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Teaching wave theory with simulations - numerical aspects

ABSTRACT: A ripple tank simulation is presented that lets the students interactively explore basic wave phenomena like the propagation of circular waves, the Doppler effect or refraction at a boundary. Moreover the artifacts of the numerical simulation that show up for special parameter values like very short or very long wave lengths can be used to demonstrate the limitations of the simulation program.
This is a good starting point for a discussion of the finite difference scheme employed for solving the two-dimensional wave equation: The consequences of the Nyquist frequency and of numerical dispersion and damping are explained as well as the sophisticated boundary scheme known as "perfectly matched layer".

1. Introduction

Simulation programs are widely used as valuable tools in physics education, large collections for many different application areas are available on the internet [1] or have been published [2]. They provide idealized *virtual experiments* that allow to explore the general behaviour of a physical system or to find precise numerical relations. For that purpose they generally emulate the precise physical laws of simplified physical situations thereby freeing the students from coping with complicated secondary effects.

For teaching wave theory a basic device that allows to demonstrate many important phenomena is the ripple tank. A simulated version can supplement true experiments by loosing some real world restrictions, e. g.

reflections at the boundaries can be suppressed,

properties of the medium can be chosen arbitrarily,

any initial conditions can be set.

Many instructive examples from basic wave theory, acoustics or optics can be easily created by simply including some point or line sources and properly shaped walls.

But when one tries to compute numerical solutions of the wave equation on a standard PC one has to restrict the accuracy of the simulation - e. g. by introducing a rather small computational grid - in order to get animations that run fluently in real time. This can lead to many different kinds of numerical artefacts that spoil the accuracy of the results. Furthermore it destroys the illusion of looking at a real-world situation.

Instead of trying to hide these problems by restricting the possible parameter ranges to values that lead to "correct" results, one can explicitly confront the students with unexpected phenomena. If the mathematical prerequisites - and the time available for off-topic themes - permit it, one can use the opportunity to explain some basic facts of the finite difference method for solving the wave equation [3]. But even if not, the students can gain a basic comprehension of the problems of numerical simulation. This is a very important point especially for engineering students, who all to often use the results of complex numerical programs without critically reflecting on the methods used and their validity for the question at hand.

The next section shows some strange-looking results from applets that are used to demonstrate circular wave propagation, the Doppler effect and refraction. In the following sections some basic features of the finite difference scheme used in the programs are presented and it is shown how they lead to the problems observed before. All values are given as dimensionless numbers, units can be provided easily if desired.

2. Examples of artefacts in a ripple tank simulation

We will now present three example programs together with their usual applications in a physics course. For certain parameter values they show rather astonishing results, which are labeled for reference in the following analysis section.
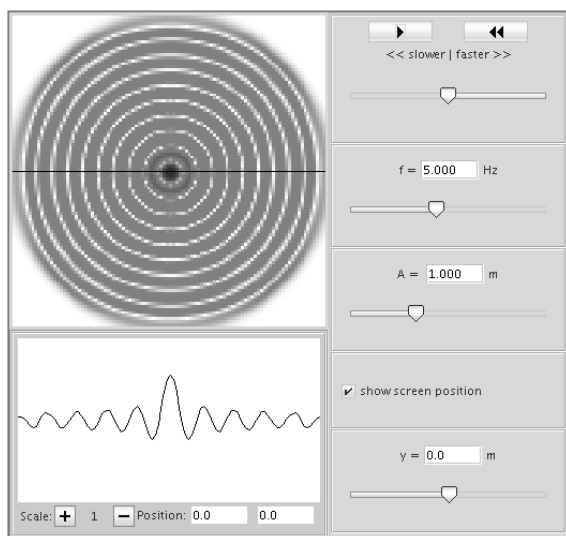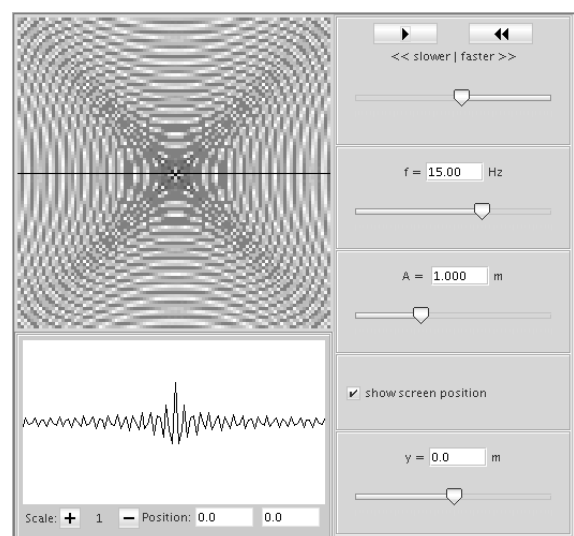

Figure 1: Regular circular wave

Figure 2: Diagonally distorted wave

Propagation of circular waves

The first program simulates circular waves spreading from a point source that oscillates harmonically. Students can measure wave lengths and amplitudes to find the form of the corresponding wave function (s. fig. 1).

Using other frequencies than the standard value f = 5 can lead to surprising phenomena:

Problem A: At f = 92 the image is the same is for f = 7. One has to assure the students that this is **not** a bug in the program!

Problem B: For f = 15 a diagonal pattern emerges (s. fig 2).

Problem C: With f = 30 no wave is shown at all, the screen is empty except for the direct vicinity of the source.

Problem D: Using f = 1, the circular pattern is deformed and contains quadratic bumps (s. fig 3).

Doppler effect of a moving source

The second example shows the waves propagating from a point source that moves with constant velocity. Together with a corresponding program for a moving receiver it shows the physical difference between these two cases and allows to measure the Doppler frequency shift.

Problem E: Setting the velocity to v = 0.8 (at a wave propagation velocity of c = 1) the bow wave is missing almost completely, instead a kind of shock wave develops in the direction of movement (s. fig 4).
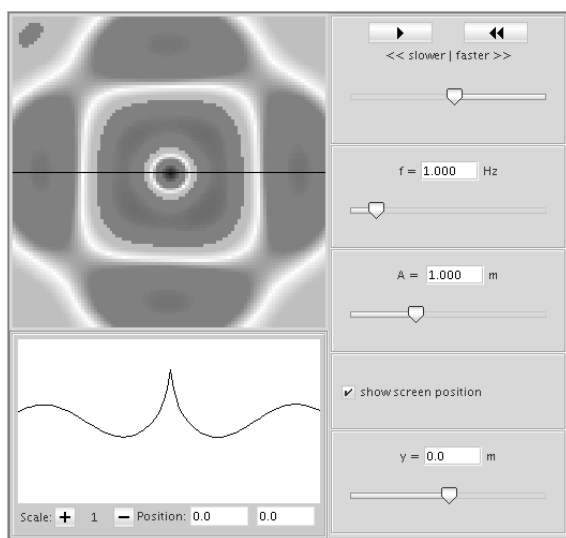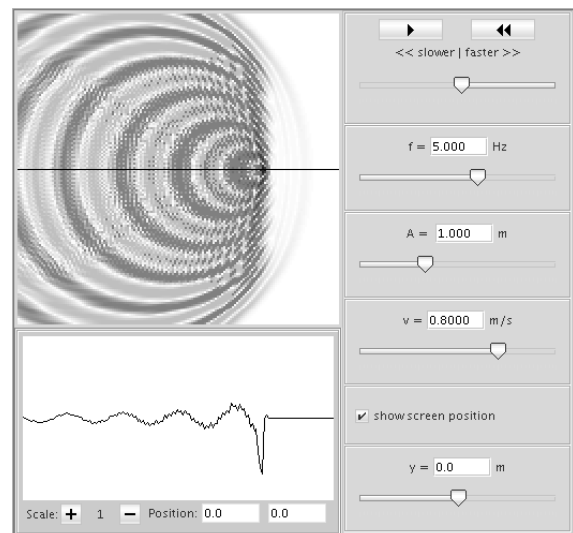
Figure 3: Circular wave with bumps   Figure 4: Doppler effect with shock wave

Wave refraction

The third applet displays a plane wave that meets a different medium. Students can change the angle of the incident wave and the propagation velocity c_2 in the second medium to find Snellius' law and the connection between c and the index of refraction (s. fig. 5).

Problem F: Using $c_2 = 0.5$ and f = 8 the wave seems to be not refracted at all, but propagates almost straight ahead through the second medium.

Problem G: For f = 10 (and again $c_2 = 0.5$) the wave doesn't intrude the second medium, but is totally reflected instead.

Numerical aspects of the wave equation

To find numerical solutions of the two-dimensional wave equation

$$\frac{\partial^2 u}{\partial t^2} - c^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = 0 \quad (1)$$

the applets use a standard finite difference scheme on a quadratic grid. Due to the limited computer speed a sufficiently smooth animation enforces a rather small grid, actually it usually has 100 grid points on the interval [-1, 1], leading to $\Delta x = 2/99$. The time step size used then is $\Delta t = 1/99$.

The next sections show how different aspects of the discretization lead to the problems listed above. Since the analysis should in principle be comprehensible by students with no beforehand knowledge of numerical mathematics, it concentrates on the most basic arguments.

Nyquist frequency

To understand the reason for problem A one only has to realize that the simulation proceeds in fixed time steps, which creates a stroboscopic effect (s. fig. 6): The sample values that result from a source oscillating with f = 92 sampled at $\Delta t = 1/99$ coincide with samples from a source with f = 7.

For students with a background in signal theory (e. g. electrical engineers) one can point at the relationship to the Nyquist–Shannon sampling theorem: The Nyquist frequency here is

$$f_N = \frac{1}{2 \Delta t} = \frac{99}{2}$$

which for a signal of f = 92 leads to an aliasing frequency

$$f_A = 2 f_N - f = 7$$
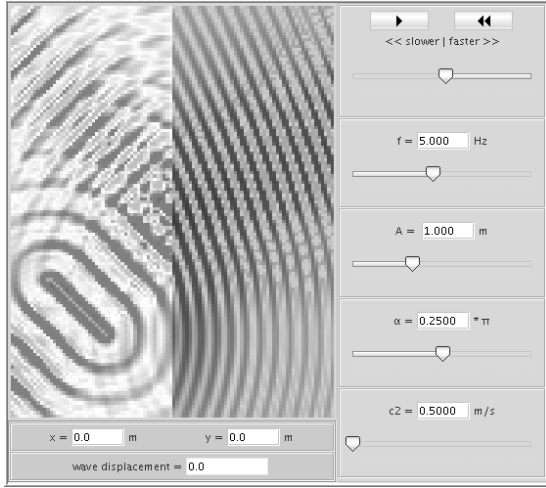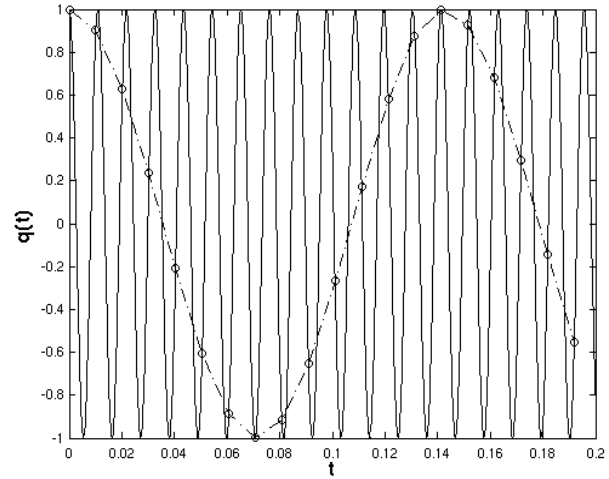
in accordance with the observations.

Figure 5: Refraction

Figure 6: Aliasing above the Nyquist frequency

Numerical dispersion

To solve the wave equation numerically one introduces the value $U_{i,j}^n$ of the wave function on the grid point (x_i, y_i) at time t_n. Replacing the second derivations by central differences

$$\frac{\partial^2 u}{\partial t^2} \quad \rightarrow \quad \frac{1}{(\Delta t)^2}(U_{i,j}^{n+1} - 2U_{i,j}^n + U_{i,j}^{n-1})$$

$$\frac{\partial^2 u}{\partial x^2} \quad \rightarrow \quad \frac{1}{(\Delta x)^2}(U_{i+1,j}^n - 2U_{i,j}^n + U_{i-1,j}^n)$$

$$\frac{\partial^2 u}{\partial y^2} \quad \rightarrow \quad \frac{1}{(\Delta x)^2}(U_{i,j+1}^n - 2U_{i,j}^n + U_{i,j-1}^n)$$

the wave equation is transformed into

$$U_{i,j}^{n+1} = (2 - 4\xi^2)U_{i,j}^n + \xi^2(U_{i+1,j}^n + U_{i-1,j}^n + U_{i,j+1}^n + U_{i,j-1}^n) - U_{i,j}^{n-1} \qquad (2)$$

where the Courant number ξ has been introduced:

$$\xi := \frac{c \Delta t}{\Delta x} \qquad (3)$$

Starting with values for U at time steps n = 0 and n = 1 and given values on the grid boundaries, one can use (2) to easily compute U at later times.

The best-known solutions of the wave equation are of course traveling waves. Therefore to analyze the properties of the numerical scheme used here we make the ansatz

$$U_{j,l}^n = e^{i(n\omega \Delta t - jk_x \Delta x - l k_y \Delta x)}$$

We insert it into (2) and get

$$\sin^2(\xi \frac{\omega}{c} \frac{\Delta x}{2}) = \xi^2 \left(\sin^2(k_x \frac{\Delta x}{2}) + \sin^2(k_y \frac{\Delta x}{2}) \right) \quad (4)$$

This is a dispersion relation, i. e. a relation between omega and $\vec{k}$. In the continuum limit $\Delta x \to 0$ it reproduces the well known formula

$$\frac{\omega}{c} = \sqrt{k_x^2 + k_y^2} = |\vec{k}| =: k \quad (5)$$

Since the (phase) velocity v of the wave is given by $v = \omega / k$, eq. (5) states that all waves travel with the same velocity c, irrespective of their frequency. But for finite Δx things are a bit more complicated.

A simple consequence of (4) is that in order to have a real valued ω for all values of k_x, k_y, we must have

$$\xi \leq \frac{1}{\sqrt{2}}$$

This is the famous CFL condition, which constrains the size of the time step for a given Δx. If it is violated, small scale fluctuations (large k) will grow up exponentially and make the simulation results completely useless. In the following we will set ξ = 1/2 as it is used in the simulation program.

Specializing to horizontal waves we set $k_x = k$, $k_y = 0$. Putting this into (4) and solving for k, one gets the velocity of waves traveling in horizontal direction:

$$v_h = \frac{\omega}{k} = \frac{\omega \Delta x}{2 \arcsin(\frac{1}{\xi} \sin(\xi \frac{\omega}{c} \frac{\Delta x}{2}))} \quad (6)$$

The same relation holds for vertical waves due to the quadratic grid.
For diagonal waves we have accordingly $k_x = k_y = k / \sqrt{2}$, which leads to

$$v_d = \frac{\omega \Delta x}{2 \sqrt{2} \arcsin(\frac{1}{\sqrt{2}\xi} \sin(\xi \frac{\omega}{c} \frac{\Delta x}{2}))} \quad (7)$$

With the values for Δx, ξ and c used in the first applet the wave propagation velocities in horizontal (or vertical) and diagonal directions are plotted as functions of the frequency f = ω/2π in fig. 7.
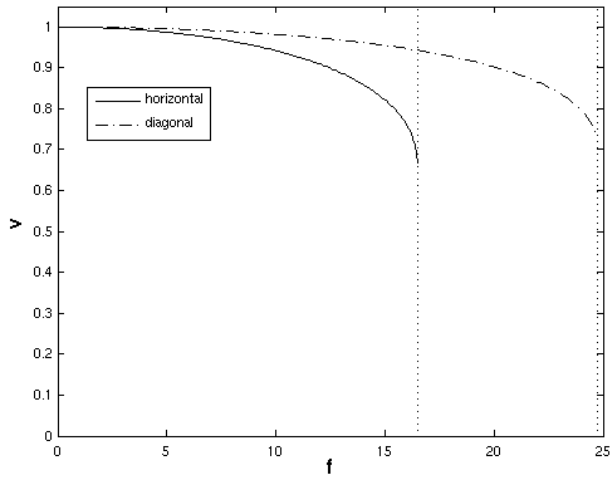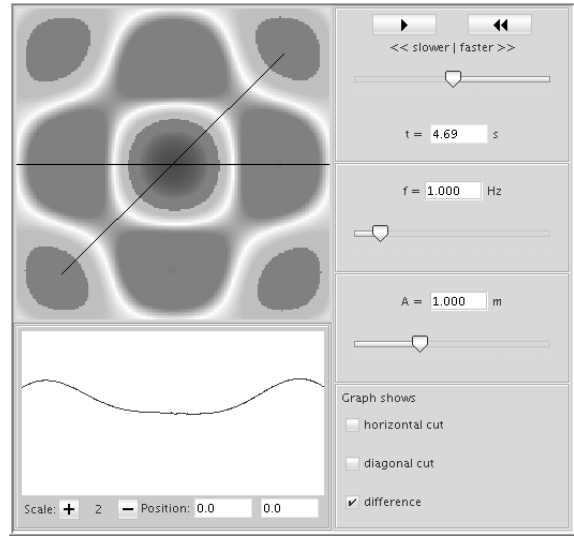
Figure 7: Numerical dispersion relations

Figure 8: Standing wave due to reflections

This easily accounts for the diagonal pattern seen in problem B: For f = 15 the velocities are

$$v_h = 0.8213, \quad v_d = 0.9548$$

i. e. the waves propagate faster in diagonal directions.

For problem F we have the same explanation: With c = 0.5 and f = 8 we get

$$v_h = 0.3802, \quad v_d = 0.4735$$

Since $v_d > v_h$, the refracted wave is bent into the diagonal direction, which leads to the physically incorrect behaviour seen above.

Numerical damping
Though the CFL condition guarantees real values of omega for all real values of k, it doesn't work in the inverse direction: For $\xi = 1/2$ the dispersion relation (4) leads to complex values for k if ω is chosen large enough. As a result the corresponding waves are damped exponentially.

Vice versa the requirement that k and accordingly the wave velocity v are real valued leads to an upper bound for the frequency. Using eq. (6)/(7) for horizontal/diagonal waves one gets

$$
\begin{aligned}
\omega_h &\leq \frac{c}{\Delta x} \frac{2}{\xi} \arcsin(\xi) \\
\omega_d &\leq \frac{c}{\Delta x} \frac{2}{\xi} \arcsin(\sqrt{2}\,\xi)
\end{aligned}
\tag{8}
$$

Setting $\xi = 1/2$ the bounds for the frequencies are simply

$$f_h \leq \frac{1}{3}\frac{c}{\Delta x}$$
$$f_d \leq \frac{1}{2}\frac{c}{\Delta x} \qquad (9)$$

With the values of problem C we have

$$f_h \leq 16.5, \quad f_d \leq 24.75$$

Since f = 30, the wave is damped and can't propagate.

The applet showing the Doppler effect uses a smaller grid size of $\Delta x = 2/149$ therefore

$$f_h \leq 24.83, \quad f_d \leq 37.25$$

The Doppler shifted frequency is given by the usual relation

$$f_D = \frac{f}{1 - v_Q/c} = 25$$

Therefore the wave doesn't propagate horizontally, whereas the diagonal part adds to the back waves and produces the "shock wave" of problem E.

In the case of problem G the grid size is $\Delta x = 2/99$, but now the velocity para-meter (on the right half) is only c = 1/2, i.e.

$$f_h \leq 8.25, \quad f_d \leq 12.375$$

Since the plane wave doesn't travel horizontally, it can't enter the medium.

Reflection at the boundaries
The remaining problem D happens for the low frequency f = 1, where the discretization scheme should work very well. Its origin is instead connected with the treatment of the boundaries, which is a much more difficult problem than one might expect.

Confronted with the question of what one should do at the boundaries, students usually propose at first to set U = 0, i. e. a simple Dirichlet condition. They have vague ideas like "There is nothing outside" and are rather surprised to see what actually happens (using another applet designed for that purpose): The outgoing wave is reflected at the boundaries, which completely destroys the circular pattern. A moments thought reveals the reason for the reflections: U = 0 is equal to a "fixed end", waves can't simply propagate "through" it. An analogue of the "loose end" doesn't help either: Waves are reflected here as well.

How to formulate boundary conditions that sustain the illusion of a virtually infinite grid, i. e. that don't lead to reflections, is actually a really hard problem and subject to a lot of - still ongoing - research. Fortunately a couple of good

practical solutions have been found [4]. The one used here is the introduction of a boundary layer of considerable thickness, which contains a clever designed absorbing material, the so-called *perfectly matched layer* (PML) due to Berenger [5]. Unfortunately the discretized version is not "perfect", but has residual reflections which increase with smaller incidence angles. A good rule of thumb is to take a boundary layer width that is at least half the wave length of the longest waves that appear.

Though the mathematical details are too complicated for an introductory course, the idea of the PML can be easily understood. To analyze further what is going on in the example, an additional applet is provided that displays the wave function in horizontal and diagonal directions together with the difference of these curves (cf. fig. 8).

When the wave meets the border at the edges, a substantial reflection happens that is difficult to recognize directly, but shows up rather clearly in the difference plot. It meets the outgoing wave, which leads to the generation of a standing wave directly visible as the already known box-shaped pulsating bumps.

The width of the boundary layer used in the applet is 0.4, which - according to the above mentioned rule - should work for waves with frequencies above 1.25. The problem at f = 1 is therefore well understood, and at f = 2 the simulated waves are almost perfectly circular.

Conclusions

The examples presented here have shown clearly that a ripple tank simulation can not only be useful for demonstrating physical problems, but displays very nicely some important features of the finite difference scheme used to solve the two-dimensional wave equation numerically.

Except for fundamental skills in algebraic, mainly trigonometric manipulations the mathematics used is restricted to a basic understanding of differentiation and a working knowledge of complex numbers, especially Euler's formula. The only exception is the formulation of the wave equation itself. Therefore it should be possible - after some hand-waving arguments to justify the wave equation - to present the details even in a freshman physics course.

But even if the mathematical details are beyond the grasp of the students, they at least can understand the basic connection between the grid size and the wave lengths that can be reasonably simulated on a grid. And most of all it can remind them of the basic law of numerics that is so often neglected in practice: Always check the prerequisites!

References

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