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Fast convolution with the free space Helmholtz Green's function ☆

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ABSTRACT

We construct an approximation of the free space Green's function for the Helmholtz equation that splits the application of this operator between the spatial and the Fourier domains, as in Ewald's method for evaluating lattice sums. In the spatial domain we convolve with a sum of decaying Gaussians with positive coefficients and, in the Fourier domain, we multiply by a band-limited kernel. As a part of our approach, we develop new quadratures appropriate for the singularity of Green's function in the Fourier domain. The approximation and quadratures yield a fast algorithm for computing volumetric convolutions with Green's function in dimensions two and three. The algorithmic complexity scales as $\mathcal{O}(\ \log\ + C(\log\ ^{-1})\ )$, where is selected accuracy, is the number of wavelengths in the problem, is the dimension, and C is a constant. The algorithm maintains its efficiency when applied to functions with singularities. In contrast to the Fast Multipole Method, as $\rightarrow 0$, our approximation makes a transition to that of the free space Green's function for the Poisson equation. We illustrate our approach with examples.

1. I

In many applied fields including acoustics, quantum mechanics, and electromagnetics, we encounter the need to compute convolutions with the free space Helmholtz Green's function. In these fields problems of interest often involve media or potentials described by functions with discontinuities or singularities. However, it is difficult to construct fast and accurate algorithms to compute convolutions with such functions entirely in spatial or entirely in the Fourier domain. In the spatial domain, a straightforward discretization of Green's function results in dense matrices, whereas in the Fourier domain slow decay of the product requires an unreasonably large computational domain to obtain accurate results. For these reasons, our

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approach to obtain a fast and accurate algorithm is based on approximating Green's function so that its application is split between the spatial and Fourier domains.

We consider the problem of convolving a given function with the free space Helmholtz Green's function G,

$$(\mathbf{x}) = \int_{\mathbb{R}} G(\mathbf{x} - \;)\,(\;) \tag{1}$$

where G satisfies

$$(\Delta + {}^2)G(\mathbf{x}) = -\delta(\mathbf{x}) \tag{2}$$

and the Sommerfeld condition

$$\lim_{|\mathbf{x}| \to \infty} |\mathbf{x}|^{\frac{-1}{2}} \left(\frac{G}{|\mathbf{x}|} - \quad G \right) = 0 \qquad 0 \tag{3}$$

We assume that $\in L\,(D)$ for some $1 \leqslant \; \leqslant \infty$, and is supported in a bounded domain D. The function is the solution to

$$(\Delta + {}^2)\;(\mathbf{x}) = -\;(\mathbf{x}) \tag{4}$$

and satisfies the Sommerfeld condition.

In dimension , the free space Helmholtz Green's function is given by

[redacted]

$$G(\mathbf{x}) = \frac{}{4} \left(\frac{}{2\;|\mathbf{x}|} \right)^{(\;-2)\;2} H^{(1)}_{(\;-2)\;2}(\;|\mathbf{x}|)$$

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where $H^{(1)}_{(\;-2)\;2}$ is a Hankel function of the first kind and $|\mathbf{x}| = \left(\sum_{=1} {}^2\right)^{1\;2}$ denotes the Euclidean norm of the vector $\mathbf{x}$. We focus our attention on dimensions $= 3$ and $= 2$, so that

[redacted]

$$G(\mathbf{x}) = \begin{cases} \frac{1}{4} \frac{|\mathbf{x}}{|\mathbf{x}|} & \text{for dimension} \;= 3 \\ \frac{}{4} H^{(1)}_0(\;|\mathbf{x}|) & \text{for dimension} \;= 2 \end{cases} \tag{5}$$

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is inversely proportional to the square of the band-limit (see [19, Corollary 3.9]). The method in [20] also constructs a band-limited version of Green's function and suffers from similar accuracy problems for discontinuous scattering potentials (see [20, Theorem 2]). The approach in [21] is based on an approximation of sufficiently smooth functions by a collection of equally spaced Gaussians of fixed width. Given such an approximation, convolutions of Gaussians with Green's function are computed analytically. However, the effectiveness of this representation (or, alternatively, the accuracy of the result) depends on the smoothness of the function (see [21, Theorems 1 and 2]), which renders the method ineffective for discontinyields the outgoing and incoming Green's functions

$$G^{\pm}(\text{[illegible]}) =$$

where

$$\widehat{F}_{\text{sing}}(\quad) = \frac{1 - \quad^{-\alpha^2(\quad^2 - \quad^2)\quad^2}}{\quad^2 - \quad^2}$$
$$\widehat{F}_{\text{oscill}}(\quad) = \frac{\quad^{-\alpha^2(\quad^2 - \quad^2)\quad^2}}{\quad^2 - \quad^2} \tag{24}$$

and α is a real parameter to be selected later. Next, we outline the approximation and application of $\widehat{F}_{\text{sing}}$ and $\widehat{F}_{\text{oscill}}$ with the details of estimates and associated parameter choices deferred to following sections.

Using

$$\frac{1 - \quad^{-\alpha^2(\quad^2 - \quad^2)\quad^2}}{\quad^2 - \quad^2} = 2\int_{-\infty}^{\log \alpha} \quad^{-(\quad^2 - \quad^2)\quad^2 + 2}$$

we transform $\widehat{F}_{\text{sing}}$ to the spatial domain to obtain

$F_{\text{sing}}(12$ δ δ δ δ α δ δ α δ δ δ δ δ δ δ δ δ δ δ δ δ δ

$\|(\mathcal{R}_e(G) - \widetilde{G}_R) * \ \|_{L\ (D)} \leqslant \ \| \ \|_{L\ (D)}$ f53154309674:03j /T[(decays)-241(rap-)]TJg-51.697-143251

$$\frac{1}{2\ \ ^{3}\ ^{2}}\lim_{\to 0^{+}}\int_{0}\quad ^{-\ ^{2}\ ^{2}+\frac{(\ +\ )^{2}}{4\ ^{2}}} \quad = \frac{1}{2\ \ ^{2}}\,\mathrm{p\,v}\int_{0}^{\infty}\frac{^{-\frac{\ ^{2}+\ ^{2}}{4\ ^{2}}}}{^{2}-\ ^{2}}\sin(\quad)\qquad+\frac{\sin(\quad)}{4}$$

Setting $\ = \ (2\alpha)$, we recover (29) and the imaginary part of Green's function and, since the integral on the interval $(\ \infty)$ is well defined for $\ = 0$, we recover (25) after the change of variable $\ = \ 2$.

We note that in dimension $\ = 2$ we may follow the same steps but starting (for) with

$$\frac{}{4}H_{0}^{(1)}((\ -\ )\ ) = \frac{1}{2}\int_{0}^{\infty}\ ^{-\ ^{2}\ ^{2}+\frac{(\ +\ )^{2}}{4\ ^{2}}}\frac{}{}$$

instead of (34).

4. E 1 2

In this section, we provide the estimates required to obtain Theorems 1 and 2. The proof is split into a sequence of propositions:

(1) Proposition 5 provides estimates for the error due to removing a small interval around the singularity at $\ =\ $ in (29) and limiting the integration to a finite region, thus exploiting the exponential decay of $\widehat{F}_{\mathrm{oscill}}$ in (24).
(2) Proposition 8 gives an estimate of the error due to the discretization of the integral defining F_{sing} in (25).
(3) Proposition 10 provides an estimate of the error of the approximation of $\widehat{F}_{\mathrm{oscill}}$ in (24) by $\widehat{\ }_{\mathrm{oscill}}$ in (27).
(4) Proposition 11 provides an estimate of the error of the approximation in the spatial domain of F_{oscill} in (29) by $\ _{\mathrm{oscill}}$ in (28).

The combination of these propositions yields a proof of Theorems 1 and 2. These estimates also allow us to select parameters and α and elucidate their meaning.

In order to estimate the contribution of $\widehat{F}_{\mathrm{oscill}}(\ )$ Fsp471and,3.6567we21(mea)-3roduce error od (S)Tj I09.833 0 Td (S)Tj T23203 0 inF

$$\widehat{F}_{\text{oscill}}(0) = -\frac{1}{{}^{2}\delta^{1\ (\ ^{2}-1)}}$$

Choosing the parameter close to 1 may cause a loss of accuracy due to numerical cancellation as F_{sing} and F_{oscill} could be large and of opposite signs (see Fig. 4

$0 \leqslant \quad \leqslant \quad - \min\{ \ \delta \ \delta\}$

$$|\widehat{F}_{\text{oscill}}(\ ) - \widehat{\ }_{\text{oscill}}(\ )| \leqslant \ _0 \frac{-\alpha^2(\ ^2 - \ ^2)\ \ ^2}{^2 - \ ^2} \tag{41}$$

$+ \min\{ \ \delta \ \delta\} \leqslant \quad \leqslant \quad . F$

$$\sum_{=1}^{M} w \ (\ + \ ) ^{- \ (\ + \ )^2} \leqslant \frac{2}{+} \tag{42}$$

$0 \leqslant \quad \leqslant$

$$\sum_{=1}^{M} w \ (\ - \ )^2 \ ^{- \ (\ - \ )^2} \leqslant 2 \tag{43}$$

$- \min\{ \ \delta \ \delta\} \leqslant \quad \leqslant \quad + \min\{ \ \delta \ \delta\}.$

Using spherical coordinates and $\mathrm{diam}(D) \leqslant 1$, Proposition 11 yields

$$\|F_{\mathrm{oscill}} - \ _{\mathrm{oscill}}\|_{L^1(D)} \leqslant 4 \quad \int_0^1 (\ ^2 + \ ) \quad = \frac{20}{6}$$

in dimension $\ = 3$, and

$$\|F_{\mathrm{oscill}} - \ _{\mathrm{oscill}}\|_{L^1(D)} \leqslant 2 \quad \int_0^1 (\ + \ ^3 \ ^2) \quad = \frac{18}{10}$$

in dimension $\ = 2$. Similarly, but using Proposition 8, we have

$$\|F_{\mathrm{sing}} - \ _{\mathrm{sing}}\|_{L^1(D)} \leqslant 4 \left(\int_0^{\delta_0} \quad + \int_{\delta_0}^1 \quad \right) \leqslant 2 \ \left(\delta_0^2 + \ \right)$$

for $\ = 3$, and

$$\|F_{\mathrm{sing}} - \ _{\mathrm{sing}}\|_{L^1(D)} \leqslant 2 \left(\int_0^{\delta_0} \log\left(1 + \frac{1}{\ ^2}\right) \quad + \int_{\delta_0}^1 \log\left(1 + \frac{1}{\ ^2}\right) \quad \right) \leqslant 2 \ \left(\delta_0^2 \log \delta_0^{-1} + \delta_0^2 + \ (\log 2 + \delta_0^2 \log \delta_0^{-1})\right)$$

for $\ = 2$. In dimension $\ = 3$ we select $\delta_0 = \sqrt{\ }$; in dimension $\ = 2$ we choose δ_0 so that $\ = \delta_0^2 \log \delta_0^{-1}$. With these choices, we combine the estimates and obtain the result. □

5. [illegible]

An algorithm to convolve with (28)

By adding and subtracting $\frac{1}{4\ ^2}\int_0^2\ \sum$

discretize them as needed. We note that the cost associated with computing the band-limited Fourier transform is described below and does not change the overall complexity of the algorithm.

I :

(1) *F* : For fixed and given accuracy , we select (which ultimately determines α in (37)) and construct $\widetilde{}_{\mathrm{oscill}}$ using the N_F-point quadrature given in (46), $N_F = \sum_{=1}^{J} L$ (or its analogue in dimension $= 3$, see Remark 16). We estimate the number of nodes as $N_F \sim (\quad) + C_0(\log {}^{-1})$, where C_0 is a constant (see Remark 13 and Tables 2 and 3 for illustration).

(2) : For fixed and given accuracy , we construct

The assumption that the band-limited Fourier transform of the input function is available does not change the overall complexity of the algorithm (even for functions with discontinuities or singularities). Due to the band-limiting nature of $\widetilde{\ }_{\mathrm{oscill}}$ (as well as of $\mathcal{I}m(G)$), we only need to compute the Fourier transform of the input function within a ball of radius . Using the USFFT [12–14] (which, in fact, was designed for this purpose), the computational cost scales at most as $\mathcal{O}((\log\ ^{-1})\ \ \log\ )$. For example, the algorithm in [12] first projects the function onto a subspace of splines where the number of splines is proportional to $(\ \log\ ^{-1})$. This step is followed by the FFT requiring $\mathcal{O}(\ \ \log\ )$ operations and the final adjustment of the computed values involving $\mathcal{O}(\ \ )$ operations. Since a typical implementation of USFFT fixes the accuracy, e.g. double precision, we estimate the overall cost of computing the band-limited Fourier transform as depend0-1.r.ayonly1.r.ayng

is expected as the number of nodes in this construction approaches optimal (i.e., effectively approaches) as gets large. For fixed , we observe J_{diam} depends weakly on and, thus, effectively $N_F \sim \log {}^{-1}$ rather than $N_F \sim (\log {}^{-1})^2$ obtained by estimates.

In Table 3, we display the number of radial quadrature nodes in the Fourier domain along the diameter in dimension $= 3$ in (52). We note that the number of quadrature nodes along the diameter in dimensions $= 2$ and $= 3$ are almost the same.

7. C

We develop an approximation of the free space Helmholtz Green's function in dimensions $= 2\ 3$ by splitting its action between the spatial and Fourier domains. Our approximation achieves:

- a spatial domain representation as a sum of Gaussians, capturing the singularity of Green's function at zero, and
- a Fourier domain representation as a smooth, radially symmetric and effectively band-limited kernel.

Using properties of this approximation, we construct a fast and accurate algorithm for computing convolutions with Green's function and illustrate its performance in dimension $= 2$. We indicate how to extend the algorithm (specifically, by using a discretization of a sphere in the Fourier domain) to dimension $= 3$. We expect our approach to be most useful for accurate computations in problems where the media or potentials are described by functions with discontinuities or singularities.

The extension of our approach to the Helmholtz Green's function with periodic or Dirichlet/Neumann boundary conditions may be found in [2].

A

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A A. *A.1. P*

Since $1\ ({}^2 - (\pm)^2)$ is radially symmetric, we apply (9) and (10).

In dimension $= 3$, using [30, 3.723 (3)], we have

$$\lim_{\to 0^+} \frac{1}{|\,|^{\frac{1}{2}}(2\ )^{\frac{3}{2}}} \int_0^\infty \frac{{}^{\frac{3}{2}} J_{\frac{1}{2}}(|\,|\ )}{{}^2 - (\pm)^2} = \lim_{\to 0^+} \frac{1}{2\ {}^2 |\,|} \int_0^\infty \frac{\sin\ |\,|}{{}^2 - (\pm)^2} = \frac{1}{4} \frac{\pm\ |\,|}{|\,|}$$

In dimension $= 2$, using [30, 6.532 (4), 28, 9.6.4], we obtain

$$\lim_{\to 0^+} \frac{1}{2} \int_0^\infty \frac{J_0(|\,|\ )}{{}^2}$$

A.3. P P 8

P . We begin by truncating the region of integration in (25) to the interval $[-\log(\alpha\ \ )\ \gamma]$ where γ will be chosen later. We claim that there exists a N-term quadrature with nodes and weights 0 (see e.g. the generalized Gaussian quadratures in [25, Section 7]), such that in dimension $= 3$ we have

$$\left|\frac{1}{4\ \ ^{3}\ ^{2}}\int_{-\log\frac{\alpha}{}}^{\gamma} \ ^{-\ ^{2}\frac{2}{4}}\ \ ^{2}\ ^{-2}+\ \ -\sum_{=1}^{N}\ \ ^{-}\ \ ^{2}\right| \leqslant \frac{}{2} \tag{56}$$

for $0 \leqslant \ \ \infty$, where $= \ \ ^{2}\ ^{-2}\ +\ \ 4\ \ ^{3}\ ^{2}$ and $= \ ^{2}\ \ 4$. Using the definition of F_{sing} (25), and noting that the integrand is positive, we have

$$\left|F_{\mathrm{sing}}(\ ) - \sum_{=1}^{N}\ \ ^{-}\ \ ^{2}\right| \leqslant \frac{}{2} + \frac{1}{4\ \ ^{3}\ ^{2}}\int_{\gamma}^{\infty} \ ^{-\ ^{2}\frac{2}{4}}\ \ ^{2}\ 4^{2}+ \tag{57}$$

Using the change of variable $= \ ^{2}\ ^{2}\ \ 4$, and estimating $\ ^{2}\ ^{-2}$ by its upper bound, we have

$$I(\ ) = \frac{1}{2\ ^{-1}\ \ \ ^{2}}\int_{\gamma}^{\infty} \ ^{-\ ^{2}\frac{2}{4}}\ \ ^{2}\ ^{-2}\ +(\ -2)$$

for $\in [\tilde{\delta}\ 1]$. Substituting $= (\ \pm\ )\ (\ (\ +1))$

To estimate (69), we split it into two terms and, in the first term, change variables $=\ -$ so that

$$|I_3(\ )| \leqslant \int_{-} \sum_{=1}^{M} w \quad - \quad ^{2} \ ($$

Thus, we have

$$\left|\frac{1}{2}\int_{-}^{+}\ \widehat{\ }_{\text{oscill}}(\ )J_0(\ )\qquad\right| \leqslant \delta\log(\ \delta^{-1})\left(\frac{58}{15}+\frac{4}{\ }\sqrt{\ }\right) \tag{81}$$

Using Proposition 5 and (79)–(81), we obtain the result. □

A.6. P

L 17. *F* 0 $\delta \leqslant 1$ 2, α, $\geqslant 0$ *w*

$$\frac{1}{2\ ^{2}}\left|\text{p v}\int_{-}^{+}\ \widehat{F}_{\text{oscill}}(\ )\sin(\ )\qquad\right| \leqslant \frac{\delta\ ^{2\alpha^2\delta}}{2\ ^{2}}(6+9\alpha^2) \tag{82}$$

$= 3$

$$\frac{1}{2}\left|\text{p v}\int_{-}^{+}\ \widehat{F}_{\text{oscill}}(\ )J_0(\ )\qquad\right| \leqslant \frac{\delta\ ^{2\alpha^2\delta}}{2}\left(\sqrt{6}\ +6\alpha^2+\frac{8}{3}\right) \tag{83}$$

$= 2$, *w* $= \min\{\ \delta\ \delta\}$.

P . In order to use Lemma 20

$$= 3,$$

$$\frac{1}{2} \int^{\infty} |\widehat{F}_{\mathrm{oscill}}(\quad) J_0(\quad)\ | \quad \leqslant \frac{-\alpha^2(\ ^2-1)}{4}$$

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