Solving Time-Harmonic Scattering Problems by the Ultra Weak Variational Formulation

Plane waves as basis functions

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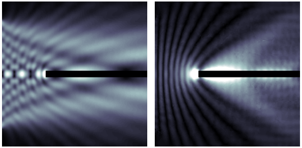
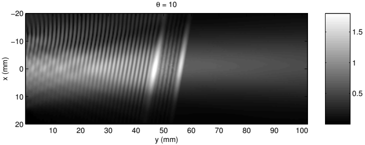
Outline

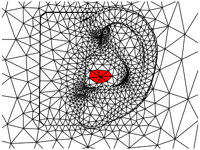
1. Introduction
   - Acoustic Problems
   - The Helmholtz Equation
   - Decisions, decisions...
2. Derivation of the UWVF
   - The Mesh and Continuity
   - Variational Formulation (UWVF)
   - The discrete UWVF
3. Numerical Results
   - 2D Results and Conditioning
   - Improving the ABC
   - Parallelization
   - FEMLAB and Another Example

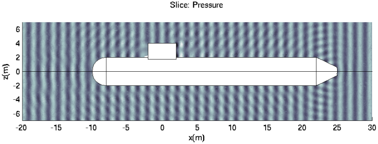
Outline

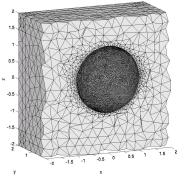
Computational Acoustics Examples [Huttunen]

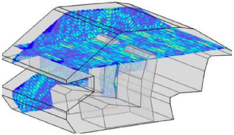












Acoustic Scattering

Given the shape and acoustic properties of an object, predict how it interacts with acoustic waves at a single frequency.

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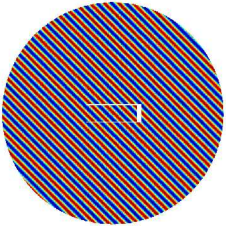

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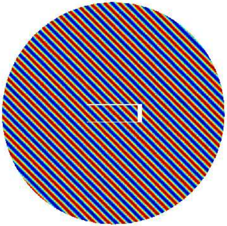
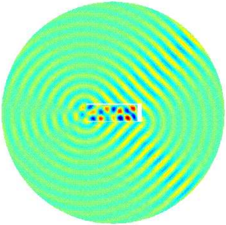


Incident



Scattered

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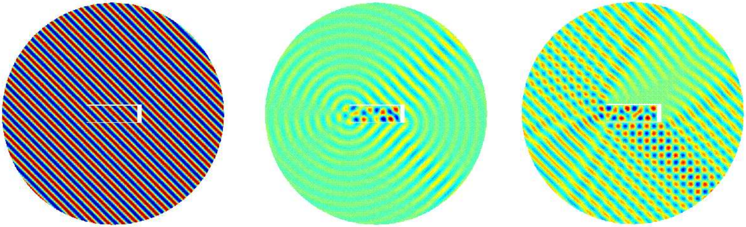


Incident Scattered Total

Outline

Helmholtz Equation

Given a bounded doman Ω the pressure field is $P(\boldsymbol{x}, t) = p(\boldsymbol{x}) \exp(i\omega t)$ where p satisfies

$$\nabla \cdot \rho^{-1} \nabla p + \kappa^2 \rho^{-1} p = 0 \text{ in } \Omega$$

where ρ is the density and the wave number (complex!) is given by $\kappa = \omega / c + i\alpha$ where c is the speed of sound and α is the absorption coefficient. Boundary condition

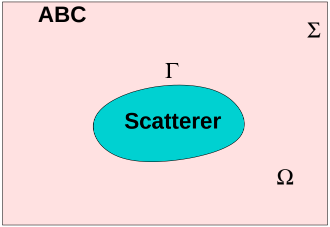
$$\left(\rho^{-1} \frac{\partial p}{\partial n} - i\sigma p \right) = Q \left(\rho^{-1} \frac{\partial p}{\partial n} + i\sigma p \right) + g$$

on the boundary $\partial\Omega$ where g is data, $|Q| \leq 1$ and $\sigma \in \mathbb{R}$

A Model Scattering Problem

Let $\Omega \subset \mathbb{R}^3$ (or $\mathbb{R}^2$) with disjoint boundaries Γ and Σ.
Approximate u which satisfies

$$\begin{aligned} \Delta u + \kappa^2 u &= 0 \text{ in } \Omega \\ u &= g \text{ on } \Gamma \; (Q = 1) \\ \frac{\partial u}{\partial \nu} - iku &= 0 \text{ on } \Sigma \; (Q = 0) \end{aligned}$$



where g describes the incoming plane wave. The region Ω is meshed with tetrahedra and the UWVF applied there.
ABC = Absorbing Boundary Condition

Outline

Possible methods

- Integral equations. Handle unbounded media, complex shapes. There are fast solvers but they are difficult to program and complex for penetrable media, coatings, narrow objects....
- **Finite elements.** Higher order needed to handle dispersion and becomes expensive at short wavelength. Geometry and complex materials handled. Difficult to solve the linear system and handle unbounded domains.

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The big decision

Motivated by medical ultrasound applications (complex structure, short wavelength) we decided on the following:

- A volume based method (finite element grid)
- Special shape functions (“basis functions”) that are solutions of the Helmholtz equation on each element.

Methods using special basis functions

- Partition of unity finite element method = PUFEM (Babuška and Melenk 1997, Keller and Giladi 2001, Huttenen, Gamallo and Astley 2005, Kim et al 2005)
- Least squares method (Trefftz, Monk and Wang 1999, Desmet 2002)
- Discontinuous enrichment method (Farhat et al. 2001, 2003, 2005)
- Plane wave augmented basis in integral equations (Darrigrand 2001, Perrey-Debain et al. 2002, Chandler-Wilde and Langdon 2004/5,...)
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The Mesh

Approximate the domain Ω by a tetrahedral finite element mesh consisting of N_h tetrahedra Ω_k, $k = 1, \cdots, N_h$ of maximum diameter h.

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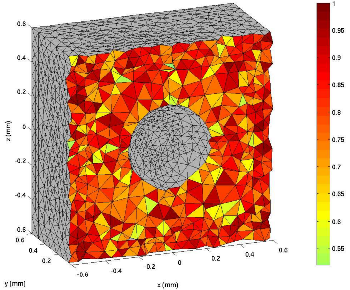

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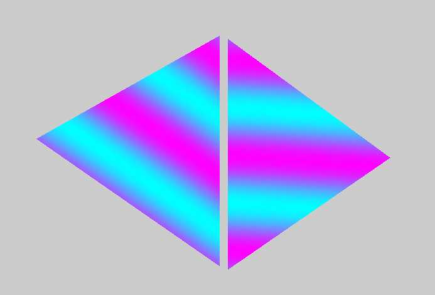

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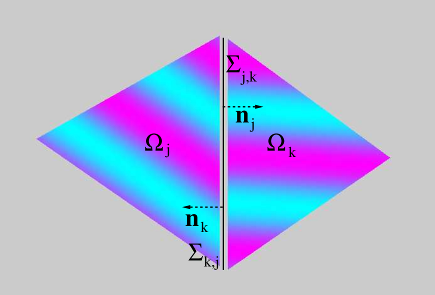

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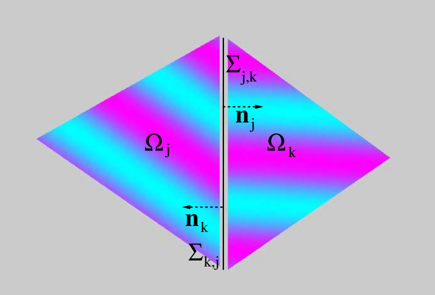

Major restriction: ρ and κ must be piecewise constant and constant on each element.

Required continuity between elements

Let $p_k = p|_{\Omega_k}$ and $p_j = p|_{\Omega_j}$ then since p is a solution of the Helmholtz equation

$$p_k = p_j \text{ and } \frac{1}{\rho_k}\frac{\partial p_k}{\partial n_k} = -\frac{1}{\rho_j}\frac{\partial p_j}{\partial n_j} \text{ on } \Sigma_{j,k}$$

In the UWVF this is achieved by demanding that Robin (one way wave equation) data agree on the interfaces, so on $\Sigma_{j,k}$

$$\frac{1}{\rho_k}\frac{\partial p_k}{\partial n_k} + i\sigma p_k = -\frac{1}{\rho_j}\frac{\partial p_j}{\partial n_j} + i\sigma p_j$$
$$\frac{1}{\rho_k}\frac{\partial p_k}{\partial n_k} - i\sigma p_k = -\frac{1}{\rho_j}\frac{\partial p_j}{\partial n_j} - i\sigma p_j$$

where $\sigma > 0$ is a parameter (function) on $\Sigma_{j,k}$ (e.g. $\sigma = \Re(\kappa)$).

Outline

Variational equations

[Cessent and Després] Let ξ_k satisfy the *adjoint* equation

$$\nabla \cdot \rho^{-1} \nabla \xi_k + \overline{\kappa^2} \rho^{-1} \xi_k = 0 \text{ in } \Omega_k$$

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then for $\sigma > 0$ (e.g. $\sigma = \Re(\kappa)$)

$$\begin{aligned} \int_{\partial\Omega_k} \frac{1}{\sigma} \left(\frac{1}{\rho} \frac{\partial p}{\partial n_k} + i\sigma p \right) \left(\overline{\frac{1}{\rho} \frac{\partial \xi_k}{\partial n_k} + i\sigma \xi_k} \right) ds \quad &= \quad \int_{\partial\Omega_k} \frac{1}{\sigma} \left(\frac{1}{\rho} \frac{\partial p}{\partial n_k} - i\sigma p \right) \left(\overline{\frac{1}{\rho} \frac{\partial \xi_k}{\partial n_k} - i\sigma \xi_k} \right) ds \\ &\quad -2i \int_{\partial\Omega_k} \left(\frac{1}{\rho} \frac{\partial p}{\partial n_k} \overline{\xi_k} - \overline{\frac{1}{\rho} \frac{\partial \xi_k}{\partial n_k}} p \right) ds \end{aligned}$$

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$$\nabla \cdot \rho^{-1} \nabla \xi_k + \overline{\kappa^2} \rho^{-1} \xi_k = 0 \text{ in } \Omega_k$$

by Green's Theorem

$$\begin{aligned}\int_{\partial\Omega_k} \frac{1}{\sigma} \left(\frac{1}{\rho} \frac{\partial p}{\partial n_k} + i\sigma p \right) \left(\overline{\frac{1}{\rho} \frac{\partial \xi_k}{\partial n_k} + i\sigma \xi_k} \right) ds \quad &= \quad \int_{\partial\Omega_k} \frac{1}{\sigma} \left(\frac{1}{\rho} \frac{\partial p}{\partial n_k} - i\sigma p \right) \left(\overline{\frac{1}{\rho} \frac{\partial \xi_k}{\partial n_k} - i\sigma \xi_k} \right) ds \\ &\quad -2i \int_{\Omega_k} \left(\nabla \cdot \frac{1}{\rho} \nabla p \, \overline{\xi_k} - \overline{\nabla \cdot \frac{1}{\rho} \nabla \xi_k} \, p \right) dV\end{aligned}$$

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by the Helmholtz and adjoint Helmholtz equations

$$\int_{\partial\Omega_k} \frac{1}{\sigma} \left(\frac{1}{\rho} \frac{\partial p}{\partial n_k} + i\sigma p \right) \left(\overline{\frac{1}{\rho} \frac{\partial \xi_k}{\partial n_k} + i\sigma \xi_k} \right) ds$$

$$= \int_{\partial\Omega_k} \frac{1}{\sigma} \left(\frac{1}{\rho} \frac{\partial p}{\partial n_k} - i\sigma p \right) \left(\overline{\frac{1}{\rho} \frac{\partial \xi_k}{\partial n_k} - i\sigma \xi_k} \right) ds$$

Variational Problem Continued

$$\int_{\partial\Omega_k} \frac{1}{\sigma}\left(\frac{1}{\rho_k}\frac{\partial p_k}{\partial n_k} + i\sigma p_k\right)\left(\overline{\frac{1}{\rho_k}\frac{\partial \xi_k}{\partial n_k} + i\sigma \xi_k}\right) ds$$

$$= \sum_j \int_{\Sigma_{k,j}} \frac{1}{\sigma}\left(-\frac{1}{\rho_j}\frac{\partial p_j}{\partial n_j} - i\sigma p_j\right)\left(\overline{\frac{\partial \xi_k}{\partial n_k} - i\sigma \xi_k}\right) ds$$

Let

$$\mathcal{X}_k = \left(\frac{1}{\rho_k}\frac{\partial p_k}{\partial n_k} + i\sigma p_k\right)\Big|_{\partial\Omega_k} \text{ and } \mathcal{Y}_k = \left(\frac{1}{\rho_k}\frac{\partial \xi_k}{\partial n_k} + i\sigma \xi_k\right)\Big|_{\partial\Omega_k}$$

and let

$$F_k(\mathcal{Y}_k) = \left(\frac{1}{\rho_k}\frac{\partial \xi_k}{\partial n_k} - i\sigma \xi_k\right)\Big|_{\partial\Omega_k}$$

Variational Problem Continued

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then, for a tetrahedron surrounded by four other tetrahedra

$$\int_{\partial\Omega_k} \frac{1}{\sigma} \mathcal{X}_k \overline{\mathcal{Y}_k}\, ds = -\sum_j \int_{\Sigma_{k,j}} \frac{1}{\sigma} \mathcal{X}_j \overline{F_k(\mathcal{Y}_k)}\, ds$$

boundary faces are handled using the boundary condition.

Outline

The Discrete UWVF

For each element Ω_k we choose p_k directions $\boldsymbol{d}_j$ on the unit sphere [Sloan et al.] and define the solution on that element to be a sum of traces of plane waves

$$\mathcal{X}_k^h = \sum_{j=1}^{p_k} x_j^k \left(\frac{1}{\rho_k} \frac{\partial \exp(i\overline{\kappa}\boldsymbol{d}_j \cdot \boldsymbol{x})}{\partial n_k} + i\sigma \exp(i\overline{\kappa}\boldsymbol{d}_j \cdot \boldsymbol{x}) \right) \Bigg|_{\partial\Omega_k}$$

The test function is, for $1 \leq r \leq p_k$,

$$\mathcal{Y}_k^h = \left(\frac{1}{\rho_k} \frac{\partial \exp(i\overline{\kappa}\boldsymbol{d}_r \cdot \boldsymbol{x})}{\partial n_k} + i\sigma \exp(i\overline{\kappa}\boldsymbol{d}_r \cdot \boldsymbol{x}) \right) \Bigg|_{\partial\Omega_k}$$

In this case $F_k(\mathcal{Y}_k^h)$ is easy to compute:

$$F_k(\mathcal{Y}_k^h) = \left(\frac{1}{\rho_k} \frac{\partial \exp(i\overline{\kappa}\boldsymbol{d}_r \cdot \boldsymbol{x})}{\partial n_k} - i\sigma \exp(i\overline{\kappa}\boldsymbol{d}_r \cdot \boldsymbol{x}) \right) \Bigg|_{\partial\Omega_k}$$

Properties of the acoustic UWVF

- [Huttunen, Monk] The UWVF is a special implementation of the upwind Discontinuous Galerkin method using plane wave basis functions.
- [Cessenat/Després, 2D] Assume $\Im(\kappa) = 0$. If $|Q| < 1$, $M = 2\mu + 1$

$$\|\mathcal{X} - \mathcal{X}_M\|_{L^2(\Gamma)} \leq Ch^{\mu-1/2}\|u\|_{\mathcal{C}^{\mu+1}(\Omega)}$$

- The discrete problem has the form $(B - C)\boldsymbol{x} = \boldsymbol{b}$ where B is Hermitian positive definite and the eigenvalues of $B^{-1}C$ lie in the closure of the unit disk excluding 1

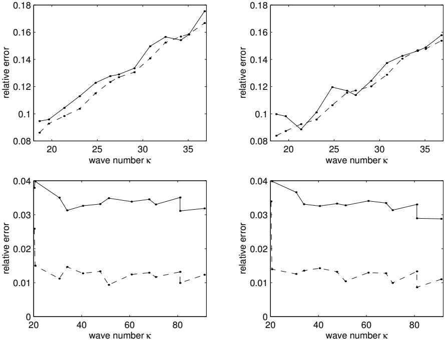
Outline

UWVF results in 2D

Domain Ω is annulus $0.4 \leq r \leq 1$

Remesh at each κ to keep $\lambda/h \approx 8$ (FEM)

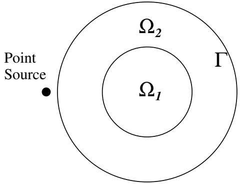
Remesh at each κ to keep $\sqrt{2p}\lambda/h \approx 4.5$ (UWVF)



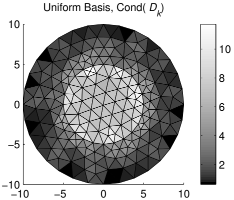
Dirichlet Neumann

Conditioning

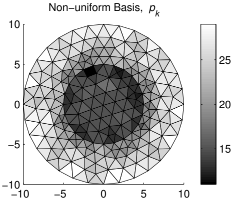
- Basic UWVF uses *p* directions/element. This can cause bad conditioning for *B* (e.g. on small elements, if κ changes,...)
- We use different p_k for element Ω_k. One possibility: chose p_k so that the condition number of the submatrix corresponding to $\int_{\partial K} \mathcal{X}\overline{\mathcal{Y}}\, ds$ is a desired maximum value.



Domain



Cond. No. Uniform p_k

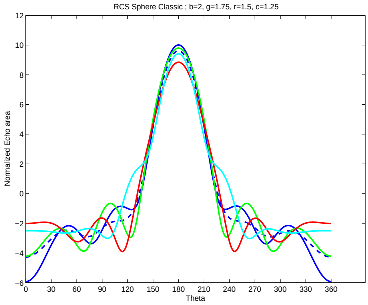


Non uniform p_k

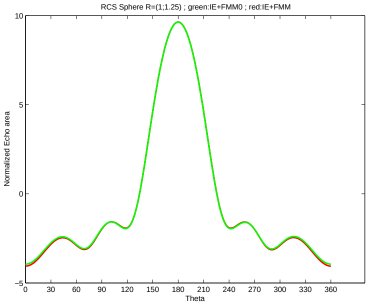
Outline

Efficiency of the ABC

Logarithm of the modulus of the far field pattern for scattering of a plane wave by a sphere $\kappa = 4$, $a = 1$, wavelength $\lambda \approx 1.6$ for different ABC boundary diameter



ABC at $r = 1.25(c), 1.5(r)$, and $r = 1.75(g), 2(b)$

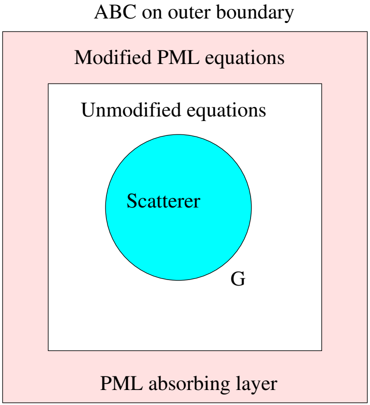


"Exact"

Note: these are electromagnetic results

The PML

The Sommerfeld absorbing boundary condition is not efficient. We want to use the “Perfectly Matched Layer” (PML) of Bérenger.



The PML layer absorbs incident waves exponentially rapidly. The only reflection is from the outer boundary (for the continuous problem).

UWVF with PML in 3D

Let us use the complex stretching of spatial variables

$$x' = \begin{cases} x + \frac{i}{\kappa} \int_{x_0}^{x} \sigma_0 (|x| - x_0)^n \, dx, & |x| \geq x_0, \\ x, & |x| < x_0 \end{cases} \quad \text{and define} \quad \frac{\partial x'}{\partial x} = d_x .$$

By using similar expression for y and z, and requiring p satisfy the Helmholtz equation in primed variables, we obtain a modified Helmholtz equation:

$$\nabla \cdot \left(\frac{1}{\rho} A \nabla \right) p + \frac{\kappa^2 \eta^2}{\rho} p = 0 \quad \text{where} \quad A = \mathrm{diag}\left(\frac{d_y d_z}{d_x}, \frac{d_x d_z}{d_y}, \frac{d_x d_y}{d_z} \right).$$

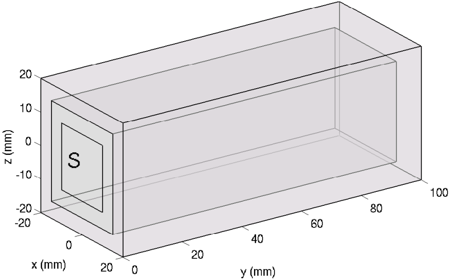
PML continued

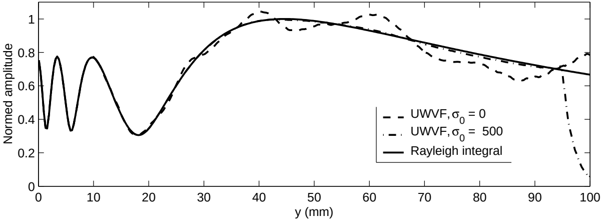
For the PML elements, the boundary function χ_k and plane wave basis function are

$$\chi_k = \Big(\big(-\frac{1}{\rho_k} n_k \cdot (A_k \nabla) - i\sigma \big) p_k \Big) \quad \text{and} \quad \varphi_{k,\ell} = e^{i\overline{\kappa}_k d_{k,\ell} \cdot \overline{r}'},$$

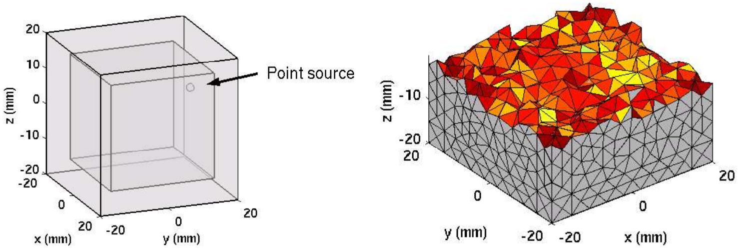
where $r' = (x', y', z')$. Surprisingly, $n = 0$ works quite well with the UWVF.

Improvement due to the PML

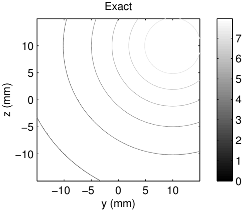




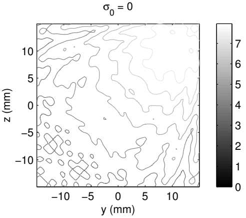
Another Test Example (point source)



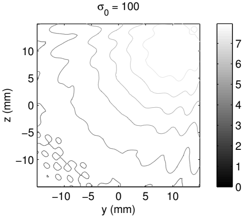
Point Source Results



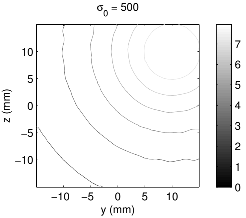
Exact



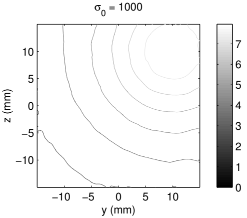
$\sigma_0 = 0$



$\sigma_0 = 100$



$\sigma_0 = 500$

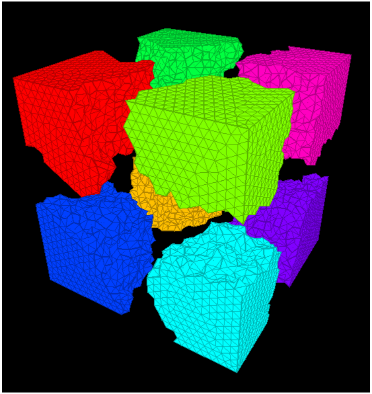


$\sigma_0 = 1000$

Outline

Parallelization

The UWVF has been parallelized using domain decomposition (METIS) and MPI. The basic tasks are assembly and the iterative solver (BiCGStab, easily parallelized). Coupling is via faces.



Left: METIS decomposition of a mesh around a sphere (!) into 8 parts.

Current problem: how to predict the number of directions per element to guarantee good conditioning and accuracy.

Choice of p_k [Caryol and Collino]

- How can we choose p_k to ensure accuracy?
- **Idea:** Good approximation of a general plane wave is necessary for convergence.
- In 2D, using $p_k = 2\mu + 1$ directions, if h is radius of the element

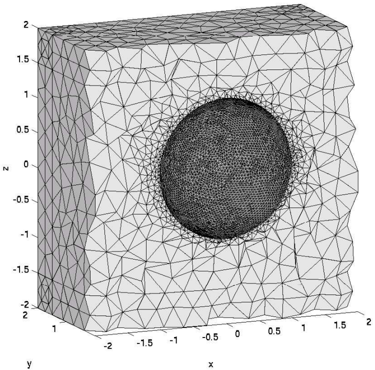
$$E \leq \frac{1}{(\mu+1)!}\left(1 + \frac{\sqrt{\mu+3}}{\mu+2}\right)\left(\frac{kh}{2}\right)^{\mu+1}$$

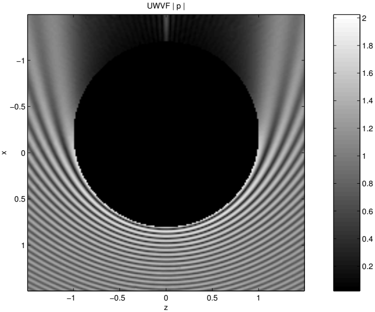
- In 2D, to obtain an interpolant with pointwise error ϵ

$$\mu \approx \kappa h + \frac{1}{2}\left(\frac{3}{2}W\left(\frac{1}{3\pi\epsilon^2}\right)\right)^{2/3}(\kappa h)^{1/3}$$

where $W(x)\exp(W(x)) = x$.

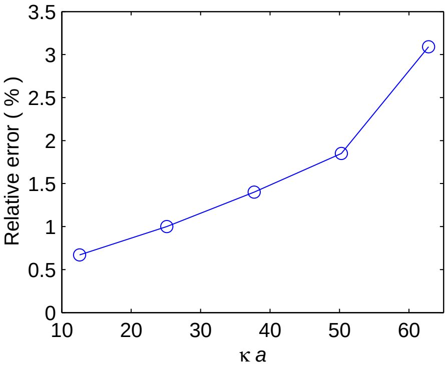
Sphere with radius $a = 1$.





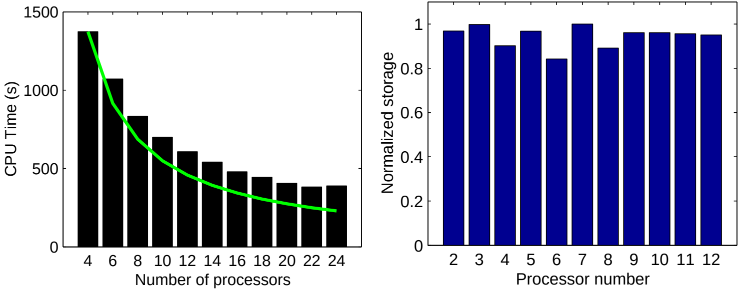
Left: The mesh. *Right:* The UWVF approximation for a plane wave at $\kappa a \approx 63$.

Error as a function of the wave number



The results are computed in the same mesh using the condition number limit Max(Cond(D_k))$< 1e6$. Note, the total error includes errors due to UWVF approximation, PML and triangulated surface of the sphere.

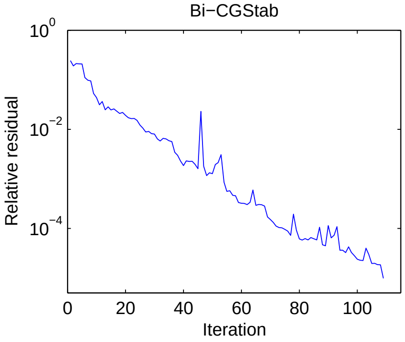
Scalability and load distribution



Left: CPU time as a function of number of processors.
Right: Storage on different processors when 12 processors are used.

Iterative solution of the linear system

The UWVF linear system can be solved by simple iterative scheme. We use BiCGStab.



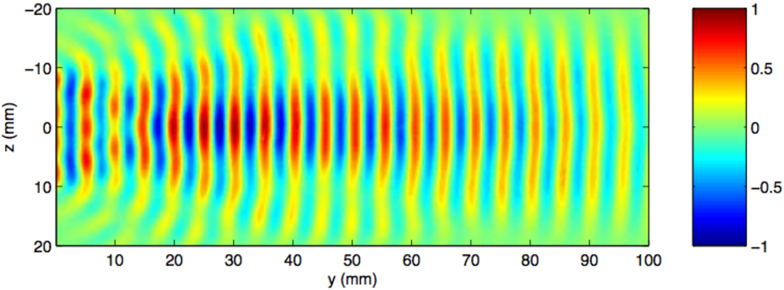
Number of DoF:	3,474, 770
Number of CPUs:	24 (2.8GHz P4)
Available Memory:	48GB
Switch:	1000BaseT

Solution time is 451s using 25.3 GB memory (109 iterations).

Outline

Comparison to FEMLAB [Huttunen]

FEMLAB P_2 FEM with low order ABC.



Comparison continued

FEMLAB (two meshes):

f (kHz)	h (mm)	Elem.	CPU (s)	Error (%)	Mem (GB)
100	3	101 978	448	30.88	1.4
150	1.8	478 471	4699	25.39	2.5
200	1.8	478 471	5321	20.64	2.5
300	1.8	478 471	5391	30.13	2.5

UWVF (one mesh, variable # directions):

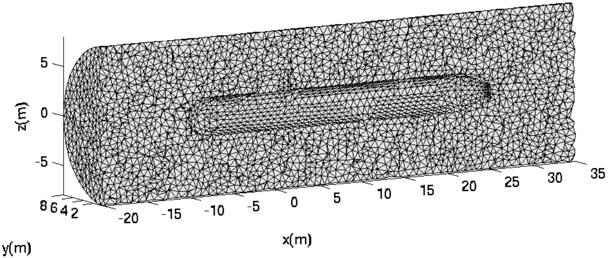
f (kHz)	h (mm)	Elem.	CPU (s)	Error (%)	Mem (GB)
100	15	16 926	275	28.56	0.2
150	15	16 926	353	23.22	0.3
200	15	16 926	449	20.07	0.4
300	15	16 926	854	18.96	1.1

FEMLAB implementation

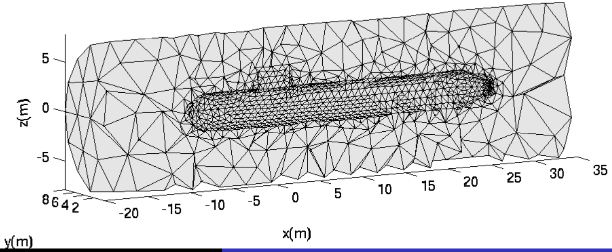
- The acoustic UWVF code will appear as part of the acoustics module in FEMLAB.
- The Maxwell and fluid-structure UWVF (in that order!) will also be added later.
- Please see *www.waveller.com*

Submarine: meshes

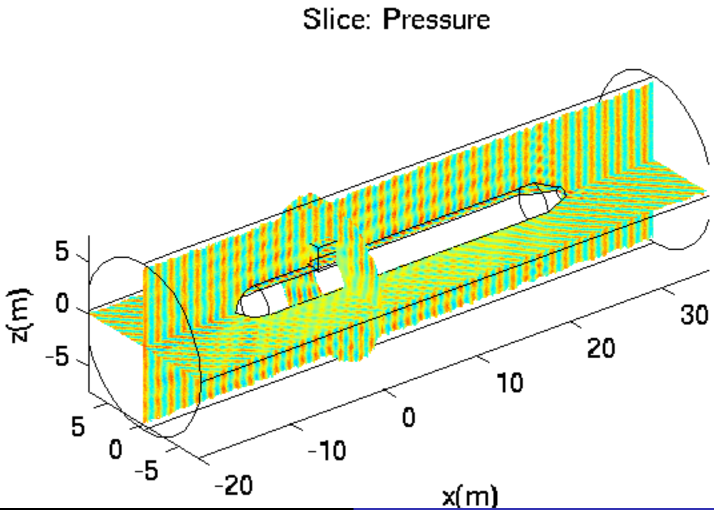
FEM:



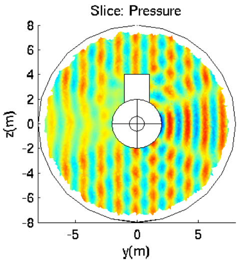
UWVF:

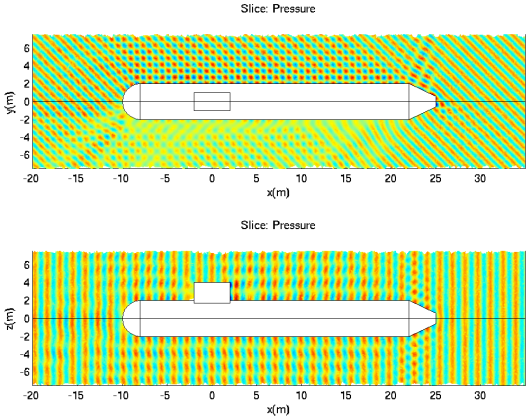


Submarine: UWVF calculation in FEMLAB



Submarine: UWVF calculation





Extensions/current work

The UWVF can be extended to certain symmetric hyperbolic systems and in particular to

- Maxwell's equations
  - PML
  - Coupled FMM and UWVF [with Eric Darrigrand, Rennes]
- Linear elasticity
- Coupled fluid-solid problem (2D only so far)
- Comparison with PUFEM [Huttunen, Gamallo and Astley]

Summary

- The FEM is the best developed volume method for practical computations. High order works best for wave problems with smooth solutions.
- The UWVF offers an alternative to PUFEM for plane wave bases. We find it competetive to FEM.
- The UWVF performs well provided the number of directions is chosen carefully and the scatterer is smooth (questions remain about performance near singularities).