An efficient Multigrid calculation of the Far field map for Helmholtz problems

11th International Conference on Mathematical and Numerical Aspects of Waves, 3-7 June 2013

TWNA Research Group, University of Antwerp

S. Cools*, B. Reps & W. Vanroose*

*Correspondence to: siegfried.cools@ua.ac.be, wim.vanroose@ua.ac.be.

Presentation contents

Quick overview

- Motivation: efficient Far field map computation
- Introduction: the Helmholtz equation
- The Far field map
- The Complex Contour method
- Solving the HH eqn. on a complex contour using multigrid
- Numerical validation & multigrid performance (2D-3D)
- Conclusions

Motivation: Far field map

Inverse scattering problems

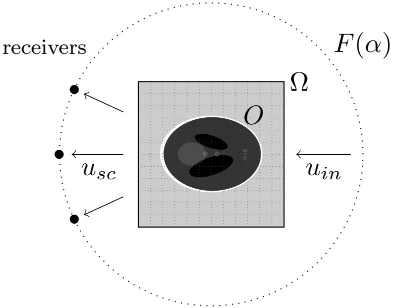
Iteratively solve

$$\min_i \|F_{data} - F_i\|,$$

where $F_i = \{$Far field maps of i-th approximation to the object for N incoming waves$\}$.

▷ Requires *many* forward problem solves = Far field map calculations from the direct scattering problem.

Far field amplitude data



Helmholtz equation

"Representation of the physics behind a wave scattering at an object χ defined on a compact area O located within a domain $\Omega \subset \mathbb{R}^d$."

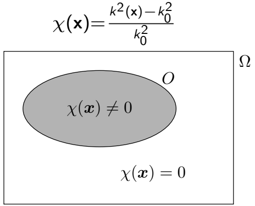
The total wave solution u_{tot} satisfies the homogeneous HH equation

$$\left(-\Delta - k^2(\mathbf{x})\right) u_{tot}(\mathbf{x}) = 0 \quad \text{on} \quad \Omega \subset \mathbb{R}^d, \quad d \geq 1,$$

with no wave source present within the domain. Space-dependent wave number function k defined as

$$k(\mathbf{x}) = \begin{cases} k(\mathbf{x}), & \text{for } \mathbf{x} \in O, \\ k_0, & \text{for } \mathbf{x} \in \Omega \setminus O, \end{cases}$$

where $k_0 \in \mathbb{R}$, $O \subset \Omega \subset \mathbb{R}^d$, O compact.



Helmholtz equation

Decomposition ($u_{in} = e^{ik_0\eta\cdot\mathbf{x}} =$ *incoming wave*, $u =$ *scattered wave*)

$$u_{tot} = u_{in} + u,$$

implies

$$\begin{aligned} & \left(-\Delta - k^2(\mathbf{x})\right) u_{tot}(\mathbf{x}) = 0 \\ \Rightarrow \quad & \left(-\Delta - k^2(\mathbf{x})\right) u(\mathbf{x}) = (\Delta + k^2(\mathbf{x}))u_{in}(\mathbf{x}) \\ \Rightarrow \quad & \left(-\Delta - k^2(\mathbf{x})\right) u(\mathbf{x}) = (k^2(\mathbf{x}) - k_0^2)u_{in}(\mathbf{x}), \end{aligned}$$

yielding the inhomogeneous *scattered wave equation*

$$\boxed{\left(-\Delta - k^2(\mathbf{x})\right) u(\mathbf{x}) = f(\mathbf{x}) \quad \text{on} \quad \Omega \subset \mathbb{R}^d,} \tag{1}$$

where $f(\mathbf{x}) = (k^2(\mathbf{x}) - k_0^2)u_{in}(\mathbf{x}) \doteq k_0^2\chi(\mathbf{x})u_{in}(\mathbf{x})$.

Helmholtz equation

Scattered wave equation (1)

$$\left(-\Delta - k^2(\mathbf{x})\right) u(\mathbf{x}) = f(\mathbf{x}) \quad \text{on} \quad \Omega \subset \mathbb{R}^d,$$

with $f(\mathbf{x}) = k_0^2 \chi(\mathbf{x}) u_{in}(\mathbf{x})$.

Solved for u on discretized subset $\Omega^N \subset \Omega$ ('numerical box') with outgoing wave boundary conditions, e.g. PML, ECS.

State-of-the-art iterative solvers:

multigrid-preconditioned Krylov methods

Elman Ernst O'Leary (2002)

Erlangga Oosterlee Vuik (2004) - Complex Shifted Laplacian (CSL)

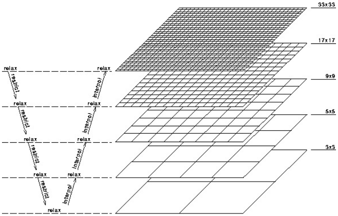
Reps Vanroose bin Zubair (2010) - Complex Stretched Grid (CSG)

Helmholtz equation & Multigrid

Two-grid correction scheme

- Relax ν_1 times on $A^h v^h = f^h$ (e.g. ω-Jacobi, Gauss-Seidel, ...).
- Compute $r^h = f^h - A^h v^h$, restrict $r^{2h} = I_h^{2h} r^h$, and solve
$$A^{2h} e^{2h} = r^{2h}.$$
- Interpolate $e^h = I_{2h}^h e^{2h}$ and correct $v^h \leftarrow v^h + e^h$.
- Relax ν_2 times on $A^h v^h = f^h$.

Multigrid V-cycle = recursion.

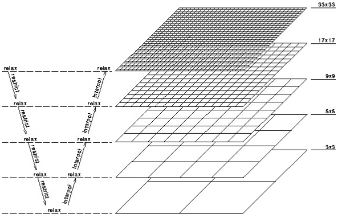


Helmholtz equation & Multigrid

Two-grid correction scheme

- Relax ν_1 times on $A^h v^h = f^h$ (e.g. ω-Jacobi, Gauss-Seidel, …).
- Compute $r^h = f^h - A^h v^h$, restrict $r^{2h} = I_h^{2h} r^h$, and solve
$$A^{2h} e^{2h} = r^{2h}.$$
- Interpolate $e^h = I_{2h}^h e^{2h}$ and correct $v^h \leftarrow v^h + e^h$.
- Relax ν_2 times on $A^h v^h = f^h$.

Multigrid V-cycle = recursion.



NOTE: multigrid cannot solve HH scattering system (1), only preconditioning systems! (CSL/CSG)

Ernst Gander (2012)

Far field mapping

Assume $$\left(-\Delta - k^2(\mathbf{x})\right) u^N(\mathbf{x}) = k_0^2 \chi(\mathbf{x}) u_{in}(\mathbf{x}) \quad \text{for } \mathbf{x} \in \Omega,$$

$$\left(-\Delta - k_0^2\right)\, u(\mathbf{x}) = g(\mathbf{x}) \qquad \text{for } \mathbf{x} \in \mathbb{R}^d,$$

where $g(\mathbf{x}) \doteq k_0^2 \chi(\mathbf{x})(u_{in}(\mathbf{x}) + u^N(\mathbf{x}))$.

Analytical solution using Helmholtz Green's function:

$$\begin{aligned} u(\mathbf{x}) &= \int_{\mathbb{R}^d} G(\mathbf{x}, \mathbf{x}')\, g(\mathbf{x}')\, d\mathbf{x}' \\ &= \int_{\Omega} G(\mathbf{x}, \mathbf{x}')\, k_0^2 \chi(\mathbf{x}') \left(u_{in}(\mathbf{x}') + u^N(\mathbf{x}')\right) d\mathbf{x}', \quad \mathbf{x} \in \mathbb{R}^d. \end{aligned}$$

▷ Calculate u in any point $\mathbf{x} \in \mathbb{R}^d$ *outside* the numerical box, using only the information *inside* the numerical box.

Far field mapping

Let $\mathbf{x} = (\boldsymbol{\alpha}, \rho)$ be given by a unit vector $\boldsymbol{\alpha} \in \mathbb{R}^d$ and length $\rho \in \mathbb{R}$. Asymptotic form of $G(\mathbf{x}, \mathbf{x}')$ (separable) yields the far field ($\rho \to \infty$) wave pattern for u

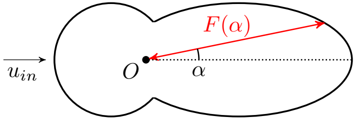
$$\lim_{\rho\to\infty} u(\rho, \boldsymbol{\alpha}) = D(\rho)F(\boldsymbol{\alpha}), \qquad \boldsymbol{\alpha} \in \mathbb{R}^d,$$

where

$$F(\boldsymbol{\alpha}) = \int_\Omega e^{-ik_0 \mathbf{x}' \cdot \boldsymbol{\alpha}} g(\mathbf{x}')\, d\mathbf{x}'. \tag{2}$$

is the *far field amplitude map*.

2D schematic:



Far field mapping

Note that the far field integral can be split into a sum of two contributions: $F(\boldsymbol{\alpha}) = I_1 + I_2$, with

$$I_1 = \underbrace{\int_\Omega e^{-ik_0 \mathbf{x}\cdot\boldsymbol{\alpha}} \chi(\mathbf{x}) u_{in}(\mathbf{x}) d\mathbf{x}}_{\text{all factors known explicitely}} \quad \text{and} \quad I_2 = \underbrace{\int_\Omega e^{-ik_0 \mathbf{x}\cdot\boldsymbol{\alpha}} \chi(\mathbf{x}) u^N(\mathbf{x}) d\mathbf{x}}_{\text{requires } u^N(\mathbf{x}) \text{ for } x \in \Omega \text{ !}}$$

Far field mapping

Note that the far field integral can be split into a sum of two contributions: $F(\boldsymbol{\alpha}) = I_1 + I_2$, with

$$\underbrace{I_1 = \int_\Omega e^{-ik_0\mathbf{x}\cdot\boldsymbol{\alpha}}\chi(\mathbf{x})u_{in}(\mathbf{x})d\mathbf{x}}_{\text{all factors known explicitely}} \quad \text{and} \quad \underbrace{I_2 = \int_\Omega e^{-ik_0\mathbf{x}\cdot\boldsymbol{\alpha}}\chi(\mathbf{x})u^N(\mathbf{x})d\mathbf{x}}_{\text{requires } u^N(\mathbf{x}) \text{ for } x\in\Omega\ !}$$

Summary: Far field map calculation in a nutshell:

- Step 1. Solve the HH eqn. (1) for u to obtain a solution u^N on a numerical domain.
- Step 2. Calculate/approximate the Fourier integral (2) on the given numerical domain.

Far field mapping

Note that the far field integral can be split into a sum of two contributions: $F(\boldsymbol{\alpha}) = I_1 + I_2$, with

$$I_1 = \underbrace{\int_\Omega e^{-ik_0\mathbf{x}\cdot\boldsymbol{\alpha}}\chi(\mathbf{x})u_{in}(\mathbf{x})d\mathbf{x}}_{\text{all factors known explicitely}} \quad \text{and} \quad I_2 = \underbrace{\int_\Omega e^{-ik_0\mathbf{x}\cdot\boldsymbol{\alpha}}\chi(\mathbf{x})u^N(\mathbf{x})d\mathbf{x}}_{\text{requires } u^N(\mathbf{x}) \text{ for } x\in\Omega\ !}$$

Summary: Far field map calculation in a nutshell:

- Step 1. Solve the HH eqn. (1) for u to obtain a solution u^N on a numerical domain.

main computational bottleneck

- Step 2. Calculate/approximate the Fourier integral (2) on the given numerical domain.

Far field mapping

Extension to χ analytical

Far field map definition (2) relies on the object of interest χ having compact support; however,

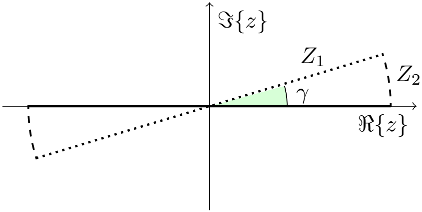
> **Theorem:** Let $U = \{f : \mathbb{R}^d \to \mathbb{R}\,\text{comp. supp.}\}$ and $V = \{f : \mathbb{R}^d \to \mathbb{R},$ f analytical $\mid \forall \varepsilon > 0, \exists K \subset \mathbb{R}^d$ compact, $\forall x \in \mathbb{R}^d \setminus K : |f(x)| < \varepsilon\}$, then $U \subset V$ dense.
>
> **Proof:** using notion of compactly supported, non-analytical, C^∞ bump functions, cf. Mead Delves (1973).

Hence, the far field mapping $F(\alpha)$ (2) is well-defined for analytical object functions χ that vanish at infinity.

Complex contour method

For u and χ analytical the far field integral

$$I_2 = \int_\Omega e^{-ik_0 \mathbf{x}\cdot\boldsymbol{\alpha}} \chi(\mathbf{x}) \underbrace{u^N(\mathbf{x})}_{\text{difficulty}} \, d\mathbf{x}$$



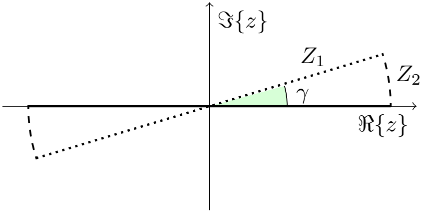
can be calculated over a **complex contour** $Z = Z_1 + Z_2$, rather than over the real domain Ω, i.e.

$$I_2 = \underbrace{\int_{Z_1} e^{-ik_0 \mathbf{z}\cdot\boldsymbol{\alpha}} \chi(\mathbf{z}) u^N(\mathbf{z}) d\mathbf{z}}_{\text{requires } u^N(\mathbf{z}) \text{ for } \mathbf{z} \in Z_1 \text{ !}} + \int_{Z_2} e^{-ik_0 \mathbf{z}\cdot\boldsymbol{\alpha}} \chi(\mathbf{z}) u^N(\mathbf{z}) d\mathbf{z}.$$

Complex contour method

For u and χ analytical the far field integral

$$I_2 = \int_\Omega e^{-ik_0 \mathbf{x}\cdot\boldsymbol{\alpha}} \chi(\mathbf{x}) \underbrace{u^N(\mathbf{x})}_{\text{difficulty}} \, d\mathbf{x}$$



can be calculated over a **complex contour** $Z = Z_1 + Z_2$, rather than over the real domain Ω, i.e.

$$I_2 = \underbrace{\int_{Z_1} e^{-ik_0 \mathbf{z}\cdot\boldsymbol{\alpha}} \chi(\mathbf{z}) u^N(\mathbf{z}) d\mathbf{z}}_{\text{requires } u^N(\mathbf{z}) \text{ for } \mathbf{z} \in Z_1 \ !} + \int_{Z_2} \cancel{e^{-ik_0 \mathbf{z}\cdot\boldsymbol{\alpha}} \chi(\mathbf{z})} u^N(\mathbf{z}) d\mathbf{z}.$$

Solving HH eqn. on complex contour

Complex Shifted Laplacian (CSL) system with $\beta \in \mathbb{R}$

$$\left(-\Delta - (1+i\beta)k^2(\mathbf{x})\right) u(\mathbf{x}) = f(\mathbf{x})$$

is efficiently solvable using multigrid. Erlangga Oosterlee Vuik (2004)
Discretized:

$$-\left(\frac{1}{h^2} L + (1+i\beta)k^2\right) u_h = b_h,$$

with L = Laplacian stencil matrix. Division by $(1+i\beta)$ yields

$$-\left(\frac{1}{(1+i\beta)h^2} L + k^2\right) u_h = \frac{b_h}{1+i\beta} \tag{3}$$

= the original HH system discretized with $\tilde{h} = \sqrt{1+i\beta}\, h \doteq \rho e^{i\gamma} h$.
Reps Vanroose bin Zubair (2010)

Solving HH eqn. on complex contour

Erlangga Oosterlee Vuik (2006)

Cools Vanroose (2013)

Rule-of-thumb for CSL

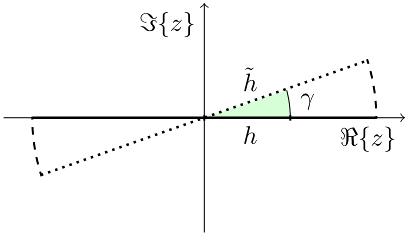
HH system (3) can be efficiently solved using multigrid for $\beta > 0.5$.

Conversion to angle γ

$$\sqrt{1+\beta i} \doteq \rho exp(i\gamma)$$

$$\tilde{h} = \sqrt{1+i\beta}\, h = \rho \exp(i\gamma) h$$

$$\Leftrightarrow \ \gamma = \frac{\arctan(\beta)}{2} \underset{\beta=0.5}{\approx} 13.28^\circ$$



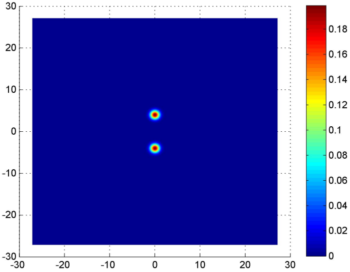
Note: softened to $\gamma \approx 9.5^\circ$ with GMRES as smoother substitute.

Numerical validation (2D)

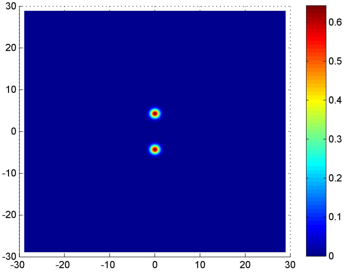
$$\chi(x,y) = -\frac{1}{5}\left(e^{-(x^2+(y-4)^2)} + e^{-(x^2+(y+4)^2)}\right)$$

Object of interest $|\chi|$ (modulus)

Real domain with ECS $|\chi(\mathbf{x})|$
($\theta_{ECS} = 45°$)



Complex contour $|\chi(\mathbf{z})|$
($\gamma = 14.6°$)

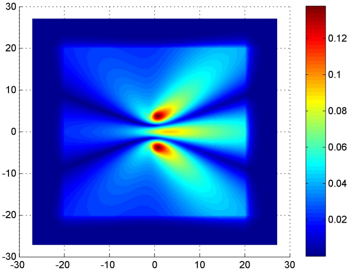


Numerical validation (2D)

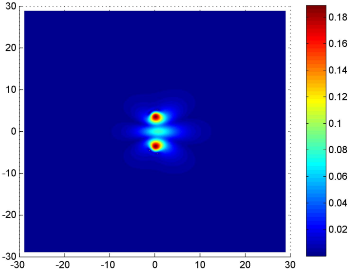
$$\chi(x,y) = -\frac{1}{5}\left(e^{-(x^2+(y-4)^2)} + e^{-(x^2+(y+4)^2)}\right)$$

Scattered wave solution $|u|$

Real domain with ECS $|u(\mathbf{x})|$
LU factorization



Complex contour $|u(\mathbf{z})|$
V(1,1) cycles ($tol_{res} = 10^{-6}$)

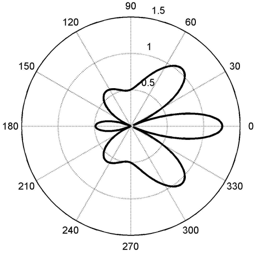


Numerical validation (2D)

$$\chi(x,y) = -\frac{1}{5}\left(e^{-(x^2+(y-4)^2)} + e^{-(x^2+(y+4)^2)}\right)$$

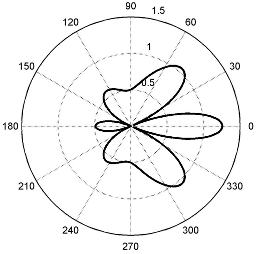
Far field amplitude map

Real domain with ECS $F(\alpha)$



$$\frac{\|F_{re} - F_{ex}\|_2}{\|F_{ex}\|_2} = \texttt{9.37e-5}$$

Complex contour $F(\alpha)$



$$\frac{\|F_{co} - F_{ex}\|_2}{\|F_{ex}\|_2} = \texttt{1.39e-4}$$

Multigrid performance (3D)

Solving the HH system - complex contour $\gamma = 10^\circ$
GMRES(3)-smoothed V(1,1) cycles ($tol_{res} = 10^{-6}$)

$n_x \times n_y \times n_z$	16^3	32^3	64^3	128^3	256^3
$k_0 = 1/4$	**10** (0.79s.) 0.24	**9** (4.65s.) 0.20	**9** (44.2s.) 0.21	**9** (352s.) 0.20	**9** (2778s.) 0.20
$k_0 = 1/2$	12 (0.92s.) 0.31	**10** (4.96s.) 0.24	**10** (48.3s.) 0.22	**10** (390s.) 0.23	**9** (2797s.) 0.21
$k_0 = 1$	7 (0.62s.) 0.13	13 (6.59s.) 0.32	**11** (54.6s.) 0.27	**10** (387s.) 0.24	**10** (3079s.) 0.24
$k_0 = 2$	2 (0.28s.) 0.00	8 (4.24s.) 0.14	13 (63.9s.) 0.33	**11** (428s.) 0.27	**10** (3006s.) 0.24
$k_0 = 4$	1 (0.20s.) 0.00	2 (1.35s.) 0.00	7 (36.1s.) 0.12	13 (503s.) 0.33	**11** (3306s.) 0.26

Multigrid performance (3D)

Solving the HH system - complex contour $\gamma = 10^\circ$

GMRES(3)-smoothed V(1,1) cycles ($tol_{res} = 10^{-6}$)

$k_0 h = 0.625$

$n_x \times n_y \times n_z$	16^3	32^3	64^3	128^3	256^3
$k_0 = 1/4$	**10** (0.79s.) 0.24	**9** (4.65s.) 0.20	**9** (44.2s.) 0.21	**9** (352s.) 0.20	**9** (2778s.) 0.20
$k_0 = 1/2$	12 (0.92s.) 0.31	**10** (4.96s.) 0.24	**10** (48.3s.) 0.22	**10** (390s.) 0.23	**9** (2797s.) 0.21
$k_0 = 1$	7 (0.62s.) 0.13	13 (6.59s.) 0.32	**11** (54.6s.) 0.27	**10** (387s.) 0.24	**10** (3079s.) 0.24
$k_0 = 2$	2 (0.28s.) 0.00	8 (4.24s.) 0.14	13 (63.9s.) 0.33	**11** (428s.) 0.27	**10** (3006s.) 0.24
$k_0 = 4$	1 (0.20s.) 0.00	2 (1.35s.) 0.00	7 (36.1s.) 0.12	13 (503s.) 0.33	**11** (3306s.) 0.26

Multigrid performance (3D)

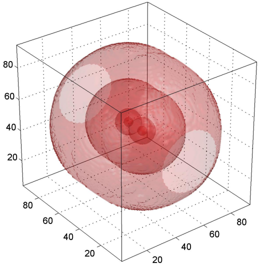
Solving the HH system $(k_0 = 1)$ - complex contour $\gamma = 10^\circ$
GMRES(3)-smoothed FMG(1,1) cycle

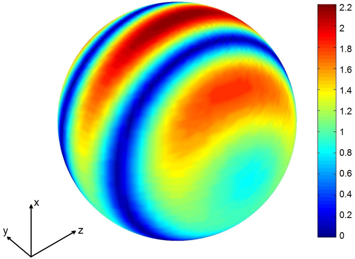
$n_x \times n_y \times n_z$	16^3	32^3	64^3	128^3	256^3
CPU time	0.20 s.	0.78 s.	6.24 s.	53.3 s.	462 s.
$\|r\|_2$	3.3e-5	7.9e-5	2.7e-5	1.1e-5	4.6e-6

Intel® Core™ i7-2720QM 2.20GHz CPU, 6MB Cache, 8GB RAM.

Multigrid performance (3D)

Solving the HH system ($k_0 = 1$) - complex contour $\gamma = 10^\circ$
GMRES(3)-smoothed FMG(1,1) cycle





Intel® Core™ i7-2720QM 2.20GHz CPU, 6MB Cache, 8GB RAM.

Conclusions

- We have developed a novel highly efficient calculation method for the far field map resulting from d-dimensional Helmholtz scattering problems
- Based on a reformulation of the classical Green's function integral to an equivalent integral over a complex valued domain
- *Advantage:* very efficient multigrid scattered wave solution of the Helmholtz problem on a complex domain (cf. CSL)

  $\rightarrow$ overcomes the main computational difficulty
- *Advantage:* increasingly performant on larger domains (k_0-scalabilty) and in higher spatial dimensions
- *Restriction:* Space-dependent wave number $k(\mathbf{x})$ analytical

Outlook

Current and future work (may) include(s):

- Optimizing the shape of the contour w.r.t. the object function. Does it work for all functions χ?

  $\rightarrow$ cf. work by D. Huybrechs (KULeuven, Belgium): path of steepest descent for oscillatory integrals

- Application of the proposed method to (other) practical scattering problem types, e.g. molecular break-up reactions (6D-9D Schrödinger's equation)

  $\rightarrow$ subsequent talk by W. Vanroose.

References

[1] Y.A. Erlangga, C.W. Oosterlee and C. Vuik. A novel multigrid based preconditioner for heterogeneous Helmholtz problems. *SIAM Journal on Scientific Computing* 27(4):1471–1492, 2006.

[2] D. Huybrechs and S. Vandewalle. On the evaluation of highly oscillatory integrals by analytic continuation. *SIAM Journal on Numerical Analysis* 44(3):1026–1048, 2006.

[3] W. Vanroose, D.A. Horner, F. Martin, T.N. Rescigno and C.W. McCurdy. Double photoionization of aligned molecular hydrogen. *Physical Review A*, 74(5):052702, 2006.

[4] B. Reps, W. Vanroose and H. bin Zubair. On the indefinite Helmholtz equation: Complex stretched absorbing boundary layers, iterative analysis, and preconditioning. *Journal of Computational Physics* 229(22):8384–8405, 2010.

[5] S. Cools, B. Reps and W. Vanroose. An efficient multigrid method calculation of the far field map for Helmholtz problems. *In preparation.* arXiv:1211.4461v2, 2013.