Imperial College London

Department of Mathematics
Imperial College London

Computational PDEs MATH60025/70025, 2024-2025
Released : 17 March 2025
Upload Deadline : 1.00 pm, 31 March 2024
The project mark, will be weighted to comprise 35% of the overall Module.

You are required to investigate the Questions below and summarise your findings in form of a well written project report – on which you will be assessed.

Please name your files in following way:

- Technical report : **CPDES_Q3_yourCID.pdf** (limit your report to 16 pages or less (including plots). **Anything beyond the 16 page limit will NOT be marked!**
- All your code(s), label as follows :
  CPDES_Q3_of_X_yourCID.m (Matlab scripts example) or
  CPDES_Q3_of_X_yourCID.py (Python scripts).
  Zip all program files and call your zipped folder: **CPDES_Q3_programs_yourCID.zip**

Where in the above **CID** will be your College ID number.

Notes: *Important*

1. Marking will consider both the correctness of your code as well as the soundness of your analysis and clarity and legibility of the technical report.
2. Exam mark will primarily be based on contents of your written technical report. You are warned that if you ONLY submit the codes for the work with **NO technical report**, you can **NOT** expect a pass mark.
3. Do **NOT** include source code listing in your technical report.
4. All figures created by your code should be well-made and properly labelled in the technical pdf report.
5. The codes **must** be submitted.

Project 3: Hyperbolic Systems

Part A: (15 Marks)

The one-dimensional wave equation for $u(x,t)$ is given by

$$u_{tt} = c^2(x)\, u_{xx}, \tag{1.1}$$

where x represents a spatial coordinate and t the time. At $t = 0$

$$u(x,0) = \exp\left(-(2x-5)^2\right)\ ; \qquad \frac{\partial u}{\partial t}(x,0) = 0. \tag{1.2}$$

The wave speed $c(x) = 1$.

1. Investigate how the solution to Eqn. 1.1 evolves for $t > 0$. Discretise the equation based on your lecture notes, such that it is second-order accurate in time and space using the Leapfrog scheme from lectures:

$$\frac{U_j^{k+1} - 2U_j^k + U_j^{k-1}}{(\Delta t)^2} = c_j^2 \left(\frac{U_{j-1}^k - 2U_j^k + U_{j+1}^k}{(\Delta x)^2} \right). \tag{1.3}$$

   At the computational end points, namely $x = \pm 10$, investigate the treatment of boundary conditions which satisfy the following:

   - Minimal numerical reflections off the left outer boundary; *i.e.* the waves pass through the boundary at $x = -10$ (also known as a transparent condition).
   - The solid wall condition on the right boundary of $\partial u / \partial x = 0$ at $x = 10$.

   Through appropriate numerical experiments investigate, discuss and demonstrate the accuracy of your numerical solution, and any dissipation and dispersive effects, as the Courant number varies, that you observe through appropriate plots, showing key features.

   Investigate how your results are affected as you vary the CFL parameter.

   Include a discussion on the"modified PDE" that Eqn.(1.4) represents, and discuss in relation to your numerical investigations.

2. Next, modify your code to set the wave speed such that it has the form

$$c(x) = (2+x)/2, \ \text{ in the region } \ -1 \le x \le 0,$$

   and $c(x) = 1$ elsewhere. Discuss and show by appropriate plots any new features you find.

Part B: (14 Marks)

The PML form of the wave equation is as follows

$$u_{tt} + 2\sigma u_t + \sigma^2 u = c^2(x) u_{xx},$$

with σ the PML absorption parameter.

1. Using a similar strategy as used earlier, namely the Leapfrog scheme, undertake a discrete dissipation-dispersion Fourier analysis to analyse the discretised equation, and investigate dissipation and dispersive behaviour. Are there any limits or bounds for σ which minimises dispersive and (or) maximises dissipative behaviour, but still provides a stable numerical scheme? Analyse and discuss for the case $c(x) = 1$.

2. Prescribing a PML layer for $x \leq -7$, devise a code to solve the above PML form of the wave equation; take $c(x) = 1$. The right boundary is prescribed to be a solid wall, satisfying the $u_x = 0$ condition at $x = 10$. At the left boundary devise an appropriate $\sigma(x)$ distribution, which allows minimal reflection off the PML interface at $x = -7$, as well as maximal dissipation of the wave prior to it reaching the left boundary at $x = -10$. Through appropriate plots show in a reasonably concise form your results, effectiveness of your PML and discuss your findings.

Part C: (6 Marks)

An implicit discretisation of the wave equation is as follows

$$\frac{U_j^{k+1} - 2U_j^k + U_j^{k-1}}{(\Delta t)^2} = c_j^2 \left(\frac{(\delta^2 U)_j^{k+1} + 2(\delta^2 U)_j^k + (\delta^2 U)_j^{k-1}}{4(\Delta x)^2} \right). \tag{1.4}$$

Here you may take $c_j = 1$.

Undertake a Fourier stability analysis to investigate stability of the scheme. Is there a CFL number bound on the numerical stability?

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Computational PDEs MATH60025/70025, 2024-2025
Project 4: Mastery (MSc, MSci only)
Released : 17 March 2025
Upload Deadline : 1.00 pm, 9 April 2025
The project mark, will be weighted to comprise Total 20% of the overall Module.

Please name your files in following way:

- Technical report : **CPDES_Q4_yourCID.pdf** (limit your report to 16 pages or less (including plots). **Anything beyond the 16 page limit will NOT be marked!**
- All your code(s), label as follows :
  CPDES_Q4_of_X_yourCID.m (Matlab scripts example) or
  CPDES_Q4_of_X_yourCID.py (Python scripts).
  Zip all program files and call your zipped folder: **CPDES_Q4_programs_yourCID.zip**

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Question 1: Implicit Wave-Equation (9 Marks)

Continuing on from project 3, part C, develop a numerical method to solve the wave equation problem defined by Eqn. 1.1–1.2, using the implicit discretisation given by Eqn. 1.4.

Demonstrate in a sufficiently concise form the results from your code, and compare the results with those you compute from those obtained earlier using the explicit method. In particular investigate how varying the Courant number affects your numerical solutions.

In your report describe in detail your numerical strategy.

Question 2: Sound and Heat Flow

You are given the following equations,

$$\frac{\partial u}{\partial t} = c\frac{\partial}{\partial x}\left(w - 2h\right), \tag{1.5a}$$

$$\frac{\partial w}{\partial t} = c\frac{\partial u}{\partial x}, \tag{1.5b}$$

$$\frac{\partial h}{\partial t} = \sigma\frac{\partial^2 h}{\partial x^2} - c\frac{\partial u}{\partial x}, \tag{1.5c}$$

where (c, σ) are constants representing the wave speed and heat conductivity respectively from the book by Richtmyer & Morton (1967), " *Difference Methods for Initial Value Problems*, pp. 264–269 (see attached copy). For what follows, take $c = 1$ and $\sigma = 0.1$.

Part A: (7 Marks)
Devise a code to solve the equations explicitly for the given values of (c, σ). This is to be solved for

$$-5 \leq x \leq 5$$

with transparent conditions for $u = 0$; and $dh/dx = 0$ at both boundaries.

As initial data at $t = 0$, take

$$u(x, 0) = 1 \text{ for } -1 \leq x \leq 1, \text{ and } u(x, 0) = 0 \text{ otherwise.}$$

For h, take as initial data

$$h(x, 0) = 1 \text{ for } -2 \leq x \leq 2, \text{ and } h(x, 0) = 0 \text{ otherwise.}$$

Further, take $w(x, 0) = 0$ as the initial data.

1. In your report discuss the step size limit required for a stable numerical solution, and the overall numerical strategy you employ.
2. Describe how you enforce conditions at the boundaries.
3. Deduce numerical stability requirements for the explicit approach. Demonstrate and confirm through usage of your code, the stability limit(s) you have deduced.
4. Present through appropriate plots how the solution fields (u, h) evolve with time.
5. Present through appropriate plots effectiveness of the conditions you impose at the boundaries and discuss your findings.
6. Choosing a range of σ (say between a relatively low and high value), investigate and report on solutions you obtain. Report on numerical aspects which become important as σ is varied.

Part B: (4 Marks)
Richtmyer & Morton suggest an implicit discretisation for one of the equations.

Describe how you thus discretise and solve the equations set in this case.

Develop your code, and thus investigate appropriate numerical correctness and report your findings. Comparing your results with those obtained in Part A.

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Both eigenvalues of G have absolute value 1, and G^*G is the unit matrix, so that *the system* (10.6) *is unconditionally stable.*

From (10.7) it is clear that the solution of this implicit system can be achieved by the algorithm given in Chapter 8 for implicit systems for the diffusion equation. Therefore, equations (10.6) provide a practically satisfactory system for the wave equation.

10.4. Coupled Sound and Heat Flow

In the flow of a compressible fluid there are often considerable differences of temperature from one point to another, and the transfer of energy by thermal conduction may have a significant effect on the motion. The parabolic equation of heat flow is then coupled to the hyperbolic equations of fluid dynamics and the two phenomena must be calculated concurrently. This effect occurs also for infinitesimal or acoustic vibrations and is responsible for absorption of ultrasonic waves.

Let the pressure, specific volume and specific internal energy be $p_0 + p$, $V_0 + V$ and $\mathscr{E}_0 + \mathscr{E}$, where p_0, V_0 and $\mathscr{E}_0$ are the ambient values and where $p \ll p_0$, $V \ll V_0$, $\mathscr{E} \ll \mathscr{E}_0$; and let the material velocity be u. $p, V, \mathscr{E}, u$ are functions of x and t. The quantity $c = \sqrt{p_0 V_0}$ is the isothermal sound speed. We take the equation of state to be

$$\mathscr{E}_0 + \mathscr{E} = (p_0 + p)(V_0 + V)/(\gamma - 1)$$

and denote by σ the ratio of thermal conductivity to specific heat at constant volume.

In terms of auxiliary dependent variables defined by $w = cV/V_0$ and $e = \mathscr{E}/c$, the differential equations, to first order of small quantities, are

$$\begin{aligned} \frac{\partial u}{\partial t} &= c\frac{\partial}{\partial x}(w - (\gamma - 1)e), \\ \frac{\partial w}{\partial t} &= c\frac{\partial u}{\partial x}, \\ \frac{\partial e}{\partial t} &= \sigma\frac{\partial^2 e}{\partial x^2} - c\frac{\partial u}{\partial x}. \end{aligned} \tag{10.8}$$

Finite-difference equations for this system can be constructed in various ways. A simple explicit system is

$$\begin{aligned} \frac{u_j^{n+1} - u_j^n}{\Delta t} &= c\,\frac{w_{j+½}^n - w_{j-½}^n - (\gamma - 1)(e_{j+½}^n - e_{j-½}^n)}{\Delta x}, \\ \frac{w_{j+½}^{n+1} - w_{j+½}^n}{\Delta t} &= c\,\frac{u_{j+1}^{n+1} - u_j^{n+1}}{\Delta x}, \\ \frac{e_{j+½}^{n+1} - e_{j+½}^n}{\Delta t} &= \sigma\,\frac{e_{j+3/2}^n - 2e_{j+½}^n + e_{j-½}^n}{(\Delta x)^2} - c\,\frac{u_{j+1}^{n+1} - u_j^{n+1}}{\Delta x}. \end{aligned} \tag{10.9}$$

The advanced values of the velocity u have been used in the second and third equations just as in the second equation (10.5) of the system without heat flow (it will be recalled that that was necessary in order to achieve a reasonable stability condition for the sound wave problem). Nevertheless, equations (10.9) are effectively explicit because the first equation can be solved first to obtain the values of u_j^{n+1} and u_{j+1}^{n+1} needed in the other two.

This system has been found satisfactory. If the sound waves and heat flow were uncoupled, the respective stability conditions would be

$$\begin{aligned} \sqrt{\gamma}c\Delta t/\Delta x &< 1, \\ \sigma\Delta t/(\Delta x)^2 &< ½. \end{aligned} \tag{10.10}$$

Surely these conditions are necessary. In the limit, as Δt and $\Delta x \to 0$, the second of these conditions always implies the first, and it is generally conjectured that it is the stability condition. In an actual calculation, one should of course choose Δx and Δt so as to satisfy the first condition as well as the second.

To avoid the small time increment required by condition (10.10) one often uses an implicit treatment of the third differential equation, for example,

$$\frac{e_{j+½}^{n+1} - e_{j+½}^n}{\Delta t} = \sigma\,\frac{e_{j+3/2}^{n+1} - 2e_{j+½}^{n+1} + e_{j-½}^{n+1}}{(\Delta x)^2} - c\,\frac{u_{j+1}^{n+1} - u_j^{n+1}}{\Delta x}. \tag{10.11}$$

The first two equations (10.9) are retained.

In the first edition of this book it was conjectured that the stability condition is $c\Delta t/\Delta x < 1$ for this system. The isothermal sound speed c

was used because instabilities generally involve very short wavelength disturbances, and for these the thermal equilibration time from crest to trough is less than the period of the wave. The equilibration time is proportional to the square of the wavelength λ, and the compressions and rarefactions in the wave motion are very nearly isothermal rather than adiabatic if $\lambda \ll \sigma/c$.

The correctness of this conjecture was confirmed in 1962 by Morimoto. In the limit $\sigma \to 0$, however, the condition is the more stringent inequality $\sqrt{\gamma}c\Delta t/\Delta x < 1$, and this suggests that, unless $\Delta x \ll \sigma/c$, there should be a practical stability condition, for a finite net, involving the two dimensionless constants

$$\nu = c\Delta t/\Delta x, \qquad \mu = \sigma\Delta t/(\Delta x)^2, \tag{10.12}$$

and also γ; it would presumably be intermediate between the two conditions above, namely, it would be of the form $\nu < \nu_0$, where ν_0 is some function of γ and μ whose values lie between $1/\sqrt{\gamma}$ and 1.

To find the practical stability condition, we adopt the principle, already stated in Section 9.7, that no Fourier component of the approximation should be allowed to grow more rapidly than the most rapid possible growth of the exact solution. Since sound waves do not grow in amplitude (in fact, they are damped out, in the present problem, by the action of the heat flow, but by a negligible amount of damping for long wavelengths), we must require the amplification factors g to be $\leqq 1$ in modulus, not merely $\leqq 1 + O(\Delta t)$. The g satisfy the equation

$$\begin{vmatrix} g-1 & -2i\nu\sin\alpha & 2i\nu(\gamma-1)\sin\alpha \\ -2ig\nu\sin\alpha & g-1 & 0 \\ 2ig\nu\sin\alpha & 0 & g-1+2\mu(1-\cos 2\alpha)g \end{vmatrix} = 0,$$

where $\alpha = \frac{1}{2}k\Delta x$. The requirement that $|g| \leqq 1$ for all α leads to the condition

$$\nu < \sqrt{(1+2\mu)/(\gamma+2\mu)}, \tag{10.13}$$

which is the practical stability condition; this condition was shown in Section 6.4 to be also sufficient for stability in the sense that a certain positive definite quadratic form in u, w, e, and $\Delta_+ e_j = e_{j+1} - e_j$ is bounded for all time if (10.13) is satisfied.

Equation (10.13) shows that, as was to be expected, stability is determined by the adiabatic sound speed for $\mu \ll 1$, by the isothermal sound speed for $\mu \gg 1$, and by an intermediate speed for $\mu \sim 1$.

In a series of numerical tests, the difference equations (the first two of (10.9) and equation (10.11)) were used to calculate the propagation of a wave which starts out as a simple jump or infinitesimal shock (infinitesimal in the sense that the linearized equations are being used). Such a wave propagates with speed $\sqrt{\gamma}c$, the profile becoming gradually rounded off so as to resemble the normal distribution curve

$$\int_{-\infty}^{x} \exp[-y^2/2]dy$$

with a width that increases as $\sqrt{t}$. An approximate (but rather good) analytic solution is known.

Figure 10.1 shows the calculated profile in a stable calculation after 165 time steps, and Figure 10.2 shows the values obtained in an unstable calculation after only five time steps; in both calculations the ordinary stability condition $c\Delta t/\Delta x < 1$ was satisfied. Figure 10.3 summarizes the series; each dot indicates the values of μ and γ of a run that was found to

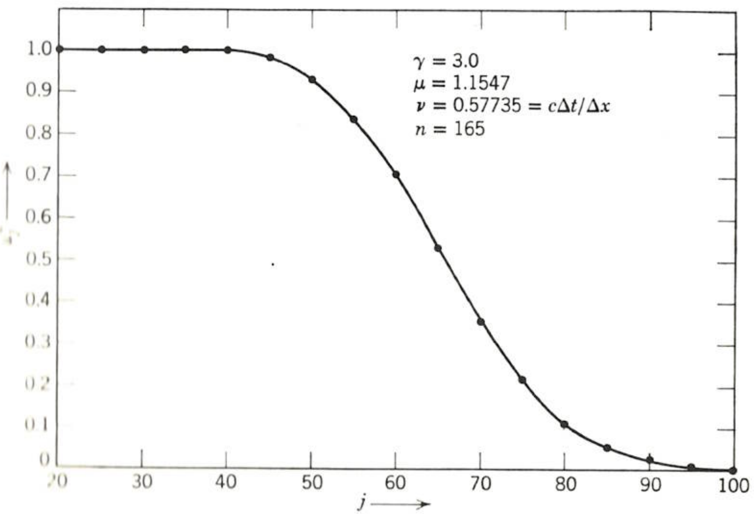

Fig. 10.1. Calculated profile after 165 cycles of an initially sharp sound wave in the presence of heat conduction.

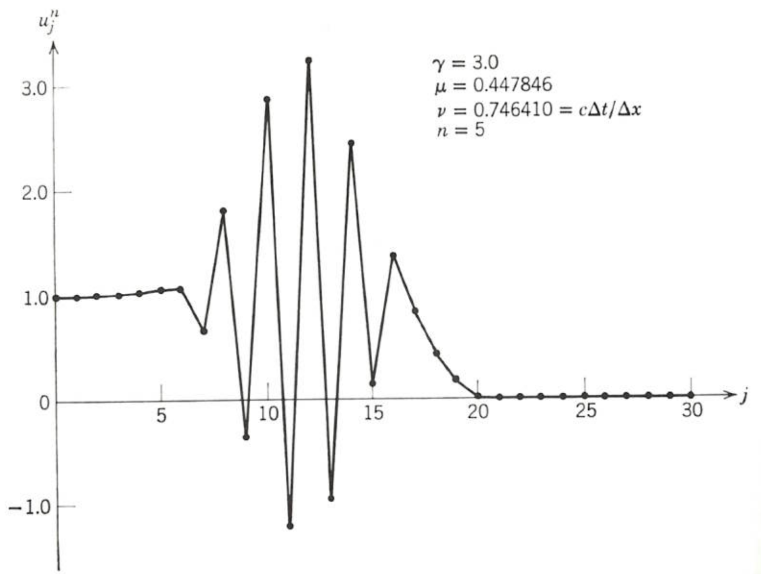

Fig. 10.2. Calculated profile after 5 cycles, in a run in which the practical criterion **(10.13)** was violated, although $c\Delta t/\Delta x < 1$.

be stable, and each cross indicates the values of a run that was found to be unstable; the curve gives the maximum permissible ν as a function of ν/μ, according to (10.13). It is seen that the observed stability condition is in agreement with the theoretical one. Two runs for which the inequality (10.13) was replaced by the equality turned out to be stable.

To understand the nature of this kind of instability, consider a calculation with $\nu = c\Delta t/\Delta x = 0.9$ and $\gamma = 3$. According to the usual criterion, this is a stable scheme, and convergence follows, for $\Delta t \to 0$. However, if Δt is such that μ is also equal to 0.9 (this case was chosen just for illustration), then, according to the determinantal equation above, $g \approx -2.6$ for the Fourier component with $k\Delta x = \pi$; therefore, this component becomes amplified a thousandfold in less than 10 time steps. To avoid this, if one wishes to keep $c\Delta t/\Delta x = 0.9$, both Δx and Δt have to be reduced by a factor ≈ 0.25, so as to satisfy (10.13).

An alternative approach is to retain the explicit character of the difference equations but to use a smaller time step, say $\Delta t/K$, where K is an integer, for the third equation than for the first two. Then each cycle

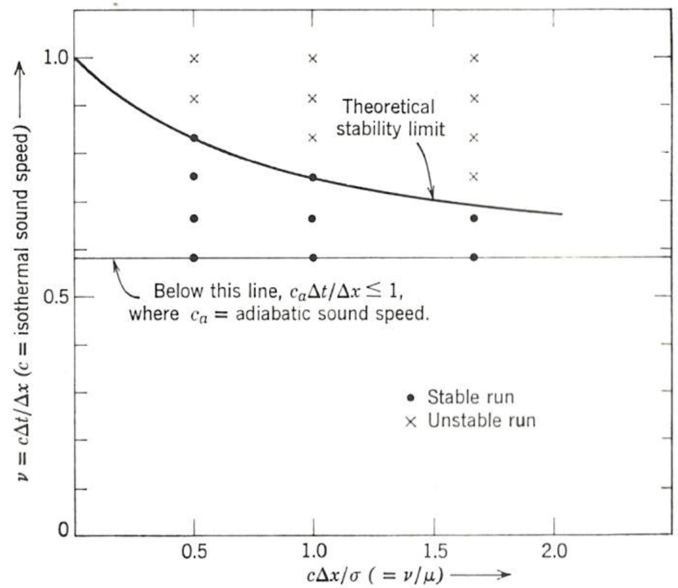

Fig. 10.3. Stability diagram for coupled sound and heat flow with $\gamma = 3$. In the numerical tests, a run was counted as stable if the profile was still smooth, as in Figure 10.1, after about 100 cycles and as unstable if the value of $|u_j^n|$ exceeded 3.0 at any point (when this happened, it happened in $\leqq 5$ cycles in every case).

of the fluid dynamic calculation is accompanied by K steps of the heat flow calculation. The procedure can be described by use of fractional superscripts:

$$\frac{e_{j+\frac{1}{2}}^{n+(m+1)/K} - e_{j+\frac{1}{2}}^{n+m/K}}{\Delta t/K} = \sigma\,\frac{e_{j+\frac{3}{2}}^{n+m/K} - 2e_{j+\frac{1}{2}}^{n+m/K} + e_{j-\frac{1}{2}}^{n+m/K}}{(\Delta x)^2} - c\,\frac{u_{j+1}^{n+1} - u_j^{n+1}}{\Delta x},$$

$$m = 0, 1, \cdots, K = 1.$$

It is conjectured that in this case the stability condition is

$$\frac{c\Delta t}{\Delta x} < 1 \quad \text{and} \quad \frac{\sigma\Delta t/K}{(\Delta x)^2} < 1/2.$$

10.5. A Practical Stability Criterion

The above example and those of Sections 9.7 and 11.6 show that stability, as usually defined, is not always adequate for the practical