Project 4: Partial differential equations (PDEs)*

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December 2022

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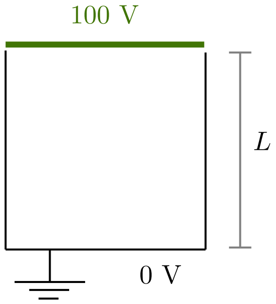
*Code for the following tasks can be found at the repository: https://github.com/VictorG20/comphysics.git

1. Laplace equation



Consider the two-dimensional setup of a square box with a side length of L, where the top edge is set to a potential of 100 V and the other three edges are grounded, i.e. at a potential of zero. Your task is to find the potential within the box, where it solves the Laplace equation

$$\Delta\phi(x, y) = 0. \tag{1}$$

a) Write a program that computes the potential $\phi(x, y)$ within the box with a discretisation length of $\Delta x = L/100$. Implement the Jacobi, Gauß–Seidel and SOR methods. As a stopping criterion, assert that the error of the discretised Laplace equation is smaller than $\epsilon_{\text{max}} = 10^{-3}$ V everywhere. The error is defined as $\epsilon_{i,j} = |\phi_{i,j} - (\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1})/4|$. Plot the average and maximum error versus the number of iterations for all algorithms. For SOR, use four different over-relaxation parameter values $\alpha = 0.5, 1.0, 1.25, 1.5, 1.75$ and 1.99. Check if it still converges for $\alpha \geq 2.0$. Discuss your results. (6 points)

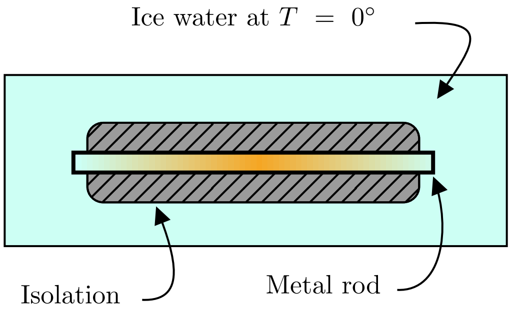
b) The solution of this problem can be written as an infinite series:

$$\phi(x, y) = \sum_{n=1,3,5,\ldots}^{\infty} \frac{400}{n\pi} \sin\left(\frac{n\pi y}{L}\right) \exp(-n\pi x). \tag{2}$$

Plot this solution for 1, 10, 100 and 1000 terms. Plot the difference between one of the iterative solutions and the "infinite" series solution using 1000 terms. Discuss your results. (4 points)

2. Diffusion

Consider a metallic rod of a finite length L and a small radius, which is isolated at its side, but not at its ends, where it is placed in contact with ice water at $0\,^{\circ}\mathrm{C}$:



To simulate the temperature flow, we will need to solve the diffusion PDE

$$\frac{\partial T(x,t)}{\partial t} = \frac{K}{C\rho}\frac{\partial^2 T(x,t)}{\partial x^2}, \tag{3}$$

with the thermal conductivity K, the heat capacity C and the density ρ. Use $L = 1$, $K = 210$, $C = 900$ and $\rho = 2700$, and, if not otherwise specified, $\Delta x = 0.01$ and $\Delta t = 0.1$ with a number of time steps $N_t = 10000$. The rod's temperature distribution is initially set to $T(x, 0) = \sin(\pi x/L)$.

a) Simulate the system using the FTCS algorithm and plot $T(x,t)$. (8 points)

Solution: The discretized equation with an FTCS scheme reads

$$T(t_{n+1}, x_j) = T(t_n, x_j) + \frac{K}{C\rho}\frac{\Delta t}{(\Delta x)^2}\left(T(t_n, x_{j+1}) - 2T(t_n, x_j) + T(t_n, x_{j-1})\right) \tag{4}$$

where the end points are given by $T(x = 0, t) = T(x = L, t) = 0$ at all times.

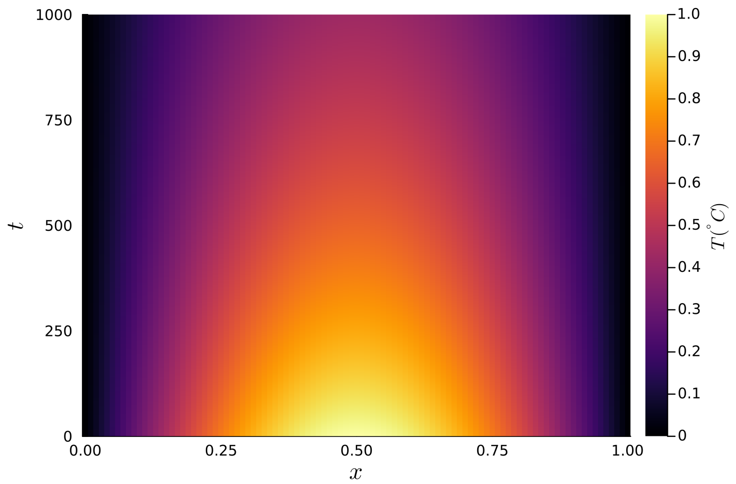


Figure 1: Heat map of the temperature along the rod at different times for the values of the parameters given.

b) The analytical solution is given by

$$T_{\text{exact}}(x,t) = \sin\left(\frac{\pi x}{L}\right)\exp\left(-\frac{\pi^2 K t}{L^2 C\rho}\right). \tag{5}$$

With that, we can define our simulation error as

$$\epsilon(t) = \frac{1}{N_x}\sum_{j=1}^{N_x-1} |T(j\Delta x, t) - T_{\text{exact}}(j\Delta x, t)|, \tag{6}$$

where $N_x = L/\Delta x$. Study the behaviour of $\epsilon(t = 100)$ varying Δt between 0.001 and 0.7 while keeping Δx fixed. What happens? Explain your finding. (4 points)

Solution: The exact solution $T_{\text{exact}}(x,t)$ is obtained in the appendix. For the FTCS method, the computed temperature values at time t, starting from $t = 0$, are given by

$$\boldsymbol{T}(t) = \begin{bmatrix} T(\Delta x, t) \\ T(2\Delta x, t) \\ \vdots \\ T([N_x - 1]\Delta x, t) \end{bmatrix} = U\lambda^{N_t}U\boldsymbol{T}(0) \tag{7}$$

where N_t is the rounded integer of the division $t/\Delta t$ and

$$U_{ij} = \sqrt{\frac{2}{N_x}}\sin\left(\frac{\pi i j}{N_x}\right), \qquad \lambda = \text{diag}\left[1 - 4\frac{K\Delta t}{C\rho(\Delta x)^2}\sin^2\left(\frac{j\pi}{2N_x}\right)\right] \tag{8}$$

for $i, j = 1, \ldots, N_x - 1$, from which one can compute the error exactly for any Δx and Δt.

A simpler analysis on the truncation error goes as follows: The forward in time scheme implies taking

$$T(x, t+\Delta t) = T(x,t) + \frac{\partial T}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 T}{\partial t^2}(\Delta t)^2 + \mathcal{O}(\Delta t^3) \tag{9}$$

and replacing

$$\frac{\partial T}{\partial t} = \frac{T(x, t+\Delta t) - T(x,t)}{\Delta t} \underbrace{-\frac{1}{2}\frac{\partial^2 T}{\partial t^2}\Delta t}_{\text{first error term}} + \mathcal{O}(\Delta t^3). \tag{10}$$

Similarly, for the spatial second derivative with a central difference we have

$$\begin{aligned} T(x \pm \Delta x, t) = T(x,t) \pm \frac{\partial T}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 T}{\partial x^2}(\Delta x)^2 \pm \frac{1}{3!}\frac{\partial^3 T}{\partial x^3}(\Delta x)^3 \\ + \frac{1}{4!}\frac{\partial^4 T}{\partial x^4}(\Delta x)^4 + \mathcal{O}(\Delta x^5) \end{aligned} \tag{11}$$

$$\frac{\partial^2 T}{\partial x^2} = \frac{T(x+\Delta x, t) - 2T(x,t) + T(x-\Delta x, t)}{(\Delta x)^2} - \frac{1}{12}\frac{\partial^4 T}{\partial x^4}(\Delta x)^2 + \mathcal{O}(\Delta x^4) \tag{12}$$

Therefore, when solving the diffusion equation with the FTCS scheme, we have a first error term given by

$$E(\Delta x, \Delta t) = \frac{1}{2}\frac{\partial^2 T}{\partial t^2}\Delta t - \frac{1}{12}\frac{K}{C\rho}\frac{\partial^4 T}{\partial x^4}(\Delta x)^2. \tag{13}$$

Since we have the exact solution for $T(x,t)$ we can evaluate this expression

$$E(\Delta x, \Delta t) = \frac{1}{2}\frac{\pi^4}{L^4}\frac{K}{C\rho}\left[\frac{K}{C\rho}\Delta t - \frac{1}{6}(\Delta x)^2\right]T(x,t). \tag{14}$$

Additionally, Von-Neumann stability analysis yields the condition

$$\Delta t \leq C\rho\Delta x^2/(2K). \tag{15}$$

These two expressions give an idea of how the error grows for different values of Δx and Δt. In particular, if Δx is fixed, we have three regions for Δt:

$$\Delta t < \frac{1}{6}\frac{C\rho}{K}(\Delta x)^2 \implies E \text{ decreases linearly with increasing } \Delta t \tag{16}$$

$$\frac{1}{6}\frac{C\rho}{K}(\Delta x)^2 < \Delta t < \frac{1}{2}\frac{C\rho}{K}(\Delta x)^2 \implies E \text{ increases linearly with increasing } \Delta t \tag{17}$$

$$\Delta t > \frac{1}{2}\frac{C\rho}{K}(\Delta x)^2 \implies \text{Method is not stable.} \tag{18}$$

Thus, for $K = 210$, $C = 900$, $\rho = 2700$ and $\Delta x = 0.01$ the above means that we start seeing different behaviors at the values $\Delta t = 0.193$ and $\Delta t = 0.579$. These results are shown in

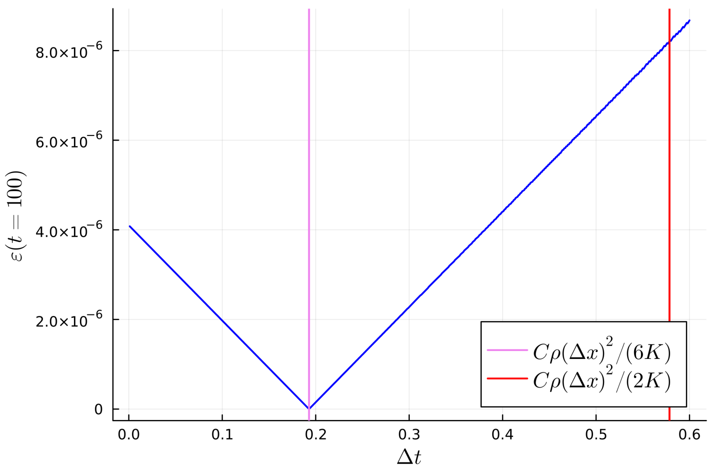


Figure 2: Simulation error obtained through the equation in (6) at a final time $t = 100$.

Although from Figure 2 it might seem that the method remains stable even slightly after the theoretical $\Delta t_{\max} = 0.57857$ for $\Delta x = 0.01$, we must understand that this is due to the fact that it might take longer for the errors to be noticeable. For example, we know from part a) that equilibrium takes $t > 1,000$ to set in, so, for $t = 1,000$ we have the situation in Figure 3.

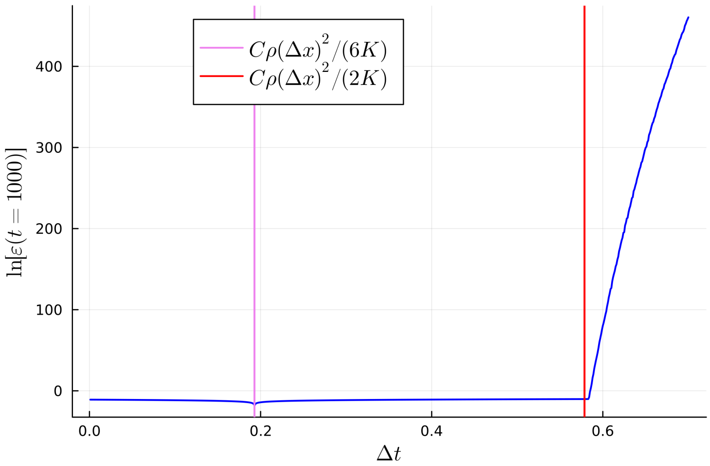


Figure 3: Approaching the theoretical value of $\Delta t = C\rho(\Delta x)^2/(2K)$ for $\Delta x = 0.01$.

Hence, we do observe that choosing a value close or bigger than Δt_{max} might lead to non-bounded error in our solutions. Thus, in choosing a method which is conditionally stable, we might still get away with breaking the stability condition for slightly larger values of Δt, as long as the final time doesn't let the error set in.

c) Now, implement the implicit Euler backward, the Crank-Nicolson and Dufort-Frankel algorithms and repeat the analysis for $\epsilon(t = 100)$ for all of them. Discuss your results comparing the four algorithms, in particular with respect to the scaling behaviour of the error with Δt. (4 points)

Solution: For each of the methods mentioned, we follow the same analysis as the one in part b) for FTCS. The results are shown in Fig.(4)

- Implicit Euler backward scheme or BTCS:

  The first error terms are

$$E(\Delta t, \Delta x) = -\frac{1}{2}\frac{\pi^4}{L^4}\left(\frac{K}{C\rho}\right)^2\left[\Delta t + \frac{1}{6}\frac{C\rho}{K}(\Delta x)^2\right]T(x,t) \tag{19}$$

  so the error grows linearly with Δt for a fixed Δx (since we take the absolute value, the sign in front is irrelevant). It is important to notice that, contrary to the case of the FTCS scheme, now the increasing is monotonous, as the term inside square brackets is always positive, whereas for the FTCS scheme we had a difference in terms which could first decrease and then increase again.

- Crank-Nicolson scheme:

  The first error terms are

$$E(\Delta t, \Delta x) = \frac{1}{12}\frac{\pi^6}{L^6}\frac{K}{C\rho}\left[\left(\frac{K\Delta t}{C\rho}\right)^2 - \left(\frac{L\Delta x}{\pi}\right)^2\right]T(x,t) \tag{20}$$

  so the error is quadratic in Δt and it has a change in sign at the value

$$\Delta t_{\text{change, CN}} = \frac{C\rho L\Delta x}{K\pi}. \tag{21}$$

  For the given values of K, C, ρ, L and Δx this implies that $\Delta t_{\text{change, CN}} = 36.83$ at which point many things in the analysis need to be reconsidered (since for $\Delta t > 1$ our Taylor expansions need special attention). We also notice that for the above values, the error $\mathcal{O}(\Delta x^2)$ has a value of $\approx 10^{-5}$, whereas for $\Delta t = 0.7$, for example, the corresponding $\mathcal{O}(\Delta t^2)$ error has a magnitude of 6×10^{-9}, so in a plot with $\Delta t \in [0.001, 0.7]$ we won't really see much change due to Δt.

- Du Fort-Frankel scheme:

  The first error terms are

$$E(\Delta t, \Delta x) = \frac{K}{C\rho}\frac{\pi^4}{L^4}\left\{\left(\frac{K}{C\rho}\Delta t\right)^2\left[\frac{1}{(\Delta x)^2} - \frac{\pi^2}{6L^2}\right] - \frac{1}{12}(\Delta x)^2\right\}T(x,t) \tag{22}$$

  so the error is quadratic in Δt and it has a change in sign at the value

$$\Delta t_{\text{change}} = \left(\frac{C\rho}{K}\Delta x\right)\sqrt{\frac{1}{12}\left[\frac{1}{(\Delta x)^2} - \frac{\pi^2}{6L^2}\right]^{-1}}. \tag{23}$$

  This implies that, for a fixed Δx, the error first decreases quadratically until Δt_{change} and afterwards it increases quadratically with Δt.

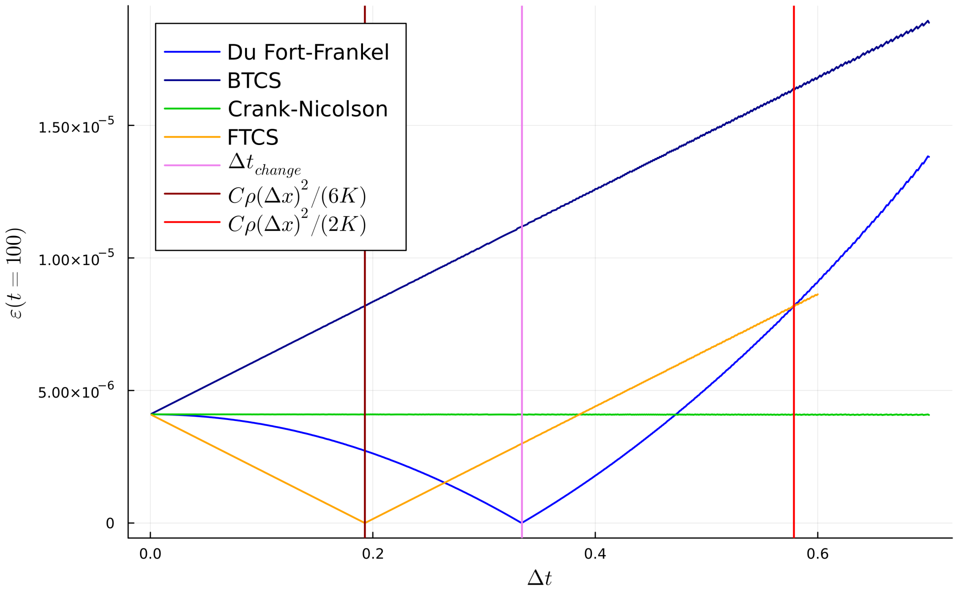


Figure 4: Error as a function of Δt for four different methods. Δt_{change} corresponds to the turning point of the Du Fort-Frankel scheme. The other two vertical lines are the same discussed for the FTCS scheme in part b).

3. Solitons

Water waves in shallow, narrow channels can be described by the Koorteweg–de Vries (KdeV) equation

$$\frac{\partial u(x,t)}{\partial t} + \epsilon u(x,t)\frac{\partial u(x,t)}{\partial x} + \mu\frac{\partial^3 u(x,t)}{\partial x^3} = 0. \tag{24}$$

The non-linear term leads to a sharpening of the wave and ultimately to a shock wave. In contrast, the $\partial^3 u/\partial x^3$ term produces broadening. For the proper parameters and initial conditions, the two effects exactly balance each other, and a stable wave is formed, which is called a "soliton". These stable solitons almost behave as particles, and appear in many areas of physics. For more details on the numerical discovery of this fascinating phenomenon, see "Computer Simulations Led to Discovery of Solitons". For a deeper dive, you can also download the original paper from Stud.IP ▸ Übung: Methods of Computational Physics ▸ Files ▸ Additional Material.

Inserting the traveling wave ansatz $u(x,t) = u(x-ct)$ gives a solvable ODE with the (non-trivial) solution

$$u(x,t) = \frac{-c}{2}\operatorname{sech}^2\left(\frac{1}{2}\sqrt{c}(\xi-\xi_0)\right), \tag{25}$$

where $\xi = x - ct$ is the phase. Note that the amplitude is proportional to the propagation speed c. Discretising the KdeV equation gives the algorithm

$$\begin{aligned} u_j^{n+1} \approx u_j^{n-1} &- \frac{\epsilon}{3}\frac{\Delta t}{\Delta x}\left[u_{j+1}^n + u_j^n + u_{j-1}^n\right]\left[u_{j+1}^n - u_{j-1}^n\right] \\ &- \mu\frac{\Delta t}{\Delta x^3}\left[u_{j+2}^n + 2u_{j-1}^n - 2u_{j+1}^n - u_{j-2}^n\right]. \end{aligned} \tag{26}$$

To calculate u_j^2, the first term on the right-hand side is not yet available, so we use a simpler forward difference scheme for the time step, which gives

$$\begin{aligned} u_j^2 \approx u_j^1 &- \frac{\epsilon}{6}\frac{\Delta t}{\Delta x}\left[u_{j+1}^1 + u_j^1 + u_{j-1}^1\right]\left[u_{j+1}^1 - u_{j-1}^1\right] \\ &- \frac{\mu}{2}\frac{\Delta t}{\Delta x^3}\left[u_{j+2}^1 + 2u_{j-1}^1 - 2u_{j+1}^1 - u_{j-2}^1\right]. \end{aligned} \tag{27}$$

In addition to the first time step, we also need to treat u_1^n, u_2^n, $u_{N_{\max}-1}^n$ and $u_{N_{\max}}^n$ separately, since also they can not be updated using Eq. (26). Given the initial state we will use below, a simple method is to use the constant boundary values $u_1^n = 1$ and $u_{N_{\max}}^n = 0$. This leaves u_2^n and $u_{N_{\max}-1}^n$. These are still to be calculated using Eqs. (26) and (27), but with the replacements $u_0^n \to u_1^n$ (when calculating u_2^n) and $u_{N_{\max}+1}^n \to u_{N_{\max}}^n$ (when calculating $u_{N_{\max}-1}^n$) on the right-hand sides.

a) Derive Eq. (26). For the first derivatives, use the central difference approximations $\partial u/\partial t \approx (u_j^{n+1} - u_j^{n-1})/(2\Delta t)$ and $\partial u/\partial x \approx (u_{j+1}^n - u_{j-1}^n)/(2\Delta x)$. To find an approximation for the third derivative expand $u(x,t)$ to including $\mathcal{O}(\Delta x^4)$ about the four points $u(x \pm \Delta x, t)$ and $u(x \pm 2\Delta x, t)$, then solve for $\partial^3 u/\partial x^3$. Finally, for the non-differentiated $u(x,t)$ in the second term of Eq. (26), use the average over three adjacent points, i.e. $u = (u_{j-1}^n + u_j^n + u_{j+1}^n)/3$. In your derivation, keep track of the truncation error, to prove that Eq. (26) is of order $\mathcal{O}(\Delta t^3) + \mathcal{O}(\Delta t \Delta x^2)$. (4 points)

Solution: Taking the expansions of $u(x \pm \Delta x, t)$ and $u(x \pm 2\Delta x, t)$ yields

$$\begin{aligned} u(x \pm \Delta x, t) = u(x,t) &\pm \frac{\partial u(x,t)}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 u(x,t)}{\partial x^2}(\Delta x)^2 \\ &\pm \frac{1}{6}\frac{\partial^3 u(x,t)}{\partial x^3}(\Delta x)^3 + \frac{1}{24}\frac{\partial^4 u(x,t)}{\partial x^4}(\Delta x)^4 + \mathcal{O}(\Delta x^5) \end{aligned} \tag{28}$$

$$\begin{aligned} u(x \pm 2\Delta x, t) = u(x,t) &\pm 2\frac{\partial u(x,t)}{\partial x}\Delta x + 2\frac{\partial^2 u(x,t)}{\partial x^2}(\Delta x)^2 \\ &\pm \frac{4}{3}\frac{\partial^3 u(x,t)}{\partial x^3}(\Delta x)^3 + \frac{2}{3}\frac{\partial^4 u(x,t)}{\partial x^4}(\Delta x)^4 + \mathcal{O}(\Delta x^5) \end{aligned} \tag{29}$$

so the differences are

$$u(x + \Delta x, t) - u(x - \Delta x, t) = 2\frac{\partial u(x,t)}{\partial x}\Delta x + \frac{1}{3}\frac{\partial^3 u(x,t)}{\partial x^3}(\Delta x)^3 + \mathcal{O}(\Delta x^5) \tag{30}$$

$$u(x + 2\Delta x, t) - u(x - 2\Delta x, t) = 4\frac{\partial u(x,t)}{\partial x}\Delta x + \frac{8}{3}\frac{\partial^3 u(x,t)}{\partial x^3}(\Delta x)^3 + \mathcal{O}(\Delta x^5) \tag{31}$$

Thus, using first and third order central differences approximation for the corresponding partial derivatives we have

$$\frac{\partial u(x,t)}{\partial x} = \frac{u(x+\Delta x,t) - u(x-\Delta x,t)}{2\Delta x} + \mathcal{O}(\Delta x^2) \tag{32}$$

$$\frac{\partial^3 u(x,t)}{\partial x^3} = \frac{u(x+2\Delta x,t) - u(x-2\Delta x,t) - 2[u(x+\Delta x,t) - u(x-\Delta x,t)]}{2\Delta x^3} + \mathcal{O}(\Delta x^2) \tag{33}$$

and similarly for time

$$\frac{\partial u(x,t)}{\partial t} = \frac{u(x,t+\Delta t) - u(x,t-\Delta t)}{2\Delta t} + \mathcal{O}(\Delta t^2). \tag{34}$$

Finally, for the term $u(x,t)$ we have (using both signs in expression (28))

$$u(x,t) = \frac{u(x,t) + u(x+\Delta x,t) + u(x-\Delta x,t)}{3} + \mathcal{O}(\Delta x^2). \tag{35}$$

Replacing the above expressions in equation (24) and solving for $u(x, t+\Delta t) \equiv u_j^{n+1}$

$$\begin{aligned} u_j^{n+1} &= u_j^{n-1} + \mathcal{O}(\Delta t^3) \\ &- 2\Delta t\epsilon \left[\frac{u_{j+1}^n + u_j^n + u_{j-1}^n}{3} + \mathcal{O}(\Delta x^2)\right]\left[\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x} + \mathcal{O}(\Delta x^2)\right] \\ &- \mu\frac{\Delta t}{\Delta x^3}\left[u_{j+2}^n + 2u_{j-1}^n - 2u_{j+1}^n - u_{j-2}^n\right] + \mathcal{O}(\Delta t \Delta x^2). \end{aligned} \tag{36}$$

The non-linear term requires special attention since in taking the product we have what appears to be a term of order $\mathcal{O}(\Delta x)$

$$\frac{1}{6\Delta x}[u^n_{j+1} + u^n_j + u^n_{j-1}][u^n_{j+1} - u^n_{j-1}] + \mathcal{O}(\Delta x^2)\frac{u^n_{j+1} - u^n_{j-1}}{2\Delta x} + \mathcal{O}(\Delta x^2) \tag{37}$$

However, according to equation (30) we have that

$$\frac{u^n_{j+1} - u^n_{j-1}}{2\Delta x} = \frac{\partial u(x,t)}{\partial x} + \mathcal{O}(\Delta x^2) \tag{38}$$

and therefore

$$\mathcal{O}(\Delta x^2)\frac{u^n_{j+1} - u^n_{j-1}}{2\Delta x} = \mathcal{O}(\Delta x^2) \tag{39}$$

from which it follows Eq. (26) with an error of order $\mathcal{O}(\Delta t^3) + \mathcal{O}(\Delta t \Delta x^2)$.

b) Implement the above algorithm solving the KdeV equation for the initial condition

$$u(x, t=0) = \frac{1}{2}\left[1 - \tanh\left(\frac{x-25}{5}\right)\right]. \tag{40}$$

The parameters are given by $\epsilon = 0.2$ and $\mu = 0.1$ and the step sizes by $\Delta x = 0.4$ and $\Delta t = 0.1$. Use 130 steps in x, such that our simulation volume is given by $L = 130\Delta x = 52$. Verify that these constants satisfy the stability condition

$$\frac{\Delta t}{\Delta x}\left[\epsilon|u| + 4\frac{\mu}{(\Delta x)^2}\right] \leq 1. \tag{41}$$

Store the solution every 250 or so time steps and run the simulation for about 2000 time steps. Plot the disturbance u versus position and versus time. Scott Russell observed in 1834 in the Edinburgh-Glasgow canal that an initial, arbitrary wave form set in motion evolves into two or more solitary waves that move at different velocities. Can you confirm his observation? Into how many solitary waves does your initial wave form break up into? (8 points)

Solution: With the given values of the parameters, the disturbance u versus position and time is shown in Fig.(5) alongside with the stability condition at each time step, evaluated with the maximum absolute value of u at the given time, in Fig.(6). Additionally, perturbance versus space at different times can be seen in Fig.(7). From them it can be seen that indeed the initial wave breaks into 7 solitary waves after 200 simulation seconds (2,000 time steps with $\Delta t = 0.1$). It is also important to note that at every time in the simulation, we remain below the boundary necessary for stability. However, if we ran the simulation for longer, the right-most wave will "collide" with the simulation wall and start producing amplitudes due to numerical error that no longer satisfy the stability criteria.

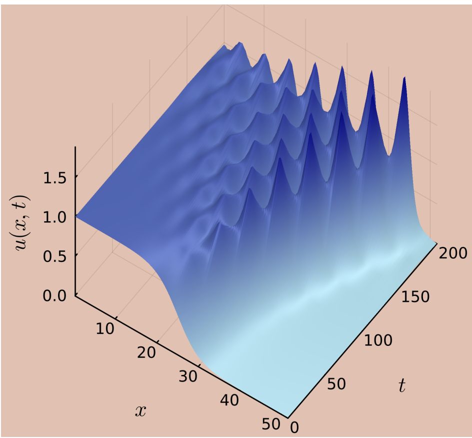


Figure 5: Surface plot of the disturbance as a function of time and space for every 250 time steps.

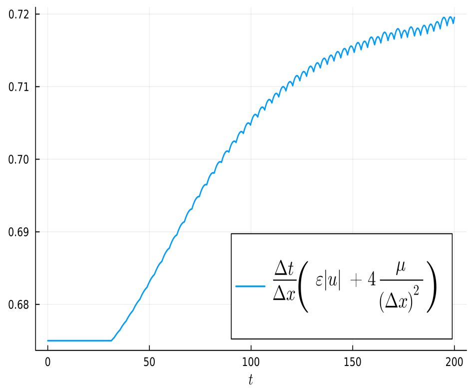


Figure 6: Values of the stability condition in (41).

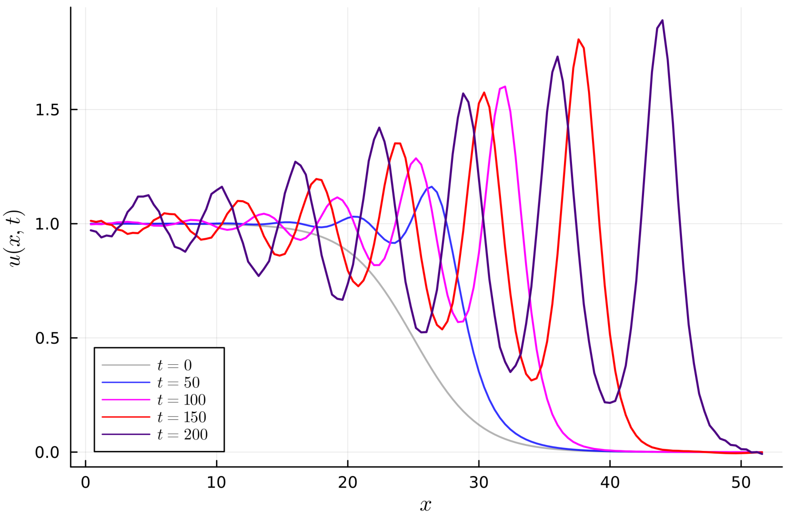


Figure 7: Perturbance u at different times in all of space.

c) Explore what happens when a tall soliton collides with a short one. Do they bounce off each other? Do they go through each other? Do they interfere? Do they destroy each other? Does the tall soliton still move faster than the short one after collision? Start off by placing a tall soliton of height 0.8 at $x = 12$, and a small soliton in front of it at $x = 26$:

$$u(x, t = 0) = 0.8\left[1 - \tanh^2\left(\frac{3x}{12} - 3\right)\right] + 0.3\left[1 - \tanh^2\left(\frac{4.5x}{26} - 4.5\right)\right]. \tag{42}$$

Make sure to adapt the constant boundary values for u_1^n and $u_{N_{\max}}^n$ for this simulation. (4 points)

Solution: As shown in appendix B, the shape of a soliton solution for the form of the equation in (24) is given by

$$u(x, t) = \frac{3c}{\epsilon}\,\mathrm{sech}^2\left(\frac{1}{2}\sqrt{\frac{c}{\mu}}(\xi - \xi_0)\right). \tag{43}$$

where c is the propagation speed. One important feature of these solutions is that, since the equation is nonlinear, they do not admit to be multiplied by an arbitrary constant in order to still be solutions of the original equation. Additionally, the sum of two solitons is not a solution of the Koorteweg-de Vries equation at all times, but yields

$$\frac{9c_1c_2}{\epsilon\sqrt{\mu}}\,\mathrm{sech}^2\eta_1\,\mathrm{sech}^2\eta_2\left(\sqrt{c_1}\tanh\eta_1 + \sqrt{c_2}\tanh\eta_2\right), \qquad \eta_i = \frac{1}{2}\sqrt{\frac{c_i}{\mu}}(x - c_it - x_{0,i}) \tag{44}$$

which, if not zero at all times, in general it is extremely small and, most importantly, it does go to zero for $t \to \infty$. Therefore, the sum of solitons is preserved after long times as a solution of the KdeV equation. For these reasons, I think that there is a mistake with the initial condition in (42), as it can't correspond to a simple sum of solitons:

$$\begin{aligned}
&\frac{1}{2}\sqrt{\frac{c_1}{\mu}} = \frac{3}{12} \implies c_1 = \frac{1}{4}\mu, \qquad \frac{3c_1}{\epsilon} = \frac{4}{5} \implies c_1 = \frac{4}{15}\epsilon \implies \mu = \frac{16}{15}\epsilon\\
&\frac{1}{2}\sqrt{\frac{c_2}{\mu}} = \frac{4.5}{26} \implies c_2 = \frac{81}{676}\mu, \quad \frac{3c_2}{\epsilon} = \frac{3}{10} \implies c_2 = \frac{1}{10}\epsilon \implies \mu = \frac{676}{810}\epsilon
\end{aligned} \tag{45}$$

It might, of course, also be the case that I am wrong and my simulation is also wrong as it doesn't display two solitons after the interaction with the above initial condition. However, if I implement as an initial condition the sum of two solitons with $c_1 = 4/75$, $x_{0,1} = 12$, $c_2 = 1/50$, $x_{0,2} = 26$ and the same parameters as in part b), I get the results in Fig.(8). The stability of the simulation can be seen in Fig.(9), where it is shown that during the whole simulation the stability condition is fulfilled, the dip corresponding to the times at which the two solitons meet, giving a single peek that has smaller amplitude than the maximum amplitude previous and after the interaction (see the attached animation).

- Do they bounce off of each other?

  No. Both of them keep moving in the same direction.

- Do they go through each other?

  Yes.

- Do they interfere?

  Yes, in the sense that they both kind of mix as one passes through the other. See also below.

- Do they destroy each other?

  No. They have some interference as they phase each other but they are still the same solitons afterwards.

- Does the tall soliton still move faster than the short one after collision?

  Yes. The speed of both solitons remains unaltered as one of them passes through the other.

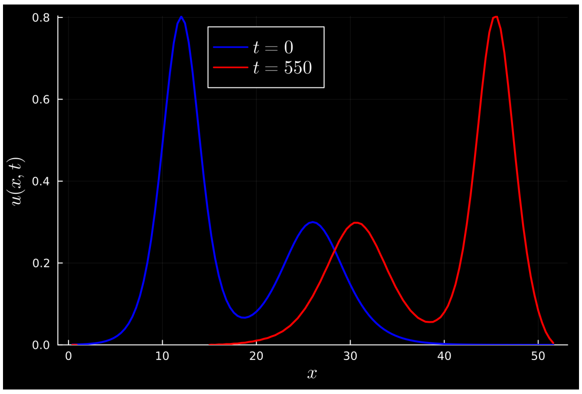


Figure 8: Initial and final states of the perturbance $u(x,t)$ using the same parameters as in part b), but after 5,500 time steps.

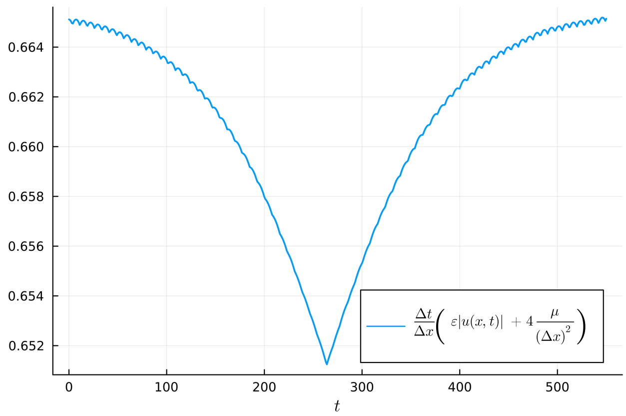


Figure 9: Stability condition for the associated simulation above. At each time, $|u|$ was taken as the maximum absolute value of the perturbance.

A. Exact solution for the diffusion equation with homogeneous boundary conditions

Since the boundary conditions are homogeneous, i.e., $T(x=0,t) = T(x=L,t) = 0$, we may attempt to solve the diffusion by proposing $T(x,t) = X(t)\Theta(t)$, in which case our equation reads:

$$\frac{\partial T(x,t)}{\partial t} = \frac{K}{C\rho}\frac{\partial^2 T(x,t)}{\partial x^2} \longmapsto \frac{C\rho}{K}\frac{1}{\Theta}\frac{\mathrm{d}\Theta}{\mathrm{d}t} = \frac{1}{X}\frac{\mathrm{d}^2 X}{\mathrm{d}x^2}. \tag{46}$$

As both sides of this equation depend on different variables, they must be equal to a constant α. Then, the spatial part can satisfy the boundary conditions for a non-trivial solution only if $\alpha = -k^2$, since

$$\frac{1}{X}\frac{\mathrm{d}^2 X}{\mathrm{d}x^2} = \alpha \implies \begin{cases} \alpha > 0: & X(x) = C_1 e^{\sqrt{\alpha}x} + C_2 e^{-\sqrt{\alpha}x} \\ \alpha = 0: & X(x) = C_1 x + C_2 \\ \alpha < 0: & X(x) = C_1 \sin(\sqrt{-\alpha}x) + C_2 \cos(\sqrt{-\alpha}x) \end{cases} \tag{47}$$

and therefore

$$X(0) = X(L) = 0 \implies \begin{cases} \alpha > 0: & C_1 = -C_2, \quad 2C_1 \sinh(\sqrt{\alpha}L) = 0 & \implies X(x) = 0 \\ \alpha = 0: & C_2 = 0, \qquad\qquad\qquad C_1 = 0 & \\ \alpha < 0: & C_2 = 0, \qquad C_1 \sin(\sqrt{-\alpha}L) = 0 & \implies \sqrt{-\alpha} = \dfrac{m\pi}{L} \end{cases} \tag{48}$$

So the spatial part reads

$$X(x) = C_1 \sin\left(\frac{m\pi x}{L}\right) \quad \text{for integers } m. \tag{49}$$

Integrating the temporal part

$$\frac{C\rho}{K}\frac{1}{\Theta}\frac{\mathrm{d}\Theta}{\mathrm{d}t} = -\left(\frac{m\pi}{L}\right)^2 \implies \Theta(t) = A\exp\left(-m^2\frac{\pi^2 K t}{L^2 C\rho}\right) \tag{50}$$

we obtain the most general solution, for the given boundary conditions, as

$$T(x,t) = \sum_{m=0}^{\infty} C_m \sin\left(\frac{m\pi x}{L}\right)\exp\left(-m^2\frac{\pi^2 K t}{L^2 C\rho}\right). \tag{51}$$

Finally, for the initial condition $T(x, t=0) = \sin(\pi x/L)$, using

$$\int_0^L \mathrm{d}x\ \sin(n\pi x/L)\sin(m\pi x/L) = \frac{L}{2}\delta_{m,n} \tag{52}$$

we get $C_m = \delta_{m,1}$ and our particular solution reads

$$\boxed{T(x,t) = \sin\left(\frac{\pi x}{L}\right)\exp\left(-\frac{\pi^2 K t}{L^2 C\rho}\right).} \tag{53}$$

B. Traveling-wave Ansatz

From the Koorteweg-de Vries (KdeV) equation

$$\frac{\partial u(x,t)}{\partial t} + \epsilon u(x,t)\frac{\partial u(x,t)}{\partial x} + \mu\frac{\partial^3 u(x,t)}{\partial x^3} = 0 \tag{54}$$

taking $u(x,t) = u(x-ct) \equiv u(\xi)$ we get the ODE

$$-c\frac{\mathrm{d}u}{\mathrm{d}\xi} + \epsilon u\frac{\mathrm{d}u}{\mathrm{d}\xi} + \mu\frac{\mathrm{d}^3 u}{\mathrm{d}\xi^3} = \frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{1}{2}\epsilon u^2 - cu + \mu\frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2}\right) = 0 \tag{55}$$

which implies

$$\frac{1}{2}\epsilon u^2 - cu + \mu\frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} = a = \text{const.} \tag{56}$$

This equation resembles the shape of Newton's second law in one dimension:

$$\mu\frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} = a + cu - \frac{1}{2}\epsilon u^2 \longmapsto m\frac{\mathrm{d}^2 x}{\mathrm{d}t} = F[x(t)] \tag{57}$$

and by analogy we can get another integral of motion if we multiply this equation by $v \equiv \mathrm{d}u/\mathrm{d}\xi$

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left(\frac{1}{2}\mu v^2 + \frac{1}{6}\epsilon u^3 - \frac{1}{2}cu^2 - au\right) = 0 \implies B \equiv \frac{1}{2}\mu v^2 + \frac{1}{6}\epsilon u^3 - \frac{1}{2}cu^2 - au = \text{const.} \tag{58}$$

The above equation can be seen as defining curves in the phase space of $u(\xi)$, for which case we have a "potential" given by

$$V[u(x,t)] = \frac{1}{6}\epsilon u^3 - \frac{1}{2}cu^2 - au. \tag{59}$$

The qualitative behaviour of $V[u(x,t)]$ can be seen from a simple analysis:

$$\frac{\mathrm{d}V}{\mathrm{d}u} = \frac{1}{2}\epsilon u^2 - cu - a = \frac{1}{2}\epsilon\left(u - \frac{c}{\epsilon}\right)^2 - a - \frac{c^2}{2\epsilon} \overset{!}{=} 0 \implies u = \frac{c}{\epsilon} \pm \sqrt{\frac{2a\epsilon + c^2}{\epsilon^2}} \tag{60}$$

If $c^2+2a\epsilon \geq 0$ the derivative of the potential vanishes. However, for the case in which $c^2+2a\epsilon = 0$, the point does not correspond to a maximum nor a minimum, but simply to an inflection point

$$\frac{\mathrm{d}^2 V}{\mathrm{d}u^2} = \epsilon\left(u - \frac{c}{\epsilon}\right) = \pm\frac{\epsilon}{|\epsilon|}\sqrt{c^2 + 2a\epsilon}. \tag{61}$$

So, if $c^2 + 2a\epsilon > 0$, we have both a local maximum and a local minimum and thus a region for which the amplitude of u oscillates between two values. If our initial conditions are such that $V_{\text{local min}} = V[u_{\text{local min}}] < B < V_{\text{local max}} = V[u_{\text{local max}}]$ and $u_{\text{local min}} < u < u_{\text{local max}}$, the amplitude will have some finite "period" T_ξ and will therefore not correspond to a soliton, since the excitations will reappear periodically. However, if we take a configuration with $B = V_{\text{local max}}$ (and, again, $u_{\text{local min}} < u < u_{\text{local max}}$), the period of these oscillations becomes infinite (think of a pendulum with an energy equal to the separatrix energy) and hence, we will have a single traveling-wave. The only thing keeping us from calling this a "soliton" is the fact that at $\xi \to \pm\infty$ the amplitude is not going to zero but to the value of the maximum amplitude. This can be fixed, however, if we require that the maximum of the potential is at $u = 0$

$$\left.\frac{\mathrm{d}^2 V}{\mathrm{d}u^2}\right|_{u=0} = -c \overset{!}{<} 0 \implies \boxed{c > 0} \quad \text{and} \quad u_{+,-} \overset{!}{=} 0 \implies 2a\epsilon = 0 \implies \boxed{a = 0.} \tag{62}$$

The first of these conditions means that the propagation speed must be positive (c being a speed already implies that it's positive) while the second one means that, at all values of ξ, we have

$$\frac{1}{2}\epsilon u^2 - cu + \mu \frac{\mathrm{d}^2 u}{\mathrm{d}\xi^2} = 0. \tag{63}$$

In particular, since we now know that at $\xi \to \pm\infty$, $u \to 0$, this implies that $\left.\mathrm{d}^2u/\mathrm{d}\xi^2\right|_{\xi\to\pm\infty} \to 0$. Similarly, the constant of motion in (58) implies that $\left.\mathrm{d}u/\mathrm{d}\xi\right|_{\xi\to\pm\infty} \to 0$. Under these conditions we finally have the physical description of a soliton and we can proceed to integrate from the constant of motion in (58):

$$B = V_{\max} = 0 = \frac{1}{2}\mu v^2 + \frac{1}{6}\epsilon u^3 - \frac{1}{2}cu^2 \implies \int_{\xi_0}^{\xi} \frac{\sqrt{3\mu}}{u\sqrt{3c-\epsilon u}} \frac{\mathrm{d}u}{\mathrm{d}\xi'}\mathrm{d}\xi' = \xi - \xi_0$$

$$s \equiv \sqrt{3c - \epsilon u} \implies \frac{\mathrm{d}s}{\mathrm{d}\xi} = \frac{-\epsilon}{2\sqrt{3c-\epsilon u}} \frac{\mathrm{d}u}{\mathrm{d}\xi} \implies \xi - \xi_0 = \int_{s_0}^{s} 2\sqrt{3\mu} \frac{\mathrm{d}s}{3c - s^2}$$

$$s = \sqrt{3c}\tanh\eta \implies \frac{\mathrm{d}s}{\mathrm{d}\eta} = \sqrt{3c}\,\mathrm{sech}^2\eta \implies \tanh\left(\frac{1}{2}\sqrt{\frac{c}{\mu}}(\xi-\xi_0)\right) = \sqrt{1 - \frac{\epsilon u}{3c}}$$

$$\boxed{u = \frac{3c}{\epsilon}\,\mathrm{sech}^2\left(\frac{1}{2}\sqrt{\frac{c}{\mu}}(\xi - \xi_0)\right).} \tag{64}$$