ACM40080 Advanced Computational Science – Assignment 1

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Instructions

This is Assignment 1 of the Module, consisting of 2 questions. This assignment is worth 20% of the module's final mark. Each question is worth 50% of the assignment's mark.

For each question, you will need to complete two parts each carrying equal marks:

- A MATLAB numerical code to solve the problem. Minimum requirements: The MATLAB code must be original and it must contain clear comments in every section. Of course, once you have created a program to solve a problem, you can use it as part of another program to solve a different problem. Figures created with MATLAB must be properly labelled (time axis, appropriate font size, etc.) and the plot region must coincide with the region of interest.

- A report describing the numerical and analytical methods used, your results, figures and conclusions. Minimum requirements: The report must be self-contained, clear and explain in detail the numerical methods used. Figures must have proper captions. Every quantity appearing in the report must be properly defined.

Please **write your name and student number** in the first page of your answers.

The answers must be sent by e-mail to the Lecturer before Friday 14th March, 2014 at 23:00 GMT. Late assignments are accepted only on that Friday but they will be penalised with a reduction of 50% of the marks.

Question 1 – The Wave Equation

We will numerically solve the wave equation

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = 0 \tag{1}$$

with $c = 1$.

1.1. Write a program to solve (1) using centre differences, i.e.

$$\frac{\partial^2 u}{\partial t^2} \approx \frac{\delta_t \delta_t u_j^n}{\tau^2}, \qquad \frac{\partial^2 u}{\partial x^2} \approx \frac{\delta_x \delta_x u_j^n}{h^2},$$

solve the equation on a grid with range $-7 \leq x \leq 7$, $t \geq 0$. Apply Dirichlet boundary conditions: $u(-7,t) = u(7,t) = 0 \, \forall \, t \geq 0$. Start with the initial conditions $u(x,0) = \exp(-x^2)\,,\ -7 < x < 7$ and $\frac{\partial u}{\partial t}(x,0) = 0\,,\ -7 \leq x \leq 7$. Evolve from $t = 0$ to $t = 14$. Plot and interpret. What do you notice?

1.2. Produce a stability analysis of the numerical method. Defining $\nu = c\frac{\tau}{h}$ as in the lectures, study the evolution of a Fourier mode $u_j^n = (\xi)^n \exp(i\,k\,h\,j)\,$, where k is the wavenumber and ξ is the amplification factor:

(i) Find the amplification factor as a function of k, h and ν. Notice that there will be two solutions, denoted $\xi_\pm$.

(ii) Explain why is that so. Are both solutions physically sensible?

(iii) For which values of ν do *both* solutions satisfy $|\xi_\pm| \leq 1$? The answer will determine the stability criterium of your numerical method. For which value of ν is there saturation of these inequalities? You should use this value of ν to obtain your numerical solution in part 1.1.

(iv) Finally, compute analytically the arguments of the complex solutions $\xi_\pm$ in terms of the product $k\,h$, and plot them as functions of $k\,h \in [0, \pi]$. Find approximate expressions for these arguments in the limit when $k\,h$ is small. Compare these expressions with the corresponding expression that is obtained from the analytical solution of the wave equation, $\arg(\xi_\pm) = \pm k\,c\,\tau$.

1.3. The choice of h in the previous numerical computation must be validated by a resolution study. Once you have fixed ν from the stability criterium, you must find an optimal value of h that resolves the wave up to $t = 10.5$. Compare the results of your simulation against halving of h. As a first attempt, you will compare the relative difference between L^2-norms of solutions at $t = 10.5$. In general, the L^2 norm of a field $u(x,t)$ is defined as $\|u(\cdot,t)\|_{L^2} = \sqrt{\int_a^b [u(x,t)]^2 \, dx}\,$, where a, b denote the boundary points of the spatial domain.

(i) Compute numerically the L^2-norm $L_h = \sqrt{h \sum_{x=-7}^{x=7} (u_h(x, 10.5))^2}$ of the solution at $t = 10.5$ obtained using a grid spacing of h (here, u_h denotes the numerical solution of the problem for a given spacing h).

(ii) Compute numerically the L^2-norm $L_{h/2} = \sqrt{h/2 * \sum_{x=-7}^{x=7} (u_{h/2}(x, 10.5))^2}$ of the solution at $t = 10.5$ obtained using a grid spacing of $h/2$, and

(iii) Define the *relative error* as $e_r(h) \equiv \frac{L_h - L_{h/2}}{L_h}$. Try different values of h and plot the relative error as a function of h. Find the largest h so that the relative error is still less than 0.001 (corresponding to an acceptable 0.1% error). This is your most optimal choice of h, which saves both computational time and computer memory, still resolving the solution. Make sure your choice of h is robust, in the sense that changing h to nearby values still produces low relative errors.

1.4. Repeat questions 1.1 and 1.3 using Neumann boundary conditions, $\frac{\partial u}{\partial x}(-7,t) = \frac{\partial u}{\partial x}(7,t) = 0$. Does anything change?

1.5. Another resolution study and a more powerful validation tool is possible in this case because of the existence of conservation laws. Define the 'Hamiltonian density',

$$\mathcal{H}(x,t) = \frac{1}{2}\left(\frac{\partial u}{\partial t}\right)^2 + \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2 .$$

The total energy $E(t)$ is defined to be the integral over x,

$$E(t) = \int_{x_{\min}}^{x_{\max}} \mathcal{H}(x,t)dx .$$

(i) Show analytically from eq.(1) that, if one uses either Dirichlet or Neumann boundary conditions at $x = x_{\min}$ and $x = x_{\max}$, then $E(t)$ is a conserved quantity, i.e., show that $dE/dt = 0$ in either case.

(ii) For both problems 1.1 and 1.4, compute numerically, using a similar approach as for the computation of L^2 norms, the total energy as a function of time $0 \le t \le 14$ (use the optimal h obtained in the previous problems). Plot, for each case, the relative error $f_r(t) \equiv \frac{E(t)-E(0)}{E(0)}$. Is this quantity bounded by a small number? Evaluate the bound. Now, repeat the computation with h replaced by $h/2$. Is the bound reduced? Quantify.

Question 2 – The Wave Equation with an External Potential

2.1. Now let us solve a wave equation with an external potential,

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + V(x)u = 0 \qquad \text{where} \quad V(x) = \frac{1}{\cosh^2(x)}\,, \tag{2}$$

with $c = 1$. Solve numerically on a grid of size $-20 \leq x \leq 20$, with Neumann boundary conditions. Start with the initial conditions $u(x,0) = u_0(x) = \exp\left(-(x-6)^2/2\sigma^2\right)$ and $\frac{\partial u}{\partial t}(x,0) = \frac{du_0}{dx}$, where $\sigma = 1$. The initial pulse should propagate leftwards towards $x = 0$, and then interact with the potential barrier. Some of the pulse will be reflected, and some will be transmitted. Plot an array of snapshots at various instances of t (properly labelled) until a time $t_{\max}$ chosen so that the reflected and transmitted pulses separate well from the barrier but are not too close to the boundaries.

2.2. Repeat the resolution study in terms of h as in part 1.3, using the corresponding solutions obtained at $t = t_{\max}$.

2.3. Define the 'Hamiltonian density',

$$\mathcal{H}(x,t) = \frac{1}{2}\left(\frac{\partial u}{\partial t}\right)^2 + \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2 + \tfrac{1}{2}V(x)u^2\,.$$

The total energy $E(t)$ is defined to be the integral over x, $E(t) = \int_{x_{\min}}^{x_{\max}} \mathcal{H}(x,t)dx\,.$

(i) Show analytically from eq.(2) that, if one uses either Dirichlet or Neumann boundary conditions at $x = x_{\min}$ and $x = x_{\max}$, then $E(t)$ is a conserved quantity, i.e., show that $dE/dt = 0$ in either case.

(ii) Compute numerically the total energy as a function of time $0 \leq t \leq t_{\max}$ (use the optimal h obtained in problem 2.2). Plot the relative error $f_r(t) \equiv \frac{E(t)-E(0)}{E(0)}$. Make sure this quantity is always bounded by a number of order 10^{-3} or smaller. Reduce h if needed.

2.4. We will quantify how much of the pulse has been reflected and how much absorbed, in terms of the pulse width σ.

(i) Compute, for the case $\sigma = 1$, the energy on the right ($E_>$) and the left ($E_<$) of the barrier, respectively:

$$E_>(t) = \int_0^{x_{max}} \mathcal{H}(x,t)dx, \qquad E_>(t) = \int_{x_{min}}^{0} \mathcal{H}(x,t)dx\,.$$

Then define dimensionless reflection and transmission coefficients, $R(t) = E_>(t)/E(t)$, $T(t) = E_<(t)/E(t)$, so that $R(t) + T(t) = 1$. Compute $T(t)$ at $t = t_{\max}$ defined as the time when the transmitted pulse has came out of the barrier $x = 0$ and is still far from the boundary.

(ii) Plot $T(t_{\max})$ as a function of σ (try several values of σ, say: $2, 1.5, 1, 0.5, 0.2, 0.1$). Make sure that $\sigma > 10h$, otherwise your pulse will not be very well resolved. Remember to test in each case that total energy is conserved within a relative error of 10^{-3}. Also, remember to check in each case the convergence with resolution studies in terms of h. Give a physical interpretation of the dependence of T on σ.