Fast Solvers for Highly Oscillatory Problems

Alex Barnett

Sound, light, and other electromagnetic waves such as microwaves surround us, enabling communication and imaging technologies both ancient and modern. Elastic waves bounce through the earth's crust, enabling us to "see" thousands of kilometers deep. Such propagating waves are highly oscillatory in time and space, and may scatter off obstacles or get trapped in resonant cavities. Accurate numerical modeling of these important phenomena is slow even on large modern computers, because linear systems involving huge numbers of unknowns must be solved. However, recent progress in designing algorithms has allowed much more rapid solutions.

1 Time harmonic waves in one and more dimensions

We are all familiar with the waves that spread out in growing circles when a raindrop hits a puddle, or a stone is thrown into a pond. This is an example of a *wave equation* in two dimensions. If x and y are Cartesian coordinates in the horizontal plane, then the height $U(x, y, t)$ of the water surface varies in space (x, y) and time t. In fact U obeys a *partial differential equation* (PDE) [1]

[1] There are many good books on PDEs; a basic one is [4] and a more mathematical one [7].

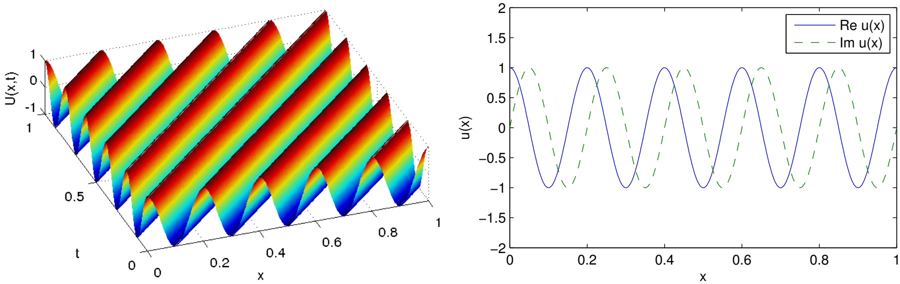

Figure 1: Simple traveling time harmonic wave in 1D with frequency $\omega/2\pi = 5$, and constant wave speed $c(x) = 1$, hence constant wavelength $\lambda = 2\pi/k = 0.2$. The left shows $U(x,t) = \mathrm{Re}[e^{ikx}e^{-i\omega t}]$ as a 3D height plot in space and time. Note that the crests all move to the right with unit speed. The right graphs the real and imaginary parts of the complex-valued spatial function $u(x) = e^{ikx}$.

relating its space and time derivatives. Let's start with a simpler case: waves in one dimension (1D). You can easily observe these by plucking a long elastic string such as a washing line, and watching the waves bounce back and forth along it. From Newton's 2nd law it is easy to derive that the displacement $U(x,t)$, where x is the coordinate along the string, obeys a "hyperbolic" PDE

$$\frac{\partial^2 U}{\partial x^2} - \frac{1}{c(x)^2}\frac{\partial^2 U}{\partial t^2} = 0 \ , \qquad \text{(1D wave equation)} \qquad (1)$$

where $c(x)$ is the local speed of waves at the point x, which may vary with position (imagine the washing line is heavy in some places, slowing down the waves, but light in others). To summarize (1), "acceleration is proportional to local spatial curvature." This 1D PDE is a decent model for the majority of musical instruments [5], including strings, guitars, wind, brass, and pianos. [2]

Often one cares about a single *frequency* of wave: this is called "time harmonic," and means that everything vibrates with the same sinusoidal function of time. Imagine continuously vibrating the washing line, in which case its response would settle into a steadily repeating pattern. A general sinusoidal function of time with frequency f (i.e. repetition period $1/f$) can be written $a\cos(\omega t) + b\sin(\omega t)$ for some constants a and b, where $\omega = 2\pi f$. Including variation in space we could write $U(x,t) = u_1(x)\cos(\omega t) + u_2(x)\sin(\omega t)$.

[2] For a fascinating reason—the irregular spacing of their resonant frequencies—most *percussion* instruments instead involve either the 2D wave equation, or wave equations for bending beams or plates (which are 4th order).

Mathematicians find it simpler to rewrite this using complex numbers,

$$U(x,t) = \mathrm{Re}[u(x)e^{-i\omega t}] \,, \qquad \text{(definition of time harmonic solution)} \quad (2)$$

where you can check that $u(x) = u_1(x) - iu_2(x)$. It is now easy to substitute (2) into (1) to give the differential equation satisfied by this complex function u,

$$u''(x) + k(x)^2 u(x) \;=\; 0 \qquad \text{(1D Helmholtz equation)} \qquad (3)$$

where the known function $k(x) = \omega/c(x)$ is called the *wavenumber*. Notice that u is a function of only one variable, so is easier to solve for than U which depended on two. Fig. 1 shows an example U and u. Also notice that $u(x) = 0$ is a (very boring!) solution to (3). In practice one adds a "source term" g which specifies the strength of vibrational driving at each point in space, so

$$u'' + k(x)^2 u \;=\; g(x) \qquad \text{(1D Helmholtz equation with source)} \,, \qquad (4)$$

or one sends in waves from far away so that they scatter or reflect. Finally, one usually cares only about a bounded region of space, such as an interval $\Omega = (0, L)$; on its endpoints one needs "boundary conditions" which enforce that waves are only radiating away from the region. Another type of boundary condition—common for washing lines—is that u is pinned down to zero at some point; this is called a Dirichlet condition.

Many more wave phenomena occur in 2D (surface waves) or in 3D (acoustic, electromagnetic, and elastic waves). These are much harder to simulate in the computer than in 1D, essentially because of all the different directions waves can travel. The generalization of (3) is then written

$$\Delta u + k(\mathbf{x})^2 u \;=\; g(\mathbf{x}) \qquad \text{(Helmholtz equation with source)} \qquad (5)$$

where $\mathbf{x} = (x, y)$ in 2D, or (x, y, z) in 3D. Here, $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$ in 2D, or $\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ in 3D, and is called the *Laplacian operator*. (5) is an "elliptic" PDE. To create a mathematically well-posed problem, boundary or radiation conditions must also be applied on a curve or surface enclosing Ω, the region of interest. Fig. 2 shows example scattering and source problems in 2D.

2 The highly oscillatory case, and real world applications

When might we care about solving the above Helmholtz equations? A key property of a time harmonic wave is its *wavelength* (repetition distance) $\lambda = 2\pi/k$, where recall k is the wavenumber. Larger k (shorter λ) means more rapid oscillations in space. Remember that we are immersed in a bath of waves: for instance everything we hear is governed by sound waves of wavelengths λ

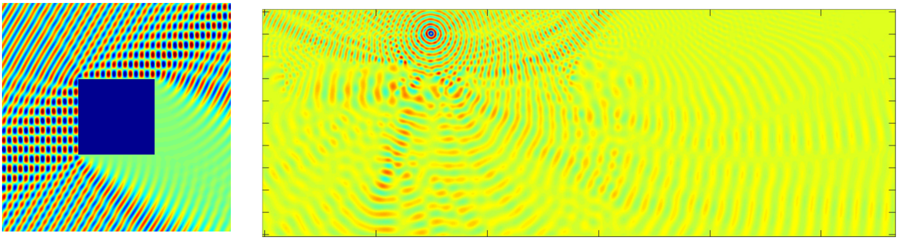

Figure 2: Highly oscillatory problems in 2D. Left: numerical computation of scattering of a "plane wave" (coming from about the 10 o'clock direction) from the unit square with Dirichlet boundary condition ($k = 50$ is constant in space), with error $\epsilon = 10^{-10}$, using the method of [1]. Note that the waves do not cast a hard shadow; they "diffract" around the corners. Right: numerical finite-difference computation of solution where g is a point source in a model for seismic wave propagation ($k(\mathbf{x})$ varies in space, causing bending and reflection of waves), from [9]. In both cases $\mathrm{Re}[u]$ is plotted using a color scale where red is positive, blue is negative, and yellow or green is around zero.

between about 0.015 m and 15 m, and everything we see is light of wavelengths between 4×10^{-7} m and 7×10^{-7} m. Imagine that you are an engineer who has been given the 3D geometry of a (small) concert hall Ω of typical dimension $L = 15$ m, and asked to predict how sound emitted by the performers will be heard by each audience member (this will involve various reflecting boundary conditions due to the materials of the walls). In this case, since the air is close to uniform, $c(x)$, and hence $k(x)$, is constant. But the ratio of the shortest wavelength we can hear ($\lambda \approx 0.015$ m) to the hall size is $L/\lambda \approx 10^3$, a big number. This regime where $L/\lambda \gg 1$ is called "highly oscillatory." We will see below why solving such a problem accurately is very challenging, even on a big computer.

We've just seen an application of highly oscillatory waves in architectural acoustics. What others are there?[3] Geology is studied, or oil searched for, using seismic (3D elastic) waves emitted by earthquakes or by special heavy vibrator trucks.[4] Here $k(\mathbf{x})$ varies in unknown ways, so in fact the goal is to reconstruct $k(\mathbf{x})$ given only a large number of reflected waves detected on

[3] In some of these examples the Helmholtz equation must be replaced by the related Maxwell or elastodynamic equations.

[4] really!

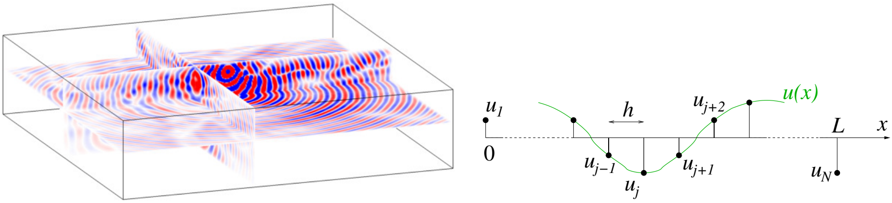

Figure 3: Left: Seismic wave solution u in a 3D domain (acoustic approximation), where g is a point source with frequency f of 6 cycles/second. The domain is 20 km × 20 km × 4.7 km. Red is positive and blue negative. Right: setup for 1D finite difference approximation in $[0, L]$. Each number u_j represents u at a gridpoint.

the earth's surface. This is called an *inverse problem*, and is even harder than solving the Helmholtz or elastic equation itself (the "forward problem"). Figs. 2 and 3 include simulated seismic wave solutions. Given an aircraft, engineers want to know the directional pattern that radar (electromagnetic waves in the 0.01 m to 1 m range) will scatter or reflect from it, or how to design its shape to minimize reflection or sound pollution.

Whales communicate using underwater sound waves that propagate hundreds of kilometers through a depth-dependent $k(\mathbf{x})$. The human body is safely imaged by ultrasound reflection (another inverse problem), yet to get the best pictures one needs accurate models of wave propagation in the varying tissues. Light pulses are guided and switched at high speeds in microscopic devices that enable the internet backbone, and may one day enable ultra-fast optical computing. The design of more efficient thin-film solar cells for renewable energy requires modeling light waves in complex geometries (dielectrics like glass which have a different k from air). Finally, at the microscopic scale, all matter is a quantum wave, described by Schrödinger's equation (a multi-dimensional complex-valued version of (1) but with a single time derivative).

This range of applications shows the importance of efficient numerical methods for solving highly oscillatory wave problems.

3 Numerical approximate solutions

The above PDEs involve mostly continuous functions: to describe them *exactly* would need their values at an infinite number of points! Of course, computers can handle only a finite, limited, number of real numbers. An art in numerical analysis is to *approximate* u only to some desired accuracy ϵ, using a reasonably small number N of discrete unknowns—this is called "discretization." This often involves relying on the fact that u is smooth. This can create a more efficient algorithm, thus faster computer solution time. Sometimes it is also possible to *prove* that the error is no larger than some ϵ.

We illustrate this with a "finite difference" discretization of (4) (see [8] for more detail). Let the values u_j, for $j = 1, \ldots, N$, represent $u(x_j)$ at points x_j on a regular grid of spacing $h = L/(N-1)$, as in the right panel of Fig. 3. The simplest way to approximate the 2nd derivative in (4) is then

$$u''(x) \approx h^{-2}(u_{j-1} - 2u_j + u_{j+1}) \qquad \text{(3-point stencil formula)} \qquad (6)$$

Enforcing (4) at each grid point and using (6), we get the linear system $A\mathbf{u} = \mathbf{g}$, where A is an $N \times N$ matrix with diagonal entries $k(x_j) + 2h^{-2}$, entries $-h^{-2}$ adjacent to the diagonal, and zero elsewhere, $\mathbf{g}$ is the vector with entries $g(x_j)$, and $\mathbf{u}$ the unknown vector with entries u_j. Since A has most entries zero it is called *sparse*. There are direct solution methods for this "tridiagonal" sparse structure that requires only $\mathcal{O}(N)$ arithmetic operations.[5] This is *much* faster than the $\mathcal{O}(N^3)$ operations usually needed for Gaussian elimination.

How accurate is this scheme? For simplicity consider a source-free region where $k(x)k$ is constant, then locally let's take $u(x) = e^{ikx}$.[6] We know $(e^{ikx})'' = -k^2e^{ikx}$, but (6) gives instead, using the Taylor series for cosine,

$$\frac{e^{i(k-h)x} - 2e^{ikx} + e^{i(k+h)x}}{h^2} = \frac{2(\cos kh - 1)}{h^2}e^{ikx} = -k^2e^{ikx}\left(1 - \frac{(kh)^2}{12} + \ldots\right)$$

The second term $-(kh)^2/12$ is thus the relative error of this discretization, so it is clear that $kh < 1$ is needed for high accuracy. In other words there must be several grid points per wavelength, meaning $N \gg L/\lambda$. A rigorous error analysis is quite tricky, but shows that this scheme must even have a growing number of grid points per wavelength to maintain the same accuracy as k grows (the "pollution" effect).

People have invented much better ways to numerically solve the 1D Helmholtz equation, but the point is that the above method easily generalizes to 2D and 3D, giving the commonly used 5-point and 7-point stencils. The resulting matrices are sparse but not tridiagonal, so are harder to solve. In 2D, $N \gg (L/\lambda)^2$, and a direct solution takes $O(N^{3/2})$. In 3D, $N \gg (L/\lambda)^3$, and a direct solution takes $O(N^2)$. Returning to the concert hall problem, where $L/\lambda = 10^3$, we see that at least a billion unknowns would be needed, and 10^{18} arithmetic operations (which would take a year on a desktop computer!) Fortunately, mathematicians and engineers have developed improved solution methods that

[5] The notation $\mathcal{O}(N)$ means that there are positive constants C and N_0 such that, for all $N > N_0$, the number of operations never exceeds CN.

[6] In fact u is a linear combination of this and its conjugate. The argument still applies.

are more efficient. Incidentally, this problem size ($N \sim 10^9$) is about the largest that can be currently solved in 3D variable-$k(\mathbf{x})$ seismic applications.

4 Modern progress and open questions

We saw above that highly oscillatory problems can lead to massive linear systems when discretized. The other standard discretization approach is called the *finite element method*, and is useful when the geometry of the domain and/or the $k(\mathbf{x})$ variations are complicated. There are plently of *iterative* methods to solve such systems that rely only on the ability to compute $A\mathbf{x}$ given a vector $\mathbf{x}$. However, the high frequency k makes these methods slow to converge. Recent progress has been made by combining direct solutions in sub-regions then using iterative methods to couple together these regions (for instance [9]), or by using so-called "sweeping preconditioners" that exploit the fact that in many applications waves do not reflect very strongly from the medium [3]. Another direction is to discretize with a higher order of accuracy, meaning $\epsilon = \mathcal{O}(h^p)$ for some large p (with k held constant the above finite difference stencils give only $p = 2$). The stencils are bigger and the linear systems trickier, but the accuracy higher. Pushing this to very large p leads to so-called spectral methods, or spectral collocation.

If $k(\mathbf{x})$ is *piecewise constant* (as in the concert hall example, or when light traveling in air hits glass), we know analytically how waves propagate each constant-k region. For example, a point source for the 3D Helmholtz equation creates a "Green's function" solution $u = e^{ikr}/r$, where r is the distance from the source. Armed with this, one can use potential theory to rephrase the problem using unknowns (grid points) living only on the *boundaries* of such regions. The result is an *integral equation* [7] with kernel involving the Green's function. The advantage is that the N needed is now "one dimension lower," for instance only $(L/\lambda)^2$ in 3D. At large k (short wavelengths) this can be a huge reduction. Careful design leads to a *well-conditioned* linear system for which iterative methods converge rapidly. This contrasts with the above direct PDE discretizations, which are always ill-conditioned. However, the $N \times N$ linear system is now *dense* rather than sparse, so computing $A\mathbf{x}$ from $\mathbf{x}$ would naively take $\mathcal{O}(N^2)$ work. Amazingly, by clever hierarchical use of the fact that the interaction between distant clusters of points using the Green's function is well approximated by a *low rank* matrix, one may reduce this work to only $\mathcal{O}(N)$, or $\mathcal{O}(N \log N)$. This is called the "fast multipole method" [6, 2]. The extension of such ideas to fast direct and "butterfly" solvers for integral equations is an active area of research.

Finally, when L/λ is huge (e.g. $\gg 10^2$) one can often get a decent solution using a ray optics approximation, or Keller's geometric theory of diffraction.

This explains why for light waves (with λ a million times shorter than for sound waves), it is very easy to predict that in a concert hall you will *see* the performers clearly, unless geometrically obstructed! Even at $k = 50$, reasonably sharp geometric shadows are seen in the left panel of Fig. 2, although to get high accuracy a full PDE solution would be needed. Thus, the numerically difficult region is actually L/λ "large but not extremely large", often between 10 and 10^4. Numerical methods that combine ray asymptotics with PDE discretizations or integral equations are an active area of research.

I end with a couple of open questions to think about that could revolutionize the solution of high frequency wave problems:

1. What is the most efficient or sparse way to numerically represent oscillatory solutions in 2D or 3D when k is constant? When $k(\mathbf{x})$ varies?
2. How can *distributed* computer architectures best be used to solve huge wave problems?
3. Is it generally believed that, when a wave is trapped in a resonant (reflective) cavity, the complexity of the numerical problem is at least $\mathcal{O}(k^3)$ in 2D, or $\mathcal{O}(k^6)$ in 3D. Can these bounds be beaten for highly oscillatory resonant cavities?

Image credits

Fig. 2, right panel Ph.D thesis of Leo Zepeda-Nuñez, MIT, 2015.

Fig. 3, left panel Seismic Laboratory for Imaging and Modelling (SLIM), UBC, https://www.slim.eos.ubc.ca/SLIM.Projects.ResearchWebInfo/Modelling/modelling.html, visited on January 7, 2017.

All other figures Produced by the author.

References

[1] A. H. Barnett and T. Betcke, *An exponentially convergent non-polynomial finite element method for time-harmonic scattering from polygons*, SIAM J. Sci. Comput. **32** (2010), no. 3, 1417–1441.

[2] H. Cheng, W. Y. Crutchfield, Z. Gimbutas, L. Greengard, F. Ethridge, J. Huang, V. Rokhlin, N. Yarvin, and J. Zhao, *A wideband fast multipole method for the Helmholtz equation in three dimensions*, J. Comput. Phys. **216** (2006), 300–325.

[3] B. Engquist and L. Ying, *Sweeping preconditioner for the Helmholtz equation: Moving perfectly matched layers*, Multiscale Mod. Sim. **9** (2011), no. 2, 686–710.

[4] S. J. Farlow, *Partial differential equations for scientists and engineers*, Dover, 1993.

[5] N. H. Fletcher and T. Rossing, *The physics of musical instruments*, 2nd edition ed., New York: Springer-Verlag, 1998.

[6] L. Greengard and V. Rokhlin, *A fast algorithm for particle simulations*, J. Comput. Phys. **73** (1987), 325–348.

[7] Ronald B. Guenther and John W. Lee, *Partial differential equations of mathematical physics and integral equations*, Prentice Hall, Englewood Cliffs, New Jersey, 1988.

[8] R. J. LeVeque, *Finite difference methods for ordinary and partial differential equations*, SIAM, 2007.

[9] L. Zepeda-Nuñez and L. Demanet, *Nested domain decomposition with polarized traces for the 2D Helmholtz equation*, 2016, submitted to *SIAM J. Sci. Comput.*, preprint available at `https://arxiv.org/abs/1510.01831`.

Alex Barnett *is an associate professor of mathematics at Dartmouth College, New Hampshire, and in the Numerical Algorithms Group at the Flatiron Institute, Simons Foundation, New York.*

Mathematical subjects
will be filled out by the editors

Connections to other fields
will be filled out by the editors

DOI
will be filled out by the editors

Snapshots of modern mathematics from Oberwolfach are written by participants in the scientific program of the Mathematisches Forschungsinstitut Oberwolfach (MFO). The snapshot project is designed to promote the understanding and appreciation of modern mathematics and mathematical research in the general public worldwide. It started as part of the project "Oberwolfach meets IMAGINARY" in 2013 with a grant by the Klaus Tschira Foundation. The project has also been supported by the Oberwolfach Foundation and the MFO. All snapshots can be found on www.imaginary.org/snapshots and on www.mfo.de/snapshots.

Junior Editor
will be filled out by the editors
junior-editors@mfo.de

Senior Editor
Carla Cederbaum
senior-editor@mfo.de

Mathematisches Forschungsinstitut
Oberwolfach gGmbH
Schwarzwaldstr. 9 – 11
77709 Oberwolfach
Germany

Director
Gerhard Huisken

Mathematisches Forschungsinstitut Oberwolfach
Member of the Leibniz Association
Klaus Tschira Stiftung gemeinnützige GmbH
KTS
oberwolfach FOUNDATION
IMAGINARY open mathematics