New Computational Tools for Wave Modeling

Tomi Huttunen

Inverse Problems Group Department of Physics University of Kuopio Finland

Outline of the talk

- Modeling of wave phenomena
- Limitations of standard methods
- Wave basis modeling methods
- Ultra-weak variational formulation
- Numerical examples

Acoustic waves



Figure 1: An instaneous particle displacement and corresponding acoustic pressure

Time-harmonic wave equations

• The model for acoustic pressure waves $P(r,t) = p(r) \overline{\exp(-i\omega t)}$

$$\nabla \cdot \left(\frac{1}{\rho}\nabla p\right) + \frac{\kappa^2}{\rho}p = 0$$

where p = acoustic pressure, $\rho = \text{density}$, c = speed of sound, $\omega = 2\pi f$ angular frequency, $\kappa = \omega/c + i\alpha = \text{wave number and } \alpha$ is the absorption coefficient.

• The electromagnetic Maxwell's equations for electric and magnetic fields (*E* and *H*)

$$-i\omega\epsilon \boldsymbol{E} - \nabla \times \boldsymbol{H} = 0$$

$$-i\omega\mu \boldsymbol{H} + \nabla \times \boldsymbol{E} = 0$$

• Elastic waves (Navier equation for displacement *u*)

 $\mu \Delta \boldsymbol{u} + (\Lambda + \mu) \nabla (\nabla \cdot \boldsymbol{u}) + \omega^2 \rho \boldsymbol{u} = 0$

Standard tools

- For the numerical approximation of the previous partial differential equations (PDE), the computational domain needs to be discretized
- In finite element methods (FEM), the solution is approximated in each element of the computational mesh using low-order polynomials
- In finite difference methods (FDM), the computational domain is covered with a set of points, and derivatives of the PDEs are approximated via numerical differences between adjacent points.
- In boundary element methods (BEM) only boundaries or material interfaces are discretized.

Limitations of standard PDE solvers

- "A rule of thumb" for low-order FEM and FDM is ten points per wavelength λ
- Due to the *numerical pollution*, even denser meshes are needed at high frequencies
- Boundary element methods (BEM) become complex for problems in inhomogeneous media
- Consequently, ray-approximations are commonly used ⇒ reduced accuracy

Example: Scattering from a submarine



Figure 2: Frequency f = 1500 Hz in water, the length of the hull L = 35 m.

Typical mesh for FEM at 400 Hz



Figure 3: The mesh consists of 224611 tetrahedra and 41110 vertices. At 400 Hz, $\lambda/h_{max} = 4$ i.e. 4 elements per wavelength.

A common problem

- Clearly, we can consider that this problem [scattering of radar waves by an aircracft] remains unsolved and a completely new method of approximation is needed to deal with the very short-wave solution
 O.C. Zienkiewicz: "Achievements and some unsolved problems of the finite element method". International Journal for Numerical Methods in Engineering, 47, 9-28 (2000)
- A SOLUTION: New wave basis methods relax the requirement of dense meshes

Methods using plane waves basis functions

- Partition of unity finite element method = PUFEM (Babuška and Melenk 1997)
- Least squares method (Monk and Wang 1999)
- Discontinuous enrichment method (Farhat et al. 2001)
- Discontinuous Galerkin method (Farhat et al. 2003)
- Plane wave basis in integral equations (Perrey-Debain et al. 2002) (also for elastic waves)
- Ultra weak variational formulation (Després 1994, Cessenat and Després 1998)

UWVF

• A new function is defined on element interfaces

$$\chi_k = \left(-\frac{1}{\rho_k}\frac{\partial p_k}{\partial n} - i\varsigma p_k\right)$$

• The function χ_k in an element K_k is approximated using a plane wave basis

$$\chi_k \approx \sum_{\ell=1}^{N_k} \chi_{k,\ell} \left(-\frac{1}{\rho_k} \frac{\partial}{\partial n_k} - i\varsigma \right) \varphi_{k,\ell} \quad \text{where} \quad \varphi_{k,\ell} = \begin{cases} e^{i\overline{\kappa}_k d_{k,\ell} \cdot r} & \text{in } K_k \\ 0 & \text{elsewhere} \end{cases}$$

• The discrete problem is written as the sparse matrix equation

$$(I - D^{-1}C)X = D^{-1}b,$$

where D is a block diagonal matrix, C is a sparse block matrix and X includes weights $\chi_{k,\ell}$ for basis functions for each element.

Typical mesh for the UWVF



Figure 4: The mesh consists of 12506 tetrahedra and 3097 vertices. At 400 Hz, $\lambda/h_{max} = 0.5$

Current status of the research

- Parallel UWVF solver for 3D Helmholtz problems (we use a 24 processor PC cluster)
- A similar parallelized solver for Maxwell's equations
- 2D Matlab-codes for elastodynamics and coupled fluid-structure problems

Our fields of application

- Focused ultrasound surgery (FUS) from 1999
- Collaboration with Kullervo Hynynen's group from Harvard Med. School
- Modeling of large-scale ultrasound fields in complex geometries
- Audio acoustic modeling with Nokia from 2003: the simulation of the head related transfer function (HRTF) for 3D virtual acoustics
- Maxwell's equations (2004) ⇒ Microwave tomography of wood with University of Oulu's Sensor and Measurement Laboratory in Kajaani (2005)

Harvard's FUS prototype



Figure 5: A Phased array for brain surgery.

A simplified simulation



Figure 6: Pressure amplitude |p| for the transmission of ultrasound beam through a layered medium at f = 531 kHz.

Audio acoustic simulations



Figure 7: The geometry for the head-and-torso model.

HRTF simulations



Figure 8: Left: Pressure at 20 kHz. Right: The field in the left ear as a function of the direction and the frequency of the incoming wave.

Other audio applications



Figure 9: A sound field in a car cabin at f = 5000 Hz.

Microwave measurements



Figure 10: A microwave antenna and the wood measurement setup.

Simulated results at 5.0 GHz



Figure 11: Left: The far-field of the antenna. Right: A simulation with the wood sample.

On-going projects

- Further development of the acoustics UWVF
- Extension of the UWVF method for 3D elastodynamics and fluid-(solid)structure problems
- Development of corresponding parallel codes
- UWVF for microwave modeling
- Development of the fully-parallelized 3D electromagnetic wave simulation tool continues

WAVELLER acoustics

- A command line software for acoustics
- Uses the parallelized UWVF with the plane wave basis
- The number of basis functions can vary from element to element based on the local wave number ⇒ the same coarse mesh can be used over a wide range of frequencies
- WAVELLER can be run through Femlab's graphical interface (an extension to Femlab's acoustic mode)
- Pre- and post-processing in Femlab
- See, www.waveller.com

Conclusions

- In comparison with standard PDE solvers (FEM and FDM), the new plane wave basis methods, such as the UWVF, lead to considerable savings in memory and CPU-time
- However, multi-processor computing is still necessary for many practical applications
- Next steps include:
 - Better understanding of the approximation properties of the plane waves
 - Extension of the method for other wave problems