

39. Finite element method Crank-Nicholson implementation of the convection equation:

$$M_x \frac{f_j^{n+1} - f_j^n}{\Delta t} + \frac{1}{2} u \left(L_x f_j^{n+1} + L_x f_j^n \right) = 0$$

(a) With Mass operator $M_x = (\delta, 1 - 2\delta, \delta)$; Multiplication with Δt and applying the operators

$$\begin{aligned} & \left(\delta f_{j-1}^{n+1} + (1 - 2\delta) f_j^{n+1} + \delta f_{j+1}^{n+1} \right) - \left(\delta f_{j-1}^n + (1 - 2\delta) f_j^n + \delta f_{j+1}^n \right) \\ & + \frac{u\Delta t}{4\Delta x} \left[\left(f_{j+1}^{n+1} - f_{j-1}^{n+1} \right) + \left(f_{j+1}^n - f_{j-1}^n \right) \right] = 0 \end{aligned}$$

Re-arranging all terms at time level $n + 1$ on the left side and all terms for time level n on the right side of the equation yields with $c = u\Delta t / \Delta x$

$$\left(\delta - \frac{1}{4}c \right) f_{j-1}^{n+1} + (1 - 2\delta) f_j^{n+1} + \left(\delta + \frac{1}{4}c \right) f_{j+1}^{n+1} = \left(\delta + \frac{1}{4}c \right) f_{j-1}^n + (1 - 2\delta) f_j^n + \left(\delta - \frac{1}{4}c \right) f_{j+1}^n$$

(b) Amplification factor

Dividing the above equation by f_j^n yields

$$\begin{aligned} & \left[\left(\delta - \frac{1}{4}c \right) \exp(-ik\Delta_x) + (1 - 2\delta) + \left(\delta + \frac{1}{4}c \right) \exp(ik\Delta_x) \right] g = \\ & \left(\delta + \frac{1}{4}c \right) \exp(-ik\Delta_x) + (1 - 2\delta) + \left(\delta - \frac{1}{4}c \right) \exp(ik\Delta_x) \end{aligned}$$

with $\exp(ik\Delta_x) + \exp(-ik\Delta_x) = 2\cos k\Delta_x$ and $\exp(ik\Delta_x) - \exp(-ik\Delta_x) = 2i\sin k\Delta_x$ such that

$$\begin{aligned} & \left[(1 - 2\delta) + 2\delta \cos k\Delta_x + \frac{i}{2}c \sin k\Delta_x \right] g = (1 - 2\delta) + 2\delta \cos k\Delta_x - \frac{i}{2}c \sin k\Delta_x \\ & \text{or } g = \frac{(1 - 2\delta) + 2\delta \cos k\Delta_x - \frac{ic}{2} \sin k\Delta_x}{(1 - 2\delta) + 2\delta \cos k\Delta_x + \frac{ic}{2} \sin k\Delta_x} \end{aligned}$$

(c) Stability:

Fast route: the numerator is the complex conjugate of the denominator. Therefore the magnitude of the numerator and the denominator are the same \Rightarrow magnitude of the ratio is 1 \Rightarrow the scheme is always stable!

Note: One can write any complex number $z = x + iy = r \exp(i\phi)$ where r is the magnitude. The division $z/z^* = \exp(i\phi) / \exp(-i\phi) = \exp(2i\phi)$ such that the magnitude must be one!

Long route: Abbreviate $G = [(1 - 2\delta) + 2\delta \cos k\Delta_x]$ and $H = \frac{c}{2} \sin k\Delta_x$

such that

$$g = \frac{G^2 - H^2 - 2iHG}{G^2 + H^2}$$

$$\begin{aligned} \text{and } |g|^2 = gg^* &= \frac{\{G^2 - H^2\}^2 + (2H)^2 G^2}{\{G^2 + H^2\}^2} \\ &= \frac{G^4 - 2G^2H^2 + H^4 + 4H^2G^2}{\{G^2 + H^2\}^2} = \frac{(G^2 + H^2)^2}{(G^2 + H^2)^2} = 1 \end{aligned}$$

Thus the scheme is unconditionally stable!

40. Simulations of the transport equation.

(a) Upwind method for the truncated sine wave.

Estimate of diffusion through the damping $f(x,t) = f_0 \exp(-p(m)t) \exp(im(x - q(m)t))$. Since initial amplitude is 1 the wave amplitude after time τ is $f_\tau = \exp(-p(m)\tau)$ yielding

$$p = -\frac{1}{\tau} \ln f_\tau$$

For $f_\tau \approx 0.45$ and $\tau = 12 \Rightarrow p \approx 0.067$
 Using the damping coefficient $p(m) = \alpha m^2$ and assuming $m = 2\pi/\lambda$ with $\lambda \approx 3$ yields

$$\alpha \approx p/m^2 = 0.017$$

which is much larger than the physical diffusion coefficient of $\alpha = 0.001$ assumed in the simulation. Note that this is only a rough estimate because the truncated sine wave consists of a spectrum of shorter and longer waves where short waves are damped faster while longer wavelengths are damped slower implying also that the damping rate changes over time if f consists of a spectrum of modes.

The numerical diffusion coefficient (truncation error associated with the 2nd derivative term) is

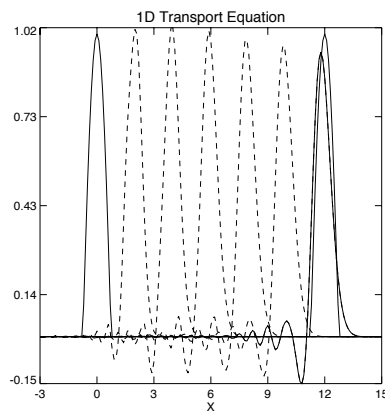
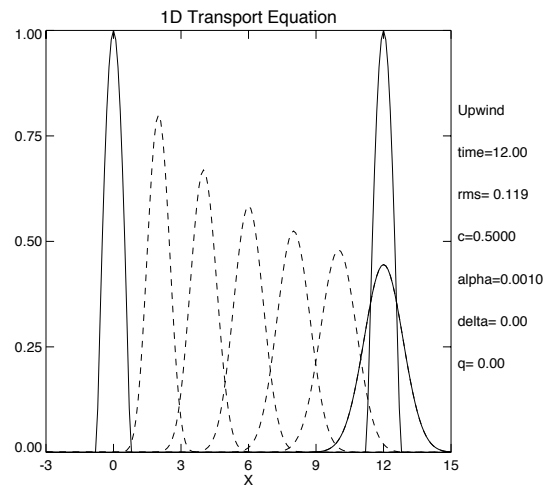
$$\alpha_{num} = \frac{1}{2} (1 - c) u \Delta x = 0.025$$

for the considered parameters. Thus the estimate actually agrees still reasonably with the numerical diffusion.

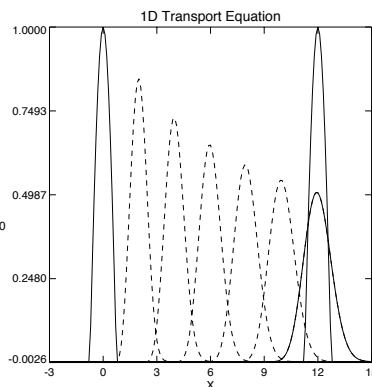
The position of the maximum agrees excellent with the expected position indicating that dispersion is very small. The numerical coefficient of the 3rd derivative is

$$\beta_{num} = c\alpha\Delta x - u\frac{\Delta x^2}{6} (1 - 3c + 2c^2) = 5 \cdot 10^{-5}$$

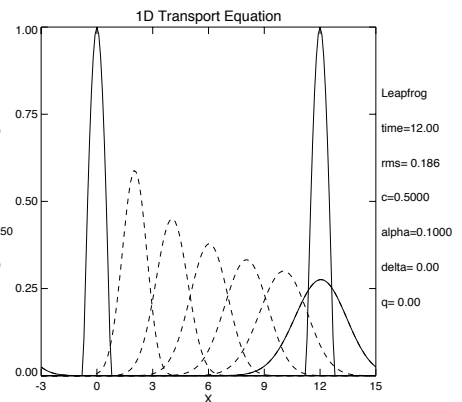
which with $q(m) = u - \beta m^2$ corresponding to a correction of $2 \cdot 10^{-4}$ to the signal speed.



Leapfrog - default



Leapfrog - $\alpha = 0.02$



Leapfrog - $\alpha = 0.1$

(b) Leapfrog method:

The Leapfrog method shows significantly less damping but the maximum is slightly shifted compared to the expected position. It also displays typical oscillations close to the grid scale. The dispersion coefficient for the chosen parameters is $\beta_{num} = 1.25 \cdot 10^{-3}$

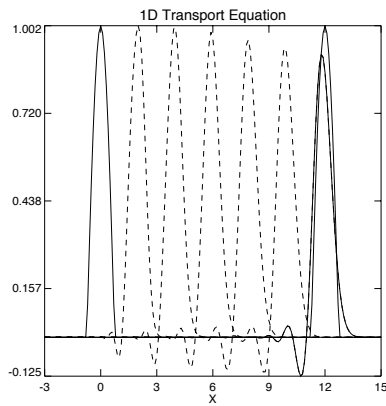
The result is as expected because the Leapfrog has no diffusion. Only the small physical diffusion acts to counter the effects of dispersion. The default diffusion coefficient is too small to suppress the oscillations. The 2nd result increases the diffusion to $\alpha = 0.25$ and suppressing the grid oscillations. Comparison with the upwind indicates that the numerical diffusion of the upwind is indeed about 0.25.

Increasing the diffusion coefficient to $\alpha = 0.1$ yields a strongly damped signal. The damping is larger than for the upwind as expected from the estimate (to yield about the same damping a diffusion coefficient of about $\alpha = 0.03$ is needed).

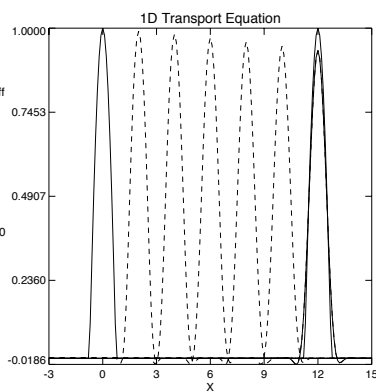
(c) Lax-Wendroff result:

Very similar to the Leapfrog case. The L-W result shows just a little more damping and slightly reduced oscillations indicating that diffusion and dispersion are very similar to the Leapfrog. Using the 4 point upwind parameter the smallest rms error is obtained for $q = 0.36$ ($q = 0.35$ plotted) in which case the oscillations are almost gone with small oscillations in front and behind the pulse (all other methods show oscillations only in the rear part of the pulse). Increasing q further generates more positive dispersion, i.e., oscillations increase at the leading edge.

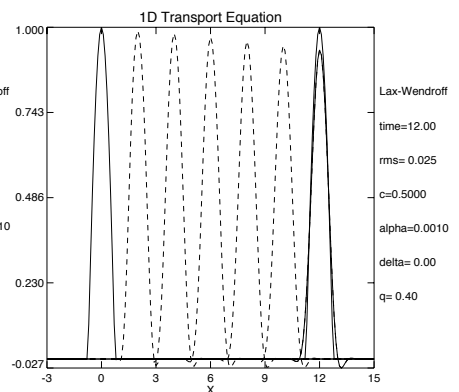
The truncation error for the 3rd derivative of f from problem 34 is $-\alpha c \Delta x - u \left(q - \frac{1-c^2}{2} \right) \frac{\Delta x^2}{3}$ requiring for the chosen parameters a value of $q = 0.36$ to render this dispersion error to 0 which is exactly what we obtained for the simulation.



Lax-Wendroff - default

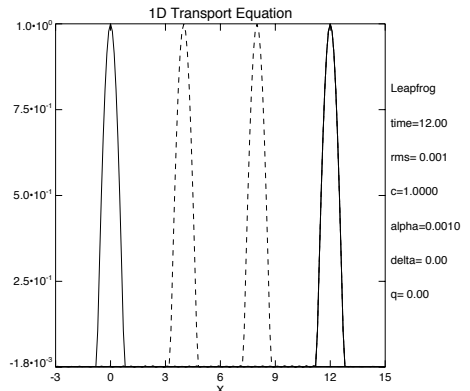


Lax-Wendroff - $q_{opt} = 0.35$



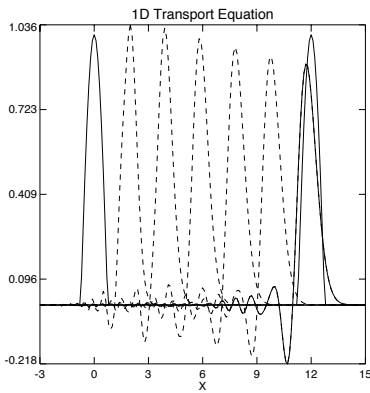
Lax-Wendroff - $q = 0.4$

The Leapfrog with $c=1$ shows an almost perfect result. (This program measures the rms error compared to the non damped signal otherwise it would be even smaller). The truncation error shows that this error (and dispersion) vanishes if $c = 1$. However, the solution lost the damping i.e., the choice of $c = 1$ eliminated the physical diffusion as well.

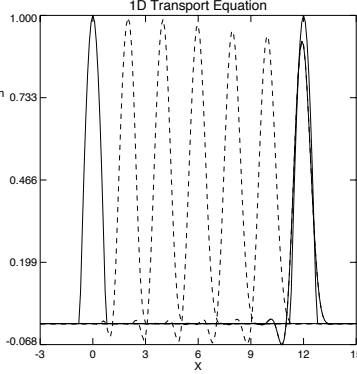


(d) Finite difference Crank-Nicholson scheme

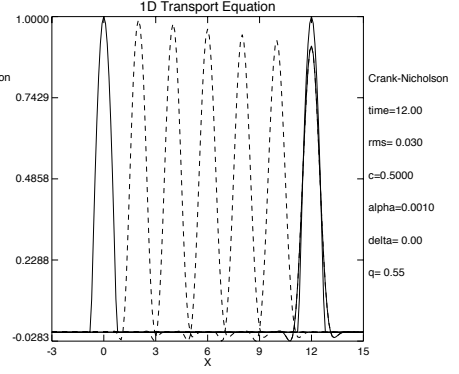
Again a result that is very similar to the Leapfrog with slightly less damping and slightly higher oscillations indicating stronger dispersion than the Leapfrog. Increasing the value of q for the 4 point forward differencing reduces the amplitude of the oscillations and provides a more accurate location of the maximum implying reduced dispersion as well. The optimum value of q is now $q = 0.55$ and larger values cause positive dispersion as in the LW case.



Crank-Nicholson - default (FDM)



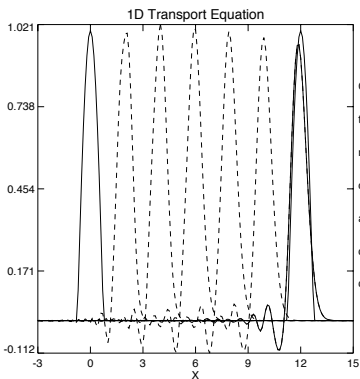
FDM Crank-Nicholson - with optimum value of $q = 0.4$



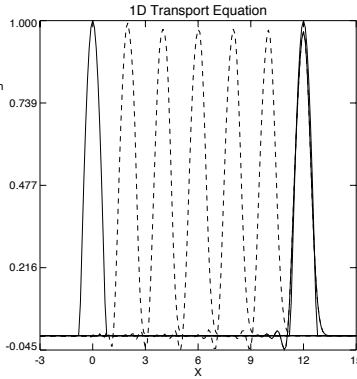
FDM Crank-Nicholson - with optimum value of $q_{opt} = 0.55$

(e) Generalized finite element Crank-Nicholson scheme

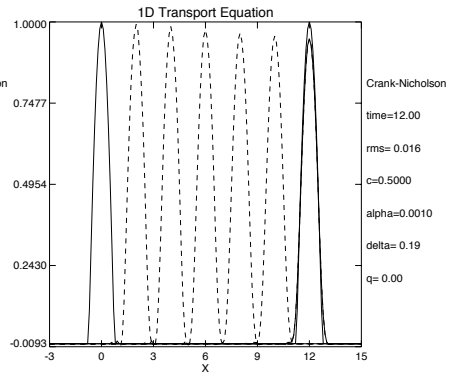
Minimum error occurs for $\delta = 0.19$. The truncation error associated with the 3rd derivative for the generalized C-N method (Fletcher, page 305 is adjustable) is $u \left(\frac{2+c^2}{12} - \delta \right) \Delta x^2$ which requires a value of $\delta = 0.1875$ to be rendered to 0 in nice agreement with the simulation. A smaller value of δ such as $\delta = 0.1$ or the FEM value $1/6$ reduces oscillations (and dispersion).



Generalized mass operator Crank-Nicholson - $\delta = 0.1$



Generalized mass operator Crank-Nicholson - $\delta = 1/6$



Generalized mass operator Crank-Nicholson - $\delta_{opt} = 0.19$

Overall, 2nd order dispersion leads to a small error in the location of the maximum of the pulse but more severely, it generates significant grid oscillations caused by the dispersion errors (severe for short wavelength), This dispersion can be balanced by enhanced diffusion, however, it may imply larger diffusion than implied by the physical diffusion of a system. To generate a solution with more accurate dispersion with the typical LW and leapfrog schemes requires higher (more appropriate spatial resolution). An alternative is the choice of a modified scheme to reduce or eliminate 3rd order derivative errors. In both the LW and the CN cases this choice lead to rather accurate propagation and strongly reduced oscillations. Similarly the FEM CN with an optimised choice of $\delta \approx 0.19$ achieved the same result. However, it is noted that the particular choices of q and δ depend on simulation parameters (u , α , Δx , Δt) and in general it is difficult to reduce errors as significantly and everywhere in the simulation (with varying velocities and diffusion).