Computational wave propagation in the spirit of the Geometrical Theory of Diffraction

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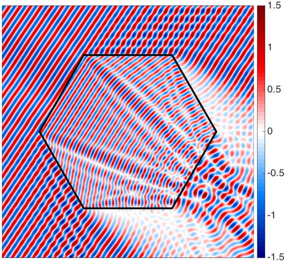
High frequency wave propagation



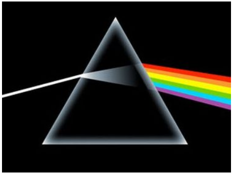
Applications in acoustics, electromagnetism, elasticity, quantum mechanics,...

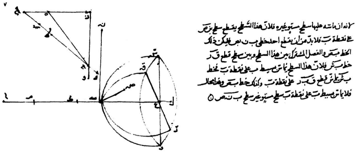
Highly oscillatory solutions, difficult to capture numerically or asymptotically.

Geometrical **ray-based approximations** have been around for centuries.

E.g., law of **refraction** often attributed to Willebrord Snellius (1580-1626) and René Descartes (1596-1650).

But the law appears in Ibn Sahl's *On Burning Mirrors and Lenses* (984), which refers to earlier Greek texts.

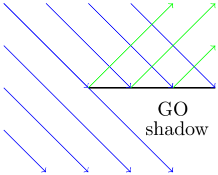


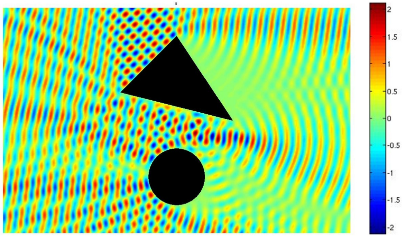


High frequency wave propagation

Geometrical optics (GO) computes only **incident**, **reflected** and **refracted** rays.

In particular, GO incorrectly predicts a zero field in shadow regions.





The propagation of waves into shadow regions is called **diffraction**.

Left: plot of $\mathrm{Re}\,[u]$, where
$\Delta u + k^2 u = 0$ in D and $u = 0$ on ∂D.

Here $k = 2\pi/\lambda > 0$ is the **wavenumber**, proportional to frequency

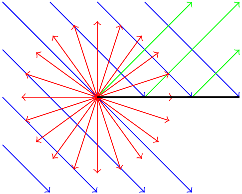
Sommerfeld (1896) and MacDonald (1902) provided the first rigorous analyses of **edge diffraction** - exact solutions for half-planes/wedges.

Fock, Leontovich, Pekeris (1940s/1950s) used asymptotic methods to study **tangent ray diffraction** for smooth scatterers.

Geometrical theory of diffraction (GTD)

Keller showed how these new results could be combined into a **ray-based theory**. Edges, corners and tangent rays give rise to new families of **diffracted rays**.

Keller's "**Geometrical Theory of Diffraction**" (GTD) provides an **accurate**, **flexible** and **physically intuitive** tool for high frequency scattering problems.



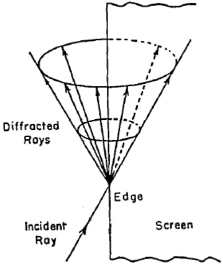
JOURNAL OF THE OPTICAL SOCIETY OF AMERICA VOLUME 52, NUMBER 2 FEBRUARY, 1962

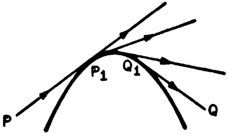
Geometrical Theory of Diffraction*

Joseph B. Keller
Institute of Mathematical Sciences, New York University, New York, New York

(Received September 13, 1961)

The geometrical theory of diffraction is an extension of geometrical optics which accounts for diffraction. It introduces diffracted rays in addition to the usual rays of geometrical optics. These rays are produced by incident rays which hit edges, corners, or vertices of boundary surfaces, or which graze such surfaces. Various laws of diffraction, analogous to the laws of reflection and refraction, are employed to characterize the diffracted rays. A modified form of Fermat's principle, equivalent to these laws, can also be used. Diffracted wave fronts are defined, which can be found by a Huygens wavelet construction. There is an associated phase or eikonal function which satisfies the eikonal equation. In addition complex or imaginary rays are introduced. A field is associated with each ray and the total field at a point is the sum of the fields on all rays through the point. The phase of the field on a ray is proportional to the optical length of the ray from some reference point. The amplitude varies in accordance with the principle of conservation of energy in a narrow tube of rays. The initial value of the field on a diffracted ray is determined from the incident field with the aid of an appropriate diffraction coefficient. These diffraction coefficients are determined from certain canonical problems. They all vanish as the wavelength tends to zero. The theory is applied to diffraction by an aperture in a thin screen diffraction by a disk, etc., to illustrate it. Agreement is shown between the predictions of the theory and various other theoretical analyses of some of these problems. Experimental confirmation of the theory is also presented. The mathematical justification of the theory on the basis of electromagnetic theory is described. Finally, the applicability of this theory, or a modification of it, to other branches of physics is explained.





My other favourite Keller papers...

IEEE TRANSACTIONS ON ANTENNAS AND PROPAGATION, VOL. AP-33, NO. 2, FEBRUARY 1985 123

One Hundred Years of Diffraction Theory

JOSEPH B. KELLER

Abstract—**The development of diffraction theory in the last 100 years is discussed from a personal viewpoint, with emphasis on the geometrical theory of diffraction. First some early work of Kirchhoff, Rayleigh, Sommerfeld, MacDonald and others is mentioned to indicate the state of the field in the 1940's. Next the author's work during World War II is described. Then the considerations that led him to the geometrical theory of diffraction are explained, and the defects of that theory are outlined. Finally the advances in the theory since its introduction, which have remedied many of these defects, are mentioned.**

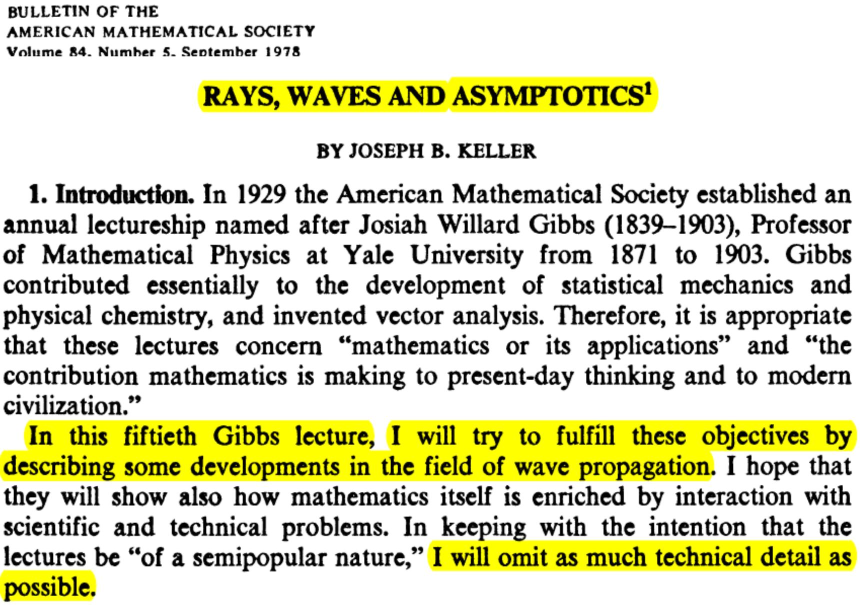
I. INTRODUCTION

DIFFRACTION IS THE process whereby light propagation differs from the predictions of geometrical optics. It can be understood qualitatively via the wave theory of light, and described quantitatively via solutions of the wave equation or of Maxwell's equations. A method for solving such equations for diffraction phenomena. Therefore Sommerfeld (1896) invented a new method for solving it, which involved a two-sheeted space. It yielded the solution in terms of Fresnel integrals, which could be evaluated easily for all parameter values, and they revealed the diffraction effects very clearly.

Unfortunately this remarkable method has found very little other use except to treat scattering by a wedge. Only Shiffman and Spencer (1947) have used it to find the potential flow around a lens, and Buslaev (1965) used the basic idea in this path integral analysis of diffraction by a convex cylinder. Consequently Karp once suggested that this method held back diffraction theory for 50 years because people tried unsuccessfully to use it, rather than try other methods.

Scattering by a wedge was solved by MacDonald (1902, 1915). Then Debye (1908) analyzed Rayleigh's solution for scattering

My other favourite Keller papers...


BULLETIN OF THE
AMERICAN MATHEMATICAL SOCIETY
Volume 84, Number 5, September 1978

RAYS, WAVES AND ASYMPTOTICS[1]

BY JOSEPH B. KELLER

1. Introduction. In 1929 the American Mathematical Society established an annual lectureship named after Josiah Willard Gibbs (1839–1903), Professor of Mathematical Physics at Yale University from 1871 to 1903. Gibbs contributed essentially to the development of statistical mechanics and physical chemistry, and invented vector analysis. Therefore, it is appropriate that these lectures concern "mathematics or its applications" and "the contribution mathematics is making to present-day thinking and to modern civilization."

In this fiftieth Gibbs lecture, I will try to fulfill these objectives by describing some developments in the field of wave propagation. I hope that they will show also how mathematics itself is enriched by interaction with scientific and technical problems. In keeping with the intention that the lectures be "of a semipopular nature," I will omit as much technical detail as possible.

Numerics vs asymptotics

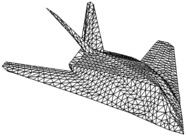
$$(\Delta + k^2)u = 0$$

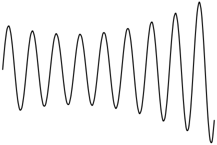
increasing k →

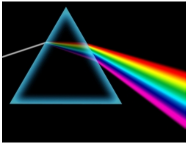
Numerical methods (FEM/BEM)

What to do in the "mid-frequency" regime??

Asymptotic methods (GO/GTD)







controllably accurate
computationally infeasible at large k

computational cost independent of k
accurate only as $k \to \infty$

Hybrid Numerical-Asymptotic (HNA) approach

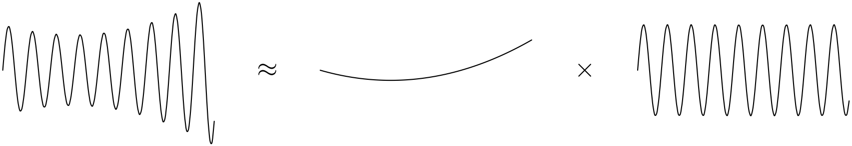
Fuse conventional FEM/BEM with high frequency asymptotics to create algorithms that are both accurate and computationally feasible over the whole frequency range.

The HNA approach

- FEM/BEM approximates u by a piecewise polynomial on a mesh.
- GO/GTD approximates u by a sum of WKB solutions (corresponding physically to incident, reflected, diffracted waves):

$$u(x) \sim \sum_{j=1}^{J} v_j(x) e^{\mathrm{i}k\phi_j(x)}, \qquad k \to \infty.$$

Phases ϕ_j and amplitudes v_j found by ray tracing, solving ODEs along rays, and asymptotic matching.



- HNA methods use a FEM/BEM approximation space incorporating **oscillatory basis functions**, with **GO/GTD phases** and **numerically computed piecewise polynomial amplitudes**.

Goal: Controllable accuracy and $O(1)$ computational cost as $k \to \infty$.

History of HNA methods

The basic idea behind the HNA approach goes back at least as far as Uncles (1976), but has developed more rapidly since the mid-1990s.

Some major contributers so far:

- FEM e.g. Giladi and **Keller** (2001).
- BEM e.g. Abboud, Anand, Asheim, Boubendir, Bruno, Chandler-Wilde, Dominguez, Ecevit, Ganesh, Geuzaine, Gibbs, Giladi, Graham, Groth, Hawkins, **Hewett**, **Huybrechs**, **Keller**, Langdon, Melenk, Mokgolele, **Moiola**, Monro, Nédélec, Parolin, Reitich, Ritter, **Smyshlyaev**, **Spence**, Twigger, Vandewalle, Zhou, ...

Keller himself was an early proponent, publishing two papers on the topic, one on FEM (2001) and one on BEM (2004).

Attraction of BEM: only need asymptotic behaviour on the **boundary**.

Nice review paper:

Chandler-Wilde, Graham, Langdon and Spence, *Numerical-asymptotic boundary integral methods in high frequency acoustic scattering*, Acta Numerica 21 (2012), pp. 89–305.

Keller and HNA BEM (smooth convex scatterer)

20th Annual Review of Progress in Applied Computational Electromagnetics

An Asymptotically Derived Boundary Element Method for the Helmholtz Equation

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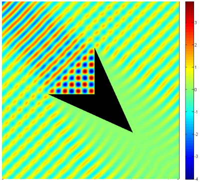
Abstract

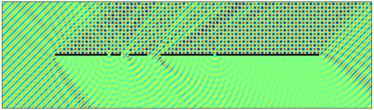
We present an asymptotically derived boundary element method for the Helmholtz equation in exterior domains, in which the basis functions are asymptotically derived. Each basis function is the product of a smooth amplitude and an oscillatory phase factor, like the asymptotic solution. The phase factor is determined a-priori by using arguments from geometrical optics and the geometrical theory of diffraction, while the smooth amplitude is represented by high order splines. Our approach accounts for all the components of the scattered field namely the reflected, shadow forming and diffracted fields, and we demonstrate that it is substantially more accurate than an approach which accounts for the reflected field only. Two types of diffracted basis functions are presented: the first accounts for the dominant oscillatory behavior in the shadow region while the second also accounts for the decay of the amplitude there. Although the method is applicable to a variety of scatterers, we focus our attention here on scattering from smooth convex bodies in two dimensions. Our computations with a conducting circular cylinder demonstrate that the number of unknowns necessary to achieve a given accuracy with this new basis is virtually independent of the wave-number.

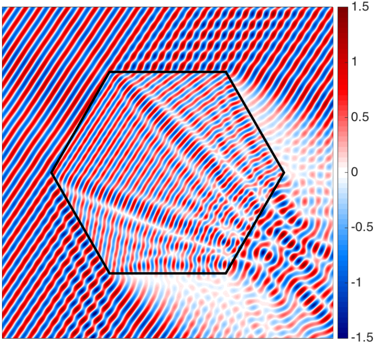
My own contribution

I am part of an extended collaboration (centred at Reading) developing HNA methods for **non-smooth scatterers**.

Our recent successes include: convex and non-convex polygons, 2D and 3D screens, and transmission problems.



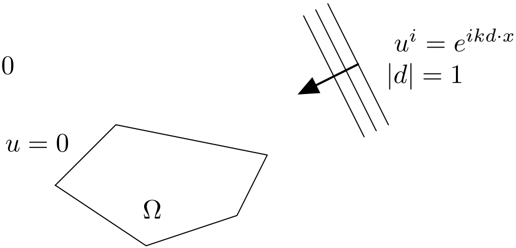




Our aim is to provide a rigorous convergence analysis whenever possible. This has led to **new rigorous results in the GTD**.

Sound-soft convex polygons

$$\Delta u + k^2 u = 0$$



$u - u^i$ outgoing
at infinity

Green's representation theorem:

$$u(x) = u^i(x) - \int_\Gamma \Phi(x,y)\,\frac{\partial u}{\partial n}(y)\,ds(y), \qquad x \in \mathbb{R}^2 \setminus \overline{\Omega},$$

$$\Phi(x,y) := \frac{\mathrm{i}}{4} H_0^{(1)}(k|x-y|), \qquad -(\Delta_y + k^2)\Phi(x,y) = \delta(x-y).$$

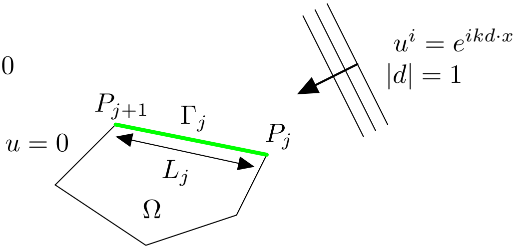
Taking boundary traces gives a **boundary integral equation** for $\partial u/\partial n$, e.g.

$$\int_\Gamma \Phi(x,y)\frac{\partial u}{\partial n}(y) ds(y) = u^i(x), \quad x \in \partial\Omega.$$

Sound-soft convex polygons

$$\Delta u + k^2 u = 0$$

$u - u^i$ outgoing at infinity



According to GTD, on a "lit" side

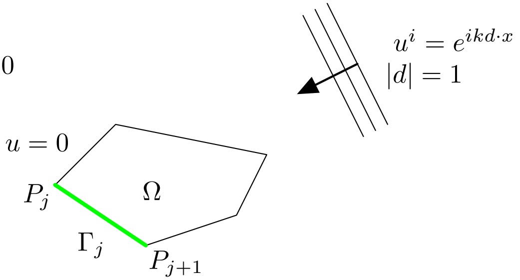
$$\frac{\partial u}{\partial n} \quad \sim \quad \underbrace{2\frac{\partial u^i}{\partial n}}_{\text{incident + reflected}} + \underbrace{Ae^{iks} + Be^{-iks}}_{\text{diffracted}}, \qquad k \to \infty$$

where s is arc length along the side, measured from P_j

Sound soft convex polygons

$$\Delta u + k^2 u = 0$$

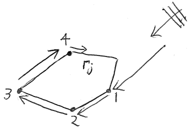
$u - u^i$ outgoing
at infinity



On an "unlit" (or "shadow") side

$$\frac{\partial u}{\partial n} \sim \underbrace{Ae^{iks} + Be^{-iks}}_{\text{diffracted}}, \qquad k \to \infty$$

Higher-order multiply-diffracted waves have the **same phases**, but **amplitudes are harder to compute**.



Regularity result ("rigorous GTD")

Theorem (Hewett, Langdon, Melenk (2013))

Let Ω be a convex polygon. Then on any side Γ_j

$$\frac{\partial u}{\partial n}(x(s)) = \underbrace{v_0(x(s))}_{GO} + \underbrace{v_j^+(s)e^{iks} + v_j^-(L_j - s)e^{-iks}}_{GTD}, \qquad 0 < s < L_j,$$

where

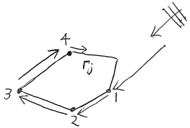
(i) $v_0 := 2\frac{\partial u^i}{\partial n}$ *if* Γ_j *is lit and* $v_0 := 0$ *otherwise,*

(ii) $v_j^\pm(s)$ *are* **analytic** *in* $\mathrm{Re}\,[s] > 0$, *with*

$$|v_j^\pm(s)| \leq C \begin{cases} k^2|ks|^{-\delta_j^\pm}, & 0 < |s| \leq 1/k, \\ k^2|ks|^{-1/2}, & |s| > 1/k, \end{cases}$$

where $\delta_j^\pm \in (0, 1/2)$ *depend on exterior angles at* P_j *and* P_{j+1} *respectively.*

Key point: $v_j^\pm$ capture **all** of the multiply-diffracted waves!



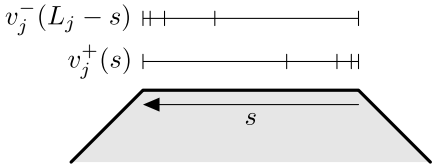
HNA approximation space V_N

On each side Γ_j we use the HNA ansatz

$$\frac{\partial u}{\partial n}(x) = v_0(x) + v_j^+(s)e^{iks} + v_j^-(L_j - s)e^{-iks}, \qquad x \in \Gamma_j,$$

where

- $v_0 := 2\frac{\partial u^i}{\partial n}$ if Γ_j is lit and $v_0 := 0$ otherwise
- $v_j^\pm$ are approximated by piecewise-polynomials on **two overlapping geometric meshes**, graded towards the corner singularities:



"hp" approximation strategy: increase polynomial degree p simultaneously with the number of layers n in the mesh ($n = cp$)

Convergence and k-dependence

Theorem (Hewett, Langdon, Melenk (2013))

If $c, k_0 > 0$ and $n \geq cp$, $k \geq k_0$, then there exists $C, \tau > 0$, independent of k, such that the Galerkin HNA BEM solution ψ_N satisfies

$$\left\| \frac{\partial u}{\partial n} - \psi_N \right\|_{L^2(\Gamma)} \leq C k^{5/2} \mathrm{e}^{-p\tau}.$$

Total number of degrees of freedom $N = \mathcal{O}\left(n(p+1)\right)$

Theorem suggests we can achieve any required accuracy of approximation with N growing only like $\log^2 k$ as $k \to \infty$, rather than like k, as for a standard BEM.

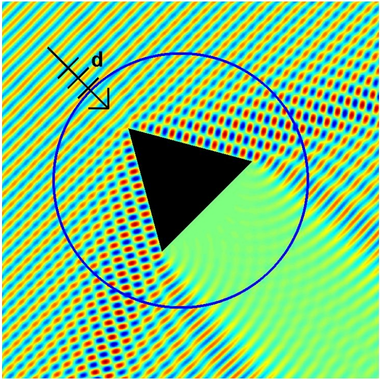
In practice, the method is effectively frequency-independent!

Analysis assumes that we use the "star-combined formulation" (Spence, Chandler-Wilde, Graham and Smyshlyaev (2011)), for which $C_{cont} = \mathcal{O}\left(k^{1/2}\right)$ and $C_{coerc} = \mathcal{O}\left(1\right)$ as $k \to \infty$. Numerical results that follow are for the standard "combined layer potential formulation".

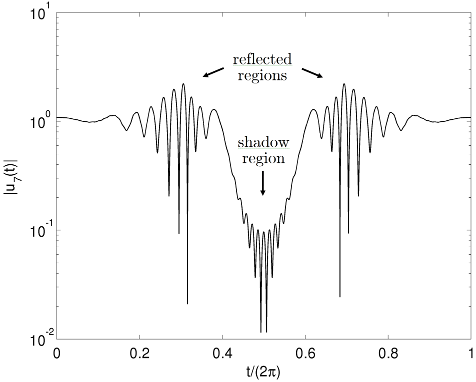
Numerical results

Given the Galerkin solution $\psi_N \approx \dfrac{\partial u}{\partial n}$, let $u_p \approx u$ be the corresponding approximation in the domain:

$$u_p(x) := u^i(x) - \int_\Gamma \Phi(x,y)\psi_N(y)\,ds(y), \qquad x \in D$$



$k = 10$



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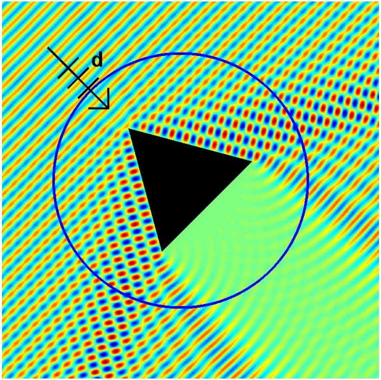

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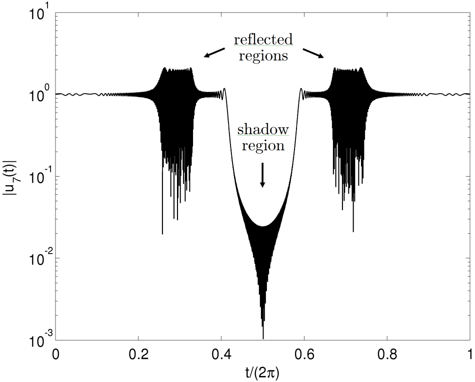
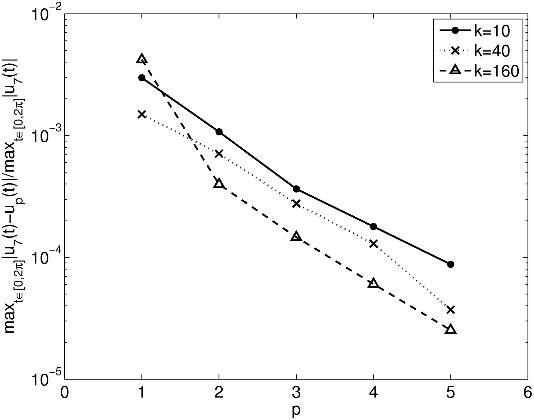


$k = 160$

Numerical results

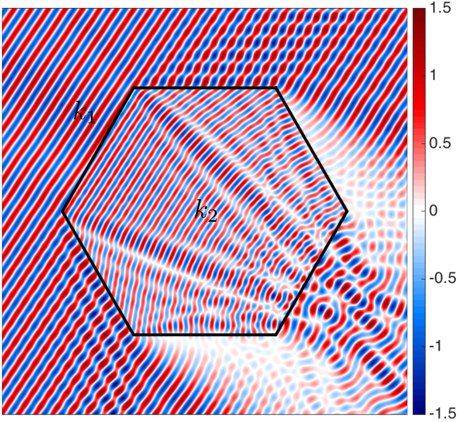
Theorem

$$\frac{\|u - u_p\|_{L^\infty(D)}}{\|u\|_{L^\infty(D)}} \le C k^{5/2}\, e^{-p\tau}, \quad k \ge k_0.$$



Exponential convergence as $p \to \infty$; Accuracy actually improves as k increases!

Transmission problems - with S. Groth and S. Langdon



- Scatterer is now a region in which the wavenumber (k_2) differs from that of the background medium (k_1)
- Transmission boundary conditions

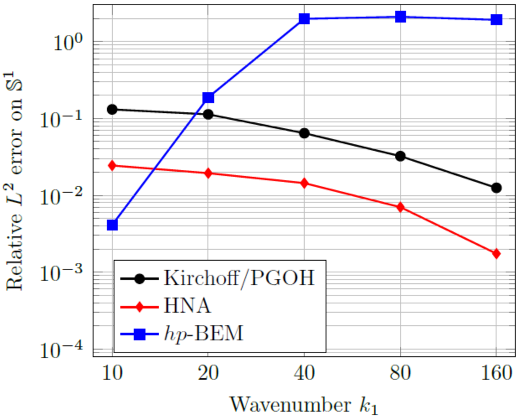
$$[u] = 0, \left[\alpha \frac{\partial u}{\partial n}\right] = 0$$

- Waves *refract* into the scatterer
- GTD not well-developed!

Infinitely many phases to consider, even for a convex polygon: incident, reflected, transmitted, diffracted, “lateral”, plus all their internal re-reflections!

We compute GO (using a beam-tracing algorithm) and incorporate **only the primary diffracted waves** into our HNA approximation space

HNA performance



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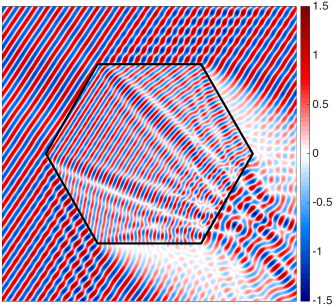
Far-field errors for GO (Kirchoff/PGOH), our HNA BEM (with fixed $N = 416$) and a conventional hp-BEM (with fixed $N = 456$), for scattering by an equilateral triangle with $\alpha = 1$ and refractive index $\mu = 1.5 + 0.003125\mathrm{i}$. ($k_2 = \mu k_1$)

At $k = 160$ our HNA achieves 0.2% error with fewer than 0.3 degrees of freedom per wavelength!

Conclusions

- High frequency scattering is a **challenging problem**
- Keller's **Geometrical Theory of Diffraction** is not just a powerful *asymptotic* method; it is influencing *computational* methods too

- Many big **open problems**:
  - GTD - transmission wedge, quarter plane, octant, inflection point, . . .
  - HNA - 3D problems, multiple scattering, . . .



References and preprints at `www.ucl.ac.uk/∼ucahdhe`