Chapter 9

Convection Equations

A physical system is usually described by more than one equation. Typical is the system of equations for an ideal gas or fluid. This requires equation for density ρ, velocity $\mathbf{u}$, and pressure p. In one dimension these equations are

$$\begin{aligned}
\frac{\partial \rho}{\partial t}+\frac{\partial \rho u}{\partial x} &= 0 \\
\frac{\partial \rho u}{\partial t}+\frac{\partial \rho u u}{\partial x} &= -\frac{\partial p}{\partial x} \\
\frac{\partial p}{\partial t}+\frac{\partial p u}{\partial x} &= (\gamma-1)\, p \frac{\partial u}{\partial x}
\end{aligned}$$

with $\gamma=5/3$ for adiabatic changes of the state of a system and u being the x component of the velocity. This system of equations is hyperbolic and the equations are of convection type. The following sections will address the discretization of convection equation and discuss properties of the discretization such as stability and accuracy of the respective schemes. An important physical aspect of the dynamics of fluids and gases is dispersion and diffusion. However, the introduction of a numerical approximation implies the introduction of numerical dispersion and diffusion. This aspect is examined in section 2. Further section in this chapter will consider extensions of a simple convection equations such as two and more dimensions, nonlinear transport, systems of equations, and steady state systems.

9.1 Linear convection equations

Let us consider the very simple one-dimensional equation

$$\frac{\partial f}{\partial t}+u \frac{\partial f}{\partial x}=0$$

where for simplicity u is assumed to be known and constant. The solution to this equation is simple. Assuming any initial condition $f((x, t_1=0)=F(x)$ the subsequent solution is given by the transport of the initial profile, i.e., f$(x, t)=F(x-u t)$.

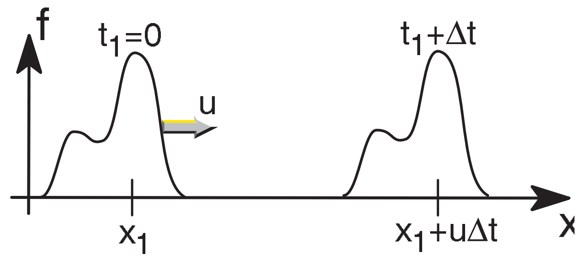


Figure 9.1: Illustration of the transport of an initial profile by a constant velocity u.

9.1.1 Simple explicit methods

FTCS scheme

In terms of a numerical scheme it would appear that the FTCS scheme is the simplest approach yielding

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

which gives an explicit equation for f_j^{n+1}

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

with $c = u\Delta t/\Delta x$. The problem with this approach is that the von Neumann stability analysis yields an amplification factor of

$$g = 1 - ic\sin(k\Delta x)$$

or for the square of the magnitude

$$|g|^2 = 1 + c^2\sin^2(k\Delta x)$$

which is always greater than 1 except for the utterly useless value of $c = 0$ implying $\Delta t = 0$. Thus although simple the FTCS scheme is always unstable for the convection equation.

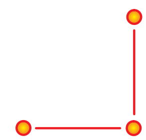
Upwind scheme and the CFL condition

Another differencing attempt can be made using upwind spatial differencing

$$\frac{f_j^{n+1}-f_j^n}{\Delta t}+\frac{u}{\Delta_x}\left(f_j^n-f_{j-1}^n\right)=0$$

yielding

$$f_j^{n+1}=(1-c)\,f_j^n+cf_{j-1}^n$$



Schematic of the upwind scheme.

Note that for negative values of u one would alter the scheme to $f_j^{n+1}=(1-|c|)\,f_j^n+|c|\,f_{j+1}^n$. Using the von Neumann stability analysis we obtain

$$\begin{aligned} g &= 1-c+c\exp(-ik\Delta x)\\ &= 1-c+c\,(\cos k\Delta x+i\sin k\Delta x)\\ &= 1+c\,(\cos k\Delta x-1)+i\sin k\Delta x \end{aligned}$$

Stability analysis:

$$\begin{aligned} gg^* &= 1+2c\,(\cos k\Delta x-1)+c^2\left(\cos^2 k\Delta x-2\cos k\Delta x+1\right)+c^2\sin^2 k\Delta x\\ &= 1+2c\,(\cos k\Delta x-1)+2c^2\,(-\cos k\Delta x+1)\\ &= 1-4c\sin^2\frac{k\Delta x}{2}+4c^2\sin^2\frac{k\Delta x}{2}=1-4c\,(1-c)\sin^2\frac{k\Delta x}{2} \end{aligned}$$

Thus stability requires $c=u\Delta t/\Delta x\leq 1$ or $\Delta t\leq\Delta x/u$. This is consistent with the condition we anticipated earlier based on the reasoning that information should travel at most one grid spacing in a single time step for any explicit method which uses updates from the immediate vicinity of any grid point.

Expanding the upwind scheme in Taylor series to determine the truncation error yields

$$\frac{\partial f}{\partial t}+u\frac{\partial f}{\partial x}-\frac{1}{2}u\Delta x\,(1-c)\,\frac{\partial^2 f}{\partial x^2}+O\left(\Delta t^2,\Delta x^2\right)=0$$

Thus the scheme is first order accurate with the leading error term as $E_j^n=-\frac{1}{2}u\Delta x\,(1-c)\,\frac{\partial^2 f}{\partial x^2}$. Which this is in principle all right for the convection equation it should be pointed out that the error involves a second derivative of f and therefore represents a numerical diffusion term with the diffusion coefficient

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

Note that the diffusion term and associated error vanish for $c=1$, however, in a more complex system with varying u and Δx such a choice is usually not possible.

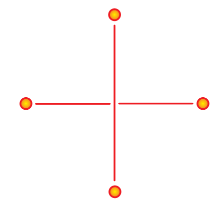
Leapfrog and Lax Wendroff schemes

A rather simple and second order accurate scheme is the so-called Leapfrog scheme

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

which yields the algebraic equation

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



Schematic of the Leapfrog scheme.

Note that this is a two level scheme. The truncation error is of order $O\left(\Delta t^2,\Delta x^2\right)$ such that the scheme is second order accurate. The amplification factor is

$$g=ic\sin\left(k\Delta x\right)\pm\sqrt{1-c^2\sin^2\left(k\Delta x\right)}$$

which yields stability for $c\leq 1$.

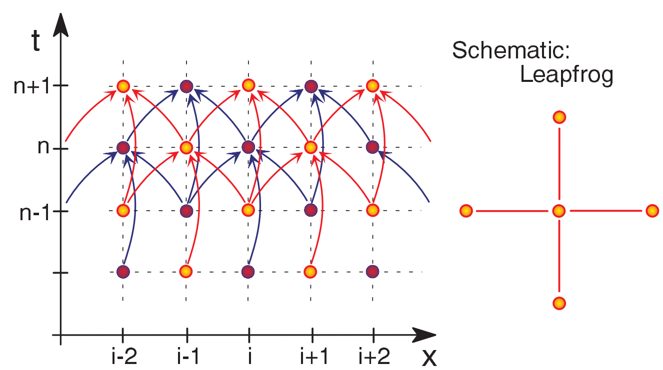


Figure 9.2: Illustration of the temporal and spatial pattern of the time stepping in the Leapfrog scheme.

The Leapfrog is, however, not without problems. The figure above illustrates that the scheme only requires either the orange or the blue indicated grid points/time levels. Thus the differencing decouples odd and even grid points at any given time step such that a solution can develop independently on the interlaced odd/even grid and thus may lead to strong oscillations on the grid scale if the two grids are combined. We will return later to this problem in connection to the issues of diffusion and dispersion.

A scheme closely related to the Leapfrog is the Lax Wendroff method. This scheme uses the forward time discretization with a correction that eliminates the lowest order error of the forward time differencing

$$\frac{\partial f}{\partial t}\approx\frac{f_j^{n+1}-f_j^n}{\Delta t}-\frac{1}{2}\Delta t\frac{\partial^2 f}{\partial t^2}=\frac{f_j^{n+1}-f_j^n}{\Delta t}-\frac{1}{2}\Delta t u^2\frac{\partial^2 f}{\partial x^2}$$

which yields for the algebraic equation

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

The resulting truncation error is $O\left(\Delta t^2, \Delta x^2\right)$. Note that the above formulation has problems in two dimensions or in general in cases where u or Δx is not constant. Therefore the Lax Wendroff scheme is typically implemented as a two step method with the steps

$$\begin{aligned}
&(\mathbf{1}) \qquad f_{j+1/2}^* = \frac{1}{2}\left(f_{j+1}^n + f_j^n\right) + \frac{1}{2}c\left(f_{j+1}^n - f_j^n\right) \\
&(\mathbf{2}) \qquad f_j^{n+1} = f_j^n + \frac{1}{2}c\left(f_{j+1/2}^* - f_{j-1/2}^*\right)
\end{aligned}$$

The first step is often addressed as auxiliary and f^* as auxiliary array for f. Note that instead of $j+1/2$ and $j-1/2$ on which the auxiliary array is defined one could just double the grid and compute the auxiliary values on the even grid indices and the actual f on the odd grid.

This two step Lax Wendroff has the same accuracy as the one step scheme and stability requires $c \leq 1$.

9.1.2 Crank-Nicholson scheme

As was the case for the diffusion equation the convection equation can be formulated in an implicit manner. Following the example of the diffusion equation the finite difference Crank-Nicholson scheme is given by

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

where $L_x = (-1, 0, 1)$ is the three point finite difference operator, i.e., $L_x f_j = \frac{1}{2\Delta x}\left(f_{j+1} - f_{j-1}\right)$. The above equation yields the following algebraic system

$$-\frac{1}{4}c f_{j-1}^{n+1} + f_j^{n+1} + \frac{1}{4}c f_{j+1}^{n+1} = \frac{1}{4}c f_{j-1}^n + f_j^n - \frac{1}{4}c f_{j+1}^n$$

The scheme is also second oder accurate and the amplification factor is

$$g = \frac{1 - i\frac{c}{2}\sin\left(k\Delta x/2\right)}{1 + i\frac{c}{2}\sin\left(k\Delta x/2\right)}$$

which demonstrates that this scheme is unconditionally stable.

Similar to the diffusion equation the crank-Nicholson approach can easily be extended to include the Galerkin linear finite element method.

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

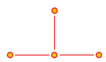
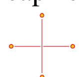
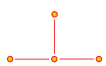
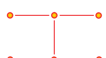
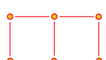
Using a general mass operator $M_x = (\delta, 1 - 2\delta, \delta)$the algebraic system becomes

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

Both the finite difference and the finite element CN schemes require the inversion of a banded tridiagonal matrix as was the case for the one-dimensional diffusion equation. As for the diffusion equation the advantage of a banded matrix is lost if the method is extended to two dimensions.

9.1.3 Summary of schemes for the one-dimensional convection equation

The following table provides an overview of various methods to solve the one-dimensional convection equation. Most properties are self explanatory. The most noteworthy differences to the diffusion equation is the fact that the FTCS scheme proves to be unstable for the convection equation.

Scheme	Algebraic equation	Truncation error	Ampl. factor g	Stability
FTCS 	$\frac{\Delta f_j^{n+1}}{\Delta t} = -uL_x f_j^n$	$E = \frac{1}{2} cu\Delta x \frac{\partial^2 f}{\partial x^2}$ $+u\frac{\Delta x^2}{6}\left(1+2c^2\right)\frac{\partial^3 f}{\partial x^3}$	$1 - ic\sin\Theta$	unstable
Upwind 	$\frac{\Delta f_j^{n+1}}{\Delta t} = -\frac{u}{\Delta x}\left(f_j^n - f_{j-1}^n\right)$	$E = -\frac{1}{2}(1-c)\,u\Delta x\frac{\partial^2 f}{\partial x^2}$ $+u\frac{\Delta x^2}{6}\left(1-3c+2c^2\right)\frac{\partial^3 f}{\partial x^3}$	$1 - c\,(1-\cos\Theta)\,ic\sin\Theta$	$c \leq 1$
Leapfrog 	$\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} = -uL_x f_j^n$	$E = u\frac{\Delta x^2}{6}\left(1-c^2\right)\frac{\partial^3 f}{\partial x^3}$	$ic\sin\Theta \pm \sqrt{1-c^2\sin^2\Theta}$	$c \leq 1$
Lax-Wendroff 	$\frac{\Delta f_j^{n+1}}{\Delta t} = -uL_x f_j^n + \frac{1}{2}uc\Delta x L_{xx} f_j^n$	$E = u\frac{\Delta x^2}{6}\left(1-c^2\right)\frac{\partial^3 f}{\partial x^3}$ $+uc\frac{\Delta x^3}{8}\left(1-c^2\right)\frac{\partial^4 f}{\partial x^4}$	$1 - ic\sin\Theta - 2c^2\sin^2(\Theta/2)$	$c \leq 1$
Crank-Nicholson 	$\frac{\Delta f_j^{n+1}}{\Delta t} = -\frac{u}{2}L_x\left(f_j^n + f_j^{n+1}\right)$	$E = u\frac{\Delta x^2}{6}\left(1+0.5c^2\right)\frac{\partial^3 f}{\partial x^3}$	$\frac{1-i0.5c\sin\Theta}{1+i0.5c\sin\Theta}$	none
FEM Crank-Nicholson 	$M_x\frac{\Delta f_j^{n+1}}{\Delta t} = -\frac{u}{2}L_x\left(f_j^n + f_j^{n+1}\right)$	$E = u\frac{\Delta x^2}{12}c^2\frac{\partial^3 f}{\partial x^3}$	$\frac{2+\cos\Theta - i1.5c\sin\Theta}{2+\cos\Theta + i1.5c\sin\Theta}$	none
Remarks	$c = \frac{u\Delta t}{\Delta x}$	$L_x = \frac{1}{2\Delta x}(-1,0,1)$ $L_{xx} = \frac{1}{\Delta x^2}(1,-2,1)$	$\Delta f_j^{n+1} = f_j^{n+1} - f_j^n$ $M_x = (1/6, 2/3, 1/6)$	

9.2 Numerical dispersion and dissipation

Central physical properties of the dynamics of many systems particularly of fluids and gases are dispersion and diffusion. Dispersion describes the properties of wave propagation, e.g., the phase and the group velocity of a sound wave of wave length λ. Note that the correct transport of waves is crucial because waves transport information, and physical properties such as mass, momentum, and energy. A closely associated property is diffusion. Diffusion in a physical system is equivalent to mixing but it also implies damping. Diffusion has different physical meanings depending on the quantity under consideration. Diffusion of the concentration or density of a substance is different from diffusion in velocity space. In the latter case the corresponding transport is called viscous and implies the loss of velocity structure and also the thermalization of directed motion. Finally diffusion of pressure or temperature implies the conduction of heat, i.e., energy transport without actual convection.

For the propagation of a wave dispersion determines the group and phases velocity of the wave whereas diffusion is associated with dissipation and damping of the wave. The effects can be expressed by the following expression for a perturbation

$$f(x,t) = f_0 \exp(-p(m)t)\exp(im(x-q(m)t)) \tag{9.1}$$

where m is the wavenumber ($= 2\pi/$wavelength), $p(m)$ describes damping, and $q(m)$ is the phase (or transport) velocity. Considering simple convection with constant velocity u we expect

$$\begin{aligned} p(m) &= 0 \\ q(m) &= u \end{aligned}$$

It is instructive to consider the following equations

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} - \alpha\frac{\partial^2 f}{\partial x^2} = 0 \tag{9.2}$$

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} + \beta\frac{\partial^3 f}{\partial x^3} = 0 \tag{9.3}$$

Substituting the plane wave approach (9.1) into the first of these equations yields the relations

$$p(m) = \alpha m^2 \quad , \quad q(m) = u$$

Thus it is seen that the effect of adding a diffusion term to the convection equation leads to damping of a perturbation with the damping rate of αm^2. Note that damping is strongest for the largest values of the wavenumber or the smallest wavelengths.

Substituting the plane wave approach (9.1) into the second equation (9.3) yields

$$p(m) = 0 \quad , \quad q(m) = u - \beta m^2$$

It is seen that the term with the third derivative added to the convection equation does not lead to damping but that it does alter the propagation speed of the perturbation. Even more important the propagation speed is now dependent on the wave number and it is lowered most for the largest wave numbers (smallest wavelength) in the system while it can be expected to be close to u for sufficiently small wave numbers or large wavelengths.

In conclusion both effects dispersion and diffusion are strongest for large wave numbers or small wavelengths. Note that the above considerations can be generalized in the sense that we can consider additional modifications of the convection equation with the result that

- all odd spatial derivative terms added to the convection equation introduce and modify dispersion
- all even derivative terms added to the convection equation introduce diffusion.

9.2.1 Fourier analysis

We can now employ this approach and conduct a Fourier analysis of the algebraic equations of a discretization. In general such a Fourier approach uses an expansion of the form

$$f(x,t) = \sum_k f_k \exp(ik(x - vt))$$

Note, k steps through wave number space, i.e., $k = 2\pi/\lambda_k$. In general v is complex such that we re-write this approach to separate imaginary and real part of the exponential

$$f(x,t) = \sum_k f_k \exp(-p(k)t) \exp(ik(x - q(k)t))$$

Substitution of this approach into a give discretization, e.g., upwind scheme yields for the amplification factor

$$g_k = \frac{f_k \exp(-p(k)(t+\Delta t)) \exp(ik(x - q(k)(t+\Delta t)))}{f_k \exp(-p(k)t) \exp(ik(x - q(k)t))}$$

or

$$g_k = \exp(-p(k)\Delta t) \exp(-ikq(k)\Delta t)$$

Since $|\exp(ikq(k)\Delta t)| = 1$ the absolution value of $g_k$is determined by the factor $\exp(-p(k)\Delta t)$ or

$$|g_k| = \exp(-p(k)\Delta t)$$

which can be solved for $p(k)$ to determine the diffusion for the respective scheme. Further the phase of g_k determines the dispersion.

Using the upwind scheme we have

$$g_k = 1 + c(\cos\Theta - 1) + ic\sin\Theta$$

where $\Theta = k\Delta x$. The phase of g_k is

$$\begin{aligned}\phi_k &= \tan^{-1}\frac{\operatorname{Im} g_k}{\operatorname{Re} g_k} = -kq(k)\Delta t \\ &= \tan^{-1}\frac{\sin\Theta}{1 + c(\cos\Theta - 1)}\end{aligned}$$

We can compare this to the exact phase which for constant velocity should be

$$\phi_{ex} = -ku\Delta t = -ck\Delta x$$

such that

$$\frac{\phi_k}{\phi_{ex}} = \frac{q(k)}{u} = -\frac{1}{ck\Delta x}\tan^{-1}\frac{c\sin\Theta}{1 + c(\cos\Theta - 1)}$$

Evaluating this expression yields for

$$\begin{aligned}&0 < c < 0.5 \qquad q(k) < u \ for\ k\Delta x \to \pi \\ &0.5 < c < 1 \qquad q(k) > u \ for\ k\Delta x \to \pi\end{aligned}$$

Example: Leapfrog

Amplification factor

$$g = ic\sin\Theta \pm \sqrt{1 - c^2\sin^2\Theta}$$

For $c \le 1$ => $|g| = 1$ such that $p = 0$ or $\alpha_{num} = 0$!

Phase:

$$\frac{q(k)}{u} = \frac{1}{ck\Delta x}\tan^{-1}\frac{c\sin\Theta}{\sqrt{1 - c^2\sin^2\Theta}}$$

Note that for small arguments of Θ and $c \leq 1$ we have sin $\approx$ tansuch that

$$\frac{q(k)}{u} \approx 1$$

Thus long wavelengths are transported with the phase velocity u as expected. The largest deviations from this correct transport occurs for short wavelength, i.e., large k.

For $\Theta = k\Delta x \approx \pi/2$ and $c \ll 1$ we obtain

$$\frac{q(k)}{u} \approx \frac{c}{c\pi/2} = \frac{2}{\pi}$$

For $\Theta = k\Delta x \approx \pi/2$ and $c \approx 1$ we obtain

$$\frac{q(k)}{u} \approx \frac{1}{c\pi/2}\frac{\pi}{2} = \frac{1}{c}$$

Summary remarks on numerical diffusion and dispersion

The prior section illustrates that a numerical approximation to the convection equation generally introduces numerical dispersion and diffusion. The amplification factor from the von Neumann stability analysis can be used to determine both of these effects. Here the amplitude of g is directly related to the numerical diffusion and the phase of the amplification factor can be used to determine the dispersion. It is worth noting that an amplification factor larger than 1 (implying instability) also implies that the numerical diffusion term is negative!

In general diffusion is caused or modified by even spatial derivatives added to the convection equation and dispersion to the odd derivatives. Since any finite difference or finite element scheme will generate higher order errors associated with even and odd derivative terms these errors in general contribute to numerical diffusion and numerical dispersion.

As a special case the high symmetry of the leapfrog method has the property that all truncation errors are due to odd derivative (all coefficients of even derivative terms are zero). Therefore the Leapfrog method has no diffusion. However, although this sounds attractive it actually poses a problem because with any diffusion the effects of dispersion can generate strong grid oscillations because wave with small wave lengths propagate different than longer wavelengths and the shortest wave length is determined by the grid spacing. Thus it is advisable to combine the leapfrog method with a diffusion term to counter the effects from dispersion.

Finally it should be noted that the insight into diffusion and dispersion can be used to correct the discussed methods by adding corrective terms which eliminate the dominant orders for diffusion and convection. This is basically equivalent to introducing higher (3rd or 4th) order methods.

9.3 One- and two-dimensional transport equations

A straightforward extension of the discussion on numerical schemes for the convection and diffusion equation is to consider a combined equation which we will address as a transport equation.

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} - \alpha\frac{\partial^2 f}{\partial x^2} = 0$$

Before discussing any discretization let us first look at properties of this equation. This is done like in the earlier example of the diffusion equation except that we will first consider the steady state transport equation

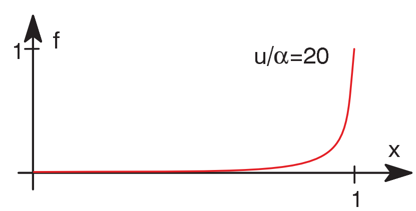
$$u\frac{\partial f}{\partial x} - \alpha\frac{\partial^2 f}{\partial x^2} = 0$$

and introduce a normalization (or scaling) of $x = L\tilde{x}$ such that after substitution the equation becomes

$$\frac{u}{L}\frac{\partial f}{\partial \tilde{x}} - \frac{\alpha}{L^2}\frac{\partial^2 f}{\partial \tilde{x}^2} = 0$$

Now we can look for the scaling where both the convection and the diffusion terms in the equation are of equal importance, i.e., $u/L = \alpha/L^2$ which yields $L_0 = \alpha/u$. Thus normalizing length scales to this length L would render both terms of equal importance. For length scales smaller than L_0 the diffusion term dominates while for length scales larger than L_0 the convection term dominates. The solution to the steady state problem with $f(0) = 0$ and $f(1) = 1$ show this 'boundary layer' characteristic for $L_0 = \alpha/u = 1/20$.

$$f(x) = \frac{\exp(ux/\alpha) - 1}{\exp(u/\alpha) - 1}$$



The cell Reynolds number is the number

$$R_{cell} = \frac{\Delta x}{L_0} = \frac{u\Delta x}{\alpha}$$

Since the numerical solution should resolves the relevant physics it is usually required that $\Delta x \le L_0$. Note that we can also re-write the cell Reynolds number as

$$R_{cell} = \frac{u}{\Delta x}\frac{\Delta x^2}{\alpha} = \frac{\tau_{\text{diff}}}{\tau_{\text{conv}}}$$

where $\tau_{\text{diff}} = \Delta x^2/\alpha$ is the diffusion time for a grid spacing (which we know already from the discussion of the diffusion equation) and $\tau_{\text{conv}} = \Delta x/u$ is the convection time over a grid spacing. An explicit method should resolve both the diffusion time (corresponding to the condition $s = \alpha\Delta t/\Delta x^2 \le 1$) and the convection time (corresponding to $c = u\Delta t/\Delta x \le 1$). Note that for actual fluid simulation u can represent a convection velocity or a typical wave speed.

9.3.1 Explicit schemes for the transport equation

FTCS method

In terms of a numerical scheme it would appear that the FTCS scheme is the simplest approach yielding

$$\frac{f_j^{n+1}-f_j^n}{\Delta t} = -\frac{u}{2\Delta_x}\left(f_{j+1}^n - f_{j-1}^n\right) + \frac{\alpha}{\Delta x^2}\left(f_{j-1}^n - 2f_j^n + f_{j+1}^n\right)$$

which gives an explicit equation for f_j^{n+1}

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

with $c = u\Delta t/\Delta x$ and $s = \alpha\Delta t/\Delta x^2$. The von Neumann stability analysis yields an amplification factor of

$$g = 1 - 2s\,(1-\cos\Theta) - ic\sin(\Theta)$$

with $\Theta = k\Delta x$ which requires

$$0 \le c^2 \le 2s \le 1$$

for stability. Note that although the FTCS method was unstable for the convection equation is is stable for this transport equation. However, another problem with the FTCS scheme is related to the truncation error. Expanding the algebraic equation in a Taylor series yields

$$\begin{aligned}\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} - \left(\alpha-\alpha'\right)\frac{\partial^2 f}{\partial x^2} - \left(\alpha u\Delta t + u^3\frac{\Delta t^2}{3} - u\frac{\Delta x^2}{6}\right)\frac{\partial^3 f}{\partial x^3} & \\ + \left(\frac{1}{2}\alpha^2\Delta t - \alpha u^2\Delta t^2 - \alpha\frac{\Delta x^2}{12} + \frac{1}{4}u^4\frac{\Delta t^3}{3} + u^2\frac{\Delta t\Delta x^2}{6}\right)\frac{\partial^3 f}{\partial x^3} &= 0\end{aligned}$$

with $\alpha' = u^2\Delta t/2$ which illustrates that the FTCS scheme modifies the diffusion term such that physical diffusion and numerical diffusion compete. For accuracy this scheme requires that

$$u^2\Delta t/2 \ll \alpha \quad \text{or} \quad c^2 \ll 2s$$

=> $R_{cell} = c/s \ll 2/c$

Upwind

Discretization:

$$\frac{\Delta f_j^{n+1}}{\Delta t} = -\frac{u}{\Delta x}\left(f_j^n - f_{j-1}^n\right) + \alpha L_{xx} f_j^n$$

which yields the equation for time level $n+1$

$$f_j^{n+1} = (s+c)\, f_{j-1}^n + (1-2s-c)\, f_j^n + s f_{j+1}^n$$

- First order accurate
- Numerical diffusion competes with physical diffusion
- Stability: $0 \leq c^2 \leq 2s \leq 1$
- Accuracy: $R_{cell} \ll 2/c$

DuFort-Frankel:

Discretization:

$$\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} = -u L_x f_j^n + \frac{\alpha}{\Delta x^2}\left(f_{j-1}^n - f_j^{n-1} - f_j^{n+1} + f_{j+1}^n\right)$$

Equation for time level $n+1$

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

Note that for very small values of s it may be of advantage to re-write this expresion as

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

- Numerical diffusion coefficient: αc^2
- Stability: $c \leq 1$; unconditional for s
- Accuracy: $c^2 \ll 1$

Lax-Wendroff:

Discretization:

$$\frac{\Delta f_j^{n+1}}{\Delta t} = -uL_x f_j^n + \alpha^* L_{xx} f_j^n$$

Equation for time level $n+1$

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

with $\alpha^* = \alpha + \frac{1}{2}uc\Delta x$

- Numerical diffusion: No 2nd order but 4th order diffusion
- Stability: $0 \le c^2 \le 2s^* \le 1$ with $s^* = \alpha^* \Delta t/\Delta x^2 = \left(\alpha + \frac{1}{2}uc\Delta x\right)\Delta t/\Delta x^2$
- Accuracy: $R_{cell} \le 2$ (to avoid spatial oscillations)

Modification of the 3pt centered difference through a four point upwind (asymmetric) approximation for $u > 0$. Using the general technique to expand

$$\frac{df}{dx} \approx af_{i-2} + bf_{i-1} + cf_i + df_{i+1}$$

yields

$$\begin{aligned} \frac{df}{dx} &= \frac{f_{i-2} - 6f_{i-1} + 3f_i + 2f_{i+1}}{6\Delta x} \\ &= \frac{f_{i+1} - f_{i-1}}{2\Delta x} + \frac{f_{i-2} - 3f_{i-1} + 3f_i - f_{i+1}}{6\Delta x} \end{aligned}$$

We can use this approximation by introducing a parameter q and separate the portion that represents the symmetric three point difference by defining the operator

$$L_x^{4+} f_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + q\frac{f_{i-2} - 3f_{i-1} + 3f_i - f_{i+1}}{3\Delta x}$$

Choosing $q = 0$ yields the usual 3 point difference approximation and increasing q from 0 to 0.5 switches the derivative to the 4 point upwind.

Note that for $u < 0$ the corresponding operator should read

$$L_x^{4-} f_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + q\frac{f_{i-1} - 3f_i + 3f_{i+1} - f_{i+2}}{3\Delta x}$$

A corresponding correction to the Lax-Wendroff algorithm is given by

$$\frac{\Delta f_j^{n+1}}{\Delta t} = -uL_x^{4+} f_j^n + \alpha^* L_{xx} f_j^n$$

for $u > 0$. The purpose of the introduction of the asymmetric upwind algorithm is an attempt to reduce the strong grid oscillations that occur for the symmetric operators.

The actual discretization ($u > 0$) in this case is

$$f_j^{n+1} = -\frac{qc}{3} f_{j-2}^n + \left(s^* + \frac{c}{2} + qc\right) f_{j-1}^n + (1 - 2s^* - qc) f_j^n + \left(s^* - \frac{c}{2} + \frac{qc}{3}\right) f_{j+1}^n$$

- with $s^* = \alpha^* \Delta t / \Delta x^2 = \left(\alpha + \frac{1}{2} uc\Delta x\right) \Delta t / \Delta x^2 = s + c^2/2$

Example of numerical constraints

Consider: $\alpha = 10^{-5}$, $u = 1$, and at least to start with $\Delta x = 0.1$.

- Diffusion: $s = \alpha \Delta t / \Delta x^2 \leq O(1)$ => $\Delta t \leq \Delta x^2 / \alpha = 10^5 \Delta x^2$
- Convection: $c = u\Delta t / \Delta x \leq 1$ => $\Delta t \leq \Delta x / u = \Delta x$
- Combined effect of diffusion and convection for accuracy:

$$R_{cell} = \frac{c}{s} = \frac{u\Delta x}{\alpha} \begin{cases} \ll 1 & first\,\mathrm{order\,(FTCS + Upwind)} \\ \leq O(1) & \mathrm{Lax - Wendroff} \end{cases}$$

=> $\Delta x \ll \alpha / u = 10^{-5}$ for FTCS and Upwind

=> $\Delta x \leq \alpha / u = 10^{-5}$ for Lax-Wendroff

- Leapfrog/Dufort-Frankel: $c^2 \ll 1$ => $\Delta t^2 \ll \Delta x^2 / u^2 = \Delta x^2 = 10^{-2}$
- Stability:
  - FTCS and Lax-Wendroff: $c^2 \leq 2s$ => $\Delta t \leq 2\alpha / u^2 = 2 \cdot 10^{-5}$
  - Leapfrog/Dufort-Frankel: $c \leq 1$ included in condition for accuracy
- Summary:
  - FTCS, Lax Wendroff: $\Delta t \leq O\left(10^{-5}\right)$; $\Delta x \leq O\left(10^{-5}\right)$
  - Leapfrog: Assume $\Delta x = 10^{-1}$ and $\Delta t = 10^{-2}$ (error in diffusion term $=10^{-2}$)

Assume final time = 100. Number of grid operations:

- FTCS and Lax Wendroff: 10^{12}
- Leapfrog: 10^5

9.3.2 Crank-Nicholson schemes

Discretization:

$$\frac{\Delta f_j^{n+1}}{\Delta t} = (\alpha L_{xx} - uL_x)\,\frac{f_j^n + f_j^{n+1}}{2}$$

Equation for time level $n+1$

$$-\frac{s+c}{2} f_{j-1}^{n+1} + (1+s)\,f_j^{n+1} - \frac{s-c}{2} f_{j+1}^{n+1} = \frac{s+c}{2} f_{j-1}^{n} + (1-s)\,f_j^{n} + \frac{s-c}{2} f_{j+1}^{n}$$

Consistency:

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} - \alpha\frac{\partial^2 f}{\partial x^2} + u\frac{\Delta x^2}{12}\left(2+c^2\right)\frac{\partial^3 f}{\partial x^3} - \alpha\frac{\Delta x^2}{12}\left(1+3c^2\right)\frac{\partial^4 f}{\partial x^4} = 0$$

- Accuracy: $O\left(\Delta t^2, \Delta x^2\right)$
- Unconditionally stable
- $R_{cell} \leq 2$for non-oscillatory solutions

Finite element Crank-Nicholson method:

$$M_x\frac{\Delta f_j^{n+1}}{\Delta t} = (\alpha L_{xx} - uL_x)\,\frac{f_j^n + f_j^{n+1}}{2}$$

Equation for time level $n+1$

$$\begin{aligned}\left(\delta - \frac{s}{2} - \frac{c}{4}\right) f_{j-1}^{n+1} + (1-2\delta+s)\,f_j^{n+1} + \left(\delta - \frac{s}{2} + \frac{c}{4}\right) f_{j+1}^{n+1} \quad &= \\ \left(\delta + \frac{s}{2} + \frac{c}{4}\right) f_{j-1}^{n} + (1-2\delta-s)\,f_j^{n} \quad &+ \quad \left(\delta + \frac{s}{2} - \frac{c}{4}\right) f_{j+1}^{n}\end{aligned}$$

with $\delta = 1/6$ for linear fem. With the generalized mass operator $M_x = (\delta, 1-2\delta, \delta)$ => consistency condition:

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} - \alpha\frac{\partial^2 f}{\partial x^2} + u\Delta x^2\left(\frac{1}{6} + \frac{c^2}{12} - \delta\right)\frac{\partial^3 f}{\partial x^3} - \alpha\Delta x^2\left(\frac{1}{12} + \frac{c^2}{4} - \delta\right)\frac{\partial^4 f}{\partial x^4} = 0$$

Dispersion (3rd order) $= 0$ for: $\delta = 1/6 + c^2/12$

- Unconditionally stable

- $R_{cell} \leq 2$for non-oscillatory solutions

Using the 4 point upwind instead of the center difference approximation (for $u > 0$)

$$L_x^{4+} f_i = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + q\frac{f_{i-2} - 3f_{i-1} + 3f_i - f_{i+1}}{3\Delta x}$$

generates the discretization:

$$\frac{qc}{6} f_{j-1}^{n+1} + \left(\delta - \frac{s}{2} - \frac{c}{4} - \frac{qc}{2}\right) f_{j-1}^{n+1} + \left(1 - 2\delta + s + \frac{qc}{2}\right) f_j^{n+1} + \left(\delta - \frac{s}{2} + \frac{c}{4} - \frac{qc}{6}\right) f_{j+1}^{n+1} = -\frac{qc}{6} f_{j-1}^{n} + \left(\delta + \frac{s}{2} + \frac{c}{4} + \frac{qc}{2}\right) f_{j-1}^{n} + \left(1 - 2\delta - s - \frac{qc}{2}\right) f_j^{n} + \left(\delta + \frac{s}{2} - \frac{c}{4} + \frac{qc}{6}\right)$$

Note that similar to the Leapfrog the convection term can be substituted by the 4 point upwind first derivative operator introduced in connection to the Lax-Wendroff method.

9.3.3 Implementation of the different methods

The explicte and implicit methods for the solution of the transport equation are impleneted in the program trans.f which can be found on the web page. Specifically the profram implements the upwind, the leapfrog/Dufort-Frankel, the Lax-Wendroff, and the Crank-Nicholson methods. The program also allows to use a mass operator with a variable choice of δ in the operator, and it allows to substitute the 4 point upwind discretization in the Lax-Wendroff and CN methods. The web page provides a readme file which is represented here for a brief summary of the program, associated files and parameters.

Program trans.f simulates the transport equation

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} - \alpha\frac{\partial^2 f}{\partial x^2} = 0$$

and as a special case with $\alpha = 0$ also the convection equation.

The fortran code require 3 files:

- trans.f - source code of the program
- transin - include fiel with parameter declarations
- trans1.dat - parameter file to select methods and parameters to run the program

Plotting: 2 idl programs

- tanim.pro - program to generate small animation from the output data. Execute this program once (.r tanim). To recycle the animation enter *xanimate, 2* at the idl prompt after running tanim. To obtain a smooth animation you may need to lower nout (in trans1.dat) and use a larger number of frames per second in xanimate: xanimate, 4

- trans.pro - program to plot (also in postscript) output from trans.f . The thick solid lines are the initial and the final solution. The thin solid line is the exact final solution. The dashed lines represent the intermediate solution. If there are to many or to few intermediate solution change the parameter nout accordingly.

The program implements 5 different methods:

- Upwind
- Leapfrog
- Lax-Wendroff
- FDM Crank-Nicholson
- FEM Crank-Nicholson

For the Lax-Wendroff and Crank-Nicholson methods a parameter q can switch between 3pt centered difference and 4pt upwind difference approx. where q (or quein trans1.dat) can be any value between $q = 0$ (=> 3pt diff) and $q = 0.5$ (=>4pt upwind). The generalized finite element Crank-Nicholson method is obtained through any non-zeror value of δ (delta in trans1.dat).

Parameters in trans1.dat:

ntmax - max number of integration steps

tmax - final time

xmin, xmax - boundaries in x

u - convection velocity

c - parameter c in convection equation

dt - time step

cordt - switch whether tiestepping is determined through c or directly through dt (note one of these is determined through the other if u and dx are fixed)

delta - mass operator weight for FEM method

que - switch for 3pt centered or 4 pt upwind difference approx

nout - number of integration steps between outputs

f0 - normalization of f

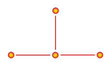
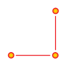
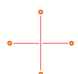
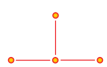
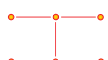
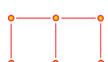
init - chooses initial condition between truncated sine wave (1), sine wave (2), or rectangular pulse (3)

lambda - wavelength or pulse size

fb(i) - boundary value at xmin and xmax

maxex - number of modes in the exact solution.

Summary of schemes for the one-dimensional transport equation:

Scheme	Algebraic equation	Truncation error	Ampl. factor g	Stab. & Accur.
FTCS 	$\frac{\Delta f_j^{n+1}}{\Delta t} = -uL_x f_j^n - \alpha L_{xx} f_j^k$	$\frac{1}{2} c u \Delta x \frac{\partial^2 f}{\partial x^2} - \left[c \alpha \Delta x \right.$ $\left. -u \frac{\Delta x^2}{6} \left(1 + 2c^2\right) \right] \frac{\partial^3 f}{\partial x^3}$	$1 - 2s\left(1 - \cos\Theta\right)$ $-ic\sin\Theta$	$0 \leq c^2 \leq 2s \leq 1$ Acc: $R_{cell} \ll 2/c$
Upwind 	$\frac{\Delta f_j^{n+1}}{\Delta t} = -\frac{u}{\Delta x}\left(f_j^n - f_{j-1}^n\right)$ $-\alpha L_{xx} f_j^n$	$-\frac{1}{2}\left(1-c\right) u \Delta x \frac{\partial^2 f}{\partial x^2} - \left[c \alpha \Delta x \right.$ $\left. -u \frac{\Delta x^2}{6} \left(1 - 3c + 2c^2\right) \right] \frac{\partial^3 f}{\partial x^3}$	$1 - \left(2s + c\right)\left(1 - \cos\Theta\right)$ $-ic\sin\Theta$	$c + 2s \leq 1$ Acc: $R_{cell} \ll 2/\left(1 - c\right)$
DuFort-Frankel  Leapfrog	$\frac{f_j^{n+1} - f_j^{n-1}}{2\Delta t} = -uL_x f_j^n$ $+\frac{\alpha}{\Delta x^2}\left(f_{j-1}^n - f_j^{n-1} - f_j^{n+1} + f_{j+1}^n\right)$	$\alpha c^2 \frac{\partial^2 f}{\partial x^2} + \left(1 - c^2\right) \cdot$ $\left(u\frac{\Delta x^2}{6} - 2\alpha^2 c^2/u\right) \frac{\partial^3 f}{\partial x^3}$	$\frac{b \pm \sqrt{b^2 - 8s(1+2s)}}{2+4s}$ $b = 1 + 4s\cos\Theta - 2ic\sin\Theta$	$c \leq 1$ $c^2 \ll 1$
Lax-Wendroff 	$\frac{\Delta f_j^{n+1}}{\Delta t} = -uL_x f_j^n + \alpha^* L_{xx} f_j^n$ $\alpha^* = \alpha + \frac{1}{2} u c \Delta x$	$-\left(c\alpha\Delta x - u\frac{\Delta x^2}{6}\right)\left(1 - c^2\right)\frac{\partial^3 f}{\partial x^3}$ $+\left[c\frac{\alpha^2}{u}\frac{\Delta x}{2} - \alpha\frac{\Delta x^2}{12}\right.$ $+uc\frac{\Delta x^3}{8}\left(1 - c^2\right)\frac{\partial^4 f}{\partial x^4}$	$1 - 4s^* \sin^2\left(\Theta/2\right) - ic\sin\Theta$ $s^* = \alpha * \Delta t/\Delta x^2$	$0 \leq c^2 \leq 2s* \leq 1$ Acc: $R_{cell} \leq 2$
Crank-Nicholson 	$\frac{\Delta f_j^{n+1}}{\Delta t} = \left(\alpha L_{xx} - uL_x\right)\frac{f_j^n + f_j^{n+1}}{2}$	$u\frac{\Delta x^2}{12}\left(2 + c^2\right)\frac{\partial^3 f}{\partial x^3}$ $-\alpha\frac{\Delta x^2}{12}\left(1 + 3c^2\right)\frac{\partial^4 f}{\partial x^4}$	$\frac{1 - s(1-\cos\Theta) - i0.5c\sin\Theta}{1 + s(1-\cos\Theta) + i0.5c\sin\Theta}$	none Acc: $R_{cell} \leq 2$
FEM Crank-N. 	$M_x \frac{\Delta f_j^{n+1}}{\Delta t} =$ $\left(\alpha L_{xx} - uL_x\right)\frac{f_j^n + f_j^{n+1}}{2}$	$uc^2 \frac{\Delta x^2}{12} \frac{\partial^3 f}{\partial x^3}$ $+\alpha\frac{\Delta x^2}{12}\left(1 - 3c^2\right)\frac{\partial^4 f}{\partial x^4}$	$\frac{2 + 3\cos\Theta - 3s(1-\cos\Theta) - i1.5c\sin\Theta}{2 + 3\cos\Theta + 3s(1-\cos\Theta) + i1.5c\sin\Theta}$	none Acc: $R_{cell} \leq 2$
Remarks	$c = \frac{u\Delta t}{\Delta x}$ $s = \frac{\alpha \Delta t}{\Delta x^2}$	$L_x = \frac{1}{2\Delta x}\left(-1, 0, 1\right)$ $L_{xx} = \frac{1}{\Delta x^2}\left(1, -2, 1\right)$	$\Delta f_j^{n+1} = f_j^{n+1} - f_j^n$ $M_x = \left(1/6, 2/3, 1/6\right)$	$R_{cell} = \frac{c}{s} = \frac{u\Delta x}{\alpha}$

9.3.4 Two-dimensional transport

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} + v\frac{\partial f}{\partial y} - \alpha_x \frac{\partial^2 f}{\partial x^2} - \alpha_y \frac{\partial^2 f}{\partial y^2} = 0$$

Explicit schemes

Similar to one dimension, e.g.

FTCS:

$$\frac{\Delta f_{jk}^{n+1}}{\Delta t} = (\alpha_x L_{xx} - uL_x) f_{jk}^n + (\alpha_y L_{yy} - vL_y) f_{jk}^n$$

Conditions for stability:

$$\begin{aligned} s_x + s_y &\leq 1/2 \\ c_x^2/s_x + c_y^2/s_y &\leq 2 \end{aligned}$$

Note: Severe diffusion for 1st order schemes.

Implicit methods

Advantage: no stability restriction

Disadvantage: Efficiency

Example FDM Crank-Nicholson:

$$\frac{\Delta f_{jk}^{n+1}}{\Delta t} = (\alpha_x L_{xx} - uL_x) \frac{f_{jk}^n + f_{jk}^{n+1}}{2} + (\alpha_y L_{yy} - vL_y) \frac{f_{jk}^n + f_{jk}^{n+1}}{2}$$

Extension to FEM Crank-Nicholson:

$$M_x \otimes M_y \left[\frac{\partial f}{\partial t}\right]_{jk} = (-uM_y \otimes L_x - vM_x \otimes L_y + \alpha_x M_y \otimes L_{xx} + \alpha_y M_x \otimes L_{yy}) \frac{f_{jk}^n + f_{jk}^{n+1}}{2}$$

Here, L_x, L_{xx}, M_x, etc as before, e.g., $M_x = (\delta, 1-2\delta, \delta)$ with $\delta = 1/6$ for linear fem.

Solution: Same as for the diffusion equation -> splitting scheme (ADI) to solve first for index j and then for index k.

Cross-stream diffusion

Cross-stream diffusion is a potential issue if the convective derivative is only 1st order accurate and flow is not aligned with one of the coordinate axes. Consider the two-dimensional steady state transport equation

$$u\frac{\partial f}{\partial x}+v\frac{\partial f}{\partial y}-\alpha\frac{\partial^2 f}{\partial x^2}-\alpha\frac{\partial^2 f}{\partial y^2}=0$$

the upwind method for the 1st derivatives and the 3 point centered approximation for the 2nd derivatives. The first order accuracy of the 1st derivative approximations leads to the modified equation

$$\begin{aligned} u\frac{\partial f}{\partial x}+v\frac{\partial f}{\partial y}-\left(\alpha-\alpha'_x\right)\frac{\partial^2 f}{\partial x^2}-\left(\alpha-\alpha'_y\right)\frac{\partial^2 f}{\partial y^2} &= 0 \\ with\ \ \alpha'_x=\frac{1}{2}u\Delta_x,\ \ \alpha'_y=\frac{1}{2}v\Delta_y \end{aligned}$$

Now let us assume the flow is not aligned with one of the coordinate axes but inclined by an angle of δ with $u=h\cos\delta$ and $v=h\sin\delta$ with the flow magnitude h. Introducing the coordinates s along the flow and n normal to the flow the transport equation transforms into

$$h\frac{\partial f}{\partial s}-\alpha\left(\frac{\partial^2 f}{\partial s^2}-\frac{\partial^2 f}{\partial n^2}\right)-\alpha'_s\frac{\partial^2 f}{\partial s^2}-\alpha'_{sn}\frac{\partial^2 f}{\partial s\partial n}-\alpha'_n\frac{\partial^2 f}{\partial n^2}=0$$

with

$$\begin{aligned} \alpha'_s &= \frac{1}{2}h\left(\Delta_x\cos^3\delta+\Delta_y\sin^3\delta\right) \\ \alpha'_{sn} &= \frac{1}{2}h\left(-\Delta_x\cos\delta+\Delta_y\sin\delta\right)\sin 2\delta \\ \alpha'_n &= \frac{1}{2}h\left(\Delta_x\cos\delta\sin^2\delta+\Delta_y\sin\delta\cos^2\delta\right) \end{aligned}$$

For uniform grid spacing $\Delta_y=\Delta_x$, the streamwise diffusion coefficient α'_s maximizes for $\delta=0°,90°$and has a minimimum at $\delta=45°$. Vice versa the cross-stream diffusion coefficient maximizes at $\delta=45°$ and is 0 for $\delta=0°,90°$. Often streamwise diffusion is less important because boundary layer flow develops strong gradient across the flow. However, cross-stream diffusion is not present if the flow is aligned with the x or y direction (because the diffusion coefficient is partly caused by the flow)!

Concluding remarks

Advective equations introduce the aspect of transport of information. This is already implicit and consistent with the hyperbolic character of the equations. The transport can occur in a variety of ways, as waves such as sound waves, or through transport of substance. In a more physical sense this also implies the transport of material, momentum, and/or energy. An inherent aspect of this transport is dispersion, i.e., the property that the speed of this transport depends on the the wave length (or structure). Clearly the proper description of this tranport requires a more rigorous model of the relevant physics which adds complexity. However the simple transport equation allows us to shed light on the influence of the numerical approximation on the transport.

The chapter has introduced the simple advection equation and the transport equation as a model to examine the influence of the numerical approximation. We have seen that the aspects of numerical diffusion and dispersion are of major importance for the accuracy of the transport and the limitations of the model. Specifically it was seen that first order accurate convection approximation introduce strong numerical diffusion which requires high resolution to miinimize these effects. A much better approximation uses at least 2nd order accurate schems which eliminate the dominant diffusion terms. However, it was also illustrated that thes methods introduce numerical dispersion with the effect that the numerical scheme alters the speed of the transport in particular for small wave lengths or high wave numbers. To compensate for this non-desired effect some diffusion may be need to damp grid oscillations which arise through the dispersion effects barticularly if strucure is not well resolved by the grid, i.e., if there are large gradients on the grid scale. Possibly the best approach might be to use 3rd order methods where the dominant error is 4th order diffusion. This reduces damping to the smallest grid scales and can be expected to dominate 5th order dispersion. Note, however, that this generates more complexity in the discretization of a complex set of basic equations and introduces also additional complexity for boundary conditions because more then a single set of boundary layer points are needed for the mathematical boundary.

9.4 Nonlinear transport

An important aspect of transport is nonlinearity. The best example for such nonlinearity is through the momentum equation of a fluid for instance in the form of Eulers equation or the Navier Stokes equation. A simple equivalent of this is Burgers equation, which contains the nonlinearity in the $u\partial u/\partial x$ term and includes a simple viscous term.

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \nu\frac{\partial^2 u}{\partial x^2} = 0$$

The the most important aspect of this nonlinearity is the aspect of wave steepening and breaking. This process is present in many physical systems. A good example is the breaking of surface waves in the shallow waters of a beach. The physics behind this wave breaking is the dependence of the wave propagation speed on the depth of the water. In deep water the wave velocity is very large and it decreases with decreasing depth of the water. Since the water is deeper for the top of the waves, these move slightly faster then the bottom of the waves. This process leads to increasing steepening of the waves as they approch the beach. A dramatic realization of this mechanism are Tsunamis where the wave travels very fast on the open ocean (with a rather small amplitude). It slows down much approaching the shallow waters of a beach and increases much in amplitude (because the energy transported is reasonably conserved). The same process exists for many other types of waves. For instance, for sound waves the speed depends on the temperature of a gas. However, the temperature is slightly enhanced in the wave region where the medium is compressed (because the pressure increase scales with a factor of γ relative to the density increase $\delta p = \gamma \delta n$). Thus compression regions in a wave travel minutely faster then expansion regions leading again to wave steepening. Note that this does not usual generate shock because of two other aspects. Sound waves expand in a three-dimensional space thereby loosing rapidly amplitude because the wave energy is distributed over and increasing area. Also, viscosity of the medium can cause damping of a wave and viscosity due to atmospheric turbulence has length scales which agree reasonably with the audible spectrum of soundwaves. The Figure below illustrates the process of wave steepening in the inviscid case (left and the case for viscous damping.

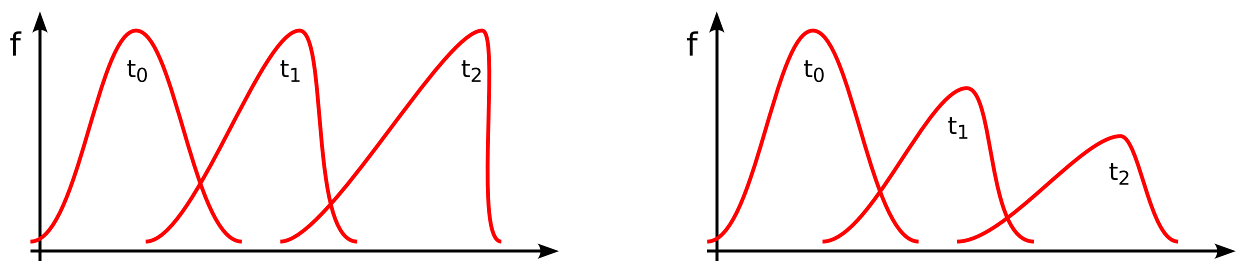


Figure 9.3: Wave breaking in the inviscid case (left and for a visous medium (right).

Note that the process of wave steepening for Burger's equation is similar to that of sound waves or surface water waves. The nonlinearity prpagates a region with larger amplitude of u faster than region with smaller values of u. The viscosity acts basically like a diffusion terms and thereby reduces the amplitude of a signal.

Burger's equation can be written in a conservative form

$$\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} = 0 \qquad (9.4)$$
$$\text{with} \qquad F = \frac{1}{2}u^2$$

which is typically beneficial to numerical discretization. Nonlinearity:

- rapid growth in spectrum of small wavelengths λ.
- energy associated with $\lambda \leq 2\Delta x$ re-appears in longer waves (conservative schemes) - aliasing

=> distortion + instability

Dissipation attenuates short wave length or high wavenumber modes.

9.4.1 Explicit schemes

FTCS:

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}+\frac{1}{2\Delta_x}\left\{\begin{array}{c} u_j^n\left(u_{j+1}^n-u_{j-1}^n\right) \\ F_{j+1}^n-F_{j-1}^n \end{array}\right\}-\frac{\nu}{\Delta x^2}\left(u_{j-1}^n-2u_j^n+u_{j+1}^n\right)=0$$

with $F=u^2/2$. Properties similar to tranport equation: 1st order accurate => large numerical dissipation competing with physical viscosity. Stability requires numerical dissipation to be smaller than numerical dissipation. Note that stability analysis requires to linearize Burgers equation.

Upwind:

A potential improvement is the substitution of convection term with a 4 point upwind approximation:

$$L_x^{(4)}F_j=\frac{1}{\Delta_x}\left(F_{j+1}-F_{j-1}\right)+\frac{q}{3\Delta_x}\left(F_{j-2}-3F_{j-1}+3F_j-F_{j+1}\right)$$

Truncation error is $O\left(\Delta_x^2\right)$ for all q except for $q=1/2$ when it is $O\left(\Delta_x^3\right)$.

Lax Wendroff: Let us first consider the inviscid case: $\partial u/\partial t+\partial F/\partial x=0$. Here the Lax-Wendroff schem should read:

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}+\frac{1}{2\Delta_x}\left(F_{j+1}^n-F_{j-1}^n\right)+T_?=0$$

where a term $T_?$ is added to eliminate the first order error. The Taylor expansion of the above equation yields

$$\frac{\partial u}{\partial t}+\frac{1}{2}\frac{\partial^2 u}{\partial t^2}\Delta t+..+\frac{\partial F}{\partial x}+O\left(\Delta_x^2\right)=0$$

where the 2nd term can be re-written as

$$\frac{\partial}{\partial t}\frac{\partial u}{\partial t}=\frac{\partial}{\partial t}\left(-\frac{\partial F}{\partial x}\right)=-\frac{\partial}{\partial x}\frac{\partial F}{\partial t}=-\frac{\partial}{\partial x}u\frac{\partial u}{\partial t}=\frac{\partial}{\partial x}u\frac{\partial F}{\partial x}$$

such that we can correct for the first order error by subtracting a sufficiently accurate (centered approximation of the term on the right of the last equation which yields

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}+\frac{1}{2\Delta_x}\left(F_{j+1}^n-F_{j-1}^n\right)-\frac{\Delta t}{2\Delta_x^2}\left[u_{j+1/2}\left(F_{j+1}^n-F_j^n\right)-u_{j-1/2}\left(F_j^n-F_{j-1}^n\right)\right]=0$$

For the case of simple nonlinear equation this is a reasonable approximation but for the full set of fluid equation F takes a more complicated form. In this case the most efficient implementation is a two step algorithm:

$$\begin{aligned} u^*_{j+1/2} &= \frac{1}{2}\left(u^n_j + u^n_{j+1}\right) - \frac{\Delta t}{2\Delta_x}\left(F^n_{j+1} - F^n_j\right) \\ u^{n+1}_j &= u^n_j - \frac{\Delta t}{\Delta_x}\left(F^*_{j+1/2} - F^*_{j-1/2}\right) \end{aligned}$$

For the full equation including the viscous term the corresponding two step scheme is

$$\begin{aligned} u^*_{j+1/2} &= \frac{1}{2}\left(u^n_j + u^n_{j+1}\right) - \frac{\Delta t}{2\Delta_x}\left(F^n_{j+1} - F^n_j\right) \\ &\quad + \frac{s}{4}\left[\left(u^n_{j-1} - 2u^n_j + u^n_{j+1}\right) + \left(u^n_j - 2u^n_{j+1} + u^n_{j+2}\right)\right] \\ u^{n+1}_j &= u^n_j - \frac{\Delta t}{\Delta_x}\left(F^*_{j+1/2} - F^*_{j-1/2}\right) + s\left(u^n_{j-1} - 2u^n_j + u^n_{j+1}\right) \end{aligned}$$

The stability constraint for this system is

$$\Delta t\left(u^2\Delta t + 2\nu\right) \le \Delta x^2$$

9.4.2 Implicit Methods

Formally it appears straightforward to cast Burgers equation (9.4) into a Crank-Nicholson formulation

$$\frac{\Delta u^{n+1}_j}{\Delta t} = -\frac{1}{2}L_x\left(F^n_j + F^{n+1}_j\right) + \frac{\nu}{2}L_{xx}\left(u^n_j + u^{n+1}_j\right)$$

with the usual definitions of the centered derivative operators L_x and L_{xx}. However, the nonlinear term F^{n+1}_j now poses a problem because it requires an implicit solution for u^{n+1} . This problem is addressed through linearization which through

$$F^{n+1}_j = F^n_j + \frac{\partial F}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 F}{\partial t^2}\Delta t + .. = F^n_j + \Delta t u\frac{\Delta u}{\Delta t} + ..$$

or $F^n_j + F^{n+1}_j = 2F^n_j + u^n_j\left(u^{n+1}_j - u^n_j\right) = u^n_j u^{n+1}_j$. Note that we obtain the same from

$$\frac{1}{2}\left(u^n_j\right)^2 + \frac{1}{2}\left(u^{n+1}_j\right)^2 = u^n_j u^{n+1}_j + \left(\Delta u^{n+1}_j\right)^2$$

with $\Delta u^{n+1}_j = u^{n+1}_j - u^n_j$ i.e., straightforward linearization. Thus the CN discretization becomes

$$u^{n+1}_j + \frac{1}{2}\Delta t L_x\left(u^n_j u^{n+1}_j\right) - \frac{1}{2}\nu\Delta t L_{xx} u^{n+1}_j = u^n_j - \frac{1}{2}\nu\Delta t L_{xx} u^n_j$$

or for the FEM CN method

$$M_x u_j^{n+1} + \frac{1}{2}\Delta t L_x \left(u_j^n u_j^{n+1}\right) - \frac{1}{2}\nu\Delta t L_{xx} u_j^{n+1} = M_x u_j^n - \frac{1}{2}\nu\Delta t L_{xx} u_j^n$$

This discretization leads to a tridiagonal matrix with coefficients

$$\begin{aligned}
c_{j,j-1} &= \delta - \frac{\Delta t}{4\Delta x} u_{j-1}^n - \frac{s}{2} \\
c_{j,j} &= 1 - 2\delta + s \\
c_{j,j+1} &= \delta + \frac{\Delta t}{4\Delta x} u_{j-1}^n - \frac{s}{2} \\
d_j &= \left(\frac{s}{2} + \delta\right) u_{j-1}^n + (1 - s - 2\delta) u_j^n + \left(\frac{s}{2} + \delta\right) u_{j+1}^n
\end{aligned}$$

and the system of equations to solve is $\sum_j c_{jk} u_k = d_j$ or

$$c_{j,j-1} u_{j-1}^n + c_{j,j} u_j^n + c_{j,j+1} u_{j+1}^n = d_j$$

Notes:

Instead uf the center first derivative we can alos use the 4th order upwind step. In this case we have

$$M_x u_j^{n+1} + \frac{1}{2}\Delta t L_x^{4+} \left(u_j^n u_j^{n+1}\right) - \frac{1}{2}\nu\Delta t L_{xx} u_j^{n+1} = M_x u_j^n - \frac{1}{2}\nu\Delta t L_{xx} u_j^n$$

with

$$L_x^{(4)} F_j = \frac{1}{2\Delta_x}\left(F_{j+1} - F_{j-1}\right) + \frac{q}{3\Delta_x}\left(F_{j-2} - 3F_{j-1} + 3F_j - F_{j+1}\right)$$

which alters the matrix to a quadridiagonal one and the coefficients to

$$\begin{aligned}
c_{j,j-2} &= q\frac{\Delta t}{6\Delta x} u_{j-2}^n \\
c_{j,j-1} &= \delta - \left(\frac{1}{4} + \frac{q}{2}\right)\frac{\Delta t}{4\Delta x} u_{j-1}^n - \frac{s}{2} \\
c_{j,j} &= 1 - 2\delta + q\frac{\Delta t}{2\Delta x} u_{j-2}^n + s \\
c_{j,j+1} &= \delta + \left(\frac{1}{4} - \frac{q}{6}\right)\frac{\Delta t}{\Delta x} u_{j-1}^n - \frac{s}{2} \\
d_j &= \left(\frac{s}{2} + \delta\right) u_{j-1}^n + (1 - s - 2\delta) u_j^n + \left(\frac{s}{2} + \delta\right) u_{j+1}^n
\end{aligned}$$

In this case the matrix first has to be reduced to tridiagonal form before using the standart Thomas algorithm for the solution.

9.4.3 Implementation of Burgers equation

The equation is similar to the linear transport equation and is implemented in the nonlinear version of trans.f which can be found on the web page. Most parameters are the same or similar to the linear version of the transport code. The program allows for 3 different initial conditions. Note that only the wave and the localized perturbation (truncated wave) are compatible with periodic boundary conditions. The step function initial condition requires Dirichlet or von Neumann conditions. For this condition the initial state is given by

$$u_0(x) = u(x,0) = \begin{cases} 1 & for\ x \leq 0 \\ 0 & for\ x > 0 \end{cases}$$

with corresponding Dirichlet boundary conditions. An exact solution for the equation is

$$\begin{aligned} u &= \frac{\int_{-\infty}^{\infty} \frac{x-\xi}{t} \exp\left[-RG(\xi,x,t)\, d\xi\right]}{\int_{-\infty}^{\infty} \exp\left[-RG(\xi,x,t)\, d\xi\right]} \\ G(\xi,x,t) &= \int^{\infty} u\left(\xi'\right) d\xi' \\ R &= 1/\nu \end{aligned}$$

Note that for the actual implementation not much changes for the upwind, leapfrog, and Lax-Wendroff methods. However, The Crank-Nicholson method changes due to the nonlinear nature of the problem which alters the method of the implicit solution as pointed out in the prior subsevtion. Addition of artificial dissipation term $0.5\nu_a \Delta t L_{xx}\left(F_j^n + F_j^{n+1}\right)$. Treating the nonlinearity the same way as before yields for the FEM CN method

$$M_x u_j^{n+1} + \frac{1}{2}\Delta t\left[L_x^{4+}\left(u_j^n u_j^{n+1}\right) - \nu L_{xx} u_j^{n+1} - \nu_a \Delta t L_{xx}\left(u_j^n u_j^{n+1}\right)\right] = M_x u_j^n - \frac{1}{2}\nu \Delta t L_{xx} u_j^n$$

9.5 Systems of Equations

As outlined in the introduction section on physical models, typically we have to solve system of equations for reasonably realistic models. In the case of fluid dynamics this set can be formulated as

$$\frac{\partial \mathbf{q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = 0$$

$$With\ \mathbf{q} = \left\{ \begin{array}{c} \rho \\ \rho u \\ \frac{p}{\gamma-1} + \frac{1}{2}\rho u^2 \end{array} \right\} \qquad \mathbf{F} = \left\{ \begin{array}{c} \rho u \\ \rho u^2 + p \\ \left(\frac{\gamma p}{\gamma-1} + \frac{1}{2}\rho u^2\right) u \end{array} \right\}$$

More generally in multi-dimensions

$$\frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \underline{\underline{\mathbf{F}}} = 0$$

where **F** becomes a 3x5 matrix because of the 3 cartesian directions and because of 5 dependent variables (note that velocity has 3 components). More generally, the equations of magnetohydrodynamics can be cast into a similar form where an additional set of equations for the magnetic field is included. The form of the equations above imply local conservation of mass, momentum and energy. They therefore also require that the system described by these equations is closed in the sense that rhs accounts for all mass, momentum, and energy density. If there is a second species of matter with which the material represented by ρ interacts, further equations and interaction terms are required for closure.

The example does not include dissipative terms but such terms can beadded in a conservative formulation, for instance by adding diffusion, e.g., a term $-\alpha\partial\rho/\partial x$ to the first term in **F**.

Some of the most straightforward discretizations of this set of equations is through the leapfrog

$$\mathbf{q}_j^{n+1} = \mathbf{q}_j^{n-1} - \frac{\Delta t}{2\Delta_x}\left(\mathbf{F}_{j+1}^n - \mathbf{F}_{j-1}^n\right) \tag{9.5}$$

or the Lax-Wendroff schemes

$$\begin{aligned} \mathbf{q}_{j+1/2}^{*} &= \frac{1}{2}\left(\mathbf{q}_j^n + \mathbf{q}_{j+1}^n\right) - \frac{\Delta t}{2\Delta_x}\left(\mathbf{F}_{j+1}^n - \mathbf{F}_j^n\right) \\ \mathbf{q}_j^{n+1} &= \mathbf{q}_j^n - \frac{\Delta t}{\Delta_x}\left(\mathbf{F}_{j+1/2}^{*} - \mathbf{F}_{j-1/2}^{*}\right) \end{aligned} \tag{9.6}$$

Both are second order accurate. Note that any dissipative terms on the rhs involve second derivative terms and should be treated in the manner descriped in the nonlinear transport for the Lax-Wendroff or using the Du-Fort-Frankel discretization for the Leapfrog method. Note also that the order of the rhs discretization can be increased through the third order upwind (4 point) method as illustrated before.

For implicit schemes the Crank-Nicholson is formally

$$\mathbf{q}_j^{n+1} - \mathbf{q}_j^n = -\frac{\Delta t}{4\Delta_x}\left[\left(\mathbf{F}_{j+1}^n - \mathbf{F}_{j-1}^n\right) + \left(\mathbf{F}_{j+1}^{n+1} - \mathbf{F}_{j-1}^{n+1}\right)\right]$$

The issue here as in the prior example of Burgers equation is the nonlinearity which is similarly resolved by linearization

$$\begin{aligned} \mathbf{F}^{n+1} &= \mathbf{F}^n + \underline{\underline{\mathbf{A}}} \cdot \Delta \mathbf{q}^{n+1} \\ \underline{\underline{\mathbf{A}}} &= \partial \mathbf{F}/\partial \mathbf{q} \end{aligned}$$

which generates

$$-\frac{\Delta t}{4\Delta_x}\underline{\underline{\mathbf{A}}}_{j-1}\cdot\Delta\mathbf{q}_{j-1}^{n+1}+\underline{\underline{1}}\cdot\Delta\mathbf{q}_{j-1}^{n+1}+\frac{\Delta t}{4\Delta_x}\underline{\underline{\mathbf{A}}}_{j-1}\cdot\Delta\mathbf{q}_{j+1}^{n+1}=-\frac{\Delta t}{4\Delta_x}\left[\left(\mathbf{F}_{j+1}^{n}-\mathbf{F}_{j-1}^{n}\right)\right]$$

This discretization represents a block tridiagonal system which can be solved in a fairly efficient manner by a generalized Thomas algorithm.

Stability:

$$\frac{\partial\mathbf{q}}{\partial t}+\frac{\partial\mathbf{F}}{\partial x}=0$$

Neumann Method is only applicable to linear systems of equations. Therefore the above system has to be linearized

$$\begin{aligned}\frac{\partial\mathbf{q}}{\partial t} &= \underline{\underline{\mathbf{A}}}\cdot\Delta\frac{\partial\mathbf{q}}{\partial t}\\ \underline{\underline{\mathbf{A}}} &= \partial\mathbf{F}/\partial\mathbf{q}\end{aligned}$$

For all components the discretization will generate a system of equations which relate $\mathbf{q}_j^{n+1}$ to $\mathbf{q}_j^n$ in a form

$$\mathbf{q}_j^{n+1}=\underline{\underline{\mathbf{G}}}\cdot\mathbf{q}_j^n$$

where $\underline{\underline{\mathbf{G}}}$ maps $\mathbf{q}_j^n$ to $\mathbf{q}_j^{n+1}$. Any amplification of one of the components of $\mathbf{q}_j$ corresponds to exponential growth. More precisely any amplification in the system of equation has an equivalent eigenvector component. Transforming the above system into the Eigenvector coordinate system implies that instability is present if any Eigenvalue λ_i of $\underline{\underline{\mathbf{G}}}$ has a magnitude larger then 1.

For instance for the Crank-Nicholson system the $\underline{\underline{\mathbf{G}}}$ is given by

$$\underline{\underline{\mathbf{G}}}=\left(\underline{\underline{1}}+\frac{i\Delta t}{2\Delta_x}\underline{\underline{\mathbf{A}}}\sin\theta\right)^{-1}\left(\underline{\underline{1}}+\frac{i\Delta t}{2\Delta_x}\underline{\underline{\mathbf{A}}}\sin\theta\right)^{1}$$

Stability regquires for all $|\lambda_i|\leq 1$.

General remarks regarding stability: Difficult issue in particular in nonhomogeneous system. Linearization even for a 1D equilibrium usually requires the solution of a higher order complicated differential euation. In addition there may be physical instabilities which would also be present in this numerical stability analysis (provided the method is appropriate for the problem) such that in addition to a demanding analytic solution one would have to distinguish between numerical and physical instability. Usually stability analysis is conduncted for homogeneous systems for these reasons. It is alo often sufficient to understand the maximum velocity for information transport, which in cases with flow would be the fastest wave speed c_{max} added to the maximum convective velocity v_{max}, such that the stability limit for information transport in a complex system is

$\Delta t \leq \Delta x / |c_{max} + v_{max}|$. Note that this represents only the time step limitation for the hyperbolic part of the system. If diffusion is present there are additional requirements (as discussed for the simple case of the FTCS scheme) and depending on the treatment of a diffusion or viscous term the limitation could be more severe. A similar additional limitation applies if source terms are present for the equations under consideration. For instance in a case where material is produced the production ration could be expressed through

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = \nu_s (\rho_s - \rho)$$

This equation could represent ionization, recombination, or chemical production rates. Typically for an explicit scheme $\nu_s \Delta t \leq 1$.

Finally it should be noted that the stability limitations for a nonhomogenous system alway apply to the location of the most severe restriction, i.e., where for instance the combination of convective flow and wave speed is largest. This also applies in the case of nonuniform grid separations. In this case the grid transport velocity $\Delta x / \Delta t$ is smallest at the location of the highest resolution (smallest grid spacing) such that often the time step limitation should be viewed $\Delta t \leq \min(\Delta x / |c_{max} + v_{max}|)$.

Group Finite Element Method

One-dimensional formulation:

Often nonlinear equations render the finite element method rather inefficient in multidimensional systems. In this case the so-called group finite element method provides a more efficient approach.

Conventional finite element method:

$$u = \sum_l \phi_l u_l$$

Group finete element formulation:

$$u = \sum_l \phi_l u_l \quad F = \sum_l \phi_l F_l$$

Example (Burgers equation, uniform grid):

$$\frac{du_j}{dt} + L_x F_j + \nu L_{xx} u_j = 0$$

where the second term in the conventional FEM becomes

$$u \frac{\partial u}{\partial x} = \frac{u_{j-1} + u_j + u_{j+1}}{3} \frac{u_{j+1} - u_{j-1}}{2\Delta x}$$

whereas the group FEM method uses:

$$
\begin{aligned}
L_x F_j &= \frac{F_{j+1}-F_{j-1}}{2\Delta x} = \frac{1}{2}\frac{u_{j+1}^2-u_{j-1}^2}{2\Delta x} \\
&= \frac{1}{2}\frac{u_{j-1}+u_j+u_{j+1}}{3}\frac{u_{j+1}-u_{j-1}}{2\Delta x}
\end{aligned}
$$

No change for linear terms.

Multi-dimensional formulation:

$$
\frac{\partial \mathbf{q}}{\partial t}+\frac{\partial \mathbf{F}}{\partial x}+\frac{\partial \mathbf{G}}{\partial x}-\nu\left(\frac{\partial^2 \mathbf{q}}{\partial x^2}+\frac{\partial^2 \mathbf{q}}{\partial y^2}\right) = 0
$$

$$
\mathbf{q}=\begin{pmatrix} u \\ v \end{pmatrix},\quad \mathbf{F}=\begin{pmatrix} u^2 \\ uv \end{pmatrix},\quad \mathbf{G}=\begin{pmatrix} uv \\ v^2 \end{pmatrix}
$$

Group finite element approximation:

$$
\begin{aligned}
u^2 &= \sum_{l=1}^{4}\left(u^2\right)_l \phi_l(\xi,\eta) \\
uv &= \sum_{l=1}^{4}(uv)_l \phi_l(\xi,\eta) \\
\ldots
\end{aligned}
$$

Which generates the equation

$$
M_x\otimes M_y \left.\frac{\partial \mathbf{q}}{\partial t}\right|_{jk} = -M_y\otimes L_x\mathbf{F}-M_x\otimes L_y\mathbf{G}+\nu\left(M_y\otimes L_{xx}-M_x\otimes L_{yy}\right)\mathbf{q}
$$

As is seen with the group finite element meth the discretisation is straightforward whereas for the conventional element method every nonlinear term has to be computed separately and generates more terms and products in the discretized equations such that the group FEM generates vewer operations and a more efficient code.

Finally it should be remarked that similar difficulties arise for multi-dimensional implicit methods as have been pointed out before. Imlicit formulations generally lead to large matricices that have to be inverted at every integrations step. As before an efficient implementation is achieved by ADI methods which generate banded matrices (tridiagonal or quadridiagonal depending on the chosen derivative operators).