A fast algorithm for simulating scattering from a radially symmetric potential

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December 5, 2020

The variable coefficient Helmholtz equation

$$\Delta u(x) + k^2(1 + q(x))u(x) = 0 \quad \text{for all} \quad x \in \mathbb{R}^2$$

can be used to model the scattering of waves from inhomogeneous media.

In many applications:

- the wavenumber k is real-valued
- the scattering potential q is smooth, positive and has compact support contained in a disk Ω of radius R centered at 0
- the solution u, which is known as the total field, is the sum of a known incident field u_i satisfying the constant coefficient Helmholtz equation

  $$\Delta u_i(x) + k^2 u_i(x) = 0$$

  and an unknown scattered field u_s which satisfies the Sommerfeld radiation condition

  $$\lim_{r\to\infty} \sup_{0\le t<2\pi} \sqrt{r} \left| \frac{\partial u_s}{\partial r}(re^{it}) - iku_s(re^{it}) \right| = 0.$$

The goal is to obtain the scattered field u_s, which is the unique solution of the boundary value problem

$$\begin{cases} \Delta u_s(x) + k^2(1+q(x))u_s(x) = -k^2 q(x) u_i(x) \quad \text{for all} \quad x \in \mathbb{R}^2 \\ \lim_{r\to\infty} \sup_{0\le t<2\pi} \sqrt{r} \left| \frac{\partial u_s}{\partial r}(re^{it}) - iku_s(re^{it}) \right| = 0. \end{cases}$$

The scattered wave u_s becomes increasingly oscillatory as k grows, and it requires $N = \mathcal{O}\left(k^2\right)$ data points to represent it using standard methods (e.g., orthogonal polynomials, finite element bases, collocation).

As a consequence, any method which using such a scheme for representing u_s has a running time which grows at least as fast as $N = \mathcal{O}\left(k^2\right)$.

In fact, most schemes have running times which grow superlinearly with N.

I will describe a method for calculating the scattered field in $\mathcal{O}\left(k\log(k)\right)$ time.

The catch is that this method — at least in its present form — only applies to **radially symmetric** potentials q.

It operates by the method of separation of variables and exploits the fact that the one-dimensional variable coefficient Helmholtz equation

$$y''(t) + k^2 q(t) y(t) = 0$$

can be solved in $\mathcal{O}\left(\log(k)\right)$ time.

The one-dimensional variable coefficient Helmholtz equation

If $y(t) = \exp(r(t))$ solves
$$y''(t) + k^2 q(t) y(t) = 0, \tag{1}$$
then r satisfies the Riccati equation
$$r''(t) + \left(r'(t)\right)^2 + k^2 q(t) = 0. \tag{2}$$

When q is positive, the solutions of (1) are **oscillatory**, with the frequency of their oscillations increasing with k. Representing such functions using standard methods (e.g., expansions in orthogonal polynomials) requires $\mathcal{O}(k)$ data points.

Under mild conditions on q, (2) admits solutions which are **nonoscillatory** and can be represented via standard methods using a number of data points which is independent of k (when q is strictly positive or negative) and slowly growing with k when q has zeros.

The one-dimensional variable coefficient Helmholtz equation

That solutions of the Riccati equation can be approximated by nonoscillatory functions is the basis of WKB approximation, and there are many examples from the theory of special functions of second order differential equations which have solutions whose logarithms are nonoscillatory.

For instance, the formula

$$w(z) := \frac{1}{z} J^2_{\nu+\frac{1}{2}}(z) + \frac{1}{z} Y^2_{\nu+\frac{1}{2}}(z) = \frac{2}{\pi} \int_0^\infty \exp(-tz) P_\nu \left(1 + \frac{t^2}{2}\right)\, dt$$

shows that the function w is completely monotone on $(0, \infty)$. It is related to a solution r of the Riccati equation corresponding to the normal form of Bessel's differential equation via

$$r'(t) = i \frac{1}{w(z)} + \frac{1}{2} \frac{w'(z)}{w(z)}.$$

The one-dimensional variable coefficient Helmholtz equation

WKB approximations are not a numerically viable approach to computing nonoscillatory solutions of the Riccati equation because:

- they require the computation of high-order derivatives of the coefficient q
- the handling of turning points is messy

There is a viable algorithm, however, which runs in time independent of the wavenumber k in the case in which q is strictly positive and in $\mathcal{O}\left(\log(k)\right)$ time in cases in which the equation has turning points:

> B—, On the numerical solution of second order differential equations in the high-frequency regime. *Applied and Computational Harmonic Analysis* **44** (2018), 312-349.

It operates by solving the Riccati equation numerically. The only difficulty is computing the correct initial conditions.

A numerical experiment

$$q(t) = \frac{\nu^2 \sin(2t)^2}{0.1 + (t-0.5)^2} + \mu^2 \exp\left(-\frac{1}{t}\right)$$

ν	μ	Solve time	Average evaluation time
10^1	10^0	1.79×10^{-03}	5.51×10^{-07}
10^2	10^0	3.10×10^{-03}	5.39×10^{-07}
10^3	10^0	2.90×10^{-03}	5.39×10^{-07}
10^4	10^0	3.06×10^{-03}	5.61×10^{-07}
10^5	10^1	3.80×10^{-03}	4.77×10^{-07}
10^5	10^2	4.62×10^{-03}	5.38×10^{-07}
10^5	10^3	3.64×10^{-03}	6.97×10^{-07}
10^5	10^4	3.81×10^{-03}	5.60×10^{-07}
10^5	10^5	3.63×10^{-03}	4.97×10^{-07}
10^4	10^5	2.72×10^{-03}	4.76×10^{-07}
10^3	10^5	3.57×10^{-03}	5.83×10^{-07}
10^2	10^5	3.15×10^{-03}	5.78×10^{-07}
10^1	10^5	2.32×10^{-03}	5.51×10^{-07}
10^7	10^7	4.33×10^{-03}	5.73×10^{-07}

Representation of u_s in the exterior of Ω

Since q is compactly supported in Ω, the scattered wave u_s is a solution of the boundary value problem

$$\begin{cases} \Delta u_s(x) + k^2 u_s(x) = 0 \quad \text{for all} \quad x \in \Omega^c \\ \lim\limits_{r\to\infty} \sup\limits_{0\le t\le 2\pi} \sqrt{r}\left|\dfrac{\partial u_s}{\partial r}(r,t) - iku_s(r,t)\right| = 0 \end{cases} \tag{3}$$

We can separate variables in (3) to see that in the exterior of Ω, u_s can be represented as

$$u_s(r,t) = \sum_{n=-\infty}^{\infty} b_n H_n(kr)\exp(int), \tag{4}$$

where H_n is the Hankel function of the first kind of order n.

Representation of u in the interior of Ω

The total field u satisfies

$$\Delta u(x) + k^2 (1 + q(r))\, u(x) = 0 \quad \text{for all} \quad x \in \Omega.$$

Separating variables shows that u can be represented in the interior of Ω via an expansion of the form

$$u(r,t) = \sum_{n=-\infty}^{\infty} a_n \psi_{|n|}(r) \exp(int), \tag{5}$$

where, for each nonnegative integer n, ψ_n is a solution of the second order differential equation

$$r^2 \psi_n''(r) + r\psi_n'(r) + (k^2(1+q(r))r^2 - n^2)\psi_n(r) = 0$$

which is nonsingular at 0. Note that ψ_n is only determined up to a nonzero multiplicative constant, but the choice of this constant does not effect the form of (5), only the value of the coefficient a_n.

Determination of the scattered field via separation of variables

From standard elliptic regularity results, we know that u and its normal derivative are continuous across the boundary $\partial\Omega$. Moreover, $u = u_s + u_i$. It follows that

$$\sum_{n=-\infty}^{\infty} a_n \psi_{|n|}(R) \exp(int) = \sum_{n=-\infty}^{\infty} b_n H_n(kR) \exp(int) + u_i(R, t)$$

and

$$\sum_{n=-\infty}^{\infty} a_n \psi'_{|n|}(R) \exp(int) = \sum_{n=-\infty}^{\infty} b_n k H'_n(kR) \exp(int) + \frac{\partial u_i}{\partial r}(R, t)$$

Determination of the scattered field via separation of variables

If we let

$$u_i(R,t) = \sum_{n=-\infty}^{\infty} c_n \exp(int) \quad \text{and} \quad \frac{\partial u_i}{\partial r}(R,t) = \sum_{n=-\infty}^{\infty} d_n \exp(int)$$

be the Fourier expansions of the restrictions of the incident wave u_i and its derivative with respect to r to the boundary $\partial\Omega$ of Ω, then we can rewrite these equations as

$$\sum_{n=-\infty}^{\infty} a_n \psi_{|n|}(R) \exp(int) = \sum_{n=-\infty}^{\infty} b_n H_n(R) \exp(int) + \sum_{n=-\infty}^{\infty} c_n \exp(int)$$

and

$$\sum_{n=-\infty}^{\infty} a_n \psi'_{|n|}(R) \exp(int) = \sum_{n=-\infty}^{\infty} b_n k H'_n(kR) \exp(int) + \sum_{n=-\infty}^{\infty} d_n \exp(int).$$

Determination of the scattered field via separation of variables

Owing to the orthogonality of the exponential functions, the equations

$$\sum_{n=-\infty}^{\infty} a_n \psi_{|n|}(R) \exp(int) = \sum_{n=-\infty}^{\infty} b_n H_n(R) \exp(int) + \sum_{n=-\infty}^{\infty} c_n \exp(int)$$

and

$$\sum_{n=-\infty}^{\infty} a_n \psi'_{|n|}(R) \exp(int) = \sum_{n=-\infty}^{\infty} b_n k H'_n(kR) \exp(int) + \sum_{n=-\infty}^{\infty} d_n \exp(int).$$

are satisfied if and only if for each integer n,

$$\begin{cases} a_n \psi_{|n|}(R) - b_n H_n(R) = c_n \\ a_n \psi'_{|n|}(R) - b_n k H'_n(kR) = d_n. \end{cases}$$

Determination of the scattered field via separation of variables

We can easily solve this system:

$$a_n = \frac{-kH_n'(kR)\,c_n + H_n(kR)\,d_n}{H_n(kR)\,\psi_{|n|}'(R) - k\ \psi_{|n|}(R)H_n'(kR)}$$

$$b_n = \frac{-\psi_{|n|}'(R)c_n + \psi_{|n|}(R)d_n}{H_n(kR)\,\psi_{|n|}'(R) - k\ \psi_{|n|}(R)H_n'(kR)}.$$

In the interior of Ω:

$$u(r,t) = \sum_{n=-\infty}^{\infty} a_n \psi_{|n|}(r) \exp(int).$$

In the exterior of Ω:

$$u_s(r,t) = \sum_{n=-\infty}^{\infty} b_n H_n(kr) \exp(int).$$

Numerical Algorithm

It is fairly straightforward to develop a numerical method based on the method of separation of variables.

We first observe that since the incident wave u_i satisfies the constant coefficient Helmholtz equation at wavenumber k, we expect to be able to represent it and its normal derivative using $\mathcal{O}(k)$ Fourier modes. That is, in typical cases, we will have high accuracy approximations

$$u_i(t, R) \approx \sum_{n=-m}^{m} c_n \exp(int)$$

$$\frac{\partial u_i}{\partial r}(t, R) \approx \sum_{n=-m}^{m} d_n \exp(int)$$

with $m = \mathcal{O}(k)$. Moreover, the coefficients in these expansions can be computed via the fast Fourier transform in $\mathcal{O}(m \log(m))$ operations.

Numerical Algorithm

The number of terms in the expansion

$$u_i(t, R) \approx \sum_{n=-m}^{m} c_n \exp(int)$$

of the incident wave dictates the number of terms in the representations of total field u and of the scattered field u_s.

For each $n = 0, \ldots, m$, we must solve the perturbed Bessel equation

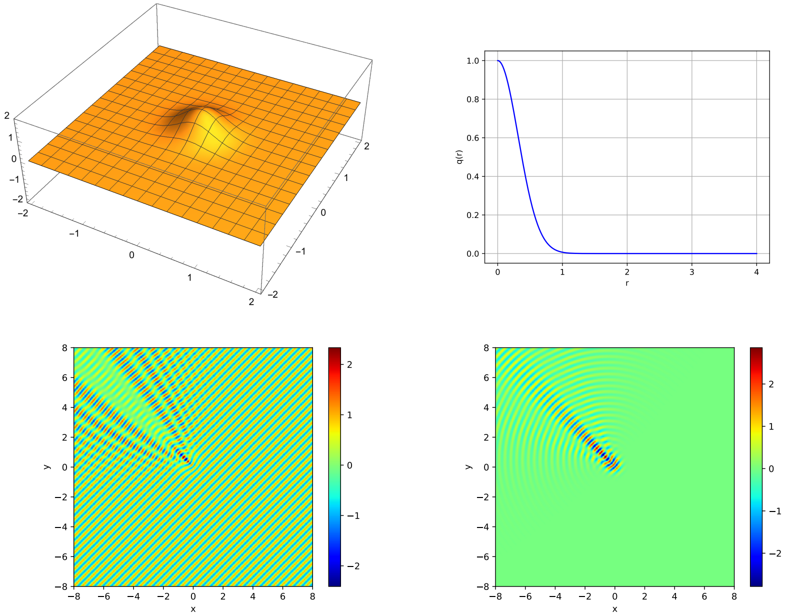
$$r^2\psi_n''(r) + r\psi_n'(r) + (k^2(1 + q(r))r^2 - n^2)\psi_n(r) = 0$$

to compute $\psi_{|n|}$. The cost for each solve is $\mathcal{O}(\log(k))$, and $m = \mathcal{O}(k)$, so the total cost to compute the functions ψ_n is $\mathcal{O}(k \log(k))$.

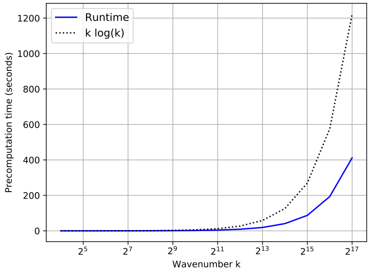
Computing the coefficients in the expansions of u and u_s requires $\mathcal{O}(k)$ operations.

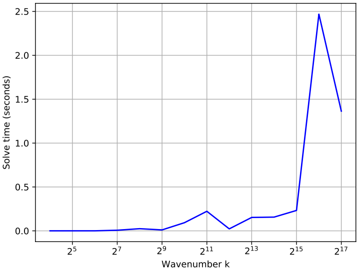
So the total running time is $\mathcal{O}(k \log(k))$.

$$q(r) = \exp(-5r^2), \quad u_i(r,t) = \exp\left(ikr\cos\left(t - \frac{\pi}{4}\right)\right)$$

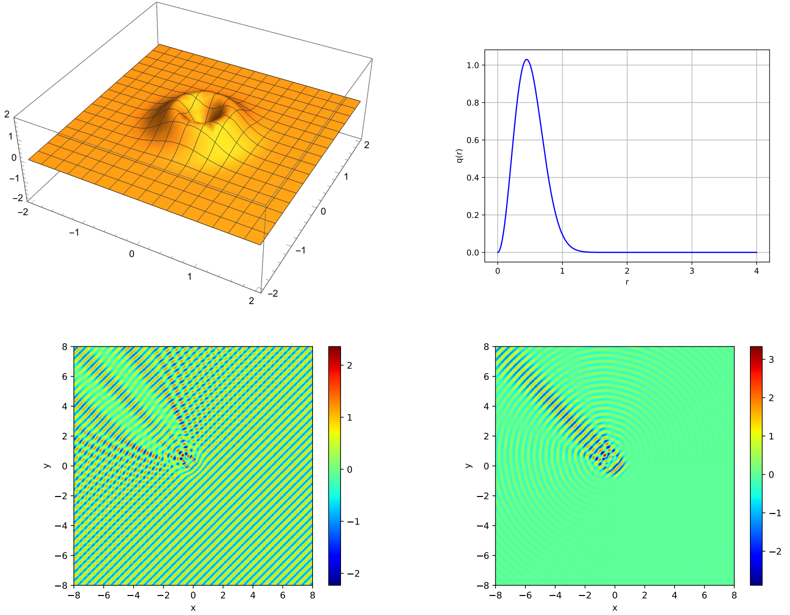


k	m	Maximum absolute error	Precomp time (in seconds)	Solve time (in seconds)
2^8	1608	2.17×10^{-12}	4.60×10^{-01}	2.44×10^{-02}
2^9	3216	4.72×10^{-12}	9.56×10^{-01}	1.06×10^{-02}
2^{10}	6433	8.54×10^{-12}	$1.96 \times 10^{+00}$	9.27×10^{-02}
2^{11}	12867	1.85×10^{-11}	$4.18 \times 10^{+00}$	2.22×10^{-01}
2^{12}	25735	6.13×10^{-11}	$8.99 \times 10^{+00}$	2.25×10^{-02}
2^{13}	51471	2.05×10^{-10}	$1.89 \times 10^{+01}$	1.52×10^{-01}
2^{14}	102943	1.51×10^{-09}	$4.08 \times 10^{+01}$	1.56×10^{-01}
2^{15}	205887	3.85×10^{-09}	$8.72 \times 10^{+01}$	2.32×10^{-01}
2^{16}	411774	2.16×10^{-08}	$1.93 \times 10^{+02}$	$2.46 \times 10^{+00}$
2^{17}	823549	1.01×10^{-07}	$4.11 \times 10^{+02}$	$1.36 \times 10^{+00}$

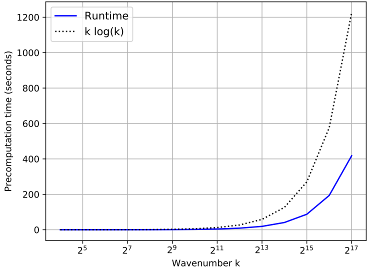


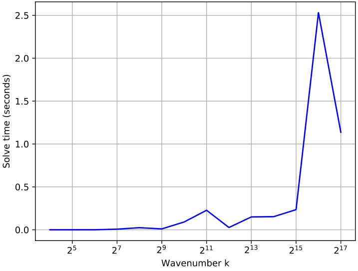


$$q(r) = 14r^2 \exp(-5r^2), \quad u_i(z) = H_0(k|z - 6i|)$$

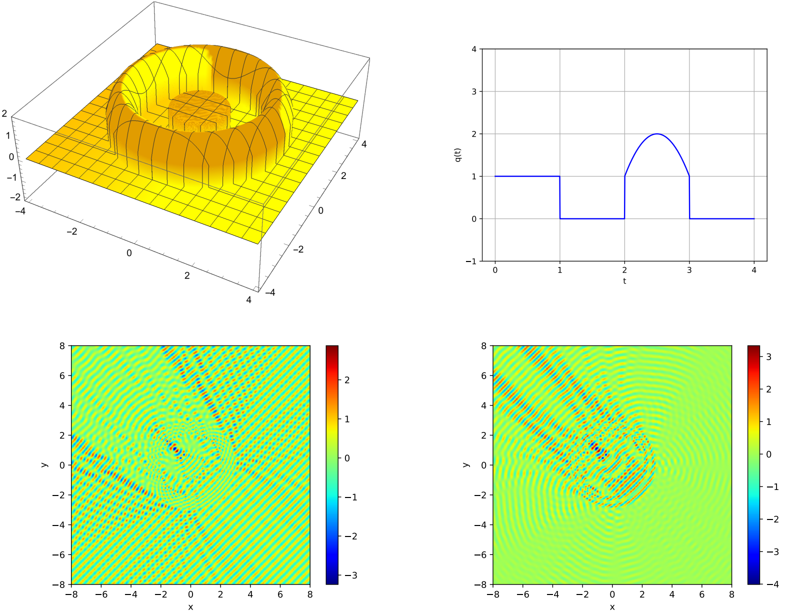


k	m	Maximum absolute error	Precomp time (in seconds)	Solve time (in seconds)
2^8	1608	2.44×10^{-12}	4.61×10^{-01}	2.44×10^{-02}
2^9	3216	5.85×10^{-12}	9.37×10^{-01}	1.03×10^{-02}
2^{10}	6433	9.34×10^{-12}	$1.98 \times 10^{+00}$	9.11×10^{-02}
2^{11}	12867	1.98×10^{-11}	$4.20 \times 10^{+00}$	2.27×10^{-01}
2^{12}	25735	4.80×10^{-11}	$9.00 \times 10^{+00}$	2.64×10^{-02}
2^{13}	51471	4.35×10^{-10}	$1.90 \times 10^{+01}$	1.49×10^{-01}
2^{14}	102943	1.91×10^{-09}	$4.09 \times 10^{+01}$	1.53×10^{-01}
2^{15}	205887	6.93×10^{-09}	$8.75 \times 10^{+01}$	2.34×10^{-01}
2^{16}	411774	3.23×10^{-08}	$1.93 \times 10^{+02}$	$2.53 \times 10^{+00}$
2^{17}	823549	1.08×10^{-07}	$4.17 \times 10^{+02}$	$1.13 \times 10^{+00}$





$$q(r) = \chi_{(0,1)}(r) + 2\chi_{(2,3)}(r), \quad u_i(z) = \exp\left(ikr\cos\left(t - \frac{\pi}{4}\right)\right)$$



k	m	Maximum absolute error	Time (in seconds)
2^8	1608	$\left(2.20 \times 10^{-12}\right)$	9.58×10^{-01}
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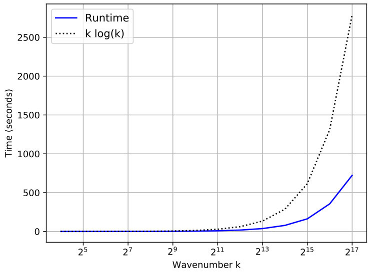

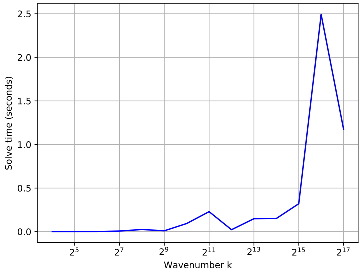

The general case?

In the two dimensional radially symmetric case, we represented the desired solution u of

$$\Delta u(x) + k^2(1 + q(x))u(x) = 0$$

in the form

$$\sum_{n=-\infty}^{\infty} a_n \psi_{|n|}(r) \exp(int)$$

with $\psi_{|n|}$ a solution of a second order differential equation whose logarithm is a nonoscillatory solution of the one-dimensional Riccati equation.

In fact, the logarithm r of $\psi_{|n|}(r) \exp(int)$ is a solution of the two-dimensional Riccati equation

$$\Delta r(x) + \nabla r(x) \cdot \nabla r(x) + k^2(1 + q(x)) = 0.$$

The general case?

In other words, we are representing the solution u of

$$\Delta u(x) + k^2 (1 + q(x))\, u(x) = 0$$

as a sum of the form

$$\sum_{n=-\infty}^{\infty} a_n \exp(\gamma_n(x))$$

where γ_n is a nonoscillatory solution of the Riccati equation

$$\Delta\gamma(x) + \nabla\gamma(x) \cdot \nabla\gamma(x) + k^2(1 + q(x)) = 0$$

such that $\exp(\gamma_n(x))$ is a multiple of $\exp(in\theta)$ on $\partial\Omega$.