Project Practikum: Summer semester 2020.

Submission & Evaluation

The projects that can take place this semester (astro, CP, theory) should be finished with either a protocol or a scientific publication draft (paper). Deadline for submission to the supervisor or in the F-Praktikum is August 31th, 2020. A digital version (PDF) should be submitted via email (`physik.f-praktikum@uni-jena.de`) or given to the F-Praktikum office.

Project: Solution of the initial boundary value problem with the wave equation

The wave equation in 1+1 dimensions for the scalar field $\phi(t,x)$

$$\partial_{tt}\phi - c^2\partial_{xx}\phi = 0 \ , \tag{0.1}$$

is the main example for hyperbolic PDEs and it is usually associated to initial or initial-boundary value problems (IVP, IVBP). In the former, one specifies an initial profile $\phi(t=0,x) = \phi_0(x)$. In the latter, one additionally specifies conditions on the boundary $\partial\Omega$ of the spatial domain $\Omega = [a,b]$ (at all times). For example, periodic boundary conditions are $\phi(t,a) = \phi(t,b)$. IVPs and IBVPs with the wave equation are *w*ell posed problems, i.e. a unique solution exist and depends continuously on the initial data.

1. **Analytical part.** Write down the general analytical solution of the IVP. Note it is composed of two "elementary waves"(or *c*haracteristic waves).

2. Rewrite the wave equation from the second order form above to a first-order in time and second-order in space system by defining the new variable $\Pi = \partial_t\phi$,

$$\partial_t\phi = \Pi \ , \tag{0.2a}$$

$$\partial_t\Pi = c^2\partial_{xx}\phi \ . \tag{0.2b}$$

   Discuss the effect of two possible choices for the the initial condition for $\Pi(t=0,x)$ in view of the analytical solution derived above.

3. Write the wave equation as a fully first order system by defining the new variables $\Pi = \partial_t\phi$ and $\chi = \partial_x\phi$.

$$\partial_t u + A\partial_x u = S \ , \tag{0.3}$$

   where A is a matrix and $u = \{\phi, \Pi, \chi\}$ is the collection of the three fields or "state vector" and S is a source term. Discuss choices for the initial data for the fields $u(t=0,x)$.

   Analyze matrix A, derive eigenvalues and eigenvectors of the matrix A. What happens to the equations if you switch to new variables $w := Ru$, where R is the matrix of eigenvectors? To answer that, first show that $AR = \Lambda R$, where $\Lambda = \mathrm{diag}\lambda_i$ and give the solution of the general IVP in these new variables.

4. **Numerical part: Finite differencing approximation.** Introduce a uniform spatial grid, $x_i = ih$ with $i = 0, ..., n-1$ and $h = 1/(n-1)$ that discretizes the domain $\Omega = [0,1]$. Call the values of a field $u(x)$ on the grid points $u(x_i) = u_i$. Show that an approximation of the first derivative at point x_i is given by

$$\frac{du}{dx} \approx \frac{u_{i+1} - u_{i-1}}{2h} + \mathcal{O}(h^2) \ . \tag{0.4}$$

   Calculate the error term $\mathcal{O}(h^2)$ of the formula above.

Hint: consider the Taylor expansions of the function at $x_i \pm h$.

The formula above is called a second-order (because of the error term) finite-differencing approximation of the derivative with centered stencil (Note you use the same number of points arounf x_i).

Similarly, show that an approximation of the second derivative at point x_i is given by

$$\frac{d^2u}{dx^2} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \mathcal{O}(h^2) \ , \tag{0.5}$$

and compute the error term.

5. Consider example functions, e.g.

$$f(x) = (x - \frac{1}{2})^2 + x \ , \tag{0.6}$$
$$f(x) = (x - \frac{1}{2})^3 + (x - \frac{1}{2})^2 + x \ , \tag{0.7}$$
$$f(x) = \sqrt{x} \ , \tag{0.8}$$
$$s(x) = \sin{(12\pi x)} \ , \tag{0.9}$$
$$s(x) = \sin^4{(12\pi x)} \ , \tag{0.10}$$
$$g_a(x) = \exp{(-ax^2)} \ , \tag{0.11}$$

and calculate the first and second derivative with the finite differencing formulas above. For each, plot the exact derivative and the finite difference approximation (top panel) and their differences (bottom panel) for a grid of say $n = 20$ points.

In some relevant cases, study the error term and **convergence**. A way to do this is to consider the difference

$$f(x) - f^{(h)}(x) = Ch^2 + \mathcal{O}(h^3) \ , \tag{0.12}$$

for a grid resolution h, and for a second grid resolution, $f(x) - f^{(h/2)}(x) = C(h/2)^2$. Note that the constant C is the same (Why? See exercise above). Thus, if one plots $(f(x) - f^{(h)}(x))/(f(x) - f^{(h/2)}(x))$ one can extract experimentally the convergence order ($p = 2$). Note, that it would be a function of x, *i.e.,* depends on the grid position.

The convergence order for the entire spatial domain can be evaluated taking the norm as

$$\frac{|f(x) - f^{(h)}(x)|}{|f(x) - f^{(h/2)}(x)|} = Q \tag{0.13}$$

where $Q = 2^p$, and p being the convergence order.

In case of oscillatory functions, it is useful to consider a different (but equivalent in meaning) plot in which one shows the difference $f(x) - f^{(h)}(x)$ superposed to the difference $Q(f(x) - f^{(h/2)}(x))$ scaled by the proper expected factor $Q = 2^2 = 4$.

Note that in absence of a known analytical solution, one can always consider a third (or more) grid resolution, say $h/4$, and compare pairs of differences $(f^{(h)}(x) - f^{(h/2)}(x))$, $Q(f^{(h/2)}(x) - f^{(h/4)}(x))$ properly scaled. This second test is called *s*elf-convergence test. Perform this test for a couple of relevant cases and compare the results obtained with the two different convergence tests.

6. **Runge-Kutta time-integration.** There exist various algorithms to perform the time integration of (a single or a system of) ODEs

$$\frac{du}{dt} = F(u) \ , \tag{0.14}$$

given an initial value $u(t = 0) = u_0$ and a r.h.s function F.

Ruge-Kutta (RK) methods are robust schemes for integrating IVP. A general formulation formulation can be given starting from the integral form of the IVP above and approximating the integrals by quadratures. The **S**-stage RK scheme reads

$$u_{n+1} = u_n + \Delta t \sum_{i=0}^{S} b_i F(t_n + c_i \Delta t \, u^{(i)}) \tag{0.15a}$$

$$u^{(i)} = \Delta t \sum_{j=0}^{S} a_{ij} F(t_n + c_j \Delta t \, u^{(j)}) \ , \tag{0.15b}$$

An equivalent form is

$$u_{n+1} = u_n + \Delta t \sum_{i=0}^{S} b_i K_i \tag{0.16a}$$

$$K_i = F(t_n + c_i \Delta t \, u_0 + \Delta t \sum_{j=1}^{S-1} a_{ij} K_j) \ . \tag{0.16b}$$

Observations: (i) a S-stage RK is defined by the set of coefficients (a_{ij}, b_i, c_i). These coefficients are usually organized in a **Butcher table**

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & ... & a_{1S} \\ c_2 & a_{21} & a_{22} & ... & a_{2S} \\ ... & ... & ... & ... & ... \\ c_S & a_{S1} & a_{S2} & ... & a_{SS} \\ \hline & b_1 & b_2 & ... & b_S \end{array} \tag{0.17}$$

(ii) $a_{ij} = 0$ with $j \geq 1$, the method is *e*xplicit; (iii) if a_{ij} has nonzero elements in the upper triangular part, the method is *i*mplicit; (iv) An S-stage RK is an Sth order accurate method, $\mathcal{O}(\Delta t^S)$.

Write a routine implementing the RK4 ($S = 4$) scheme

$$\begin{array}{c|cccc} 0 & & & & \\ 1/2 & 1/2 & & & \\ 1/2 & 0 & 1/2 & & \\ 1 & 0 & 0 & 1 & \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array} \tag{0.18}$$

and test it using the *Hamilton equations for the harmonic oscillator* $H(q,p) = 1/2(p^2/m + q^2 m)$ (where $q = \omega x$). Note that for this specific set of equations the convergence is not $\mathcal{O}(\Delta t^4)$ but higher due to cancellations in the error term. Use $u = \{q, p\}$ and test convergence of the solution, say $q(t)$, against the exact solution and conservation of energy over long timescales (several periods).

Hint Do not store all the time steps in memory! For N timesteps that would require $8N$ doubles (or, in general, $4 \times m \times N$ with 4 stages and m variables). Memory usage should be kept constant ($= 4m$) by overwriting memory when updating the state vector, and by writing to file every given number of iterations.

Hint Try not to use too complex programming for these tasks. Sophisticated codes with classes, inheritance, etc., are difficult to navigate through and debug and are most useful in large projects.

7. **Numerical solution to the Wave equation with periodic boundary condition** Consider now the wave equation in first-order in time form, say 0.2 (but the exercise can be repeated with 0.3). Discretize the space with a uniform grid and represent the derivatives on the r.h.s at each point x_i with the finite differencing expressions derived above. Schematically, the r.h.s. discretization at each point can be indicated as $L[\{u_j\}]$ and collected in the array r_i. The wave equation 0.2 is then discretized in its *s*emi-discrete form

$$\frac{du_i}{dt} = r_i = L[\{u_j\}] \ , \tag{0.19}$$