# Time-domain Numerical Solution of the Wave Equation

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**Abstract**

This paper presents an overview of the acoustic wave equation and the common time-domain numerical solution strategies in closed environments. First, the wave equation is presented and its qualities analyzed. Common principles of numerical approximation of derivatives are then reviewed. Based on them, the finite difference (FD) and the finite element methods (FEM) for the solution of the wave equation are presented along with algorithmic and practical considerations.

## 1 Introduction and Preliminaries

The sensation of sound is due to small variations in air pressure. The variations are governed by the three-dimensional *wave equation*, a second-order linear partial differential equation, which relates the temporal and spatial derivatives of the pressure field. This paper presents an overview of the wave equation (section 2) and outlines the most common time-domain[1] methods for its numerical solution; namely the *finite difference* and the *finite element* methods.

Section 3 describes the approximation of continuous functions and their derivatives by finite differences and presents methods for discretizing the wave equation using these approximations. Section 4 introduces methods for solving the resulting ordinary differential equations by time-stepping. We also present the finite element discretization of the wave equation in section 5, and conclude with some comparisons between the methods in section 6.

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[1] as opposed to frequency-domain

## 2 The Wave Equation

This section presents the wave equation and some of its qualities. We first introduce the nature of the solutions, then discuss the equation of motion along with boundary and initial conditions, and conclude with a note on the Helmholtz equation.

### 2.1 Introduction

When determining the acoustic properties of an environment, we are actually interested in the "propagation of sound", given the properties and location of a sound source. Sound waves themselves are small fluctuations in air pressure. In simple cases (in the absence of temperature gradients, for instance) these small fluctuations can be treated as small perturbations of an ambient pressure field. The propagation of these fluctuations is governed by the *wave equation*, which can be derived from purely mechanical considerations (springs and masses with certain linearizations, see e.g. Eirola, 2002) or from suitable simplifications of the more general equations of fluid dynamics (Pierce, 1991). Solution of the complete, non-linear equations of fluid dynamics is generally not required for acoustic purposes.

The solution of the wave equation is a time-dependent pressure field $u(t, \mathbf{x})$, with $\mathbf{x} \in \Omega$ and $t > 0$. Here $\Omega$ denotes the set of points inside the environment to be simulated; in realistic situations $\Omega$ is three-dimensional, but we shall often resort to lower-dimensional examples for easier presentation. We stress that the solution $u$ to the equation is a scalar function over three spatial dimensions and time; the function describes the acoustic sound pressure for each point $\mathbf{x}$ in the environment for each $t$. This is the key difference between solutions of "normal" algebraic equations and differential equations[2]; roughly speaking, the solutions of differential equations are themselves functions, while the solutions of normal algebraic equations are points within the domain of some equation-dependent function.

### 2.2 The Equation of Motion and Boundary Conditions

The wave equation is a second-order linear partial differential equation

$$u_{tt} = c^2 \Delta u + f \tag{1}$$

with

$$u_{tt} = \frac{\partial^2 u}{\partial t^2}, \quad \Delta = \nabla \cdot \nabla = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}, \tag{2}$$

whese $u$ is the pressure field (as described above) and $c$ is the speed of sound, which we assume to be constant in the whole environment. The equation thus relates the second

[2] Actually, we should be talking about *operator equations* instead of just differential equations.

time derivative of the pressure to its spatial *Laplacian* $\Delta u$. $f = f(t, \mathbf{x})$ represents time dependent force terms, which we discuss soon. The equation is called a *partial* differential equation because it involves derivatives of the solution function $u$ with respect to more than one variable.

Equation (1) is in itself not uniquely solvable. In addition to this equation of motion, the behaviour of the solution on the boundaries of the environment, which we denote by $\partial\Omega$, needs to be determined. These so-called boundary conditions (BCs) dictate how the walls of the environment reflect sound waves. Elementary types of boundary conditions prescribe either the solutions' values or the values of the solution's normal derivatives[3] on the boundary. In this paper we leave out most details on boundary conditions. We mention in passing that it is possible to construct so-called *absorbing* BCs, which do not reflect any of the waves striking the boundary, and the waves appear to just leave the domain. Absorbing boundary conditions are useful in analyzing enclosures partly bounded but connected to a "large" open space.

In addition to boundary conditions, *initial conditions* need to be specified. This means that for $t = 0$, an initial pressure distribution $u(0, \mathbf{x})$ and an initial velocity $u_t(0, \mathbf{x})$ distribution are required.

The force term $f(t, \mathbf{x})$ represents sources of disturbations in air pressure; these are the sound sources.[4] Usually, an acoustics application solves the wave equation with $f$ describing an initial impulse. The solution of the wave equation then describes the time-dependent propagation of the impulse in the environment. The solution $u$ is an univariate function (in $t$) for each $\mathbf{x}$ in the environment, and can be used as an impulse response in an auralization system.

## 2.3 Dispersion

In the case of wave propagation, *dispersion* means that waves either travelling to different directions or having different frequencies propagate with different speeds. Dispersion can occur both naturally (in a dispersive medium) and artificially. The "pure" wave equation presented above is nondispersive, i.e. in the exact solution all waves, regardless of direction or frequency, propagate with the speed $c$. Unwanted artificial dispersion occurs in all numerical methods. The effects often include waves travelling along coordinate axes propagating slower than in diagonal directions, and high-frequency waves propagating slower than lower-frequency waves. It is possible to analyze the dispersion introduced by a numerical method either directly by substituting certain "test waves" into the discretized equation (Eirola, 2002) or by frequency domain analysis, see Savioja (1999).

[3] Normal derivative: $\nabla u \cdot \mathbf{n}$, where $\mathbf{n}$ is the outward unit normal on the boundary

[4] Another way of describing sources is to use time-dependent boundary conditions, which we will not cover.

## 2.4 The Helmholtz Equation

We briefly mention that separating variables in the wave equation, that is, searching for the solution $u$ in the form

$$u = \Psi(\mathbf{x})e^{i\omega t} \tag{3}$$

leads to the so-called *Helmholtz equation*, sometimes called the *reduced wave equation*

$$\Delta\Psi_k + k^2\Psi_k = 0, \tag{4}$$

where $\omega$ is the frequency of an *eigenmode* and $k^2 = \omega^2/c^2$ is the *wave number*. Mathematically, the problem is about the eigenvalues of the Laplacian operator (Eriksson *et al.* , 1996). For closed domains, solutions only exist for a countable set of different $\omega$; the solutions $\Psi_k$ for the corresponding wave numbers are the *standing waves* inherent to the geometry of the domain. The Helmholtz equation is the basis for a large number of numerical methods for computational acoustics; they are called *spectral methods* since they do not simulate time-dependent pressure fields but the responses of the environment to different frequencies instead. Since the focus on this paper is in explicit time-domain methods, we do not discuss this further.

# 3 Finite Differences

The exact solutions to the wave equation discussed in the previous section are infinite dimensional, that is, no finite number of parameters can fully describe the solution, except in a very limited set of special cases. Since computers work with finite memories and perform only finite calculations, approximations must be made in order to solve the wave equation numerically. Here we stress that the complete, correct solution is generally unavailable to us in closed form. *Numerical analysis* deals, among other problems, with issues concerning discrete approximations to continuous problems; these include the methods used to discretize the solutions domains in both time and space, methods of solving the discretized versions of the equations, and error analysis.

## 3.1 Discretized derivatives

In this section we describe the simplest possible ways of discretizing derivatives of functions. We work in one dimension for simplicity.

As an example we look at continuous, bounded, real-valued functions defined on the interval $[0, 1]$. In order to represent general functions, we might scatter a large but finite number $N$ of equidistant points $x_i$, with $i = 1, \ldots, N$, inside the interval and store the value of the function in those points only. Even though this representation does obviously not correspond to a continuous function (generally speaking), we do have some idea of what the function is like. We denote the distance between two node points by $h$. Now,

suppose that we are interested in the derivatives of the function which we have represented by point samples. Since we only know the function's values at the node points $x_i$, we must somehow combine those values to obtain an estimate for the derivative. The simplest methods are suggested by the usual difference quotient that is used to define the derivative in the continuous case. This yields the approximations

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{h}, \tag{5}$$

$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{h}, \qquad \text{and} \tag{6}$$

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{2h}, \tag{7}$$

which are called *forward difference*, *backward difference* and *central difference*, respectively (Atkinson & Han, 2001).

The Taylor series provides us an elegant approximation for the second derivative. The expansion gives us

$$f(x+h) = f(x) + \frac{h^1}{1!}f'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + O(h^4), \tag{8}$$

$$f(x-h) = f(x) - \frac{h^1}{1!}f'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + O(h^4), \tag{9}$$

from where adding the approximations side by side and dividing through with $h^2$ we get

$$f''(x) = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} + O(h^2). \tag{10}$$

This is an accurate approximation; for smooth functions the error drops according to $h^2$. We also note that the central difference scheme in eq. (7) follows from neglecting also the second order terms and subtracting the equations from each other.

Figure 1 shows a comparison of the first order difference approximations of the function $\sin(1/x)$, plotted in blue, on the interval $[-0.2, -0.1]$. The example is arbitrary, with the function and range chosen so that the function is smooth (infinitely differentiable) on the interval. The figure illustrates the derivative approximations' nature as linear combinations of samples from the original function, and that the central difference scheme is more accurate than the other two. The original function has been artificially scaled up to show its form.

## 3.2 Discrete differential operators

By writing values of the point samples of a function $u$ as an $N$-dimensional vector $\mathbf{u}_h$, the difference approximations of the last section can be written in a matrix form so that multiplication of the vector $\mathbf{u}_h$ of function values with the matrix produces a new vector

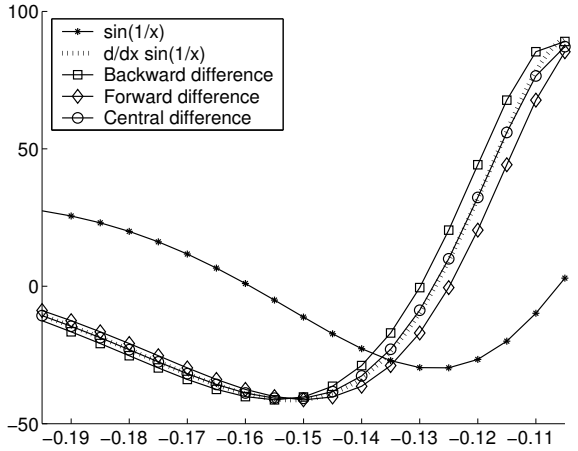



Figure 1: Comparison of several difference approximations of $\sin(1/x)$ on the interval $[-0.2, -0.1]$.

approximating the values of the derivative (or second derivative) at the node points. These matrices have banded structure; on each row, nonzero elements are only found on the diagonal and/or its immediate neighbors. As an example, the central difference and the second derivative approximations result in the matrices

$$\mathbf{D}_h = \frac{1}{2h}\begin{bmatrix} & 1 & & & & \\ -1 & & 1 & & & \\ & -1 & & 1 & & \\ & & \ddots & & \ddots & \\ & & & -1 & & 1 \\ & & & & -1 & \end{bmatrix} \quad \text{and} \quad \mathbf{\Delta}_h = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix},$$

so that $\mathbf{D}_h\,\mathbf{u}_h$ is a central difference approximation to the first derivative of the function $u$ with samples placed $h$ units apart and $\mathbf{\Delta}_h\mathbf{u}_h$ is the approximation of the second derivative in a similar fashion. Here the zero elements of the matrices have been left blank. The values for the ends of the interval are dependent on the initial and boundary conditions of the differential equation at hand, and some special care needs to be taken in order to get the boundary values right. We not discuss this further.

This point of view clearly demonstrates the fact that differentiation can be seen as an operator that acts on a function and produces another function, that is, the derivative of the original "input" function. When we deal with functions discretized as described earlier, the discretized differentiation operator is represented by a matrix. This is a consequence of differentiation being a linear operation in the continuous case[5].

[5] *Functional analysis* deals with properties of general linear operators – such as differentiation – which may be defined on infinite-dimensional spaces of functions.

## 3.3 Spatial discretization of the wave equation by finite differences

Here we show how finite difference approximations can be used for discretizing the wave equation. We work in one dimension, but we keep in mind that the development is essentially the same for higher dimensions.

By using the discretized representation $\mathbf{\Delta}_h$ for the second derivative we derive a *semidiscrete* version of the one-dimensional wave equation; by substituting $\mathbf{u}_h$ for $u$ and $\mathbf{\Delta}_h \mathbf{u}_h$ for $\Delta u$ and noting that $u_{xx} = \Delta u$ in one dimension we obtain

$$\mathbf{u}_h'' = c^2 \mathbf{\Delta}_h \mathbf{u}_h + \mathbf{f}_h, \tag{11}$$

where $\mathbf{f}_h$ denotes the values of the function $f$ in the node points, and primes denote differentiation with respect to time. Remarkably, this semidiscretized form of the wave equation is no longer a partial differential equation, since the spatial Laplacian has been "reduced" into a matrix multiply; it is an ordinary differential equation in $N$ unknowns with the unknown vector $\mathbf{u}_h$, whose elements are the values of the solution function $u$ at the node points $x_i$. This equation can be solved with any standard method for integrating differential equations with respect to time. These methods are discussed in the following section.

We also mention the *digital waveguide methods* for the solution of the wave equation. These methods are finite difference schemes with a digital signal processing point of view. The signal processing approach has many favorable qualities; these include e.g. the possiblity of using frequency-dependent boundary conditions implemented by digital filters. The interpolated waveguide mesh of Savioja *et al.* bears some resemblance to the finite element method. See (Savioja, 1999) for an in-depth treatment of digital waveguide methods.

## 3.4 Two- and three-dimensional problems

The one-dimensional difference approximations discussed in the previous sections are easily extended to two or more dimensions. For instance, the gradient operator, defined as $\nabla = \left(\frac{\partial}{\partial x} \frac{\partial}{\partial y}\right)$ in 2D and $\nabla = \left(\frac{\partial}{\partial x} \frac{\partial}{\partial y} \frac{\partial}{\partial z}\right)$ in 3D, is easily implemented with one-dimensional finite differences along each coordinate axis. In a similar fashion, the Laplacian operator – see equation (2) – takes the form

$$\begin{aligned} \Delta u|_{(ih,jh)} &\approx \frac{\mathbf{u}_h(i+1,j) - 2\mathbf{u}_h(i,j) + \mathbf{u}_h(i-1,j)}{h^2} \\ &\quad + \frac{\mathbf{u}_h(i,j+1) - 2\mathbf{u}_h(i,j) + \mathbf{u}_h(i,j-1)}{h^2} \\ &= \frac{\mathbf{u}_h(i+1,j) + \mathbf{u}_h(i-1,j) + \mathbf{u}_h(i,j+1) + \mathbf{u}_h(i,j-1) - 4\mathbf{u}_h(i,j)}{h^2} \end{aligned} \tag{12}$$

in two dimensions, where we have assumed that the two-dimensional domain has been discretized into a regular grid of points, so that the values of the function $u$ are now stored in a matrix (in stead of a vector) $\mathbf{u}_h$, so that $u_h(ih, jh) \approx \mathbf{u}(i, j)$. For simplicity, we have assumed the same discretization parameter $h$ for both dimensions. The three-dimensional case is analoguous.

Writing the difference approximation from equation (12) into a matrix form (as above) presents some difficulty due to $\mathbf{u}_h$ now being a matrix in stead of a vector as in the one-dimensional case. Still, as the approximation is again a linear combination of the elements of $\mathbf{u}_h$, a similar matrix representation does exist (Eirola, 2002). This is achieved by first stacking the columns of $\mathbf{u}_h$ into a long column vector, after which it is straightforward to derive the required matrix expressions. After this modification the semidiscretized wave equation in two or more dimensions is exactly the same as equation (11), the one-dimensional case.

## 4 Time Integration

This section presents the necessary tools for obtaining a fully discrete solution of the wave equation by time stepping. The process is called *integrating* the differential equation. To this end, we first write the semidiscretized equation as a first-order system of differential equations, and after that present different time-stepping methods for solving the first-order system. We conclude by some remarks on stability of the numerical solutions.

We first recall the semidiscretized equation

$$\begin{cases} \mathbf{u}_h'' = c^2 \boldsymbol{\Delta}_h \mathbf{u}_h + \mathbf{f}_h, & \mathbf{x} \in \Omega \text{ (equation of motion)} \\ \mathbf{u}_h(0, \mathbf{x}) = \mathbf{u}_h^0(\mathbf{x}), & \text{(initial condition for } \mathbf{u}_h\text{)} \\ \mathbf{u}_h'(0, \mathbf{x}) = \mathbf{v}_h^0(\mathbf{x}), & \text{(initial condition for } \mathbf{u}_h'\text{)}, \end{cases}$$

where $\mathbf{u}_h^0$ and $\mathbf{v}_h^0$ are predefined functions defined over the spatial discretization. In addition, the problem-dependent boundary conditions need to be specified. This is a second-order system of ordinary differential equations in $N$ unknowns.

Most integration methods work on first-order differential equations. This poses no problems, since all higher-order problems can be transformed into first-order ones by introducing new variables. To transform the semidiscretized wave equation into a first-order system, we define a new variable $\mathbf{v}_h = \frac{d\mathbf{u}_h}{dt}$ so that equation (11) takes the form

$$\begin{cases} \frac{d\mathbf{v}_h}{dt} = c^2 \boldsymbol{\Delta}_h \mathbf{u}_h + \mathbf{f}_h \\ \frac{d\mathbf{u}_h}{dt} = \mathbf{v}_h. \end{cases} \tag{13}$$

This has the effect of doubling the number of unknowns, since we are now left with *two* vectors of length $N$ to solve for. We can further simplify the system (13) by concatenating

the vectors $\mathbf{u}_h$ and $\mathbf{v}_h$ into a new vector $\mathbf{w}$ so that we get

$$\frac{d\mathbf{w}}{dt} = \mathbf{A}\mathbf{w} + \mathbf{g}, \quad \text{with} \tag{14}$$
$$\mathbf{w} = \begin{bmatrix}\mathbf{u}_h \\ \mathbf{v}_h\end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix}0 \\ \mathbf{f}_h\end{bmatrix}, \quad \mathbf{A} = \begin{bmatrix}\mathbf{0} & \mathbf{I} \\ c^2\boldsymbol{\Delta}_h & \mathbf{0}\end{bmatrix}, \quad \text{and } \mathbf{w}(0) = \begin{bmatrix}\mathbf{u}_h^0 \\ \mathbf{v}_h^0\end{bmatrix},$$

where each element of $\mathbf{A}$, printed in bold, denotes a $N \times N$ submatrix, and $\mathbf{I}$ denotes the identity matrix. This is the simplest possible form for a first-order, linear system of differential equations.

The numerical solution of the above system is a discrete sequence $\mathbf{w}^k$, $k \in \mathbb{N}$, of vectors corresponding to values of the solution $\mathbf{w}$ at different timesteps. We choose to use a constant timestep $\delta$ for simplicity, so that we have $\mathbf{w}^k \approx \mathbf{w}(t_k)$, where $t_k = \delta k$. Similarly, we denote $\mathbf{g}(\delta k)$ by $\mathbf{g}^k$.

To make description of the integration methods in the next subsections still simpler, we make use of a more abstract formulation. In general, any first-order system of differential equations[6] can be written as

$$\mathbf{w}'(t) = \mathbf{d}(t, \mathbf{w}(t)). \tag{15}$$

Equation (14) maps to this representation by

$$\mathbf{d}(t, \mathbf{w}(t)) = \mathbf{A}\mathbf{w}(t) + \mathbf{g}(t). \tag{16}$$

This more abstract form (15) is most suitable for describing integration methods.

## 4.1 Explicit methods

The most obvious integration method for the system (15) is the *Euler method*. It follows from substituting the forward difference scheme from section 3.1 into (15), yielding

$$\begin{aligned}\frac{\mathbf{w}^{k+1} - \mathbf{w}^k}{\delta} &= \mathbf{d}(t_k, \mathbf{w}^k) \\ \Leftrightarrow \mathbf{w}^{k+1} &= \delta\, \mathbf{d}(t_k, \mathbf{w}^k) + \mathbf{w}^k.\end{aligned}$$

Substituting for $\mathbf{d}$ from (16) we have

$$\mathbf{w}^{k+1} = \delta\left(\mathbf{A}\mathbf{w}^k + \mathbf{g}^k\right) + \mathbf{w}^k = (\delta\mathbf{A} + \mathbf{I})\,\mathbf{w}^k + \delta\mathbf{g}^k. \tag{17}$$

This method has the advantage of simplicity, but in practice it is not used much, because it is highly *unstable*. We come back to stability issues in the end of the section.

The Euler method is the simplest one in the class of methods generally referred to as explicit Runge-Kutta methods. The classical Runge-Kutta method, often referred to as *the* Runge-Kutta method, is one of them. All the higher-order R-K methods work by subdividing the time interval into smaller sub-timesteps, achieving variable orders of accuracy. The Euler method performs worst of these methods.

[6] also non-linear systems

## 4.2 Implicit methods

So-called implicit methods help overcome stability problems often associated with explicit schemes. The difference between explicit and implicit methods is best illustrated by the *implicit Euler* method, which follows from substituting the bacward difference approximation into (15):

$$\frac{\mathbf{w}^k - \mathbf{w}^{k-1}}{\delta} = \mathbf{d}(t_k, \mathbf{w}^k) \quad \Leftrightarrow \quad \mathbf{w}^k = \delta\, \mathbf{d}(t_k, \mathbf{w}^k) + \mathbf{w}^{k-1},$$

and after manipulating the indices we have

$$\mathbf{w}^{k+1} = \delta\, \mathbf{d}(t_{k+1}, \mathbf{w}^{k+1}) + \mathbf{w}^k, \tag{18}$$

and substituting for $\mathbf{d}$ we finally get

$$\begin{aligned} \mathbf{w}^{k+1} &= \delta \left( \mathbf{A}\mathbf{w}^{k+1} + \mathbf{g}^{k+1} \right) + \mathbf{w}^k \\ \Leftrightarrow (\mathbf{I} - \delta\mathbf{A})\ \mathbf{w}^{k+1} &= \mathbf{w}^k + \delta\mathbf{g}^{k+1} \\ \Leftrightarrow \mathbf{w}^{k+1} &= (\mathbf{I} - \delta\mathbf{A})^{-1} \left( \mathbf{w}^k + \delta\mathbf{g}^{k+1} \right). \end{aligned} \tag{19}$$

The scheme works by "borrowing" the future value for $\mathbf{w}$ in the evaluation of the function $\mathbf{d}$. The seemingly innocent switching from forward to backward differences has yielded a significantly different difference scheme; one that requires a matrix inversion. (Note that when the timestep $\delta$ is constant, the inversion only has to be done once.) The implicit Euler method is still simple, and has the virtue of unconditional stability.

The most accurate first-order implicit scheme is the Crank-Nicolson method[7]. It is an application of the central difference scheme, and its idea is to evaluate the function $\mathbf{d}$ in the middle of the timestep, with respect to both time and the solution $\mathbf{w}$. The scheme is defined as

$$\frac{\mathbf{w}^{k+1} - \mathbf{w}^k}{h} = \mathbf{d}(\tfrac{1}{2}(t_k + t_{k+1}), \tfrac{1}{2}(\mathbf{w}^k + \mathbf{w}^{k+1})).$$

Substituting $\mathbf{d}$ from (16) as before we have

$$\begin{aligned} \mathbf{w}^{k+1} &= \mathbf{w}^k + \tfrac{1}{2}\delta\mathbf{A} \left( \mathbf{w}^k + \mathbf{w}^{k+1} \right) + \delta\mathbf{g}(t_k + \tfrac{\delta}{2}) \\ \Leftrightarrow \left( \mathbf{I} - \tfrac{1}{2}\delta\mathbf{A} \right) \mathbf{w}^{k+1} &= \left( \mathbf{I} + \tfrac{1}{2}\delta\mathbf{A} \right) \mathbf{w}^k + \delta\mathbf{g}(t_k + \tfrac{\delta}{2}) \\ \Leftrightarrow \mathbf{w}^{k+1} &= \left( \mathbf{I} - \tfrac{1}{2}\delta\mathbf{A} \right)^{-1} \left[ \left( \mathbf{I} + \tfrac{1}{2}\delta\mathbf{A} \right) \mathbf{w}^k + \delta\mathbf{g}(t_k + \tfrac{\delta}{2}) \right]. \end{aligned} \tag{20}$$

As is obvious, the increased accuracy over the implicit Euler method comes at the price of a more laborious timestep, since one additional matrix multiply now has to be performed. Again, if $\delta$ is constant, the matrices have to be formed (and the other inverted) only once.

[7] Finnish "implisiittinen keskipistesääntö"

## 4.3 Stability

The continuous, exact solutions of the wave equation have the property of energy conservation. That is, if the boundaries of the environment are fully reflecting, the solution oscillates infinitely, with its energy content[8] staying constant, if we let $f \equiv 0$. This is an important property, and numerical methods perform differently with respect to it.

If a numerical method allows the energy of the discretized solution to grow without bound as time passes, the method is called *unstable*. We only state briefly that the magnitudes of the eigenvalues of the matrices used in the explicit iteration schemes determine constraints on the maximum possible timestep size. The eigenvalues' magnitudes have a dependence on $h$, so that these constraints usually dictate the maximum allowable timestep for a given level of discretization. With larger timesteps the solution is soon ruined by high-magnitude noise as calculation errors build up in an uncontrollable fashion. Implicit methods are unconditionally stable. See (Eirola, 2002) for a treatment.

In practice, the timestep restrictions imposed on explicit methods are so stringent that the additional computation per time step required by implicit methods is outweighed by the gains from using larger timesteps.

# 5 The Finite Element Method

The Finite Element Method (FEM) is a general method for solving both ordinary and partial differential equations. In this section we show how it can used for solving the wave equation. Our approach is not the only possible one, since our derivation ends up (again) in a system of ordinary differential equations, which we solve by the methods presented earlier – another approach would be to use a FEM formulation also for the time-dependent ordinary differential equation.

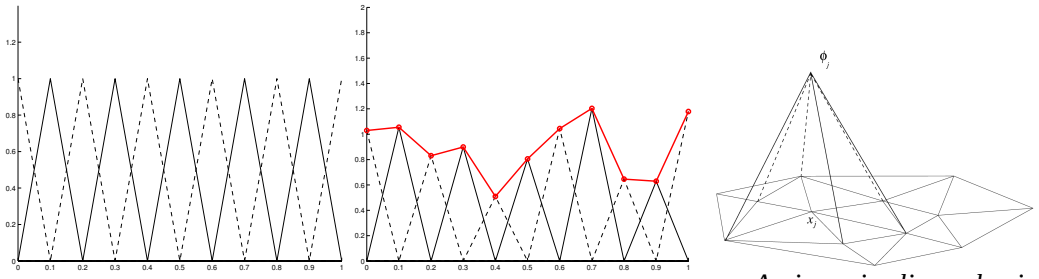
The general ideas behind the FE method rely heavily on concepts of so-called Hilbert and Sobolev spaces. We develop the method from bottom up and do not present these more advanced concepts.

## 5.1 Introduction

FEM takes a fundamentally different approach from the point-evaluation based finite difference methods described earlier. The idea is to seek for the solution as a finite linear combination of *basis functions*, so that the linear combination is, in a sense, the "best approximation" to the real solution from this finite-dimensional set of functions.

Basis functions are best described by an example, again in univariate functions on the interval $[0, 1]$. Suppose that we have scattered $N$ node points $x_i$ onto the interval, just as before. Now, we define a "hat" function $\phi_i(x)$ corresponding to each $x_i$; the hat function

[8] We skip the details of defining the energy content in a formal way.



*"Hat" functions on* $[0, 1]$

*An example linear combination of hat functions*

*A piecewise linear basis function in a triangulation (from Eirola, 2002)*

Figure 2: Illustration of piecewise linear "hat" functions on the interval $[0, 1]$ and their linear combinations. The hat functions themselves are nonzero only at their corresponding nodes and between the adjacent nodes to both directions. Their linear combinations (in red), on the other hand, define piecewise linear functions on the whole interval.

takes the value $1$ at $x_i$ and ramps linearly to $0$ towards $x_{i-1}$ and $x_{i+1}$. Now, define an N-vector $\boldsymbol{\xi}$, with its components denoted $\xi_i$, and let

$$\mathbf{u}(x) = \sum_{i=1}^{N} \xi_i \, \phi_i(x). \tag{21}$$

Figure 2 shows an example with eleven nodes, the corresponding piecewise linear basis functions, and an example linear combination of the basis functions. The *linear span* of the basis functions is a vector space in the sense that the sum of any two such functions is again a function which can be represented in the same way.

By the *support* of a function we mean the smallest set outside which the function is identically zero. The functions in the previous example are defined piecewise, and they have small supports. This has computational advantages, as will become obvious after we have formulated the full finite element method in the next sections. However, the development itself does not rule out use of functions with global supports, meaning functions that are nonzero on the whole domain. For instance, all polynomials on the whole interval $[0, 1]$ have global supports, as well as the usual trigonometric polynomials $\sin(2\pi kx)$, with $k \in \mathbb{N}$. Also, *piecewise polynomial* functions find common use in FEM applications; the "hat" functions of the example are 1st order piecewise polynomials. To be completely precise, the name *finite element method* is used only if locally supported basis functions are used; the more general case is the *Galerkin method*.

The two- and three-dimensional analogue to our hat function example is to scatter points inside the domain $\Omega$ and construct a triangulation of them in 2D or a tetrahedralization in 3D. The piecewise linear functions now take a form where the functions have value $1$ at the corresponding node and ramp to zero linearly inside the triangles (or tetraedra) associated with the node. Also higher-order piecewise polynomials can be used. (Globally

supported basis functions cannot be used in non-simple higher-dimensional geometries because of incompatibilities with the boundary conditions. This is a more advanced topic, and will not be pursued here.)

We also mention that triangles or tetraedrae are not the only possible geometrical primitives that can be used for constructing the basis functions. For instance, quadrilaterals and parallelepipedon may be used with piecewise bilinear or bicubic functions, respectively.

## 5.2 Variational Formulation of the Wave Equation

In this section we will show how to search for the solution to the wave equation as a linear combination of basis functions. Since the solutions are time-dependent, we will make the coefficient vector $\boldsymbol{\xi}$ time-dependent also, so that the spatially discretized solution has the form

$$u_h(t, \mathbf{x}) = \sum_{i=1}^{N} \xi_i(t)\, \phi_i(\mathbf{x}) \approx u. \tag{22}$$

To start off, we move all the terms of the wave equation onto the other side and get

$$u_{tt} - \Delta u - f = 0. \tag{23}$$

Now, let $V$ denote the set of bounded, continuous functions defined on $\Omega$ having piecewise continuous first derivatives (gradients in higher dimensions) and fulfilling the spatial boundary conditions of the problem. (We note that the "hat" functions, used as examples in the previous section, are members of $V$, when $\Omega = [0, 1]$, neglecting boundary conditions.) $V$ is obviously infinite-dimensional, and the exact solution $u$ to (23) is also a member of this space[9]. The fundamental theorem of calculus of variations (Guenther & Lee, 1996) states that if we multiply equation (23) by *any* function in $V$ and integrate the product over $\Omega$, we must still get $0$:

$$\int_\Omega (u_{tt} - \Delta u - f)\, v \, d\mathbf{x} = 0, \qquad \forall\, v \in V. \tag{24}$$

The goal of the following development is to simplify this equation in this general case, and then in the end to switch focus to a finite-dimensional subspace $V_h$ of $V$ spanned by the basis functions $\phi_i(\mathbf{x})$. This will allow us to write out a linear system of equations for the unknown coefficients $\boldsymbol{\xi}(t)$.

It is easy to verify by Gauss' divergence theorem[10] that

$$\int_\Omega v \Delta u \, d\mathbf{x} = -\int_\Omega \nabla v \cdot \nabla u \, d\mathbf{x} + \int_{\partial\Omega} v \nabla u \cdot \mathbf{n} \, d\sigma, \tag{25}$$

[9] In addition, its first derivative along with its Laplacian are continuous.

[10] $\int_\Omega \nabla \cdot \mathbf{F}\, d\mathbf{x} = \int_{\partial\Omega} \mathbf{F} \cdot \mathbf{n}\, d\sigma$, where $\mathbf{F}$ is a vector field over $\Omega$; just substitute $\mathbf{F} = v\nabla u$ to get (25).

where $d\sigma$ is an area element on $\partial\Omega$. Applying this result to equation (24) we have

$$\int_\Omega (u_{tt}v + \nabla u \cdot \nabla v - fv)\, d\mathbf{x} - \int_{\partial\Omega} v\nabla u \cdot \mathbf{n}\, d\sigma = 0, \qquad \forall\, v \in V, \tag{26}$$

which is called the *variational formulation* of the wave equation. The solutions to (26) are called *weak solutions* to the wave equation. Classical theory of partial differential equations shows that any sufficiently smooth $u$ that solves (26) is also a classical solution of the wave equation (Eirola, 2002).

Now we approach the heart of the matter. Substituting the approximation (22) into (26) *and* requiring that (26) *only holds for the members $\phi_k$ of $V_h$* (and not the "full" $V$) yields

$$\sum_{i=1}^N \xi_i'' \int_\Omega \phi_i(\mathbf{x})\, \phi_k(\mathbf{x})\, d\mathbf{x} + \sum_{i=1}^N \xi_i \int_\Omega \nabla\phi_k(\mathbf{x}) \cdot \nabla\phi_i(\mathbf{x})\, d\mathbf{x} - \tag{27}$$

$$\sum_{i=1}^N \xi_i \int_{\partial\Omega} \phi_k(\mathbf{x})\, \nabla\phi_i(\mathbf{x}) \cdot \mathbf{n}\, d\sigma = \int_\Omega f(\mathbf{x})\, \phi_k(\mathbf{x})\, d\mathbf{x}, \qquad \forall\, \phi_k \in V_h, \tag{28}$$

where we have used

$$u_h'' = \sum_{i=1}^N \xi_i(t)''\phi_i(\mathbf{x}), \qquad \nabla u_h = \sum_{i=1}^N \xi_i(t)\, \nabla\phi_i(\mathbf{x}),$$

with primes denoting differentiation with respect to time. We have also switched the order of summation and integration in the terms. Because $V_h$ is finite dimensional, (27) is actually a set of $N$ linear equations (one for each $\phi_k$, with $k = 1, \ldots, N$) for the coefficient vector $\boldsymbol{\xi}$. Hence it can be written in a matrix form as

$$\boldsymbol{\xi}''\mathbf{A} + \boldsymbol{\xi}\mathbf{S} - \boldsymbol{\xi}\mathbf{B} = \mathbf{f}, \tag{29}$$

with

$$A_{ij} = \int_\Omega \phi_i(\mathbf{x})\, \phi_j(\mathbf{x})\, d\mathbf{x}, \qquad S_{ij} = \int_\Omega \nabla\phi_i(\mathbf{x}) \cdot \nabla\phi_j(\mathbf{x})\, d\mathbf{x}, \tag{30}$$

$$B_{ij} = \int_{\partial\Omega} \phi_i(\mathbf{x})\, \nabla\phi_j(\mathbf{x}) \cdot \mathbf{n}\, d\sigma, \text{ and} \qquad f_j = \int_\Omega f(\mathbf{x})\, \phi_j(\mathbf{x})\, d\mathbf{x}. \tag{31}$$

Again, we are left with a linear system of ordinary differential equations, for which all the time integration methods described in section 4 apply directly.

As mentioned before, the sizes of the supports of the basis functions affect the computational load associated with FEM. The cost of evaluating the integrals in the expressions for the above matrices' elements benefits from locally supported functions, since small supports mean small nonzero regions in the integrands.

## 5.3 A Teaser

In the previous section we derived a spatial discretization of the wave equation as a linear combination of a finite number of prescribed basis functions. We have left out most of the mathematical structure that helps to understand the FE method from a more geometrical viewpoint because of lack of space. We do still mention a remarkable property; the finite element solution to the wave equation is *optimal* in the sense of a certain squared difference between the real solution and the approximate one, which means that no other linear combination of the basis functions could achieve a smaller error in this least squares -sense. This is quite surprising, considering that we do not have knowledge of the exact solution! This fact is best explained by stating (albeit cryptically) that the finite element solution is an *orthogonal projection* of the exact solution onto the finite dimensional linear span of the basis functions. For more information on vector spaces of functions, see for instance (Kreyszig, 1989).

# 6 Discussion

The previous sections have shown how the wave equation can be reduced into a system of ordinary differential equations either by finite difference approximations or by the finite element method. This section discusses some practical aspects of the methods presented above and outlines some differences between them.

## 6.1 Solution of large linear systems

In general, time integration requires solution of linear systems at each timestep. These systems are generally very large, routinely in the order of several millions of unknowns[11]. It is clear that direct solution, e.g. by Gaussian elimination, of the resulting equations is not feasible. The rescue lies in *iterative methods*, which do not manipulate the matrix (as Gaussian elimination does), but instead work by starting from an initial guess vector for the solution and then improving upon it in a successive series of iterations, until some degree of convergence is reached. Classical iterative methods include the Jacobi and Gauss-Seidel iterations. So-called *Krylov subspace* methods, such as the *conjugate gradient method*, search for the solution in the span of $\{x, Ax, A^2x, \ldots\}$, where $x$ is the initial guess and $A$ is the matrix in the problem. See Golub and van Loan (1996) for an in-depth review of iterative methods.

[11] Happily, the matrices obtained from the finite difference and FEM approximations are *sparse*, so that only a small fraction of the matrices' elements are nonzero.

## 6.2 Differences between the methods

The key difference between the finite difference method and FEM lies in the composition of the matrices. Once the matrices have been formed, the time stepping solution to the wave equation proceeds similarly.

Generally, the matrices inherent to the finite difference method have regular coefficients for nodes inside the domain; that is, all the nodes behave numerically in the same way. The matrices of FEM are more irregular, since their elements are integrals of the basis functions' products, and in general domains the basis functions do not form a regular structure. This makes construction of the FEM matrices much more involved than that of finite difference matrices.

Boundary conditions need special treatment in the finite difference method; detailed calculations on how to discretize different types of BCs are required. As stated earlier in the FEM section, the space $V$, from where the solutions are being searched for, is defined such that the basis functions "fulfill the boundary conditions" in a certain way; the rest of the BCs are enforced *weakly* in the form of the boundary integral in equation (27). In other words, FEM incorporates boundary conditions into its formulation in a unified way that alleviates some of the need for their special treatment.

Also, generation of the triangulations and tetraedralizations used frequently in FEM applications is far from trivial, and a wealth of research on the construction and quality of the subdivisions exists. Finite difference methods rely on structured grids, and hence are not dependent on such algorithms.

## 6.3 Practical considerations

The methods presented above solve for the sound field inside an enclosure in a rigorous way, i.e. the error in the solution can be made arbitrarily small (bound, of course, by machine precision) by adding more discretization nodes, using higher-order basis functions (FEM) or higher-order derivative approximations (FD) and using better time integrators.

Despite the correctness of the algorithms, direct application of these methods does *not* yield a practical system for solving for the impulse responses, at least if the whole frequency range of human hearing is to be simulated. This is obvious from geometry alone; depending on the particular method used, the spatial discretization needs 6-10 nodes per wavelength in order to resolve the frequencies faithfully (Svensson & Kristiansen, 2002). At 22 kHz one wavelength is approx. 1.5 cm, and thus the spacing between the nodes needs to be 1.5-2.5 mm. Thus, one cubic meter of space needs to be filled with 64-300 million nodes, and this translates directly to the same number of unknowns to solve for in the simulator. Herefrom it is obvious that full frequency range simulation of spaces of realistic size is as of yet completely unfeasible, and some hybrid methods combining direct numerical simulation by wavefield decomposition techniques (such as the image source method) must be utilized. For reference, modern scientific computing uses meshes with up to ten million elements. If a rectangular room with a 45 $m^3$ volume

was discretized with ten million elements, the average density of mesh points would be approx. 15 cm, corresponding to a maximum frequency of 220-370 Hz only. Clearly, direct numerical simulation of acoustic phenomena in the whole frequency range remains out of our grasp at present. This is perhaps not too unfortunate, since for instance the image source method augmented by edge diffraction sources produces an exact solution for planar geometries[12].

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[12] Albeit at the cost of exponential growth in computation time as the sound field becomes more and more diffuse.