Wave Theory II — Numerical Simulation of Waves — (1) Weve Equations and Numerical Simulation of Waves

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This course describes the fundamental theories of the numerical simulation methods of wave phenomena by using computers.

In this first lecture, wave equations in different areas are briefly reviewed, and are generalized into the common equation. Then, the purposes and the advantages of the numerical simulation are described. Finally, the methods which are described in this course are introduced and classified.

Syllabus

Plan :

1. Helmholtz equation, Numerical simulation of waves
2. Representation of wave function by using Green function (1) — Green's theorem, Free space Green function
3. Representation of wave function by using Green function (2) — Eigenfunction expansion to derive the Green function in bounded region
4. Boundary element method (1) — Boundary integral equation
5. Boundary element method (2) — Discretization of integral equation
6. Finite element method
7. Physical optics approximation
8. TBD (time domain solution, computing tools, examples, new methods, etc.)

Textbook : Handouts are available via the web page.
`http://www.mobile.ss.titech.ac.jp/~takada/waves/`

Evaluation : Weekly reports including some programming : 100 %

1 Wave Equations

1.1 Acoustic Waves

The following D'Alembert wave equation is satisfied for the small amplitude acoustic wave in the air.

$$\nabla^2\phi = \frac{1}{c^2}\cdot\frac{\partial^2\phi}{\partial t^2}, \tag{1}$$

where ϕ is the velocity potential and is related to the velocity vector $\mathbf{v}$ as

$$\mathbf{v} = -\nabla\phi. \tag{2}$$

The velocity c is related to the pressure of the air without the acoustic wave p_0 and the density ρ_0 as

$$c^2 = \frac{p_0\gamma}{\rho_0}, \tag{3}$$

where

$$\gamma = \frac{\text{Specific Heat at Constant Pressure}}{\text{Specific Heat at Constant Volume}}.$$

1.2 Electromagnetic Waves

When the media is linear, isotropic and nondispersive, the electric and the magnetic fields satisfy the following Maxwell's equations.

$$\nabla \times \mathbf{H} = \mathbf{J} + \varepsilon \frac{\partial \mathbf{E}}{\partial t}, \tag{4}$$

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t}, \tag{5}$$

where $\mathbf{J}$ is the primary current density, $\mathbf{E}$ is the electric field, $\mathbf{H}$ is the magnetic field, ε is the permittivity and μ the permiability. By substituting (4) and (5) to each other to substitute $\mathbf{E}$ or $\mathbf{H}$, the following equations are obtained.

$$\nabla \times \nabla \times \mathbf{E} + \varepsilon\mu \frac{\partial^2 \mathbf{E}}{\partial t^2} = -\mu \frac{\partial \mathbf{J}}{\partial t}, \tag{6}$$

$$\nabla \times \nabla \times \mathbf{H} + \varepsilon\mu \frac{\partial^2 \mathbf{H}}{\partial t^2} = \nabla \times \mathbf{J}. \tag{7}$$

Here, let us define the vector potential $\mathbf{A}$ and the scalar potential ϕ as

$$\mathbf{H} = \frac{1}{\mu} \nabla \times \mathbf{A}, \tag{8}$$

$$\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} = -\nabla \phi. \tag{9}$$

When Lorenz condition

$$\nabla \cdot \mathbf{A} = -\varepsilon\mu \frac{\partial \phi}{\partial t} \tag{10}$$

is applied, Eqs. (4) and (5) result in the following relations with respect to $\mathbf{A}$ and ϕ as

$$\nabla^2 \mathbf{A} - \varepsilon\mu \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\mu \mathbf{J}, \tag{11}$$

$$\nabla^2 \phi - \varepsilon\mu \frac{\partial^2 \phi}{\partial t^2} = -\frac{\rho}{\varepsilon}, \tag{12}$$

where ρ is the charge density and is related to $\mathbf{J}$ as

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}, \tag{13}$$

which is known as the continuity relation.

1.3 Quantum Theory

The probability of existence of quantum is expressed as the wave function Ψ, which satisfies the following Schrödinger equation.

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi, \tag{14}$$

where $\hbar = \frac{h}{2\pi}$ is Dyrac's constant and h is Pranck's constant, m is the mass of the quantum, $V(\mathbf{r})$ is the potential with respect to the external force. The probability of existence of quantum is given as

$$|\Psi(\mathbf{r})|^2 . \tag{15}$$

2 Purposes and Advantages of Numerical Simulation of Waves

2.1 Common Nature of Wave Equations — Helmholtz Equation

When the wave phenomenon is analytically treated, Time-harmonic expression or sinusoidal vibration at a single frequency is useful. By using the time-harmonic expression, arbitrary periodic waveform can be expressed in the Fourier series.

Wave equations for the acoustic wave (1) the electromagnetic wave (11, 12) and the wave function of quantum (14) are in the common form if the temporal variation of the wave functions are expressed by $e^{\mathrm{j}\omega t} = e^{-\mathrm{i}\omega t}$ as[1]

$$\nabla^2 \Phi + k^2 \Phi = -\rho \tag{16}$$

Equation (16) is called *scalar Helmholtz equation*[2] or simply *Helmholtz equation*, where Φ is a scalar wave function, ρ is a scalar source. This course mainly discusses the numerical solutions of the scalar Helmholtz equation.

2.2 Purposes and Advantages of Numerical Simulation of Waves

Since the wave equations and the Helmholtz equations are the partial differential equations, they shall be solved together with the boundary conditions. Only when the shape of the boundary is simple such as plane, circular or rectangular, the separation of the variables are possible, so that the equations are analytically solved. In the most of practical cases, however, the shape of the boundary is more complicated and the equations can not be solved analytically.

Contrary, the numerical solutions of the equations are always available for *any kind of the boundary shape.*

3 Introduction to Numerical Simulation Techniques

There exist a lot of numerical simulation techniques for the wave propagation. In this section, the techniques are classified into three categories, i.e. semi-analytical methods, boundary methods, and domain methods.

3.1 Semi-Analytical Methods

In the semi-analytical methods, the equations are not directly solved to satisfy the given boundary conditions. Instead, solutions of some certain canonical problems are substituted for the approximation. In particular, the techniques known as high frequency approximation techniques give the good accuracy when the scatters are much bigger than the wavelength so that the numerical discretization methods such as boundary methods and domain methods fail to treat.

Geometrical Optics Approximation, Ray-Tracing In the geometrical optics approximation (GO), the law of the reflection at the infinite plane boundary[3] is used to the boundary of any arbitrary shape to compute the scattered wave.

Advantages :

- The implementation is relatively simple.

Disadvantages :

- Edge diffraction effect can not be considered.
- Polarization rotation is not accurately considered.

Physical Optics Approximation, Kirchoff Approximation Kirchoff-Huygens' Principle guarantees that the wave function at the observation point can be always described as the sum of the radiation from the source within the closed surface (primary source) and the radiation from the fictitious

[1] In electrical engineering, the temporal variation is expressed as $e^{\mathrm{j}\omega t}$ by using the imaginary unit j. On the other hand, in physics, it is usually expressed as $e^{-\mathrm{i}\omega t}$ by using the imaginary unit i. The two expressions are related by $\mathrm{j} = -\mathrm{i}$, as far as concerning with the exponential functions. However, care shall be taken when treating Hankel functions in the cylindrical coordinates. For example, an outward traveling wave is expressed as $H_0^{(2)}(k\rho)$ in the former, and as $H_0^{(1)}(k\rho)$ in the latter.

[2] Equations (6) and (7) are expressed by the vector Helmholtz equation

$$\nabla \times \nabla \times \mathbf{A} - k^2 \mathbf{A} = \mathbf{J}, \tag{17}$$

where $\mathbf{A} = \mathbf{E}$ or $\mathbf{H}$ is a vector wave function, and $\mathbf{J}$ is a vector source. The solution of the vector Helmholtz equations are not described in this course, but two alternative approaches are possible:

1. Use of potential functions in the formulation
2. Modification and extension of simulation concept

[3] This is the canonical problem.

source on the closed surface (secondary source). However, the secondary source is usually unknown on the boundary. Therefore, the secondary source value is approximated by the incident wave in Kirchoff approximation.
Contrary, the secondary source value is approximated by the value of the secondary source when the boundary is infinite plain[4] in physical optics (PO) approximation.

Advantage :

- The accuracy is moderate.
- Diffraction effects can be considered to some extent.

Disadvantages :

- Evaluation of diffraction is accurate only in the near-axis region where the law of the reflection is satisfied.

Geometrical Theory of Diffraction When the frequency is high or the scatter is much bigger than the wavelength, the diffracted waves from the edges of the scatter, as well as the creeping waves propagating along the curved surfaces are the dominant propagation mechanisms. They both satisfy the Fermat's principle so that the diffraction paths are determined as the locally longest or shortest paths between source–scatterer–observation point. Next, the diffraction coefficients are approximated by those for infinite wedge or infinite cylinder[5] This technique is known as the Geometrical Theory of Diffraction.

Advantages :

- Diffracted waves can be evaluated very well.

Disadvantages :

- The wave function is divergent for some specific observer direction.

3.2 Boundary Methods

The problem is formulated based on the boundary condition in the boundary methods, and the Green's function plays an important role in the formulation. Hence, it is advantageous that the unknowns are assumed only on (or near) the boundary, which results in the less number of unknowns compared with the domain methods. However, the coefficient matrix becomes dense due to the remote interaction of Green's function.

Method of Moments, Boundary Element Method The method of moments (MoM) is also known as the boundary element method (BEM). The former term is used for the electromagnetic waves, while the latter is popular in the acoustics, due to the historical reasons. Boundary conditions are expressed as the integral equations with respect to the unknown surface fields. Then both the unknown surface fields and integral equations are discretized to obtain a set of linear equations.

Advantages :

- The coefficient matrix is usually well-conditioned so that the solution is robust.

Disadvantages :

- Some special analytical treatments are necessary when the source point and the observation point coincides.
- Coefficient matrix is always dense, which results in relatively larger CPU time and memory consumption.

Recently, an iterative approach called the fast multipole method (FMM)[6] is extensively studied. The unknown surface fields are approximated by the multipoles to save the computation time drastically in FMM. Therefore, it is now known as one of the fastest methods.

Generalized Multipole Technique In the generalized multipole technique (GMT), contrary to MoM/BEM, fictitious multipole point sources are assumed outside the domain and the coefficients of them are optimized so that the boundary condition is satisfied.

[4] This is the canonical problem.
[5] This is the canonical problem.
[6] There is no direct relation to the generalized multipole technique which is described next.

Advantages :

- The source points and the observation points can not be identical, and no analytical treatment is necessary with respect to the poles.
- Higher order multipoles do not generate the far field, which results in relatively sparse coefficient matrix.

Disadvantages :

- The selection of the multipole source positions are arbitrary, but is a kind of know-how.
- The coefficient matrix is usually ill-conditioned, and the number of matching points shall be bigger than the number of unknown coefficients of multipoles, and least square method shall be used. Time consuming singular value decomposition (SVD) is necessary.

Measured Equation of Invariance Measured equation of invariance (MEI) method is yet another boundary method. The so-called Mei postulates assume the local linear equations on the boundary which are invariant of the excitation. These local linear equations can be "measured" by utilizing this invariance through the tests with different excitations.

Advantages :

- In spite of a boundary method, MEI results in the sparse coefficient matrix, which can be solved efficiently in terms of memory and CPU time.
- MEI coefficients are insensitive to the perturbation of the scatterer shape so that they can be reused.

Disadvantages :

- The computation of the MEI coefficients is rather time-consuming.
- Applicability is unclear since the method is based on the postulates. By now, concave structures are known to be difficult to treat.

3.3 Domain Methods

In the domain methods, differential equations in the domain are directly or indirectly discretized so that the wave functions satisfy the boundary condition. It is advantageous that Green's function is not used in the formulation. Therefore, they are applicable to more complicated problems in which Green's function can not be derived. Traditionally, it was the drawback that the open domain problems can not be treated due to the difficulty of the domain truncation. However, good absorbing boundary conditions (ABCs) have been proposed so that the domain methods can now easily implemented to open domain problems.

Beam Propagation Method (Optics) The beam propagation method (BPM) is popularly used in the analyses of optical waveguides. The cross section of the waveguide is described in spectral domain by Fourier transform, and the longitudinal propagation is sequentially computed in section by section. In other words, the high frequency approximation is used in the longitudinal direction.

Advantages :

- The domain is discretized only along the longitudinal direction, i.e. one-dimensional discretization. The computational cost is relatively low.

Disadvantages :

- It can not be used in case the cross section changes drastically within the order of a wavelength.

Finite Difference Method, Finite Volume Method, Finite Integral Method The domain is first divided into the orthogonal grids. In the finite difference method (FDM), the finite difference approximation of the differential equation is applied. In the finite volume method (FVM) or the finite integral method (FIM), the equivalent integral equation is applied.

Advantages :

- Concept and implementation are both simple, compared with the finite element method.
- The coefficient matrix is structured, and fast computational techniques exist.

Disadvantages :

- The grid structure is limited due to the nature of finite difference approximation (for FDM).

Finite Element Method This method is named the finite element method (FEM) since the domain is discretized into triangle or tetrahedral elements. The original formulation is based on the variational method to minimize the total energy of the system which is described as the functional. Now, the direct discretization of the local volume integral equation derived from the differential equation is also known as FEM.

Advantages :

- The mesh can be generated conformal to the boundary by using triangular or tetrahedral elements.
- Efficient mesh generation algorithms exist such as Delaunay triangulation.

Disadvantages :

- The coefficient matrix is unstructured and more inefficient in the solution.

Finite Difference Time Domain Method In the finite difference time domain (FDTD) method, the time-harmonic oscillation $e^{\mathrm{j}\omega t} = e^{-\mathrm{i}\omega t}$ is not assumed. Instead, the finite difference approximation is also applied to the time domain, and the transient response of the wave function is computed. For the electromagnetic waves, the symmetrical forms of the electric and magnetic fields are utilized to implement the leap-from algorithm which result in the second order accuracy.

Advantages :

- It is applicable to nonlinear or time-variant problems.

Disadvantages :

- It has the same disadvantages as the finite difference method in the frequency domain.

Report

Tokyo Tech students are requested to submit by e-mail before the next lecture. Do not forget to fill out the student ID, your department and lab names, as well as your name. KMITL students shall follow the instruction of Dr. Chuwong.

The handouts as well as the copies of the slides can be downloaded from the web.

`http://mobile.ss.titech.ac.jp/~takada/waves/`

Exercises

1. Solve the source-free Helmholtz equation

$$\nabla^2\Phi + k^2\Phi = 0 \tag{18}$$

   in 3D Cartesian $(x,\ y,\ z)$ coordinates, 3D cylindrical coordinates $(\rho,\ \theta,\ \varphi)$, and spherical coordinates $(r,\ \theta,\ \varphi)$ by using the separation of variables.

2. Point out an example of the application of the numerical simulation of wave propagation.