Numerical Methods for High Frequency Scattering

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- EPSRC Career Acceleration Fellowship for Timo

Durham, July 2010

Aim of Our High Frequency Wave Projects

Develop numerical methods which use oscillatory basis functions to represent solutions with hugely reduced numbers of degrees of freedom.

Domain-based formulations (Plane wave DG, UWVF. etc.). Timo Betcke, Joel Phillips, Ivan Graham, Steve Langdon, SNCW, Charlotta Howarth + PhD at Bath + 3 PhDs at Reading + see talk by **Peter Monk**.

BEM-based methods. Timo Betcke, SNCW, Ivan Graham, Dave Hewett, Tatiana Kim, Steve Langdon, Euan Spence, Ashley Twigger + talks by **Markus Melenk**, **Bjorn Engquist** + **Jon Trevelyan** and colleagues at Durham

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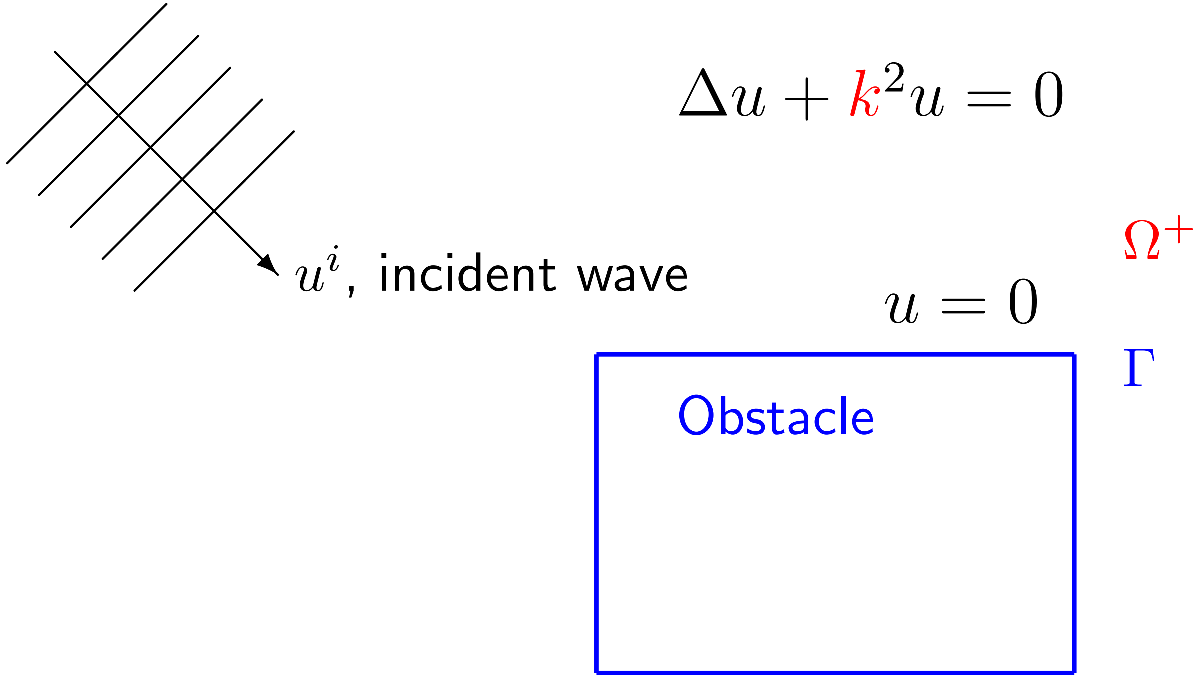
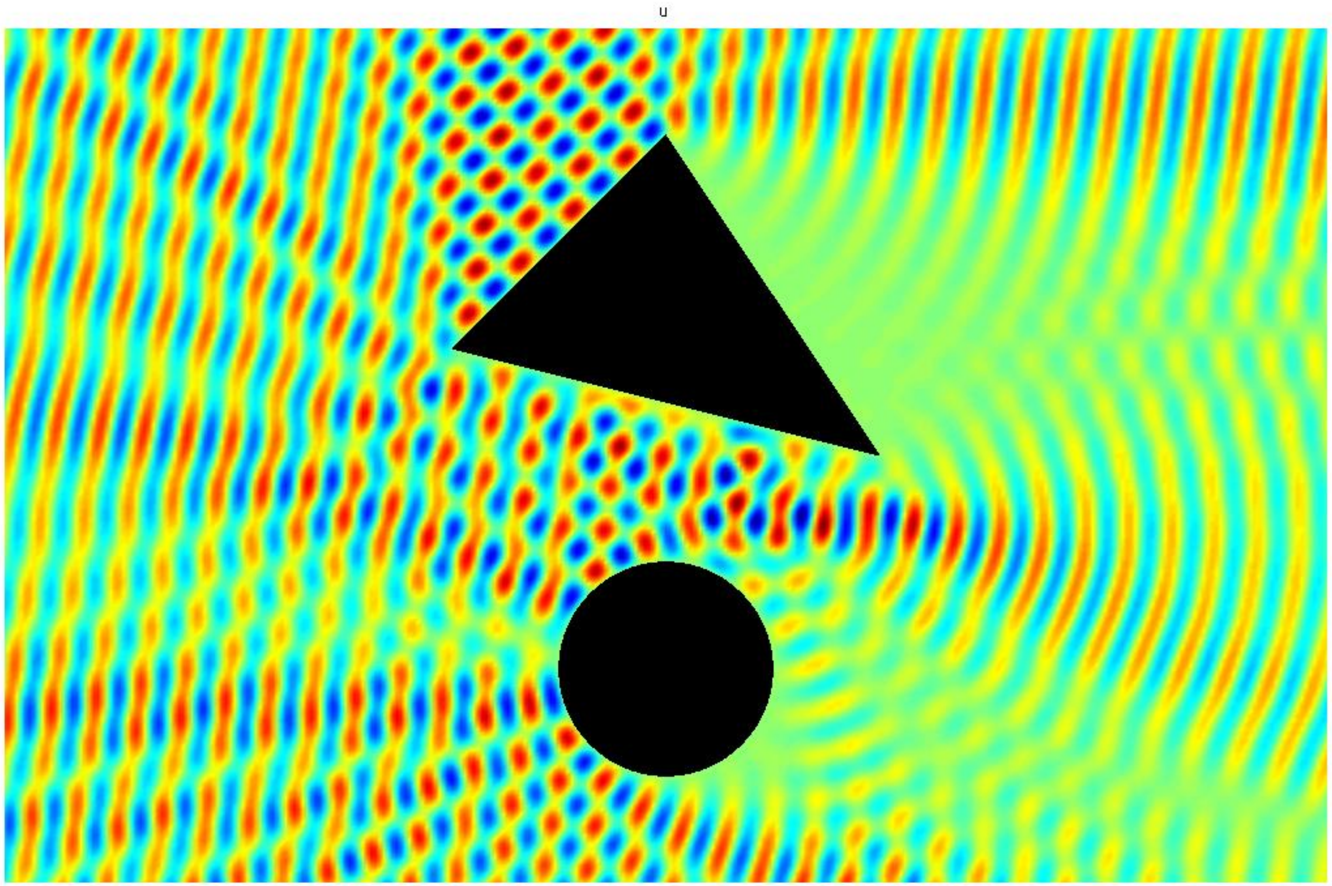
A Simple Generic Time Harmonic Scattering Problem

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



$k = \dfrac{2\pi}{\lambda} > 0$ is the **wave number** and λ the corresponding **wavelength**.

Why am I here at a **multiscale** conference??



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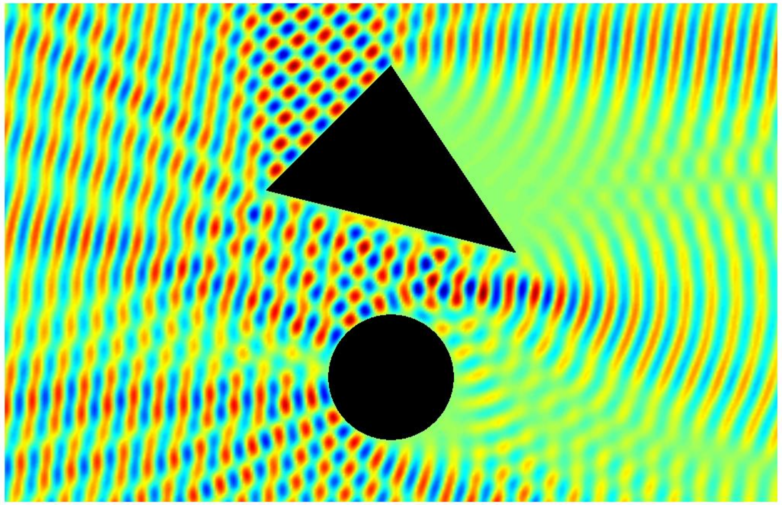

- At least one **scatterer length scale** - usually many, see e.g. Jill Ogilvy BAE Systems talk
- **Wavelength** $\lambda = 2\pi/k$ - k^{-1} scale
- Many other **scales in the solution**, $k^{-1/2}$, $k^{-1/3}$

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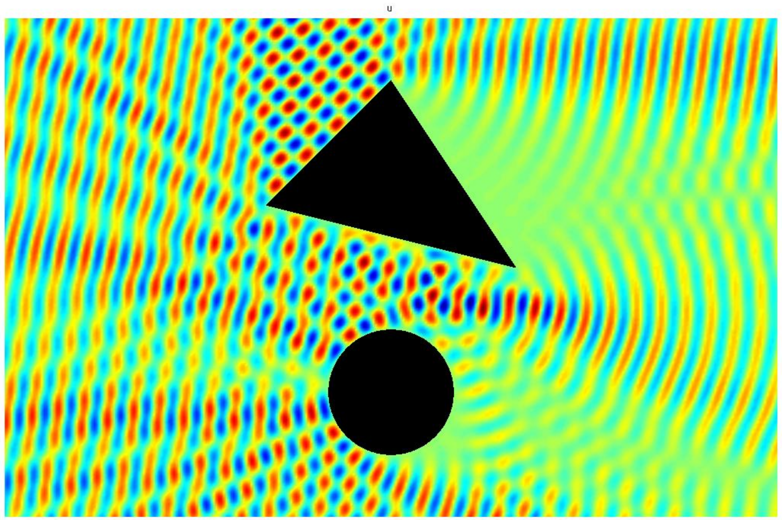

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- **Wavelength** $\lambda = 2\pi/k$ - k^{-1} scale
- Many other **scales in the solution**, $r(kr)^{-1/2}$, $R(kR)^{-1/3}$

A Simple Generic Time Harmonic Scattering Problem

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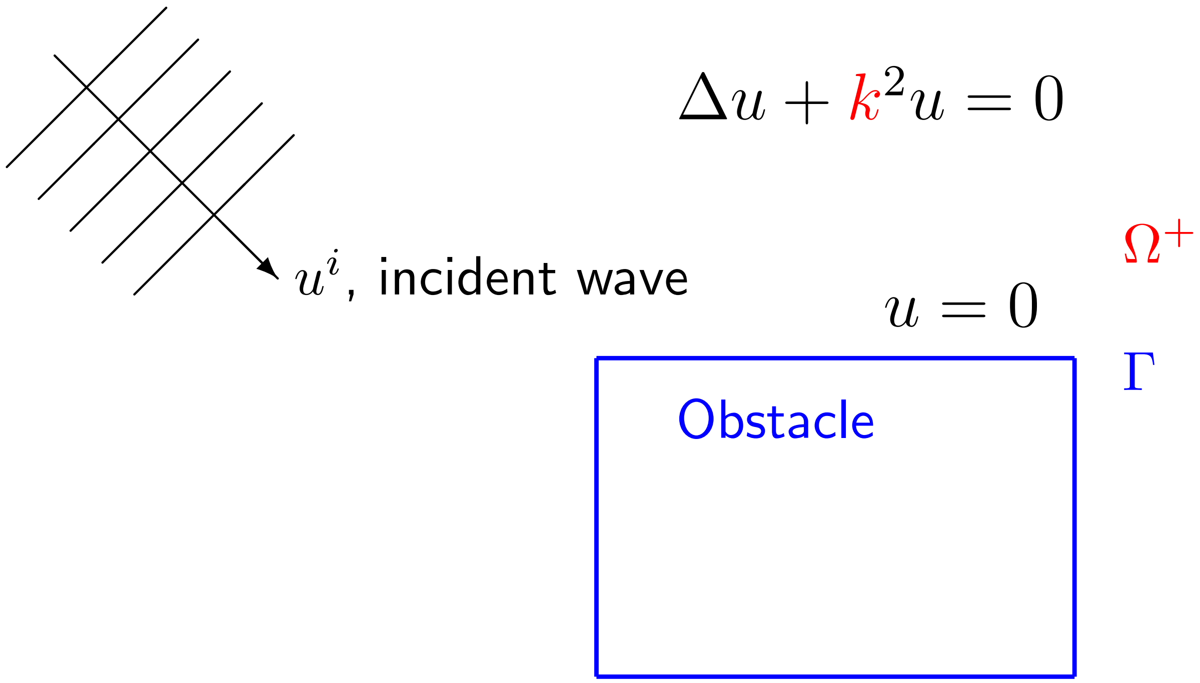

$k = \dfrac{2\pi}{\lambda} > 0$ is the **wave number** and λ the corresponding **wavelength**.

Background

When solving the **Helmholtz equation**

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

the degrees of freedom in a conventional BEM of FEM needs to increase as the **wave number** $k = \dfrac{2\pi}{\lambda}$ increases.

See e.g. the talks by **Bjorn Engquist** or **Markus Melenk**.

Today's Talk

When solving the **Helmholtz equation**

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

the degrees of freedom in a conventional BEM or FEM needs to increase as the **wave number** $k = \frac{2\pi}{\lambda}$ increases.

- In the BEM, can we avoid this by using clever basis functions, e.g. solutions of the Helmholtz equation or solutions of the Helmholtz equation multiplied by standard basis functions?
- By doing this, is a solver achievable with $O(1)$ cost in the limit as $k \to \infty$?

The Computational Challenge

In fact, can we achieve

‘prescribed error tolerances within fixed computational times for scattering problems of arbitrarily high frequency’

to quote from the title of Bruno, Geuzaine, Monro, and Reitich, Phil Trans R Soc Lond A (2004)

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Answer:

1. **YES** for some classes of 2D and 3D problems.

2. For more general classes significant improvements possible and promising research area.

The Associated Mathematical Challenge ... PROVING EVERYTHING!

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- Best approximation results using novel approximation spaces
- Stability
- Convergence
- Error estimates for fully discrete schemes

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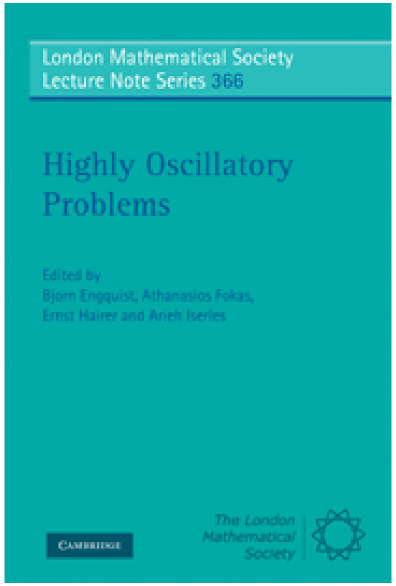
THE (HUGE) NOVELTY IS THAT WE NEED TO DO THIS IN THE LIMIT AS $k \to \infty$ with N fixed (not the classical $N \to \infty$ with k fixed).

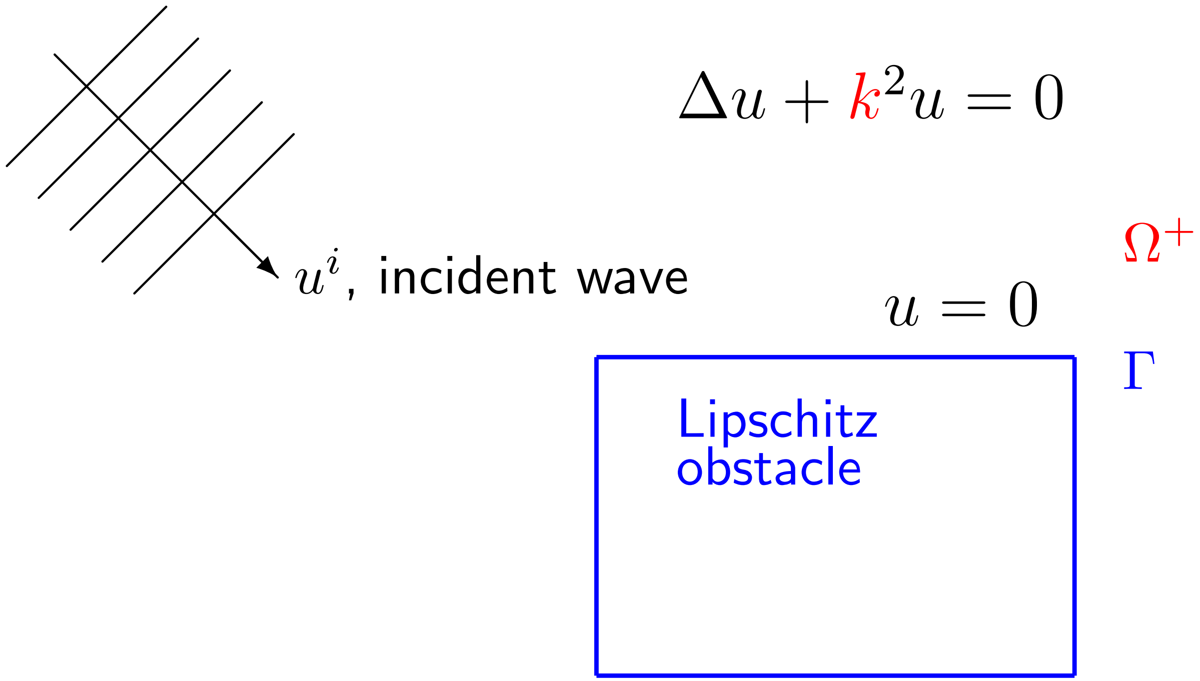
I will only scrape the surface today. For more details:

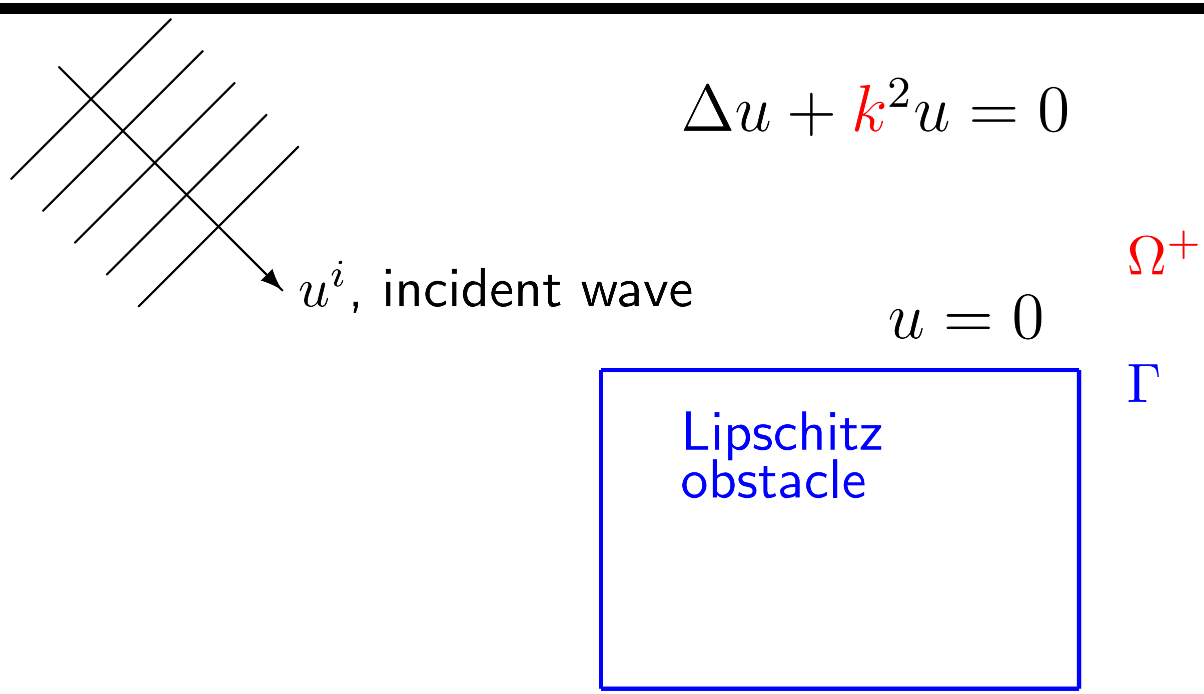
- Talk to: **Betcke, Ganesh, Graham, Hewett, Kim, Langdon, Melenk, Smyshlyaev, Spence, Trevelyan, Twigger**



- Read survey article by C-W & Graham (and related articles by Huybrechs & Olver, Monk, Motamed & Runborg) in **Highly Oscillatory Problems**, CUP, July 2009, £33.25 on amazon.co.uk.

The Scattering Problem



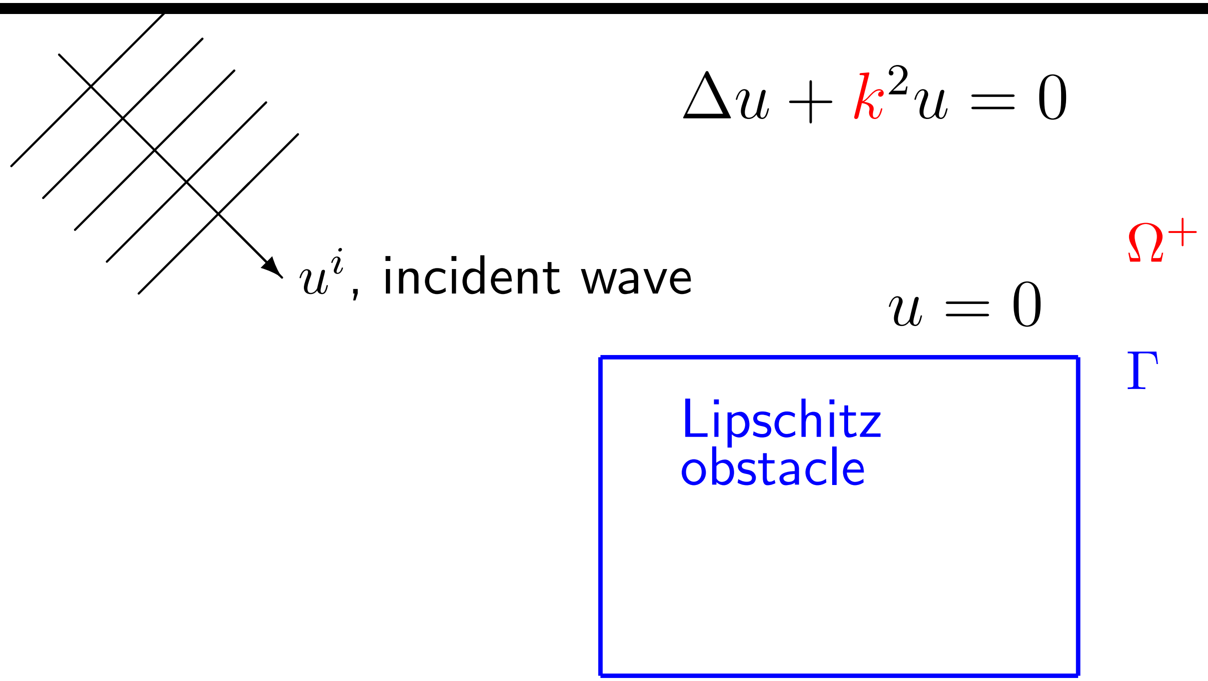


Green's representation theorem:

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

where

$$G(x,y) := \tfrac{\mathrm{i}}{4} H_0^{(1)}(k|x-y|) \text{ (2D)}, \qquad := \frac{1}{4\pi} \frac{\mathrm{e}^{\mathrm{i}k|x-y|}}{|x-y|} \text{ (3D)}.$$



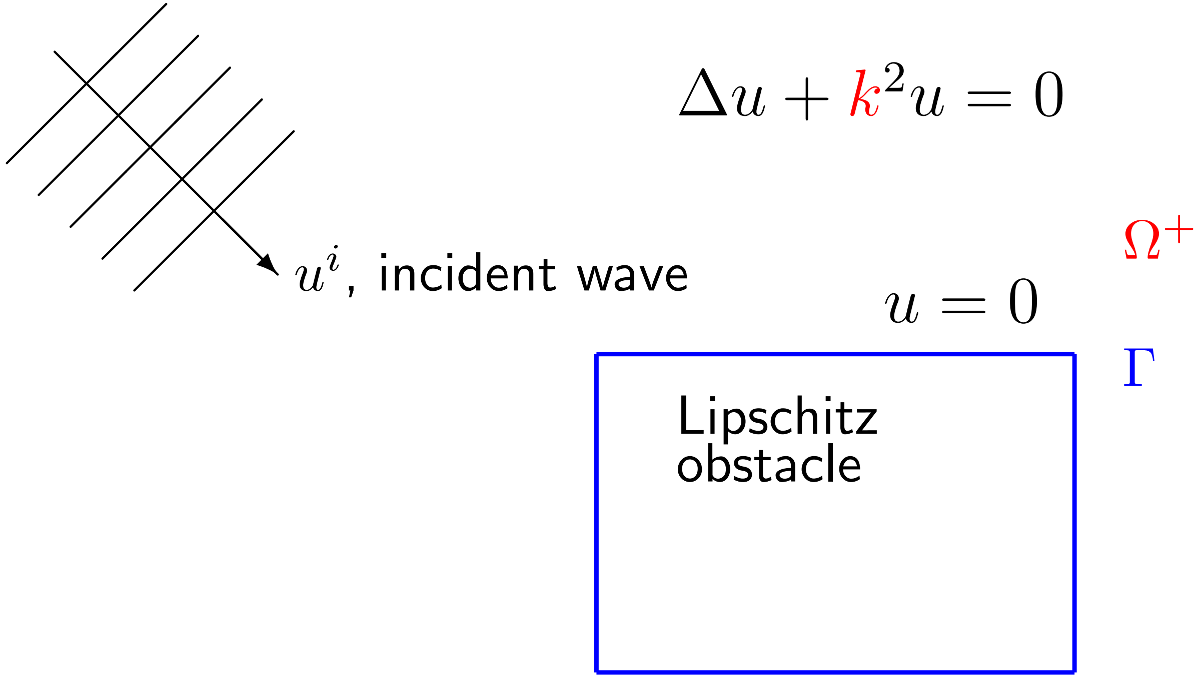
Taking a linear combination of Dirichlet and Neumann traces of the previous equation, we get the **boundary integral equation**

$$\frac{1}{2}\frac{\partial u}{\partial n}(x) + \int_\Gamma \left(\frac{\partial G(x,y)}{\partial n(x)} + \mathrm{i}\eta G(x,y) \right) \frac{\partial u}{\partial n}(y) ds(y) = f(x), \quad x \in \Gamma,$$

where

$$f(x) := \frac{\partial u^i}{\partial n}(x) + \mathrm{i}\eta u^i(x).$$

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



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Theorem (Mitrea 1996, C-W & Langdon 2007) If $\eta \in \mathbb{R}$, $\eta \neq 0$, then this integral equation is uniquely solvable in $L^2(\Gamma)$.

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in operator form

$$A\,\frac{\partial u}{\partial n} = f.$$

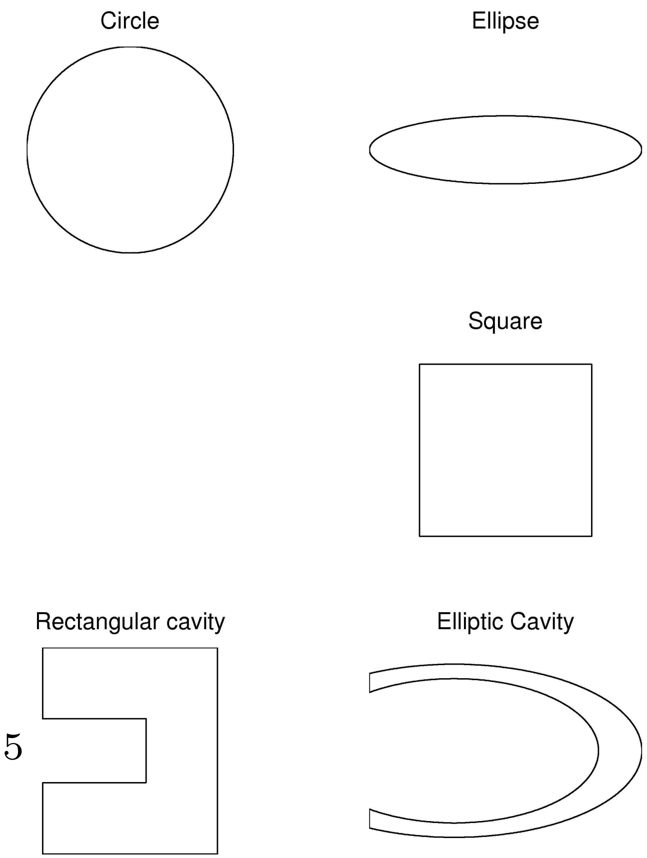
Theorem If $\eta \in \mathbb{R}$, $\eta \neq 0$, then this integral equation is uniquely solvable in $L^2(\Gamma)$.

In fact (C-W & Monk 2008, C-W, Graham, Langdon, Lindner 2009), if scatterer is **starlike** and $\eta = (1+k)$ then (in 3D)

$$\|A^{-1}\| \leq C, \quad \|A\| \leq Ck, \quad \mathrm{cond}\, A \leq Ck.$$

See **Melenk** lecture 3 for smoothing mapping properties of A and A^{-1} when Γ is analytic.

The Subtlety of Behaviour of $\|A\|$ and $\|A^{-1}\|$



$\sim k^{1/3}$, ~ 1

$\sim k^{1/2}$, ~ 1

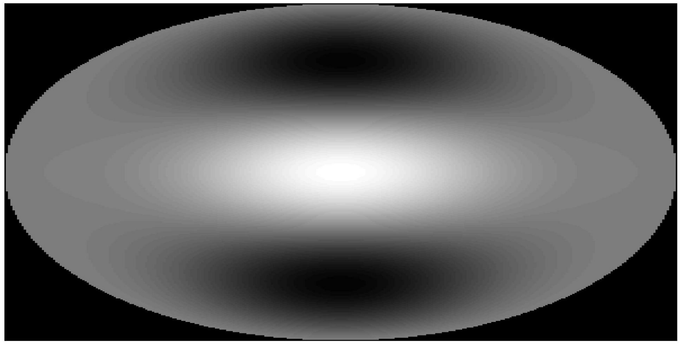
$\sim k_m^{1/2}$, $\sim k_m^{7/5}$

$\sim k_m^{1/2}$, $\sim \mathrm{e}^{\gamma k_m}$

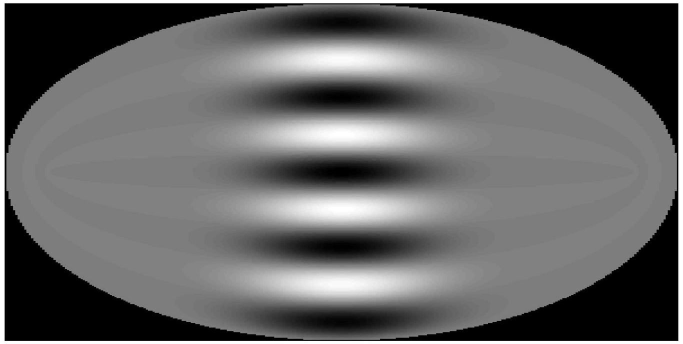
Details: see C-W et al (2009), **Betcke** et al (preprint), **Runborg** in progress.

Mechanism for Exponential Growth: Exponential Localization of Eigenmodes

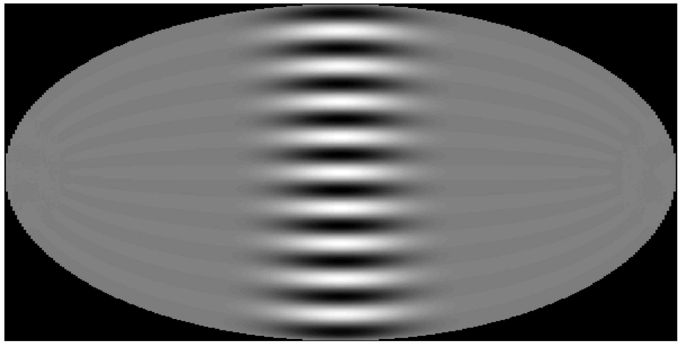
$k_{1,0}$=9.9771201566136298



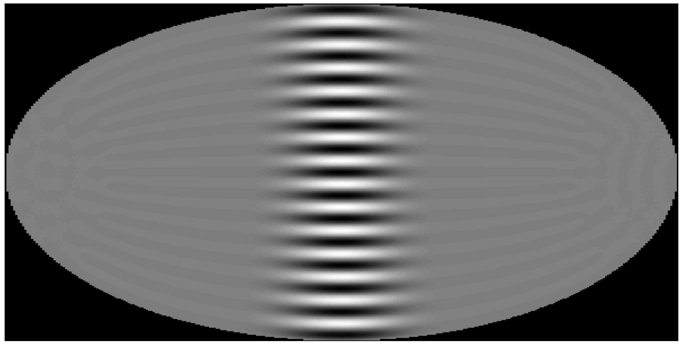
$k_{4,0}$=28.807002784875433



$k_{9,0}$=60.218097688523919



$k_{14,0}$=91.632551202864647



$$\frac{1}{2}\frac{\partial u}{\partial n}(x) + \int_\Gamma \left(\frac{\partial G(x,y)}{\partial n(x)} + \mathrm{i}\eta G(x,y)\right)\frac{\partial u}{\partial n}(y)ds(y) = f(x), \quad x \in \Gamma.$$

Conventional BEM: Approximate $\partial u/\partial n$ by a piecewise polynomial, i.e.

$$\frac{\partial u}{\partial n}(x) \approx \sum_{j=1}^{N} a_j \mathbf{b}_j(x),$$

where $\mathbf{b}_1(x), \ldots, \mathbf{b}_N(x)$ are the piecewise polynomial basis functions (precisely, if boundary curved, these functions are images of FEM basis functions under a mapping from reference element in $\mathbb{R}^{d-1}$ to Γ).

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Applying a **Galerkin method** or a **collocation method** we get a linear system to solve with N degrees of freedom, namely the unknown values of $a_1, \ldots, a_N$.

$$\frac{1}{2}\frac{\partial u}{\partial n}(x) + \int_\Gamma \left(\frac{\partial G(x,y)}{\partial n(x)} + \mathrm{i}\eta G(x,y) \right) \frac{\partial u}{\partial n}(y) ds(y) = f(x), \quad x \in \Gamma.$$

Conventional BEM: Apply a Galerkin method, approximating $\partial u/\partial n$ by a piecewise polynomial of degree p, leading to a linear system to solve with N degrees of freedom.

Problem: N of order of k^{d-1} if 'pollution' avoided (**Melenk**, Lecture 3) and cost is ... close to $O(N)$ if a fast multipole method is used (e.g. talk by **Engquist**.

This is **fantastic**, but still infeasible as $k \to \infty$.

Alternative: Reduce N by using new **oscillatory basis functions** which can represent the solution well. Specifically, let's try

$$\frac{\partial u}{\partial n}(x) \approx \sum_{i=1}^{M} \sum_{j=1}^{N_i} a_{ij} \exp(\mathrm{i} k g_i(x)) \mathbf{b}_{ij}(x),$$

with $a_{ij} \in \mathbb{C}$ the unknown coefficients,

$g_1(x), \ldots, g_M(x)$ known **phase functions**,

$\mathbf{b}_{ij}(x)$ **conventional BEM basis functions**.

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Moreover, let's have #dof $N = \sum_{i=1}^{M} N_i$ much less than conventional BEM, ideally $N = O(1)$ as $k \to \infty$, the **'high frequency $O(1)$ algorithm'** holy grail.

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$$\frac{\partial u}{\partial n}(x) \approx \sum_{i=1}^{M} \sum_{j=1}^{N_i} a_{ij} \exp(\mathrm{i}kx \cdot d_i) \mathbf{b}_{ij}(x),$$

with $a_{ij} \in \mathbb{C}$ the unknown coefficients,

$d_1, \dots d_M$ known **plane wave directions**,

$\mathbf{b}_{ij}(x)$ **conventional BEM basis functions**.

The Plan: let's have #dof $N = \sum_{i=1}^{M} N_i$ which is $N = O(1)$ as $k \to \infty$,

and then we will achieve the **'high frequency $O(1)$ CPU time algorithm'** holy grail.

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No! Unfortunately, $N = O(1) \not\Rightarrow$ CPU time $= O(1)$.

The Snag: our N^2 matrix entries are highly oscillatory integrals

When we use the **Galerkin method**, typical matrix entries in 3D are

$$\int_{\Gamma_{ij}} \int_{\Gamma_{mn}} \frac{1}{4\pi|x-y|} \exp[\mathrm{i}k(|x-y|+y\cdot d_i - x\cdot d_m)]\mathbf{b}_{ij}(y)\mathbf{b}_{mn}(x)\, ds(y)ds(x).$$

Each entry is a 4-dimensional, increasingly oscillatory integral as $k \to \infty$.

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Recent research on evaluation of oscillatory integrals is developing new tools – Filon quadrature-type methods and numerical stationary phase and steepest descent methods. See Iserles et al. 2006, Levin 1997, Bruno et al. 2004,2007, Huybrechs et al. 2006, Ganesh, Langdon, Sloan 2007, talks/poster by **Kim, Melenk** and preprints of **Melenk** and of **Dominguez, Graham, Smyshlyaev**.

How are people choosing d_i and b_{ij}??

$$\frac{\partial u}{\partial n}(x) \approx \sum_{i=1}^{M} \sum_{j=1}^{N_i} a_{ij} \exp(\mathrm{i}kx \cdot d_i)\mathbf{b}_{ij}(x),$$

with $a_{ij} \in \mathbb{C}$ the unknown coefficients,

$d_1, \ldots, d_N$ distinct unit vectors,

$\mathbf{b}_{ij}(x)$ **conventional BEM basis functions**.

Approach 1. M large – see e.g. work by **Trevelyan** et al. and cf. talk by **Monk**

Approach 2. $M = 1$.

Approach 3. M small, directions d_i carefully chosen to match high frequency solution behaviour.

How are people choosing d_i and b_{ij}??

$$\frac{\partial u}{\partial n}(x) \approx \exp(\mathrm{i}kx \cdot \hat{d}) \sum_{j=1}^{N^*} a_j \mathbf{b}_j(x),$$

with $\mathbf{b}_j(x)$ conventional BEM basis functions.

Approach 2. $M = 1$, with d the direction of the incident plane wave.

How are people choosing d_i and b_{ij}??

$$\frac{\partial u}{\partial n}(x) \approx \exp(\mathrm{i}kx \cdot d) \sum_{j=1}^{N^*} a_j \mathbf{b}_j(x),$$

with $\mathbf{b}_j(x)$ conventional BEM basis functions.

Approach 2. $M = 1$, with d the direction of the incident plane wave.

In other words, we remove oscillation by **factoring out the oscillation of the incident wave**. A slight variant is to write

$$\frac{\partial u}{\partial n}(y) = \frac{\partial u^i}{\partial n}(y) \times \mu(y)$$

and then approximate μ by a conventional BEM.

Approach 2. Remove oscillation by **factoring out the oscillation of the incident wave**, i.e.

$$\frac{\partial u}{\partial n}(y) = \frac{\partial u^i}{\partial n}(y) \times \mu(y) \quad (*)$$

and then approximate μ by a conventional BEM.

For **smooth convex obstacles** this should work well: equation $(*)$ holds with $F(y) \approx 2$ on the illuminated side and $F(y) \approx 0$ in the shadow zone (this is the high frequency **Kirchhoff** or **physical optics** approximation).

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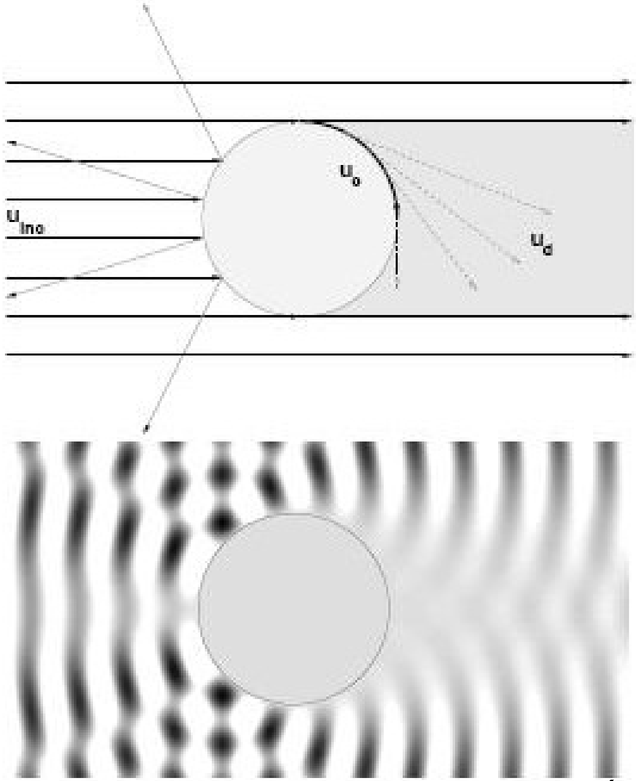
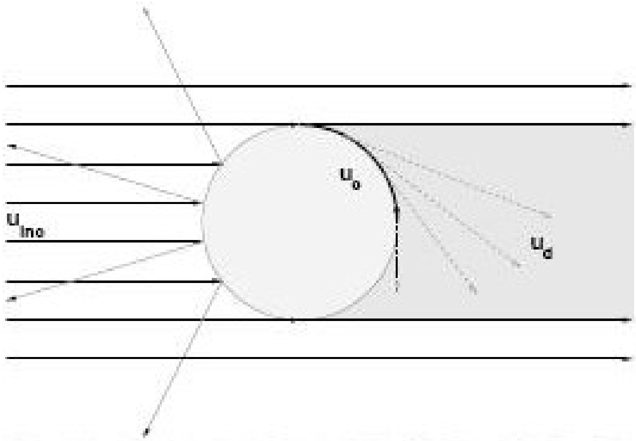
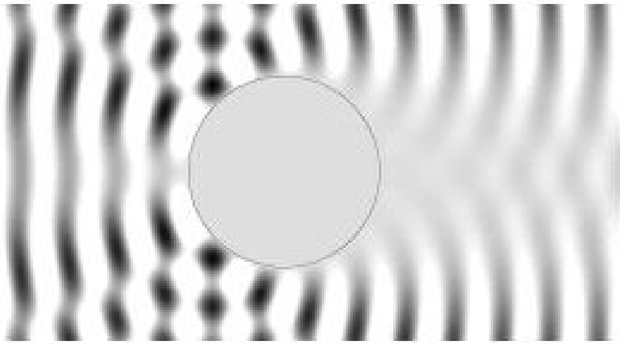
(Fig. from Motamed & Runborg (2007).)



Rigorous justification needs rigorous asymptotics (Melrose & Taylor 1985) which predicts on Γ:

- Kirchhoff approximation works on illuminated side, i.e. $\dfrac{\partial u}{\partial n} \approx 2\dfrac{\partial u^i}{\partial n}$ (for $u = 0$).





- on the shadow side there are creeping rays, with

$$\frac{\partial u^{creep}}{\partial n}(x) = A \exp(\mathrm{i}(ks - C_0 F(s) k^{1/3} s)) \exp(-C_1 F(s) k^{1/3} s),$$

  where C_0 and C_1 are known positive constants, s is arc-length, and $c_1 s \leq F(s) \leq c_2 s$

Approach 2. Remove oscillation by **factoring out the oscillation of the incident wave**, e.g.

$$\frac{\partial u}{\partial n}(y) = \frac{\partial u^i}{\partial n}(y) \times \mu(y) \quad (*)$$

and then approximate μ by a conventional BEM.

Dominguez, Graham Smyshlyaev 2007, **ignore the deep shadow zone (where field is zero), use a spectral approximation on the illuminated side, + extra spectral approximations in the transition zones of width $k^{-1/3}$.**

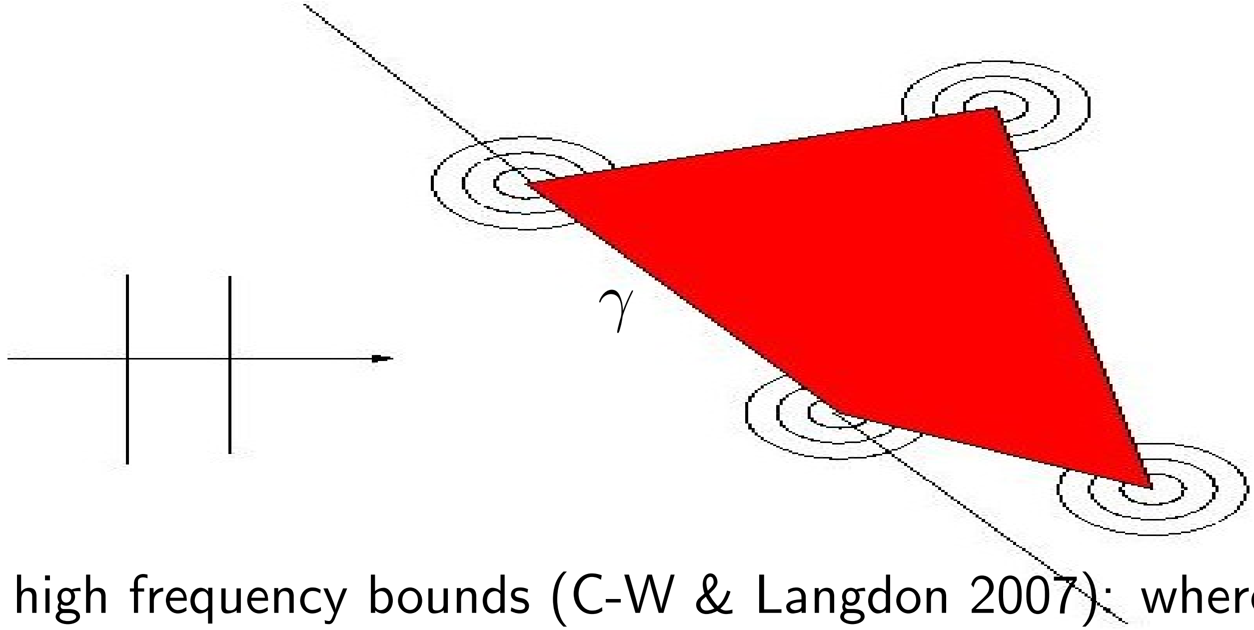
Numerics suggest $N = O(1)$ maintains accuracy as $k \to \infty$, and Dominguez et al. prove $N = O(k^{1/9+\epsilon})$ works.

How are people choosing d_i and $\mathbf{b}_{ij}$??

$$\frac{\partial u}{\partial n}(x) \approx \sum_{i=1}^{M} \sum_{j=1}^{N_i} a_{ij} \exp(\mathrm{i}kx \cdot d_i)\mathbf{b}_{ij}(x),$$

with $a_{ij} \in \mathbb{C}$ the unknown coefficients,
$d_1, \ldots, d_N$ distinct unit vectors,
$\mathbf{b}_{ij}(x)$ **conventional BEM basis functions**.

Approach 3 (2D so far). M small, directions d_i carefully chosen on the basis of the geometrical theory of diffraction to match high frequency solution behaviour.



Rigorous high frequency bounds (C-W & Langdon 2007): where s is distance along γ,

$$\frac{\partial u}{\partial n}(s) = 2\frac{\partial u^i}{\partial n}(s) + e^{iks}v_+(s) + e^{-iks}v_-(s)$$

where

$$k^{-n}|v_+^{(n)}(s)| \le \begin{cases} C_n(ks)^{-1/2-n}, & ks \ge 1, \\ C_n(ks)^{-\alpha-n}, & 0 < ks \le 1, \end{cases}$$

where $\alpha < 1/2$ depends on the corner angle.

$$\frac{\partial u}{\partial n}(s) \quad = \quad 2\frac{\partial u^i}{\partial n}(s) + \mathrm{e}^{\mathrm{i}ks}v_+(s) + \mathrm{e}^{-\mathrm{i}ks}v_-(s)$$

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Thus approximate

$$\frac{\partial u}{\partial n}(s) \quad \approx \quad 2\frac{\partial u^i}{\partial n}(s) + \mathrm{e}^{\mathrm{i}ks}V_+(s) + \mathrm{e}^{-\mathrm{i}ks}V_-(s),$$

where V_+ and V_- are piecewise polynomials on graded meshes, i.e. linear combinations of standard boundary element basis functions.

$$k^{-n}|v_+^{(n)}(s)| \leq \begin{cases} C_n(ks)^{-1/2-n}, & ks \geq 1, \\ C_n(ks)^{-\alpha-n}, & 0 < ks \leq 1, \end{cases}$$

Thus approximate

$$\frac{\partial u}{\partial n}(s) \quad \approx \quad 2\frac{\partial u^i}{\partial n}(s) + \mathrm{e}^{\mathrm{i}ks}V_+(s) + \mathrm{e}^{-\mathrm{i}ks}V_-(s),$$

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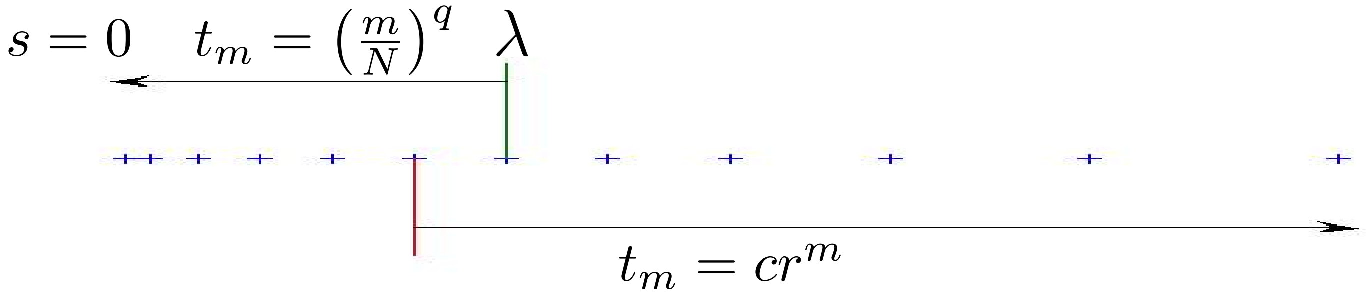

Thus approximate

$$\frac{\partial u}{\partial n}(s) \quad \approx \quad K.O. + \mathrm{e}^{\mathrm{i}ks} V_+(s) + \mathrm{e}^{-\mathrm{i}ks} V_-(s),$$

where V_+ and V_- are piecewise polynomials on graded meshes.

Theorem Where $\phi = \frac{\partial u}{\partial n}$, ϕ_N is the best L_2 approximation to ϕ from the approximation space, n is the number of sides, N the degrees of freedom, p the polynomial degree, and L the total arc-length,

$$k^{-1/2} ||\phi - \phi_N||_2 \leq C \sup_{x \in D} |u(x)| \frac{[n(1 + \log(kL/n))]^{p+3/2}}{N^{p+1}},$$

where C depends (only) on the corner angles and p.

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Use this approximation in a Galerkin method for

$$\frac{1}{2}\frac{\partial u}{\partial n}(x) + \int_\Gamma \left(\frac{\partial G(x,y)}{\partial n(x)} + \mathrm{i}\eta G(x,y) \right) \frac{\partial u}{\partial n}(y) ds(y) = f(x), \quad x \in \Gamma.$$

Table 1: Relative errors, $k = 10$

k	N (#dof)	$\|\phi - \phi_N\|_2 / \|\phi\|_2$	EOC
10	24	$1.12\times10^{+0}$	1.5
	48	4.05×10^{-1}	0.7
	88	2.55×10^{-1}	0.9
	176	1.40×10^{-1}	1.3
	360	5.52×10^{-2}	0.9
	712	3.04×10^{-2}	

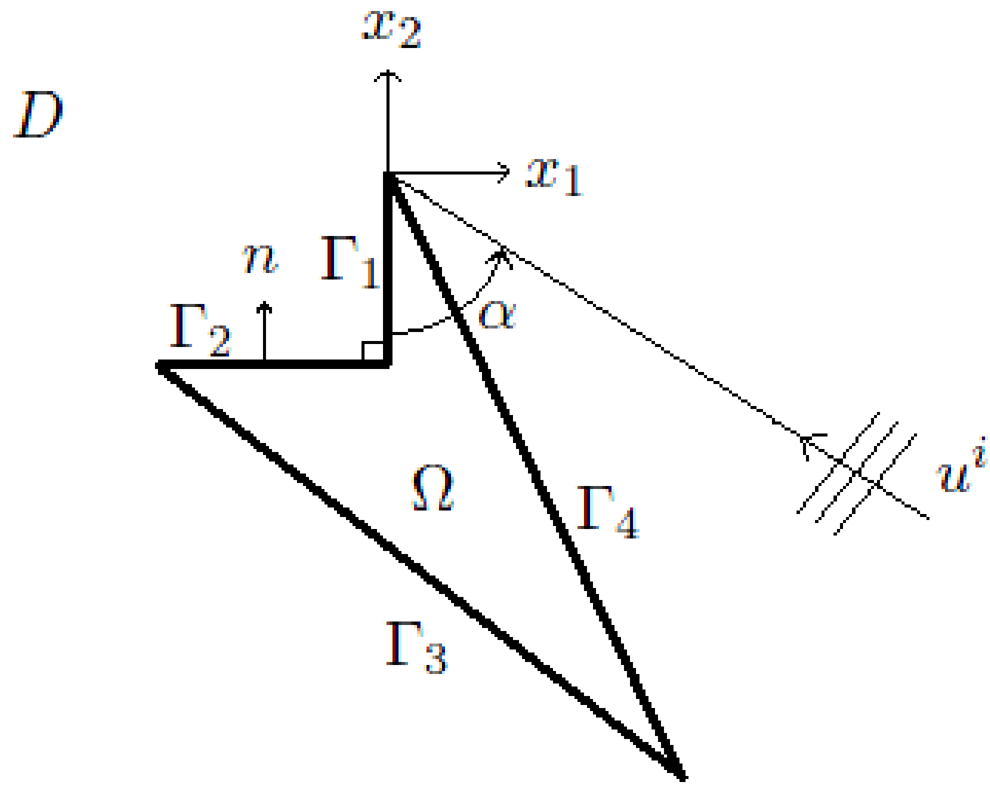
Table 2: Relative errors, $k = 160$

k	N (#dof)	$\|\phi - \phi_N\|_2 / \|\phi\|_2$	EOC
160	32	$1.04\times10^{+0}$	1.3
	56	4.24×10^{-1}	0.5
	120	3.04×10^{-1}	0.6
	240	2.05×10^{-1}	1.5
	472	7.38×10^{-2}	1.0
	944	3.70×10^{-2}	

Fully discrete hp-scheme of Langdon & Melenk with $N = 192$

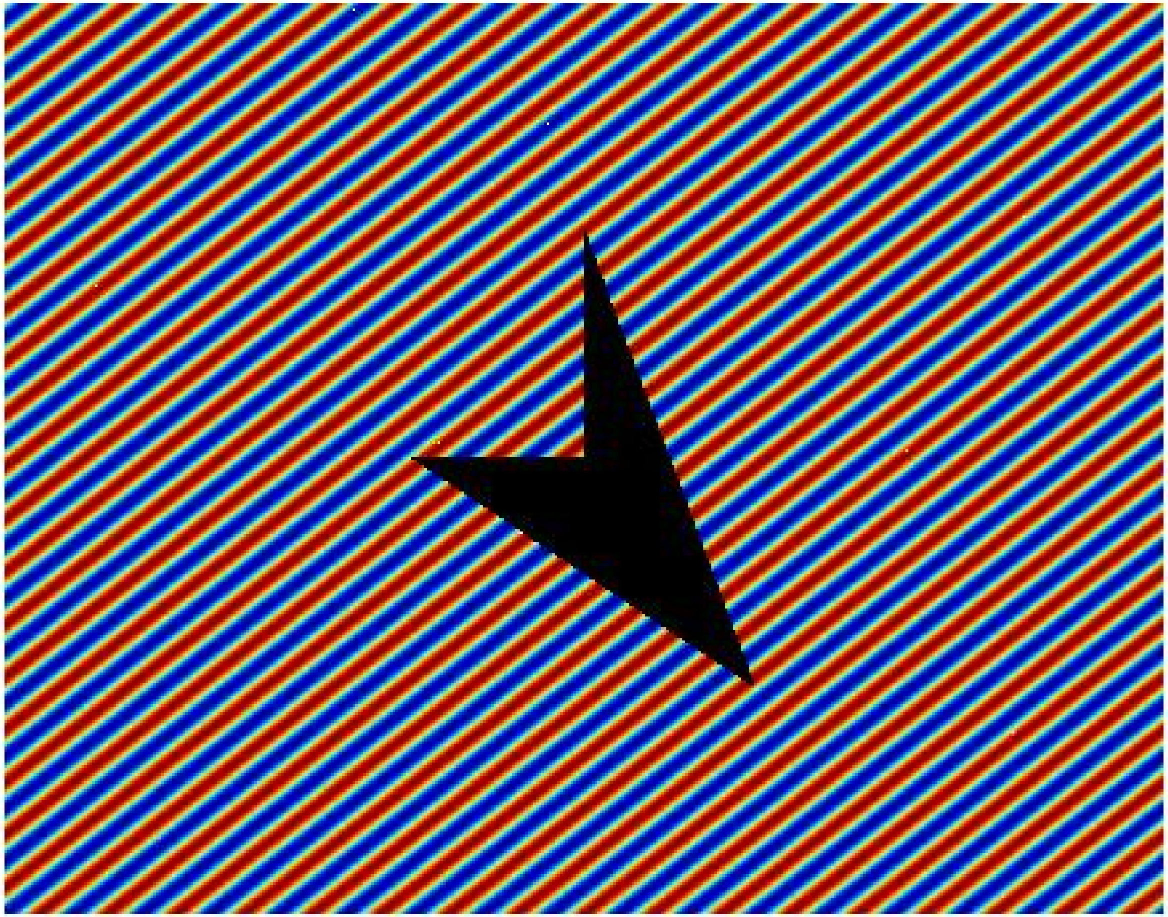
k	Relative L^2 error in $\dfrac{\partial u}{\partial n}$	Time (s)
10	1.46×10^{-2}	461
40	1.50×10^{-2}	615
160	1.55×10^{-2}	615
640	1.58×10^{-2}	732
2560	1.73×10^{-2}	844
10240	1.74×10^{-2}	940

Extension to Non-Convex Polygon (with Hewett, Langdon, Twigger)

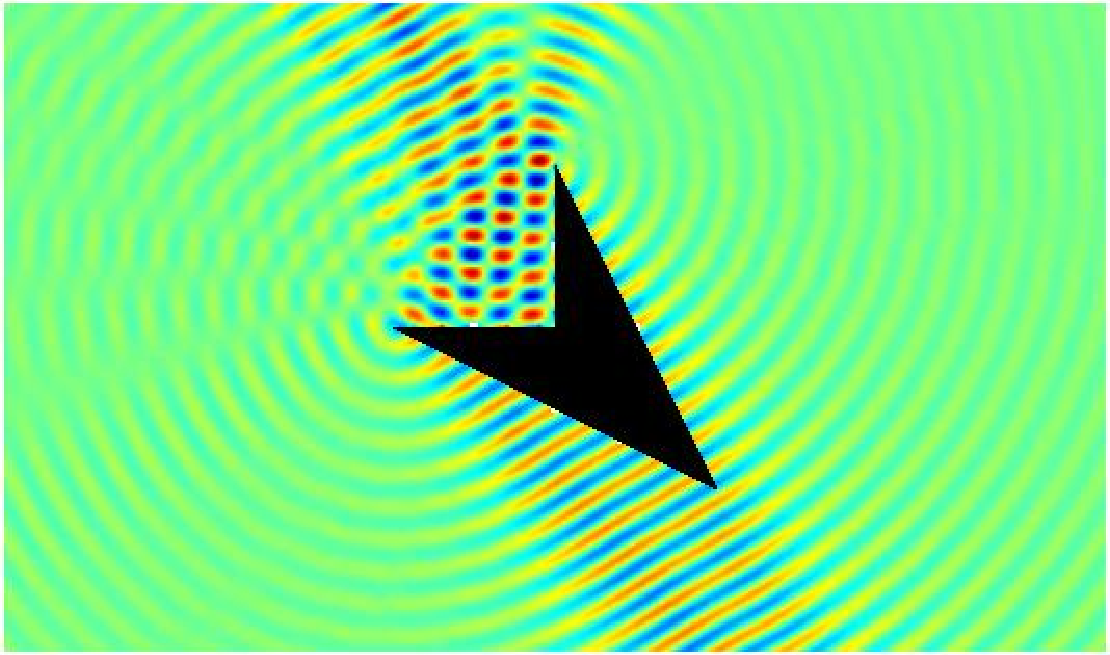


Can we understand the solution behaviour on the **'non-convex'** side Γ_2 and design an approximation space for $\dfrac{\partial u}{\partial n}$ on Γ_2 which needs $O(1)$ degrees of freedom as $k \to \infty$?

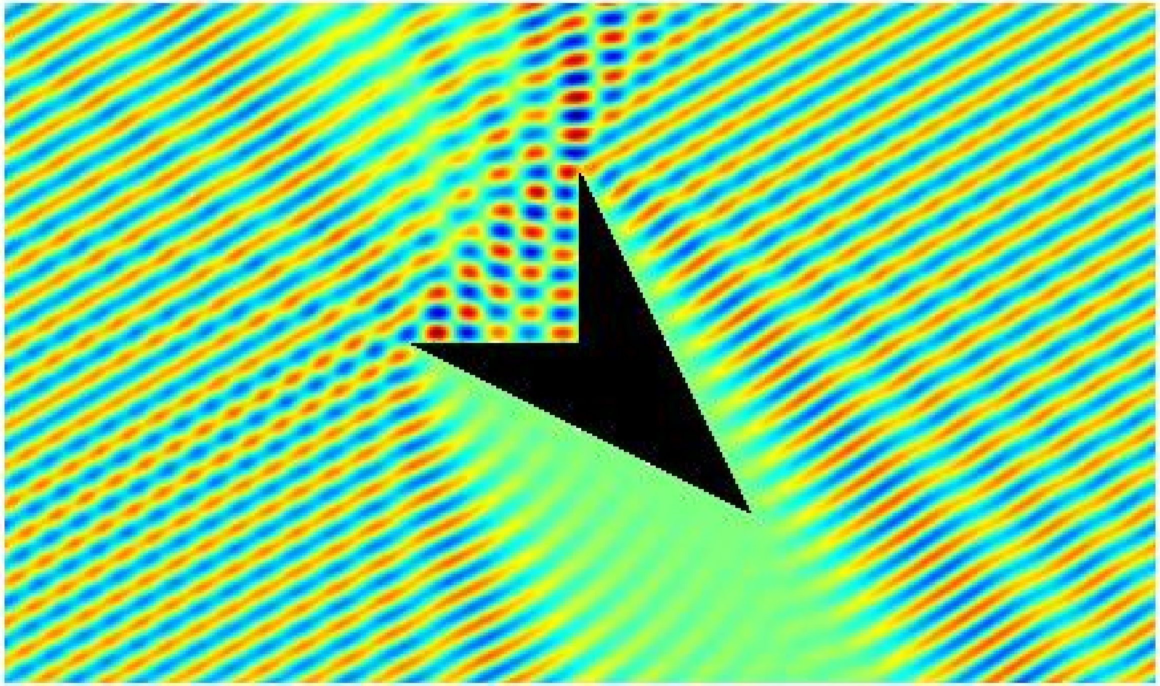
Solution Behaviour: Incident Field



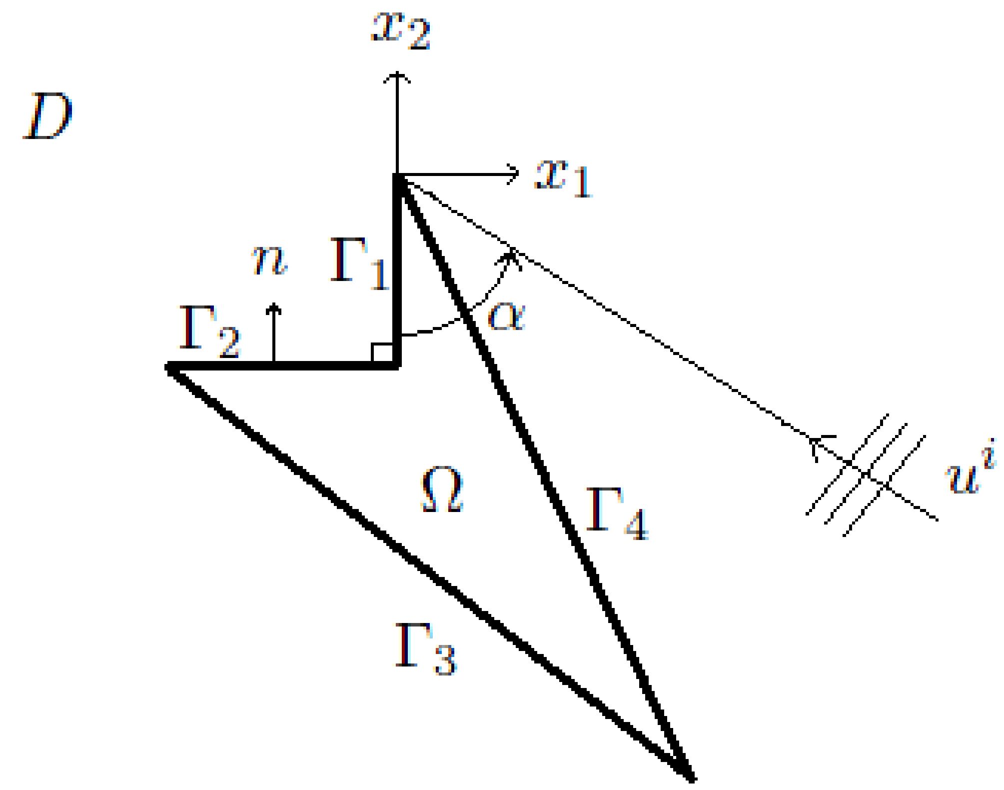
Solution Behaviour: Scattered Field



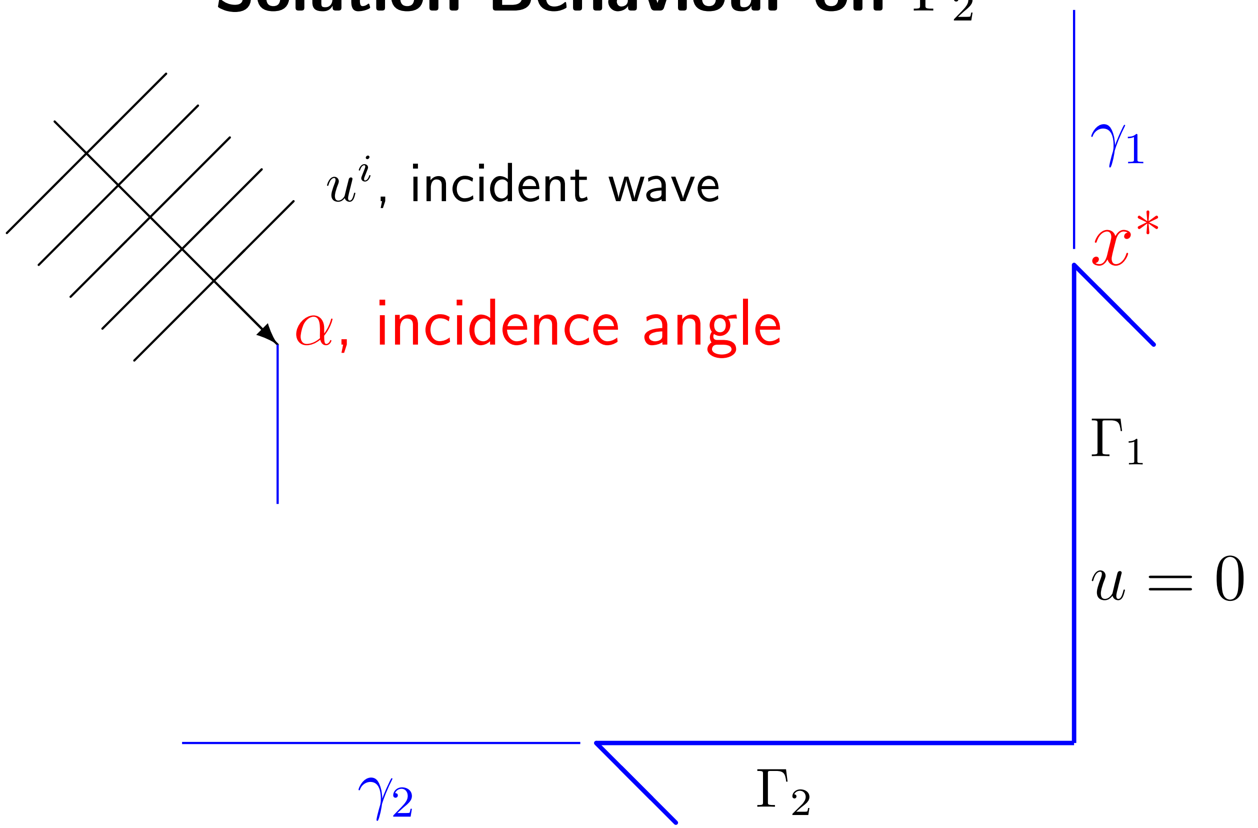
Solution Behaviour: Total Field



Solution Behaviour on Γ_2?



Solution Behaviour on Γ_2



On Γ_2,

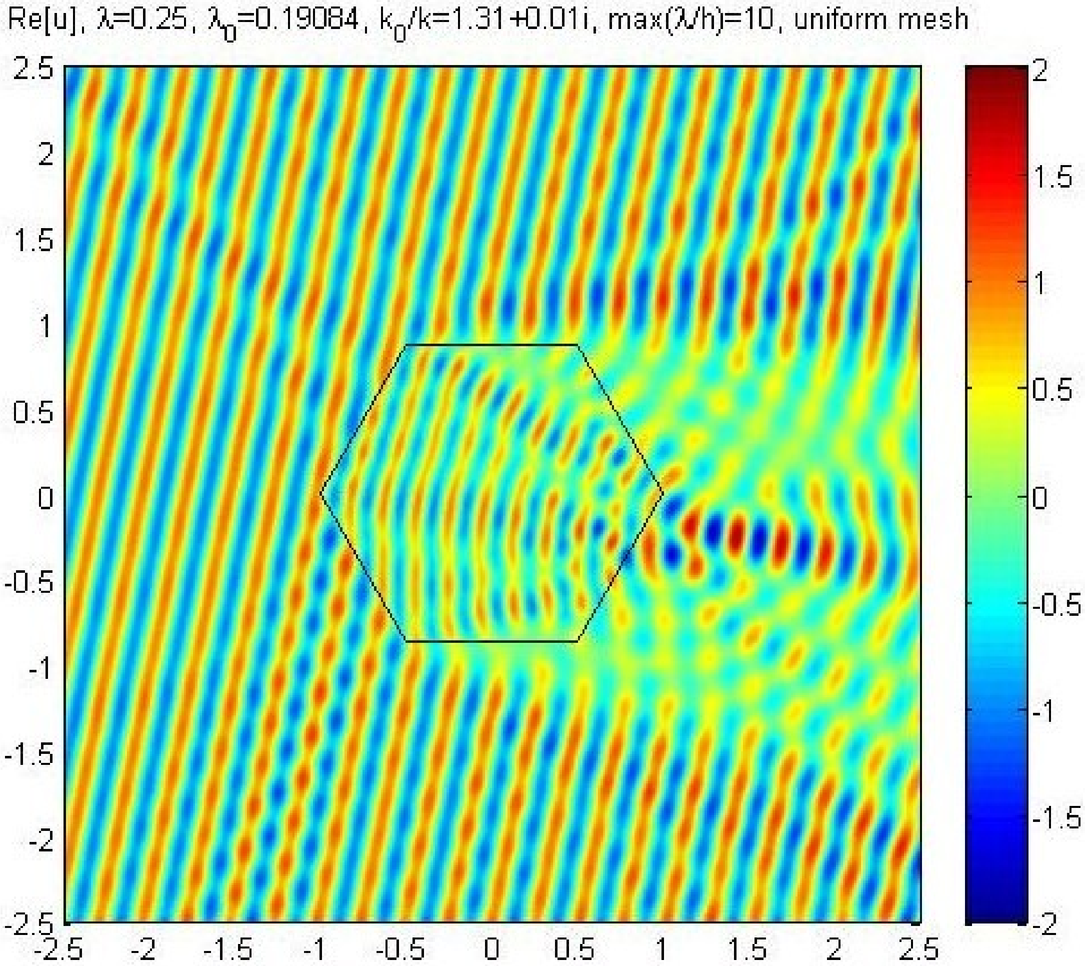
$$\frac{\partial u}{\partial n} = \text{known} + \mathrm{e}^{\mathrm{i}k|x-x^*|}F(x_1) + \mathrm{e}^{\mathrm{i}kx_1}v_+(x_1) + \mathrm{e}^{-\mathrm{i}kx_1}v_-(x_1)$$

where F and $v_\pm$ are analytic with bounds which grow only mildly with k, so that $N = O(\log k)$ as $k \to \infty$ is enough.

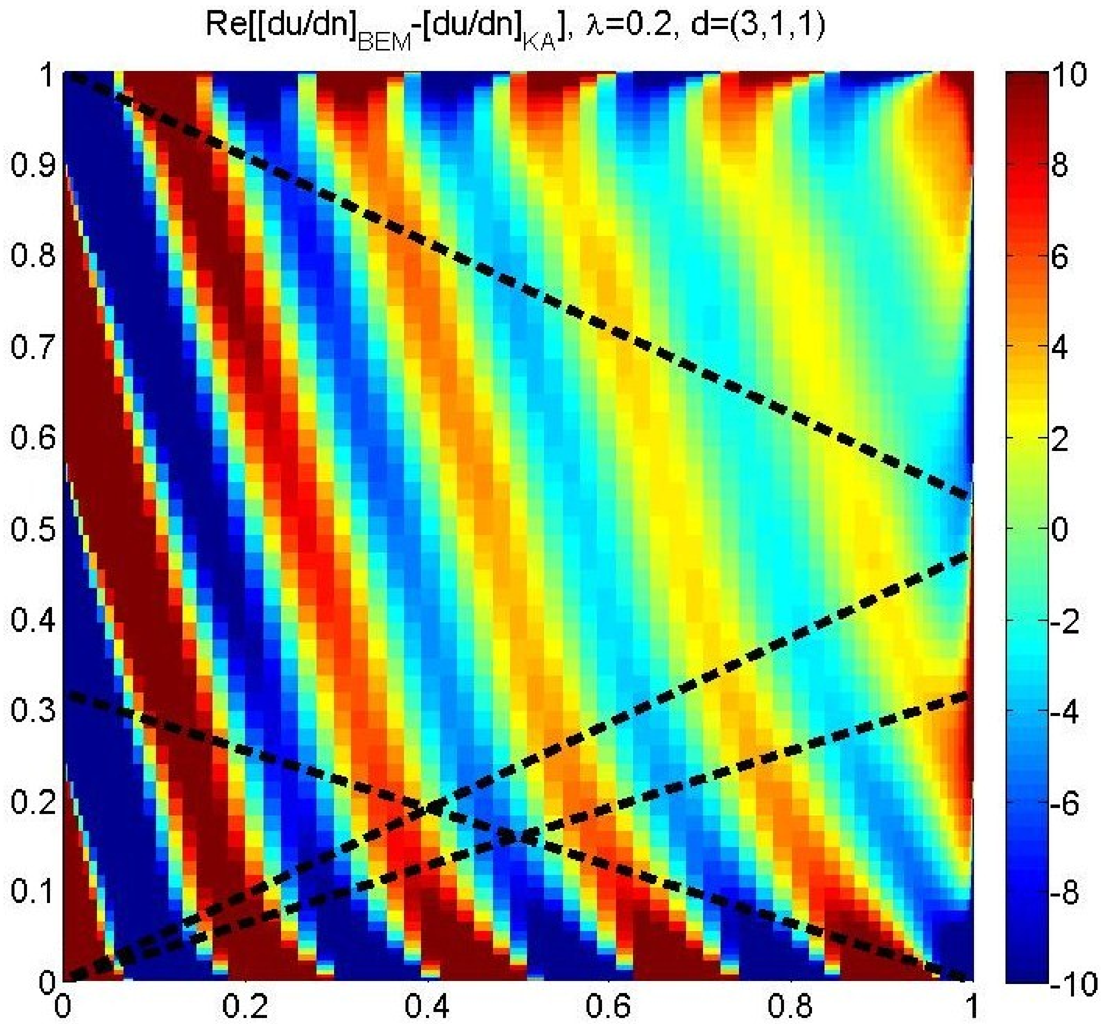
Preliminary Results: hp-BEM Based on this Ansastz

k	dof	dof per λ	L^2 error	Relative L^2 error
5	320	10.7	2.09e-2	1.51e-2
10	320	5.3	1.07e-2	1.11e-2
20	320	2.7	4.60e-3	6.91e-3
40	320	1.3	3.13e-3	6.83e-3

Extension to Transmission Problems - Motivated by Baran Talk (Betcke, Hewett, Langdon)



Extension to 3D - Square Plate (C-W, Hewett, Langdon)



Summary/Conclusions

We've reviewed recent work on BEM high frequency scattering that:

- Reduces the # D.O.F. by using oscillatory basis functions, e.g. plane waves $\times$ polynomials
- In many cases uses high frequency asymptotics, at least to deduce the **phases/oscillation** of components of the field
- Requires novel methods (e.g. numerical stationary phase) to evaluate the oscillatory integrals that arise
- Needs knowledge of rigorous high frequency asymptotics of solution and e.g. norms of integral operators and their inverses to prove complete numerical analysis results