1 D models

Damián Ginestar Peiró

Departamento de Matemática Aplicada

Universitat Politècnica de València

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Outline

Finite Difference Equations

Consider a function $u(x)$ and its derivative at point x,

$$\frac{\partial u}{\partial x}(x) = \lim_{\Delta x \to 0} \frac{u(x+\Delta x) - u(x)}{\Delta x},$$

Using Taylor's expansion

$$u(x+\Delta x) = u(x) + \Delta x \frac{\partial u}{\partial x}(x) + \frac{\Delta x^2}{2!}\frac{\partial^2 u}{\partial x^2} + \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3} + \cdots .$$

This implies that

$$\frac{\partial u}{\partial x} = \frac{u(x+\Delta x) - u(x)}{\Delta x} + O\left(\Delta x\right).$$

The approximation of the derivative $\frac{\partial u}{\partial x}$ is of first order in Δx.

Finite Difference Equations

Using

$$u(x-\Delta x) = u(x) - \Delta x \frac{\partial u}{\partial x}(x) + \frac{\Delta x^2}{2!}\frac{\partial^2 u}{\partial x^2} - \frac{\Delta x^3}{3!}\frac{\partial^3 u}{\partial x^3} + \cdots .$$

for a generic point x_i, $x_{i+1} = x_i + \Delta x$, $x_{i-1} = x_i - \Delta x$ and we have:
The forward difference

$$\boxed{\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_i}{\Delta x} + O\left(\Delta x\right)}$$

The backward difference

$$\boxed{\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_i - u_{i-1}}{\Delta x} + O\left(\Delta x\right)}$$

Finite Difference Equations

A central difference

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O\left(\Delta x^2\right)$$

For the second derivative

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2} + O\left(\Delta x^2\right)$$

Other approximations:

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{3u_i - 4u_{i-1} + u_{i-2}}{2\Delta x} + O\left(\Delta x^2\right)$$

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{-3u_i + 4u_{i+1} - u_{i+2}}{2\Delta x} + O\left(\Delta x^2\right)$$

$$\left(\frac{\partial^2 u}{\partial x^2}\right)_i = \frac{u_i - 2u_{i-1} + u_{i-2}}{\Delta x^2} + O\left(\Delta x\right)$$

Finite Difference Equations

When nonuniform meshes are used, we can obtain approximations

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_{i+1} - u_i}{\Delta x_{i+1}} + O\left(\Delta x_{i+1}\right) \ ,$$

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{u_i - u_{i-1}}{\Delta x_i} + O\left(\Delta x_i\right) \ ,$$

$$\left(\frac{\partial u}{\partial x}\right)_i = \frac{1}{\Delta x_i + \Delta x_{i+1}} \left(\frac{\Delta x_i}{\Delta x_{i+1}} \left(u_{i+1} - u_i\right) + \frac{\Delta x_{i+1}}{\Delta x_i} \left(u_i - u_{i-1}\right)\right) + O\left(\Delta x_i \Delta x_{i+1}\right) \ ,$$

where $\Delta x_i = x_i - x_{i-1}$.

Finite Difference Equations

Approximations with higher order accuracy can be constructed.

With fourth order accuracy we have

$$
\begin{aligned}
u_i' &= \frac{1}{12\Delta x}\left(u_{i-2} - 8u_{i-1} + 8u_{i+1} - u_{i+2}\right) \\
u_i'' &= \frac{1}{12\Delta x^2}\left(-u_{i-2} + 16u_{i-1} - 30u_i + 16u_{i+1} - u_{i+2}\right)
\end{aligned}
$$

As an example, we consider a bounded domain $\Omega =]0,1[$ and the non-homogeneous problem

$$\begin{cases} -u''(x) + c(x)u(x) = f(x), \quad x \in]0,1[\\ u(0) = \alpha, \; u(1) = \beta \end{cases}$$

We introduce the equidistributed grid points $(x_j)_{0 \leq j \leq N+1}$ given by $x_j = j\Delta x$, where N is an integer and the spacing is given by $\Delta x = 1/(N+1)$.
Introducing the approximation of the second order derivative:

$$\begin{cases} -\frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2} + c(x_j)u_j = f(x_j), \quad j = 1, \ldots, N \\ u_0 = \alpha, \; u_{N+1} = \beta \end{cases}$$

In matrix form, it can be written as,

$$Au = b \ ,$$

where A is the tridiagonal matrix

$$A = A^{(0)} + \begin{pmatrix} c\left(x_1\right) & 0 & \cdots & \cdots & 0 \\ 0 & c\left(x_2\right) & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & c\left(x_{N-1}\right) & 0 \\ 0 & \cdots & \cdots & 0 & c\left(x_N\right) \end{pmatrix}$$

with

$$A^{(0)} = \frac{1}{\Delta x^2}\begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix}, \quad \text{and} \quad b = \begin{pmatrix} f\left(x_1\right) + \frac{\alpha}{\Delta x^2} \\ f\left(x_2\right) \\ \vdots \\ f\left(x_{N-1}\right) \\ f\left(x_N\right) + \frac{\beta}{\Delta x^2} \end{pmatrix}.$$

If $c > 0$, the the matrix A is symmetric and positive definite.

Elliptic equations

For Neumann boundary conditions we can consider the problem

$$\begin{cases} -u''(x) + c(x)u(x) = f(x), & x \in]0,1[\\ u'(0) = \alpha, \ u'(1) = \beta \end{cases}$$

The first derivative of u can be discretized by a difference scheme as follows:

$$u'(0) \approx \frac{u(\Delta x) - u(0)}{\Delta x}, \quad u'(1) \approx \frac{u(1) - u(1 - \Delta x)}{\Delta x},$$

and we obtain the numerical scheme

$$-\frac{u_{j+1} - 2u_j + u_j - 1}{\Delta x^2} + c_j u_j = f(x_j), \quad j = 1, \ldots, N$$
$$u_0 = u_1 - \Delta x \alpha, \ u_{N+1} = u_N + \Delta x \beta,$$

Leading to the linear system

$$Bu = b$$

where

$$B = B^{(0)} + \begin{pmatrix} 0 & \cdots & \cdots & \cdots & 0 \\ \vdots & c(x_1) & & & \vdots \\ \vdots & & \ddots & & \vdots \\ \vdots & & & c(x_N) & \\ 0 & \cdots & \cdots & \cdots & 0 \end{pmatrix}$$

and

$$B^{(0)} = \frac{1}{\Delta x^2} \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 1 \end{pmatrix}, \quad b = \begin{pmatrix} -\frac{\alpha}{\Delta x^2} \\ f(x_1) \\ \vdots \\ \vdots \\ f(x_N) \\ -\frac{\beta}{\Delta x^2} \end{pmatrix}.$$

This scheme is first order accurate. To improve the accuracy of the solution, we can use a central difference scheme for the Neumann boundary conditions:

$$u'(0) \approx \frac{u(\Delta x) - u(-\Delta x)}{2\Delta x}, \quad u'(1) \approx \frac{u(1+\Delta x) - u(1-\Delta x)}{2\Delta x},$$

however, this requires introducing additional fictitious unknowns corresponding to the data u_{-1} and u_{N+2}, thus increasing the size of the linear system to be solved.

This leads to define the following numerical scheme:

$$-\frac{u_{j-1} - 2u_j + u_{j+1}}{\Delta x^2} + c_j u_j = f_j \ , \quad j = 0, \ldots, N+1$$
$$u_{-1} = u_1 - 2\Delta x\alpha, \ u_{N+2} = u_N + 2\Delta x\beta,$$

which is a second order accurate scheme.

Elliptic equations

Example

We want to study the following boundary values problem

$$\frac{\partial^2 u}{\partial x^2} = -2 \ , \quad x \in (0, 10) \ ,$$

with $u(0) = 0$ and $u(10) = 1$.

We use the finite differences approximation

$$\frac{\partial^2 u}{\partial x^2}(x_i) \approx \frac{u_{i-1} - 2u_i + u_{i+1}}{\Delta x^2} \ ,$$

Making use of 11 nodes in the mesh $x_0, x_1, \ldots, x_{10}$, we have that $\Delta x = 1$ and the equation can be approximated as

$$u_{i-1} - 2u_i + u_{i+1} = -2 \ .$$

Varying $i = 1, \ldots, 9$, we obtain the system

$$\begin{pmatrix} -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 & \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \end{pmatrix} = \begin{pmatrix} -2 \\ -2 \\ -2 \\ -2 \\ -2 \\ -2 \\ -2 \\ -2 \\ -3 \end{pmatrix}.$$

To solve this system, we can use the following instructions:

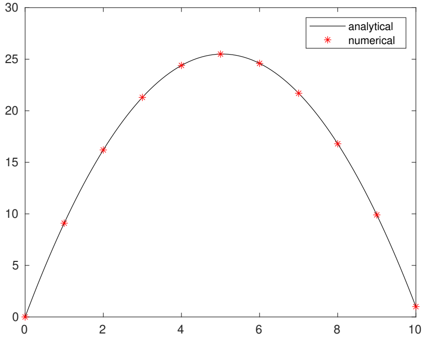
```
v1=ones(1,8);
v2=-2*ones(1,9);
A=diag(v2)+diag(v1,-1)+diag(v1,1);
b=-2*ones(9,1);
b(9)=-3;
solu=A\b;
solu=[0;solu;1];
```

The analytical solution of this problem is

$$u(x) = -x^2 + \frac{101}{10}x$$

Elliptic equations

The obtained result is



Parabolic equations: Explicit schemes

We consider the diffusion equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \ .$$

An explicit finite difference scheme may be written in the forward difference in time and central difference in space (FTCS) as,

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2} + O\left(\Delta t, \Delta x^2\right)$$

or

$$\boxed{u_i^{n+1} = u_i^n + d\left(u_{i-1}^n - 2u_i^n + u_{i+1}^n\right)}$$

where the diffusion number is

$$d = \frac{\alpha \Delta t}{\Delta x^2} \ .$$

Explicit schemes

- The concept of stability of a numerical scheme is concerned with the growth or decay of errors introduced at any stage of the computation.
- In practice, each calculation made on the computer is carried out to a finite number of significant figures which introduces a round-off error at every step of the computation.
- A particular method is stable if the cumulative effect of all the round-off errors produced in the application of the algorithm is negligible.

Explicit schemes

- In order to determine the stability of the solution of finite difference equations, it is convenient to expand the difference equation into a discrete Fourier series.
- Decay or growth of an amplification factor indicates whether or not the numerical algorithm is stable. This is known as the von Neumann stability analysis.

Explicit schemes

Assuming that at any time step n, the computed solution u_i^n is the sum of the exact solution $\bar{u}_i^n$ and error ε_i^n,

$$u_i^n = \bar{u}_i^n + \varepsilon_i^n,$$

equation associated with FTCS scheme is

$$\frac{\varepsilon_i^{n+1} - \varepsilon_i^n}{\Delta t} = \frac{\alpha}{\Delta x^2}\left(\varepsilon_{i-1}^n - 2\varepsilon_i^n + \varepsilon_{i+1}^n\right) \ .$$

If the boundary conditions are considered as periodic, the error ε_l can be decomposed into a discrete Fourier series in space at each time level n,

$$\varepsilon_l^n = \sum_{j=-N}^{N} \bar{\varepsilon}_j^n e^{ijl\frac{\pi}{N}} \ ,$$

where the domain considered is $[-L, L]$ and $\Delta x = L/N$.

Explicit schemes

Introducing the spatial phase angle

$$\phi_j = \frac{j\pi}{N} \ ,$$

for each one of the components

$$\frac{\bar{\varepsilon}_j^{n+1} - \bar{\varepsilon}_j^n}{\Delta t} e^{il\phi_j} = \frac{\alpha}{\Delta x^2} \left(\bar{\varepsilon}_j^n e^{i(l-1)\phi_j} - 2\bar{\varepsilon}_j^n e^{il\phi_j} + \bar{\varepsilon}_j^n e^{i(l+1)\phi_j} \right)$$

that is

$$\bar{\varepsilon}_j^{n+1} - \bar{\varepsilon}_j^n = d\bar{\varepsilon}_j^n \left(e^{-i\phi_j} - 2 + e^{i\phi_j} \right)$$

Explicit schemes

The computational scheme is said to be stable if the amplitude of any error harmonic $\bar{\varepsilon}_j^n$ does not grow in time, that is, if the following ratio holds:

$$|g| = \left| \frac{\bar{\varepsilon}_j^{n+1}}{\bar{\varepsilon}_j^n} \right| \leq 1 \ ,$$

where g is the amplification factor

$$g = 1 - 2d(1 - \cos(\phi_j))$$

The stability conditions are

$$g \leq 1, \quad g \geq -1 \ ,$$

Since the maximum value of $1 - \cos(\phi_j)$ is 2, we have the stability condition (Courant-Friedrich-Lewy (CFL) condition)

$$\boxed{0 \leq \frac{\alpha \Delta t}{\Delta x^2} \leq \frac{1}{2}}$$

Explicit schemes

Example

Let us assume that we have a bar with a length of 0.5 m that initially has a temperature of 25 degrees Celsius. The right end is set at a temperature of 100 degrees Celsius, while the other end is kept at 25 degrees Celsius. We want to know how the temperature evolves at different points of the different points of the bar using the heat equation

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \; ; \quad \alpha = 10^{-2}\,\mathrm{m}^2/\mathrm{s} \; .$$

Explicit schemes

We use the explicit scheme

$$u_i^{n+1} = u_i^n + \frac{\alpha \Delta t}{\Delta x^2} \left(u_{i-1}^n - 2u_i^n + u_{i+1}^n \right) \ ,$$

We choose, for example, $\Delta x = 0.1$, that is, 6 spatial nodes. If we choose $\Delta t = 0.1$s, the Courant condition (CFL)

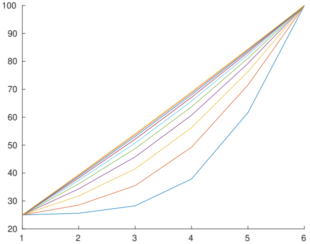
$$0 < \frac{10^{-2}}{10^{-2}} \Delta t < 0.5 \ ,$$

is satisfied.

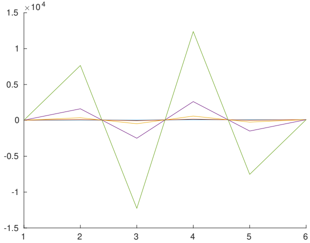
Explicit schemes

```
close all
% geometry
deltat=0.1;
deltax=0.1;
alpha=1e-2;
% initial conditions
u0=25*ones(6,1);
u0(6)=100;
%
it=1;
pasost=100;
nprint=10;
hold on
% time loop
for n=1:pasost
   tiempo=n*deltat;
   u(1)=25;
   for i=2:5
      u(i)=u0(i)+alpha*deltat/(deltax^2)*...
      (u0(i-1)-2*u0(i)+u0(i+1));
   end
   u(6)=100;
   if(it==nprint)
   it=0;
   plot(u);
   end
   it=it+1;
   u0=u;
end
```

Explicit schemes



$$\Delta t = 0.1$$



$$\Delta t = 0.6$$

Explicit schemes

Other explicit schemes are:

- The Richardson method

$$\frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t} = \alpha \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2}$$

  which is unconditionally unstable.

- The Dufort-Frankel method

$$\frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t} = \alpha \frac{u_{i-1}^n - 2\frac{u_i^{n+1} + u_i^{n-1}}{2} + u_{i+1}^n}{\Delta x^2} \,,$$

  which is unconditionally stable.

Implicit schemes

An implicit method for the parabolic equation is

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{\Delta x^2} + O\left(\Delta t, \Delta x^2\right)$$

This scheme is unconditionally stable.

$$-ru_{i-1}^{n+1} + (1+2r)u_i^{n+1} - ru_{i+1}^{n+1} = u_i^n \ , \quad r = \frac{\alpha \Delta t}{\Delta x^2}$$

Implicit schemes

If we assume homogeneous boundary conditions, for each time step it is necessary to solve a system of linear equations.

$$\begin{pmatrix} (1+2r) & -r & & & & \\ -r & (1+2r) & -r & & & \\ & & \cdots & & & \\ & & & -r & (1+2r) & -r \\ & & & & -r & (1+2r) \end{pmatrix} \begin{pmatrix} u_1^{n+1} \\ \vdots \\ u_{N_x}^{n+1} \end{pmatrix} =$$

$$\begin{pmatrix} u_1^n + r u_0^{n+1} \\ \vdots \\ u_{N_x}^n + r u_{N_x+1}^{n+1} \end{pmatrix}.$$

Implicit schemes

Another possibility is the **Crank-Nicolson method**

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{\alpha}{2}\left(\frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{\Delta x^2} + \frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2}\right)$$

or, in general,

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha\left(\beta\frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{\Delta x^2} + (1-\beta)\frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2}\right)$$

For $1/2 \leq \beta \leq 1$, the method is unconditionally stable.

Exercises

Diffusion equation

We study the heat conduction in a bar. In particular, we have a bar with an initial temperature of 0 ℃ and we apply temperatures of 100 ℃ at both extremes of the bar. We assume that the length of the bar is 1 and the thermal diffusivity is α. Compute its numerical solution using the β method (Crank-Nicolson)

Exercises

- Study the stability of the BTCS scheme for the diffusion equation

$$u_i^{n+1} = u_i^n + d\left(u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}\right)$$

- Study the stability of the CTCS scheme for the diffusion equation

$$u_i^{n+1} = u_i^{n-1} + 2d\left(u_{i-1}^n - 2u_i^n + u_{i+1}^n\right)$$

Hyperbolic equations

Given a wave equation

$$\frac{\partial^2 u}{\partial t^2} = a^2 \frac{\partial^2 u}{\partial x^2}$$

We can look for solutions of the form

$$u(x,t) = G(t)e^{ikx}$$

This implies

$$\frac{\partial^2 G}{\partial t^2} e^{ikx} = (ika)^2 \, G(t)e^{ikx}$$

That is

$$G'' = (ika)^2 \, G(t)$$

Hyperbolic equations

The solutions of the differential equation are

$$G_l = e^{ikat} \;,\quad G_r = e^{-ikat}$$

and we obtain the waves

$$u_l(x,t) = e^{ik(x+at)} \;,\quad u_r(x,t) = e^{ik(x-at)}$$

Superposition of these waves, gives

$$u(x,t) = F_1(x+at) + F_2(x-at)$$

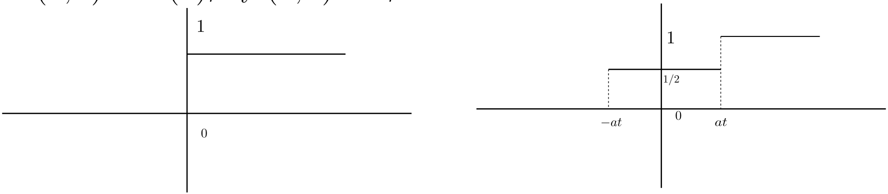
At $t = 0$,

$$\begin{aligned} u(x,0) &= F_1(x) + F_2(x) \\ \frac{\partial u}{\partial t}(x,0) &= aF_1'(x) - aF_2'(x) \end{aligned}$$

Solving for F_1 and F_2,

$$u(x,t) = \frac{1}{2}\left(u(x+at,0) + u(x-at,0)\right) + \frac{1}{2a}\int_{x-at}^{x+at} \frac{\partial u}{\partial t}(x,0)\,dx$$

$u(x,0) = H(x)$, $\partial_t u(x,0) = 0$,



Hyperbolic equations

Given a wave equation

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

it can be factorised as

$$\left(\frac{\partial}{\partial t} + a \frac{\partial}{\partial x} \right) \left(\frac{\partial}{\partial t} - a \frac{\partial}{\partial x} \right) u = 0$$

which is equivalent to

$$\begin{cases} \frac{\partial u}{\partial t} - a \frac{\partial u}{\partial x} = v \\ \frac{\partial v}{\partial t} + a \frac{\partial v}{\partial x} = 0 \end{cases}$$

Hyperbolic equations, in general, represent wave propagation. They are given by either first order or second order differential equations, which may be approximated in either explicit or implicit forms of finite difference equations.

Explicit schemes

Let us consider a first order wave equation (transport equation or convection eqution)

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial t} = 0, \quad a > 0.$$

The Euler forward method (FTFS) is

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -a\frac{u_{i+1}^n - u_i^n}{\Delta x} \ .$$

If we repeat the Von Neuman stability analysis, we obtain for the amplification factor

$$g_j = 1 - C\left(e^{i\phi_j} - 1\right) = 1 + 2C\sin^2\left(\frac{\phi_j}{2}\right) - iC\sin\left(\phi_j\right)$$

with C the Courant number

$$C = \frac{a\Delta t}{\Delta x} \ .$$

Explicit schemes

Hence, it is satisfied

$$\begin{aligned} |g|^2 &= \left(1 + 2C\sin^2\left(\frac{\phi}{2}\right)\right)^2 + C^2\sin^2(\phi) \\ &= 1 + 4C\left(1 + C\right)\sin^2\left(\frac{\phi}{2}\right) \geq 1. \end{aligned}$$

and the scheme is unconditionally unstable.

The Euler's Forward Time and Central Space (FTCS) scheme is

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -a\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} \; .$$

This is also an unconditionally unstable scheme.

Explicit schemes

The Euler's forward time and backward space (FTBS) approximations (also known as upwind method) is given by

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -a\frac{u_i^n - u_{i-1}^n}{\Delta x} \ .$$

The amplification factor takes the form

$$\begin{aligned} g &= 1 - C\left(1 - e^{-i\phi}\right) = 1 - C\left(1 - \cos(\phi)\right) - iC\sin(\phi) \\ &= 1 - 2C\sin^2\left(\frac{\phi}{2}\right) - iC\sin(\phi) \ , \end{aligned}$$

that is,

$$g = \xi + i\eta \ ,$$

with

$$\begin{aligned} \xi &= 1 - 2C\sin^2\left(\frac{\phi}{2}\right) = (1 - C) + C\cos(\phi), \\ \eta &= -C\sin(\phi) \ , \end{aligned}$$

Explicit schemes

The stability condition states that the curve representing g for all values of ϕ should remain within the unit circle.

$$\begin{aligned} |g|^2 &= (1 - C + C\cos(\phi))^2 + C^2\sin^2(\phi) \\ &= 1 - 2C(1-C)(1-\cos(\phi)) \\ &= 1 - 4C(1-C)\sin^2\left(\frac{\phi}{2}\right) \leq 1 \end{aligned}$$

This implies

$$4C(1-C))\sin^2\left(\frac{\phi}{2}\right) > 0$$

that is

$$0 < C < 1$$

Courant-Friedrich-Lewy (CFL) condition.

Explicit schemes

In numerical solutions of finite difference equations, we are also concerned with dispersion (phase) error. They should be as small as possible

The phase Φ, given by

$$\Phi = \arctan\left(\frac{\eta}{\xi}\right) = \arctan\left(\frac{-C\sin(\phi)}{1 - C + C\cos(\phi)}\right) \; .$$

The phase angle is defined as

$$\tilde{\Phi} = ka\Delta t = C\phi,$$

and the dispersion error or relative phase error is defined as

$$\varepsilon_\phi = \frac{\Phi}{\tilde{\Phi}} = \frac{1}{C\phi}\arctan\left(\frac{\eta}{\xi}\right) = \frac{1}{C\phi}\arctan\left(\frac{-C\sin(\phi)}{1 - C + C\cos(\phi)}\right) \; ,$$

that can be approximated by

$$\varepsilon_\phi \approx 1 - \frac{1}{6}\left(2C^2 - 3C + 1\right)\phi^2 \; .$$

The Lax method

$$u_i^{n+1} = \frac{1}{2}\left(u_{i+1}^n + u_{i-1}^n\right) - \frac{C}{2}\left(u_{i+1}^n - u_{i-1}^n\right)$$

which is stable for $0 < C \leq 1$.

The Midpoint Leapfrog method

$$\frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t} = -\frac{a\left(u_{i+1}^n - u_{i-1}^n\right)}{2\Delta x}$$

This scheme is stable for $0 < C \leq 1$ and it is second order accurate in time and space but it requires two sets of initial values.

Explicit schemes

The Lax-Wendroff method is obtained using the Taylor expansion

$$u(x, t + \Delta t) = u(x, t) + \frac{\partial u}{\partial t}\Delta t + \frac{1}{2!}\frac{\partial^2 u}{\partial t^2}\Delta t^2 + O\left(\Delta t^3\right)$$

Differentiating convection equation with respect to time

$$\frac{\partial^2 u}{\partial t^2} = -a\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial t}\right) = a^2\frac{\partial^2 u}{\partial x^2} \ .$$

The Taylor expansion is written as

$$u_i^{n+1} = u_i^n + \Delta t\left(-a\frac{\partial u}{\partial x}\right) + \frac{\Delta t^2}{2}\left(a^2\frac{\partial^2 u}{\partial x^2}\right)$$

Using central differencing of the second order for the spatial derivatives, we obtain

$$\boxed{u_i^{n+1} = u_i^n - a\Delta t\left(\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}\right) + \frac{1}{2}(a\Delta t)^2\left(\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}\right)}$$

which is a stable method if $0 < C \leq 1$.

Implicit schemes

Two typical implicit methods for the convection equation are, the Euler's BTCS method

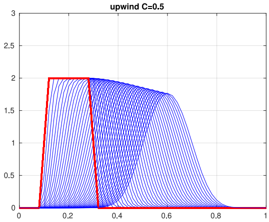
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{a}{2\Delta x}\left(u_{i+1}^{n+1} - u_{i-1}^{n+1}\right)$$

and the Crank-Nicolson method

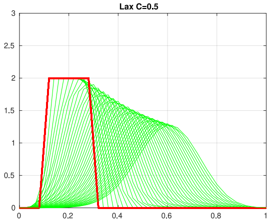
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{a}{2}\left(\frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2\Delta x} + \frac{u_{i+1}^{n} - u_{i-1}^{n}}{2\Delta x}\right)$$

These schemes are unconditionally stables.

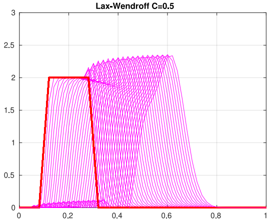
Implicit schemes



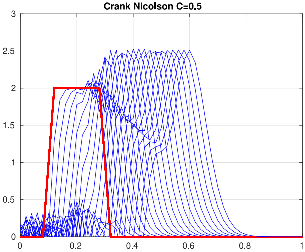
Diffusion



Diffusion



Dispersion



Dispersion

Matrix stability for finite differences method

Given a time-dependent boundary problem, once a spatial discretization is used, we obtain the semi-discrete system

$$\frac{dU}{dt} = AU + b$$

An approximate solution

$$V(t) = U(t) + \varepsilon(t)$$

The error $\varepsilon(t)$ satisfies the homogeneous equation

$$\frac{d\varepsilon}{dt} = A\varepsilon$$

Matrix stability for finite differences method

Using a time-discretization, we end up with a homogeneous difference equations system of the form

$$E^{n+1} = BE^n$$

This system is stable if all the eigenvalues of matrix B, λ, satisfy that $|\lambda| < 1$.

Matrix stability for finite differences method

Matrix stability

Use the matrix stability method to analyse the stability of the FTCS scheme for the linear convection equation

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

if periodic boundary conditions are assumed.

Solution:

The FTCS scheme is given by

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -a\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}$$

that is

$$u_i^{n+1} = u_i^n + \frac{C}{2}\left(u_{i-1}^n - u_{i+1}^n\right)$$

Matrix stability for finite differences method

For the errors, we have

$$e_i^{n+1} = e_i^n + \frac{C}{2}\left(e_{i-1}^n - e_{i+1}^n\right)$$

Evaluating the difference equation for the nodes $i = 0, 1, \ldots, N$ and using the periodicity we obtain a system of the form

$$E^{n+1} = BE^n$$

where matrix B is

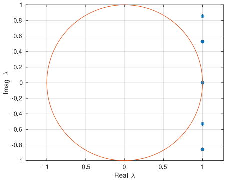
$$B = \begin{pmatrix} 1 & -D & 0 & \cdots & D \\ D & 1 & -D & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & D & 1 & -D \\ -D & \cdots & 0 & D & 1 \end{pmatrix}, \quad D = \frac{C}{2}$$

Matrix stability for finite differences method

Program to compute the eigenvalues of B

```
clear all, close all;
format long

% Number of points
Nx = 10;
x = linspace(0,1,Nx+1);
dx = 1/Nx;
% velocity
v = 1;
% Set timestep
CFL = 1;
dt = CFL*dx/abs(v);

D=dt*v/(2*dx);

v1=D*ones(1,Nx-1);
v2=ones(1,Nx);
v3=-v1;
B=diag(v2)+diag(v1,-1)+diag(v3,1);
B(1,Nx)=D;
B(Nx,1)=-D;

% Calculate eigenvalues of A
lambda = eig(B)

%for i=1:length(lambda)
%    norm(lambda(i))
%end
```

```
plot(lambda,'*');

xlabel('Real \lambda');
ylabel('Imag \lambda');

% unit circle
th = linspace(0,2*pi,101);
hold on;
plot(sin(th),cos(th));
hold off;
axis('equal');
grid on;
```



Multistep methods

Computational stability, convergence, and accuracy may be improved using multistep (intermediate step between n and $n+1$) schemes, as the Richmyer scheme

$$\frac{u_i^{n+\frac{1}{2}} - \frac{1}{2}\left(u_{i+1}^n + u_{i-1}^n\right)}{\Delta t/2} = -a\frac{\left(u_{i+1}^n - u_{i-1}^n\right)}{2\Delta x} \ ,$$

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -a\frac{\left(u_{i+1}^{n+\frac{1}{2}} - u_{i-1}^{n+\frac{1}{2}}\right)}{2\Delta x} \ .$$

These equations can be rearranged as

$$u_i^{n+\frac{1}{2}} = \frac{1}{2}\left(u_{i+1}^n + u_{i-1}^n\right) - \frac{C}{4}\left(u_{i+1}^n - u_{i-1}^n\right) \ ,$$

$$u_i^{n+1} = u_i^n - \frac{C}{2}\left(u_{i+1}^{n+\frac{1}{2}} - u_{i-1}^{n+\frac{1}{2}}\right) \ .$$

This scheme is stable for $0 < C \leq 2$.

The Lax-Wendroff scheme can be rewritten as

$$u_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}\left(u_{i+1}^n + u_{i-1}^n\right) - \frac{C}{2}\left(u_{i+1}^n - u_{i-1}^n\right)$$
$$u_i^{n+1} = u_i^n - C\left(u_{i+\frac{1}{2}}^{n+\frac{1}{2}} - u_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right)$$

The stability condition is $0 < C \leq 1$.

Conservation laws

Given the linear advection equation

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \quad x \in [0,1] \ .$$

If we define the total mass

$$M = \int_0^1 u\,dx \ ,$$

and we assume that u has periodic boundary conditions $u(0,t) = u(1,t)$, we have

$$\begin{aligned} \frac{dM}{dt} &= \frac{d}{dt}\left(\int_0^1 u dx\right) = \int_0^1 \frac{du}{dt}\,dx \\ &= -\int_0^1 a\frac{du}{dx}\,dx = -a\int_0^1 du = -a\,[u]_0^1 = 0 \ . \end{aligned}$$

Then the mass M is conserved.

Conservation laws

If we consider the FTBS scheme

$$u_i^{n+1} = u_i^n - C\left(u_i^n - u_{i-1}^n\right) \ ,$$

we calculate

$$\begin{aligned} M^{n+1} &= \sum_{i=1}^{n_x} \Delta x u_i^{n+1} = \Delta x \sum_{i=1}^{N_x} \left(u_i^n - C\left(u_i^n - u_{i-1}^n\right)\right) \\ &= M^n - C\Delta x \left(\sum_{i=1}^{N_x} u_i^n - \sum_{i=1}^{N_x} u_{i-1}^n\right) \\ &= M^n - C\Delta x \left(\sum_{i=1}^{N_x} u_i^n - \sum_{i=0}^{N_x-1} u_i^n\right) \\ &= M^n - C\Delta x \left(u_{N_x}^n - u_0^n\right) = M^n \ . \end{aligned}$$

Thus, this scheme conserves the mass with homogeneous or periodic boundary conditions.

Conservation laws

Now we consider a higher moment such as the variance

$$V = \int_0^1 u^2\, dx - M^2 \ .$$

Then we calculate

$$\frac{dV}{dt} = \int_0^1 \frac{du^2}{dt}\, dx = \int_0^1 2u\frac{du}{dt}\, dx = -2a\int_0^1 u\, du = -u\left[u^2\right]_0^1 = 0.$$

If we again consider the FTBS scheme, we calculate

$$\begin{aligned} V^{n+1} &= \sum_{i=1}^{N_x} \Delta x \left(u_i^{n+1}\right)^2 = \Delta x \sum_{i=1}^{N_x} \left(u_i^n - C\left(u_i - u_{i-1}^{n-1}\right)\right)^2 \\ &= V^n - 2C(1-C)\left(V^n - \Delta x \sum_{i=1}^{N_x} u_i^n u_{i-1}^n\right) \ . \end{aligned}$$

It can be seen that the variance always decreases when using FTBS.

Nonlinear problems

A classical nonlinear first order hyperbolic equation is the Euler's equation

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x}\ , \quad \text{or} \quad \frac{\partial u}{\partial t} = -\frac{\partial F}{\partial x}\ , \quad F = \frac{u^2}{2}$$

The Lax method can be applied to this equation. Using the FTCS differencing scheme

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{F_{i+1}^n - F_{i-1}^n}{2\Delta x}\ ,$$

and to maintain the stability, we replace u_i^n by its average,

$$\boxed{u_i^{n+1} = \frac{1}{2}\left(u_{i+1}^n + u_{i-1}^n\right) - \frac{\Delta t}{2\Delta x}\left(F_{i+1}^n - F_{i-1}^n\right)}$$

This sheme is stable if

$$\left|\frac{\Delta t}{\Delta x}u_{\max}\right| \leq 1.$$

-

Nonlinear problems

The Lax-Wendroff method for the Euler equation is derived form the Taylor expansion

$$u_i^{n+1} = u_i^n + \frac{\partial u}{\partial t}\Delta t + \frac{1}{2!}\frac{\partial^2 u}{\partial t^2}\Delta t^2 + \cdots \ .$$

We have that

$$\frac{\partial^2 u}{\partial t^2} = -\frac{\partial}{\partial t}\left(\frac{\partial F}{\partial x}\right) = -\frac{\partial}{\partial x}\left(\frac{\partial F}{\partial t}\right) \ .$$

and

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

Nonlinear problems

Thus,

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(A\frac{\partial F}{\partial x}\right) \; .$$

Substituting in the Taylor expansion,

$$u_i^{n+1} = u_i^n + \left(-\frac{\partial F}{\partial x}\right)\Delta t + \frac{\partial}{\partial x}\left(A\frac{\partial F}{\partial x}\right)\frac{\Delta t^2}{2} + O\left(\Delta t^3\right) \; ,$$

that can be approximated by

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{F_{i+1}^n - F_{i-1}^n}{2\Delta x} + \frac{\Delta t}{2\Delta x}\left(\left(A\frac{\partial F}{\partial x}\right)_{i+\frac{1}{2}}^n - \left(A\frac{\partial F}{\partial x}\right)_{i-\frac{1}{2}}^n\right)$$

Nonlinear problems

The last term of this equation is approximated as,

$$\frac{\left(A\frac{\partial F}{\partial x}\right)^n_{i+\frac{1}{2}} - \left(A\frac{\partial F}{\partial x}\right)^n_{i-\frac{1}{2}}}{\Delta x} = \frac{A_{i+\frac{1}{2}}\frac{F^n_{i+1}-F^n_i}{\Delta x} - A_{i-\frac{1}{2}}\frac{F^n_i - F^n_{i-1}}{\Delta x}}{\Delta x}$$

$$= \frac{\frac{1}{2\Delta x}\left(A^n_{i+1} + A^n_i\right)\left(F^n_{i+1} - F^n_i\right) - \frac{1}{2\Delta x}\left(A^n_i + A^n_{i-1}\right)\left(F^n_i - F^n_{i-1}\right)}{\Delta x}.$$

That is,

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{2\Delta x}\left(F^n_{i+1} - F^n_{i-1}\right)$$
$$+ \frac{\Delta t^2}{4\Delta x^2}\left(\left(u^n_{i+1} + u^n_i\right)\left(F^n_{i+1} - F^n_i\right) - \left(u^n_i + u^n_{i-1}\right)\left(F^n_i - F^n_{i-1}\right)\right)$$

This is second order accurate with the stability requirement,

$$\left|\frac{\Delta t}{\Delta x} u_{\max}\right| \leq 1.$$

Nonlinear problems

A multilstep scheme (MacCormack method) for the Euler equation is the following one,

$$
\begin{aligned}
u_i^* &= u_i^n - \frac{\Delta t}{\Delta x}\left(F_{i+1}^n - F_i^n\right), \\
u_i^{n+1} &= \frac{1}{2}\left(u_i^n + u_i^* - \frac{\Delta t}{\Delta x}\left(F_i^* - F_{i-1}^*\right)\right) .
\end{aligned}
$$

Because of the two-level splitting, the solution performs better than the Lax method or the Lax-Wendroff method.

Nonlinear problems

One of the most widely used implicit schemes is the Beam-Warming method, discussed below.
Let us consider the Taylor expansions

$$u(x,t+\Delta t) = u(x,t) + \Delta t \frac{\partial u}{\partial t}(x,t) + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2}(x,t) + O\left(\Delta t^3\right) \ , \quad (1)$$

and

$$u(x,t) = u(x,t+\Delta t) - \Delta t \frac{\partial u}{\partial t}(x,t+\Delta t) + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2}(x,t+\Delta t) + O\left(\Delta t^3\right) \ , \quad (2)$$

Substracting (1) and (2),

$$\begin{aligned} 2u(x,t+\Delta t) =& 2u(x,t) + \Delta t \frac{\partial u}{\partial t}(x,t) + \Delta t \frac{\partial u}{\partial t}(x,t+\Delta t) \\ & \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2}(x,t) + \frac{\Delta t^2}{2}\frac{\partial^2 u}{\partial t^2}(x,t+\Delta t) + O\left(\Delta t^3\right) \ , \end{aligned}$$

or

$$
\begin{aligned}
u_i^{n+1} &= u_i^n + \frac{1}{2}\left(\left(\frac{\partial u}{\partial t}\right)_i^n + \left(\frac{\partial u}{\partial t}\right)_i^{n+1}\right)\Delta t \\
&\quad + \frac{1}{2}\left(\left(\frac{\partial^2 u}{\partial t^2}\right)_i^n - \left(\frac{\partial^2 u}{\partial t^2}\right)_i^{n+1}\right)\frac{\Delta t^2}{2!} + O\left(\Delta t^3\right).
\end{aligned}
$$

We have that

$$
\left(\frac{\partial^2 u}{\partial t^2}\right)_i^{n+1} = \left(\frac{\partial^2 u}{\partial t^2}\right)_i^n + \frac{\partial}{\partial t}\left(\frac{\partial^2 u}{\partial t^2}\right)_i^n \Delta t + O\left(\Delta t^2\right),
$$

and we arrive at

$$u_i^{n+1} = u_i^n + \frac{1}{2}\left(\left(\frac{\partial u}{\partial t}\right)_i^n + \left(\frac{\partial u}{\partial t}\right)_i^{n+1}\right) + O\left(\Delta t^3\right).$$

For the equation

$$\frac{\partial u}{\partial t} = -\frac{\partial F}{\partial x}$$

we have

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -\frac{1}{2}\left(\left(\frac{\partial F}{\partial x}\right)_i^n + \left(\frac{\partial F}{\partial x}\right)_i^{n+1}\right) + O\left(\Delta t^2\right) \; .$$

Nonlinear problems

The resulting finite difference equation in implicit formulation is nonlinear, and a procedure is used to linearize it.
To this end, we write a Taylor series for $F(t+\Delta t)$ in the form

$$\begin{aligned} F(t+\Delta t) &= F(t) + \frac{\partial F}{\partial t}\Delta t + O\left(\Delta t^2\right) \\ &= F(t) + \frac{\partial F}{\partial u}\frac{\partial u}{\partial t}\Delta t + O\left(\Delta t^2\right) \end{aligned}$$

and

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{2}\left(2\left(\frac{\partial F}{\partial x}\right)_i^n + \frac{\partial}{\partial x}\left(A\left(u_i^{n+1} - u_i^n\right)\right)\right)$$

Using a second order central differencing approximation

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{2}\left(\frac{2\left(F_{i+1}^n - F_{i-1}^n\right)}{2\Delta x} + \frac{A_{i+1}^n u_{i-1}^{n+1} - A_{i-1}^n u_{i-1}^{n+1}}{2\Delta x} - \frac{A_{i+1}^n u_{i+1}^n - A_{i-1}^n u_{i-1}^n}{2\Delta x}\right) ,$$

This scheme is second order accurate, unconditionally stable, but dispersion errors may arise. To prevent this, a fourth order smoothing (damping) term is explicitly added:

$$D = -\frac{\omega}{8}\left(u_{i+2}^n - 4u_{i+1}^n + 6u_i^n - 4u_{i-1}^n + u_{i-2}^n\right) ,$$

with $0 < \omega < 1$.

Since the added damping term is of fourth order, it does not affect the second order accuracy of the method, that is of the form

$$
\begin{aligned}
&-\frac{\Delta t}{4\Delta x}A_{i-1}^{n}u_{i-1}^{n+1}+u_{i}^{n+1}+\frac{\Delta t}{4\Delta x}A_{i+1}^{n}u_{i+1}^{n+1}\\
&=u_{i}^{n}-\frac{\Delta t}{2\Delta x}\left(F_{i+1}^{n}-F_{i-1}^{n}\right)+\frac{\Delta t}{4\Delta x}A_{i+1}^{n}u_{i+1}^{n}-\frac{\Delta t}{4\Delta x}A_{i-1}^{n}u_{i-1}^{n}+D\ .
\end{aligned}
$$

The Burger's equation

The Burgers' equation is a special form of the momentum equation for irrotational, incompressible flows in which pressure gradients are neglected. Consider the Burgers' equation written in various forms,

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} \ ,$$

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

$$\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} = \nu\frac{\partial^2 u}{\partial x^2} \ .$$

These equations are mixed hyperbolic, elliptic, and parabolic types. If steady state is considered, then they become mixed hyperbolic and elliptic equations. Because of these special properties, various solution schemes have been tested.

The Burger's equation

Consider the Navier Stokes equations

$$\vec{\nabla}\vec{v} = 0$$
$$\rho\frac{\partial\left(v_i\right)}{\partial t} + \rho\vec{v}\,\vec{\nabla}\left(v_i\right) = -\vec{\nabla}\left(p\vec{e}_i\right) + \mu\nabla^2 v_i$$

that describe the dynamics of an incompressible flow where gravitational effects are negligible.

If we consider a 1D problem with no pressure gradient, the above equations reduces to

$$\boxed{\rho\frac{\partial u}{\partial t} + \rho u\frac{\partial u}{\partial x} - \mu\frac{\partial^2 u}{\partial x^2} = 0}$$

The Burger's equation:linear equation

The FTCS explicit scheme is obtained by using forward differences in time and central differences in space,

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = \nu\frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2} \ .$$

The central difference for the convective term tends to introduce significant damping.
The FTBS explicit scheme is the same as in FTCS except that backward differences are used for the convective term,

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\frac{u_i^n - u_{i-1}^n}{\Delta x} = \nu\frac{u_{i-1}^n - 2u_i^n + u_{i+1}^n}{\Delta x^2} \ .$$

The Burger's equation: linear equation

- The first order approximation of the convective term may introduce an excessive diffusion error.
- A compromise is to use higher order schemes. An example is the following one,

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a \left(\frac{11u_i^n - 18u_{i-1}^n + 9u_{i-2}^n - 2u_{i-3}^n}{6\Delta x} \right)$$
$$= \nu \frac{u_{i+1} - 2u_i^n + u_{i-1}^n}{\Delta x^2} \, .$$

The Burger's equation: linear equation

Another explicit scheme is the DuFort-Frankel method,

$$\frac{u_i^{n+1} - u_i^{n-1}}{2\Delta t} + a\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} = \nu \frac{u_{i+1}^n - 2\left(\frac{u_i^{n-1}+u_i^{n+1}}{2}\right) + u_{i-1}^n}{\Delta x^2} \ ,$$

that is

$$\boxed{u_i^{n+1} = \left(\frac{1-2d}{1+2d}\right) u_i^{n-1} + \left(\frac{C+2d}{1+2d}\right) u_{i-1}^n - \left(\frac{C-2d}{1+2d}\right) u_{i+1}^{n-1}}$$

where

$$C = \frac{a\Delta t}{\Delta x} \ , \quad d = \frac{\nu \Delta t}{\Delta x^2} \ .$$

This scheme is stable if $0 < C \leq 1$.

The Burger's equation: linear equation

The MacCormack explicit scheme is a two-step method, which can be formulated as,

Step 1

$$\Delta u_i^n = -a\frac{\Delta t}{\Delta x}\left(u_{i+1}^n - u_i^n\right) + \frac{\nu \Delta t}{\Delta x^2}\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right)$$
$$u_i^* = u_i^n + \Delta u_i^n$$

Step 2

$$\Delta u_i^* = -a\frac{\Delta t}{\Delta x}\left(u_i^* - u_{i-1}^*\right) + \frac{\nu \Delta t}{\Delta x^2}\left(u_{i+1}^* - 2u_i^* + u_{i-1}^*\right)$$
$$u_i^{n+1} = \frac{1}{2}\left(u_i^n + u_i^* + \Delta u_i^*\right) \ .$$

This scheme is stable if

$$\Delta t \leq \frac{1}{\frac{a}{\Delta x} + \frac{2\nu}{\Delta x^2}} \ .$$

The MacCormack implicit scheme is

Step 1

$$\left(1+\lambda\frac{\Delta t}{\Delta x}\right)\Delta u_i^* = \Delta u_i^n + \lambda\frac{\Delta t}{\Delta x}\Delta u_{i+1}^*$$
$$u_i^* = u_i^n + \Delta u_i^n$$

Step 2

$$\left(1+\lambda\frac{\Delta t}{\Delta x}\right)\Delta u_i^{n+1} = \Delta u_i^* + \lambda\frac{\Delta t}{\Delta x}\Delta u_{i+1}^{n+1}$$
$$u_i^{n+1} = \frac{1}{2}\left(u_i^n + u_i^* + \Delta u_i^{n+1}\right)$$

where

$$\lambda \geq \text{máx}\left(\frac{1}{2}\left(|a| + \frac{2\nu}{\Delta x} - \frac{\Delta x}{\Delta t}\right), 0\right)$$

The Burger's equation: Nonlinear equation

The non linear equation is considered

$$\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} \ .$$

The FTCS scheme for this equation is

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + \frac{F_{i+1}^n - F_{i-1}^n}{2\Delta x} = \nu \frac{u_{i-1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \ .$$

The Burger's equation: Nonlinear equation

A potentially more accurate treatment of the convective term

$$\frac{F_{i+1} - F_{i-1}}{2\Delta x}$$

is provided by replacing it by a four-point upwind discretisation:
For u positive

$$L_x^{(4)} = \frac{F_{i+1} - F_{i-1}}{2\Delta x} + \theta \frac{F_{i-2} - 3F_{i-1} + 3F_i - F_{i+1}}{3\Delta x}$$

and if u is negative

$$L_x^{(4)} = \frac{F_{i+1} - F_{i-1}}{2\Delta x} + \theta \frac{F_{i-1} - 3F_i + 3F_{i+1} - F_{i+2}}{3\Delta x}$$

These discretizations have a truncation error $O\left(\Delta x^2\right)$ for any θ except for $\theta = 0.5$ when they are $O\left(\Delta x^3\right)$.

The Burger's equation: Nonlinear equation

The Lax-Wendroff scheme is

$$u_i^{n+1} = u_i^n - \frac{\Delta t}{2\Delta x}\left(F_{i+1}^n - F_{i-1}^n\right) + \frac{1}{2}\left(\frac{\Delta t}{\Delta x}\right)^2 \Big(A_{i+\frac{1}{2}}\left(F_{i+1}^n - F_i^n\right) - A_{i-\frac{1}{2}}\left(F_i^n - F_{i-1}^n\right)\Big) + \nu \frac{u_{i-1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2},$$

where $A_{i+\frac{1}{2}} = u_{i+\frac{1}{2}} = \frac{1}{2}\left(u_i + u_{i+1}\right)$.

The scheme is stable if $|u_{\max}\Delta t/\Delta x| \leq 1$.

The Crank-Nicolson method is

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} = -\frac{1}{2}\left(\frac{-F_{i-1}^n+F_{i+1}^n}{2\Delta x}+\frac{-F_{i-1}^{n+1}+F_{i+1}^{n+1}}{2\Delta x}\right) + \frac{1}{2}\left(\frac{u_{i-1}^n-2u_i^n+u_{i+1}^n}{\Delta x^2}+\frac{u_{i-1}^{n+1}-2u_i^{n+1}+u_{i+1}^{n+1}}{\Delta x^2}\right) \ ,$$

which can be rewritten as,

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

where

$$\Delta u_i^{n+1} = u_i^{n+1}-u_i^n \ , \ \ L_x F_i^n = \frac{F_{i+1}^n-F_{i-1}^n}{2\Delta x} \ , \ \ L_{xx}u_i^n = \frac{u_{i-1}^n-2u_i^n+u_{i+1}^n}{\Delta x^2}$$

The appearance of the nonlinear implicit term F_i^n poses a problem. To overcome it we use the Taylor expansion

$$F_i^{n+1} = F_i^n + \Delta t \left(\frac{\partial F}{\partial t}\right)_i^n + \frac{1}{2}\Delta t^2 \left(\frac{\partial^2 F}{\partial t^2}\right)_i^n + \cdots$$

that is,

$$F_i^{n+1} = F_i^n + A\Delta u_i^{n+1} + O\left(\Delta t^2\right) \ .$$

We obtain the following tridiagonal algorithm,

$$\frac{\Delta u_i^{n+1}}{\Delta t} = -\frac{1}{2}L_x\left(2F_i^n + u_i^n \Delta u_i^{n+1}\right) + \frac{1}{2}L_{xx}\left(u_i^n + u_i^{n+1}\right) \ ,$$

which can be rewritten as,

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

Systems of equations

For example, we can consider unsteady compressible inviscid flow, which is governed by a system of three equations: continuity, x-momentum and energy. After a suitable non-dimensionalisation the system of equations can be written as

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

where

$$\vec{q} = \begin{pmatrix} \rho \\ \rho u \\ \frac{p}{\gamma(\gamma-1)} + \frac{1}{2}\rho u^2 \end{pmatrix} \ , \quad \vec{F} = \begin{pmatrix} \rho u \\ \rho u^2 + \frac{p}{\gamma} \\ \left(\frac{p}{\gamma-1} + \frac{1}{2}\rho u^2\right) u \end{pmatrix} \ ,$$

where q is the density, u is the velocity, p is the pressure and γ is the specific heat ratio.

Systems of equations

For this problem, the two-stage Lax-Wendroff method is of the form

$$
\begin{aligned}
\vec{q}^{\,*}_{i+\frac{1}{2}} &= \frac{1}{2}\left(\vec{q}^{\,n}_i + \vec{q}^{\,n}_{i+1}\right) - \frac{\Delta t}{2\Delta x}\left(\vec{F}^n_{i+1} - \vec{F}^n_i\right) \ , \\
\vec{q}^{\,n+1}_i &= \vec{q}^{\,n}_i - \frac{\Delta t}{\Delta x}\left(\vec{F}^*_{i+\frac{1}{2}} - \vec{F}^*_{i-\frac{1}{2}}\right)
\end{aligned}
$$

At each stage of the solution development, ρ, u and p are evaluated from $\vec{q}$ in such a way that the components of $\vec{F}$ can be determined.

Modified schemes to correct the dispersion error of the Lax-Wendroff method can be also applied.

Systems of equations

A crank Nicolson scheme will be

$$\vec{q}_i^{n+1} - \vec{q}_i^{n} = -\frac{\Delta t}{4\Delta x}\left(\left(\vec{F}_{i+1}^{n} - \vec{F}_{i-1}^{n}\right) + \left(\vec{F}_{i+1}^{n+1} - \vec{F}_{i-1}^{n+1}\right)\right) \ .$$

Making use of a multidimensional Taylor expansion

$$\vec{F}^{n+1} = \vec{F}^{n} + A\Delta\vec{q}^{n+1} + \cdots \ ,$$

the following scheme is obtained,

$$-\frac{1}{4}\frac{\Delta t}{\Delta x}A_{i-1}\Delta\vec{q}_{i-1}^{n+1} + I\Delta\vec{q}^{n+1} + \frac{1}{4}\frac{\Delta t}{\Delta x}A_{i+1}\Delta\vec{q}_{i+1}^{n+1}$$
$$= -\frac{1}{4}\frac{\Delta t}{\Delta x}\left(\vec{F}_{i+1}^{n} - \vec{F}_{i-1}^{n}\right) \ ,$$

which is a tridiagonal system for $\Delta\vec{q}_i^{n+1}$. The solution in the next step is

$$\vec{q}_i^{n+1} = \vec{q}_i^{n} + \Delta\vec{q}_i^{n+1}$$