast Solution of Boundary Integral Formulations of Elliptic Problems

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26.1 Introduction

Discretizations of boundary integral equations lead to dense linear systems. If an iterative method, such as conjugate gradients or GMRES, is used to solve such a system, the matrix-vector product has \(O(n^2)\) complexity, where \(n\) is the number of degrees of freedom in the discretization. The rapid growth of the quadratic term severely limits the size of tractable problems.

In the past two decades, a variety of methods have been developed to reduce the complexity of the matrix-vector product. These methods exploit the fact that the Green's function can be approximated by truncated series expansions when the source and the field point are sufficiently well separated. Typical examples of such methods are the fast multipole method (FMM) and wavelet-based discretizations.

The additional error introduced by the series approximation must be controlled; ideally, this error should be of the same order as the discretization error. Wavelets and the FMM have been shown to be asymptotically optimal in many situations. That is, the complexity of a matrix-vector multiplication is order \(n\), while the convergence rate of the discretization scheme is preserved (see, for example, [1]–[3]).

In this paper, we explore a spectral method to reduce the complexity of the matrix-vector product. Here, the Green's function is replaced by a trigonometric expansion, which is valid globally for all positions of source- and field-points. Spectral techniques have been applied previously by Greengard and Strain to the heat equation [4]. In this work we consider elliptic equations where the Green's function is singular and the convergence of the Fourier series is slow. To overcome this difficulty, we split the Green's function into a local part, which is evaluated directly, and a smooth part, which will be treated with the Fourier series approach. We will also develop nonequispaced fast Fourier transforms for computing the matrix-vector product efficiently.

Although the methodology can be applied to a large class of Green's functions, we limit the discussion in this paper to the Laplace equation. Our focus in this paper is on the presentation of the algorithm. A more detailed analysis of the error will be discussed elsewhere.
26.2 A Fast Algorithm for Smooth, Periodic Kernels

Consider the fast evaluation of a surface integral operator with a generic smooth and periodic kernel \( G \)

\[
\Phi(x) := \int_S G(x - y)g(y)\,dS_y, \quad x \in S, \tag{26.1}
\]

where \( S \) is a surface that is contained in the unit cube \([0,1]^3\) and \( G(\cdot) \) is a \( C^\infty \)-function that has period two in all three variables. The kernel can be approximated by the truncated Fourier series

\[
G_N(r) := \sum_{|k| \leq N} \hat{G}_k \exp(\pi i k^T r), \quad r \in [-1,1]^3, \tag{26.2}
\]

where the summation index \( k \) is in \( \mathbb{Z}^3 \) and \( |k| := \max\{k_1, k_2, k_3\} \). Under the assumptions on the kernel, the convergence of (26.2) is super-algebraic in \( N \). The resulting approximate potential is given by

\[
\Phi_N(x) = \int_S G_N(x - y)g(y)\,dS_y = \sum_{|k| < N} \exp(\pi i k^T x) \hat{d}_k, \tag{26.3}
\]

where \( \hat{d}_k = \hat{G}_k \hat{g}_k \) and

\[
\hat{g}_k = \int_S \exp(-\pi i k^T y)g(y)\,dS_y. \tag{26.4}
\]

This simple computation suggests the following approach to evaluate the potential in (26.1).

1. Compute the Fourier coefficients \( \hat{g}_k \) in (26.4).
2. Multiply \( \hat{d}_k := \hat{G}_k \hat{g}_k \) for \( |k| \leq N \).
3. Evaluate the Fourier series (26.3) for \( x \in S \).

The choice of the truncation parameter \( N \) depends on the approximation properties of the Fourier series (26.2) and can be selected to be much smaller than the size of the linear system \( n \). Stage 2 obviously involves \( O(N^3) \) operations; the other two stages can be executed efficiently using nonequispaced fast Fourier transforms (FFTs). This will be discussed next.

26.2.1 Computation of the \( \hat{g}_k \)

In this section, we describe how FFTs can be used to efficiently compute the Fourier coefficients of the function \( g \). To that end, the three-space is divided into small cubes \( G_l, l = (l_1, l_2, l_3) \in \mathbb{Z}^3, 0 \leq l_j < N \). These cubes have centers \( x_l = l/N \) and side length \( 1/N \). Note that \( N \) is the same as in (26.3) and therefore the cubes get smaller if more terms in the Fourier series expansion of the Green’s function are retained. We assume that \( S \) is
contained in the union of all cubes, and set $S_l = C_l \cap S$ to denote the piece of the surface that intersects with the $l$th cube (see Fig. 1).

![Diagram](image)

**Fig. 1.** Two-dimensional illustration of the geometry.

From (26.4) it follows that the Fourier coefficients of $g$ can be written as

$$
\hat{g}_k = \sum_l \exp \left( -\frac{\pi ik^T l}{N} \right) \int_{S_l} \exp(-\pi ik^T (y - x_l)) g(y) \, dS_y. \quad (26.5)
$$

The frequency and the spatial variable in the integral can be separated using the Jacobi–Anger expansion

$$
\exp(-i\xi t) = \sum_{\nu=0}^{\infty} (-i)^\nu (2\nu + 1) j_\nu(\xi) P_\nu(t), \quad -1 \leq t \leq 1
$$

(see, for example, [5]). Here, $j_\nu(\cdot)$ is the spherical Bessel function of order $\nu$ and $P_\nu(\cdot)$ is the Legendre polynomial of degree $\nu$. This formula can be easily applied to the integrand in (26.5); this leads to

$$
\exp(-\pi ik^T (y - x_l)) \approx \sum_{|\alpha| \leq p} (-i)^{|\alpha|} (2\alpha + 1) j_{\alpha}(\pi kH) P_\alpha \left( \frac{y - x_l}{H} \right), \quad (26.6)
$$

where $\alpha$ is the expansion order, $H = 1/(2N)$, $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ is a multi-index, $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3$, $j_{\alpha}(x) = j_{\alpha_1}(x_1) j_{\alpha_2}(x_2) j_{\alpha_3}(x_3)$, and $P_\alpha(x)$ is defined similarly. Substitution of (26.6) into (26.5) leads to the approximation

$$
\hat{g}_k \approx \sum_{|\alpha| \leq p} (-i)^\alpha (2\alpha + 1) j_{\alpha}(\pi kH) \sum_l \exp \left( -\frac{\pi ik^T l}{N} \right) m^\alpha_l (g).
$$
where
\[ m_i^\alpha(g) = \int_{S_i} P_\alpha \left( \frac{y - x_i}{H} \right) g(y) \, dS_y \]
is a moment for which exact formulas can be derived if the function and the
surface are discretized. In particular, if \( g \) is piecewise polynomial, then the
moments are linear transformations of the coefficients of \( g \) corresponding to
the nodal basis. The matrix that maps the coefficients to the \( \alpha \)th moments
is denoted by \( M_\alpha \). The number of nonzero entries in \( M_\alpha \) is \( n \).

In matrix form, the (approximate) coefficient vector \( \hat{g} \) is given by
\[ \hat{g} = \sum_{\alpha \leq p} K_\alpha F M_\alpha \hat{g}, \quad (26.7) \]

where \( F \) is the 3D FFT, \( \hat{g} \) the vector of coefficients of \( g \), and \( K_\alpha \) is a
diagonal matrix with the factors \((-i)^\alpha (2\alpha + 1) j_\alpha (\pi k H)\). The computation
of \( \hat{g} \) involves \( (p + 1)(p + 2)(p + 3)/6 \) FFTs. Since \( C_\ell \) is smaller than a
wavelength of the highest Fourier mode, it suffices to use a small value of
\( p \).

### 26.2.2 Evaluation of the Fourier Series

In the Galerkin discretization, the \( \ell \)th component of the matrix product
\( \Phi_i \) is the inner product of the potential \( \Phi \) in (26.1) with the \( \ell \)th nodal
basis function \( \varphi_i \). For the fast method, the potential is replaced with the
approximated potential \( \Phi_N \) in (26.3). In order to evaluate the potential
efficiently, the Jacobi–Anger approximation (26.6) is used again, just as in
the previous section. This is shown in the following computation:

\[ \Phi_i = \int_S \varphi_i(x) \Phi_N(x) \, dS_x \]
\[ = \sum_k \exp \left( \frac{\pi i kT}{N} \right) \int_S \exp(\pi i kT (y - x)) \varphi_i(x) \, dS_x \, d_k \]
\[ \approx \sum_{\alpha \leq p} \sum_k \exp \left( \frac{\pi i kT}{N} \right) i^{|\alpha|} (2\alpha + 1) j_\alpha (\pi k H) m_i^\alpha (\varphi_i) \, d_k. \]

In matrix notation, the above can be written as
\[ \tilde{\Phi} = \sum_{\alpha \leq p} M_\alpha^T F K_\alpha^* \tilde{d}. \quad (26.8) \]

Hence, \((p + 1)(p + 2)(p + 3)/6\) FFTs are necessary to compute the vector
\( \tilde{\Phi} \). Furthermore, it is evident that the operation (26.8) is the adjoint of
operation (26.7).
26.3 Extension to Singular Kernels

If the spectral method is applied to the Green’s function of an elliptic equation, then the convergence with respect to the truncation parameter \( N \) will be slow due to the singularity at \( r = 0 \). We will therefore split the Green’s function into a smooth and a local part.

26.3.1 Smooth Part

The following discussion is directed at the Laplace kernel, whose Fourier transform is \( 1/\xi^2 \). That is, for \( r \in \mathbb{R}^3 \),

\[
G(r) = \frac{1}{4\pi |r|} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{1}{|\xi|^2} \exp(i \xi^T r) d^3 \xi.
\]

A smooth approximation of this function can be obtained by multiplying the Fourier transform by the exponential \( \exp(-\delta |\xi|^2) \), where \( \delta > 0 \) is the mollification parameter which is at our disposal. The smooth Green’s function is given by

\[
\tilde{G}_\delta(r) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \frac{\exp(-\delta |\xi|^2)}{|\xi|^2} \exp(i \xi^T r) d^3 \xi.
\]

This kernel can be expressed in closed form, and we find that

\[
\tilde{G}_\delta(r) = \frac{1}{4\pi |r|} \text{erf} \left( \frac{|r|}{2\sqrt{\delta}} \right), \tag{26.9}
\]

where \( \text{erf}(\cdot) \) is the error function. The kernel \( \tilde{G}_\delta \) is in \( C^\infty(\mathbb{R}^3) \), but not periodic. Therefore, we introduce an offset parameter \( 0 < \mu \ll 1 \), re-scale (26.1) so that \( S \) is contained in the cube \( [0, 1 - \mu]^3 \), and define a smooth cut-off function

\[
\chi_\mu(r) = \begin{cases} 1 & \text{for } r \in [-1 + \mu, 1 - \mu]^3, \\ 0 & \text{for } r \text{ outside } [-1, 1]^3, \\ \geq 0 & \text{otherwise}. \end{cases} \tag{26.10}
\]

Thus, the kernel \( G_\delta := \chi_\mu \tilde{G}_\delta \) is smooth and periodic and generates the same potential in (26.1) as the kernel \( G_\delta \).

In stage 2 of the spectral method, the Fourier coefficients of the function \( \hat{g}_k \) are multiplied by the Fourier coefficients of the kernel \( \tilde{G}_k \). Since there are no analytic expressions of \( \tilde{G}_k \) available, these coefficients must be computed numerically, using FFTs and the Jacobi–Anger series. Since this algorithm is completely analogous to the computation of the function coefficients described in Section 26.2.1, we omit the details.
26.3.2 Local Part

Due to the behavior of the error function, the smooth part is a good approximation of the actual Green's function if $\delta$ is small and $r$ is large. In the neighborhood of the origin, the two functions are very different and therefore the contribution of this local part must be accounted for. The potential in (26.1) can be decomposed as $\Phi = \Phi_\delta + \Psi_\delta$, where

$$\Phi_\delta(x) := \int_S G_\delta(x - y)g(y)\,dS_y, \quad x \in S,$$

is the smooth part and

$$\Psi_\delta(x) := \int_S E_\delta(x - y)g(y)\,dS_y, \quad x \in S,$$

is the local part. Here, $E_\delta = G - G_\delta$. In what follows we show that the local part has an expansion with respect to the mollification parameter $\sqrt{\delta}$ and indicate how to compute the expansion coefficients.

Because of (26.5), the function $E_\delta$ decays exponentially away from the origin. We introduce another cut-off function $\chi_\nu$ for some $0 < \nu < 1$, which is small enough so that the surface has a parameterization of the form $y(t) = x + At + nh(t)$ in the $\nu$-neighborhood of $x$. Here, $n$ is the normal to the surface at the point $x$, $A \in \mathbb{R}^{3 \times 2}$ has two orthogonal columns that span the tangent plane at $x$, and $h(t) = O(t^2)$ is some scalar function in $t \in \mathbb{R}$. The local potential $\Psi_\delta(x)$ can be written in the form

$$\Psi_\delta(x) = \int_S E_\delta(x - y)g(y)\,dS_y$$

$$= \int_S E_\delta(x - y)\chi_\nu(x - y)g(y)\,dS_y + O\left(\exp\left(-\frac{\nu}{\delta}\right)\right) \quad (26.11)$$

$$= \int_{S^2} E_\delta(t)\hat{g}(t)\,d^2t + O\left(\exp\left(-\frac{\nu}{\delta}\right)\right).$$

Here, $E_\delta(t) = E_\delta(x - y(t))$, $\hat{g}(t) = \chi_\nu(x - y(t))g(t)J(t)$, and $J(t)$ is the Jacobian of the parameterization. For simplicity, we assume that the function $h(t)$ in the parameterization of the surface is analytic, that is,

$$h(t) = \sum_{|a| \geq 2} h_a t^a. \quad (26.12)$$

Thus, there are $C^\infty$-functions $H_n$ such that

$$r(t) := |x - y(t)| = |t| \sum_{n=0}^{\infty} |t|^n H_n(\hat{t}), \quad (26.13)$$
where \( \hat{t} := t/|t|, H_0(\hat{t}) = 1, \) and \( H_1(\hat{t}) = 0. \) In the neighborhood of the point \( x, \) the kernel has the form

\[
E_3(t) = \frac{1}{\sqrt{\delta}} E \left( \frac{r(t)}{\sqrt{\delta}} \right) \quad \text{where} \quad E(z) = \frac{1}{4\pi z} \left( 1 - \text{erf} \left( \frac{z}{\sqrt{2}} \right) \right).
\]

Note that \( E(z) \) is singular at \( z = 0 \) and decays exponentially as \( z \to \infty. \) Substituting (26.13) in (26.11) results in

\[
\Psi_3(x) = \frac{1}{\sqrt{\delta}} \int_{\mathbb{R}^2} E \left( \frac{r(t)}{\sqrt{\delta}} \right) \hat{g}(t) d\hat{t} + O \left( \exp \left( -\frac{\nu}{\delta} \right) \right)
\]

\[
= \sqrt{\delta} \int_{\mathbb{R}^2} E \left( |t| \sum_{n=0}^{\infty} (\sqrt{\delta}|t|)^n H_n(\hat{t}) \right) \hat{g}(\sqrt{\delta}t) d\hat{t} + O \left( \exp \left( -\frac{\nu}{\delta} \right) \right),
\]

where the second integral is the result of the change of variables \( t \to t/\sqrt{\delta}. \)

It is easy to see that \( H_n(-t) = (-1)^n H_n(t), \) which implies that the integral in the last expression is an even function of \( \sqrt{\delta}. \) Furthermore, the integral as a function of \( \sqrt{\delta} \) is \( C^\infty, \) and can be expanded in a Taylor series. Since the exponential term does not contribute to the expansion, we obtain

\[
\Psi_3(x) = \delta^+ \Psi_0 + \delta^+ \tilde{\Psi}_1 + \delta^+ \tilde{\Psi}_2 + \cdots \tag{26.14}
\]

A more detailed analysis shows that the first two expansion coefficients \( \Psi_k \)

are given by

\[
\Psi_0 = \frac{1}{\sqrt{\pi}} \tilde{g}(0),
\]

\[
\Psi_1 = \frac{1}{3\sqrt{\pi}} \left[ \Delta \tilde{g}(0) - (3h_{20}^2 + 3h_{22}^2 + 2h_{20}h_{c2} + h_{11}^2) \tilde{g}(0) \right],
\]

where \( h_{ij} \) are the coefficients in the expansion (26.12).

### 26.4 Numerical Example and Conclusions

We present numerical results pertaining to the single-layer equation

\[
\int_{S} \frac{1}{4\pi} \frac{1}{x - \hat{y}} g(y) dS_y = f(x),
\]

where \( S \) is the ellipsoid

\[
\left( \frac{x}{2} \right)^2 + \left( \frac{y}{3} \right)^2 + \left( \frac{z}{3} \right)^2 = 1
\]

and the right-hand side is \( f(x) = 1. \) This problem has an analytic solution in closed form, and we compute the \( L^2(S) \)-error of the numerical solution.
\[ \|e_h\| \text{ for various values of the meshwidth and the parameters } N \text{ and } \delta. \] 
To compute the local potential \( \Psi_h \), the expansion (26.14) is truncated after the first term. Thus, the local potential is replaced by

\[ \Psi_h(x) \approx \sqrt{\frac{\delta}{\pi}} g(x). \]  

(26.15)

This approximation is of order \( \delta^{3/2} \). The initial triangulation of the ellipsoid consists of 320 panels, which is several times uniformly refined. The finite element space is the piecewise constant functions on this triangulation. Standard convergence analysis implies that the discretization error of the direct Galerkin method is order \( h \), that is, the error is halved in every refinement step. Our goal is to choose the parameters \( N \) and \( \delta \) in such a way that the spectral scheme exhibits the same convergence behavior when refining the mesh. At the same time, the scheme should be efficient, with complexity that is linear or almost linear in the number of panels \( n \). Since the complexity of the FFT is order \( N \log N \), we set \( N \approx n^{1/3} \) to obtain almost linear complexity.

The parameter \( \delta \) affects the accuracy in two ways. If \( \delta \) is small, then the truncation error in (26.15) is small, but on the other hand, the Green’s function of the smooth part will be peaked at the origin, which increases the error of the Fourier series approximation. Table 1 displays the behavior of the error when the mesh is refined. In this table, the parameter \( \delta \) has been determined experimentally to minimize the error. Table 2 displays the effect of \( \delta \) on the error for the finest mesh.

| \( n \) | 320 | 1220 | 5120 | 20,480 | 81,920 | 327,680 |
| \( N \) | 8 | 12 | 18 | 32 | 48 | 72 |
| \( \delta \) | 1.6(-3) | 8.0(-4) | 4.0(-4) | 2.0(-4) | 1.0(-4) | 5.0(-5) |
| \( \|e_h\| \) | 0.3015 | 0.1549 | 0.08819 | 0.04151 | 0.02036 | 0.01004 |

Table 2. Errors for the finest mesh \( (n = 327,680, N = 72) \) for different values of the mollification parameter.

| \( \delta \) | 1.0(-3) | 1.0(-4) | 2.5(-5) | 1.3(-5) | 6.0(-6) | 3.0(-6) |
| \( \|e_h\| \) | 0.08540 | 0.01168 | 0.01214 | 0.02276 | 0.04004 | 0.06116 |

The hardest problem \( (n = 327,680, \delta = 3 \cdot 10^{-6}) \) took 22 GMRES iterations to converge, the overall time was about 23 minutes on an AMD Athlon64-3200 processor, and the memory allocation was about 500MB. The package FFTW [6] was used for the computation of the FFTs. The order \( p \) in (26.7) and (26.8) was set to 4 in all experiments.

The numerical results presented suggest that the parameters in the spectral method can be selected so that the resulting scheme is nearly asymptotically optimal, that is, optimal up to logarithmic factors. Currently we are working on error estimates, trying to confirm this assertion.
References


