Numerical Methods for time-dependent Partial Differential Equations

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Abstract
This is a summary of the course “Numerical Methods for time-dependent Partial Differential Equations” by P.A. Zegeling of spring 2009.

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1 General

1.1 Classification of PDEs

Second order equations of the form
\[ au_{xx} + bu_{xy} + cu_{yy} = f(u_x, u_y, x, y) \] (1)
can be categorized on the basis of the discriminant \( b^2 - 4ac \):

- \( b^2 < 4ac \): elliptic, e.g. a Poisson equation \( u_{xx} + u_{yy} = f(x, y) \)
- \( b^2 > 4ac \): hyperbolic, e.g. wave equation \( u_{tt} - u_{xx} = 0 \)
- \( b^2 = 4ac \): parabolic, e.g. (advection-)diffusion \( u_t + cu_x = \kappa u_{xx} \)

Parabolic equations often use a mixed set of conditions, namely an initial condition combined with a boundary condition. In order to solve a hyperbolic equation, two sets of initial conditions must be specified. Elliptic equations differ from the other two types of PDEs in that they typically involve only spatial coordinates. Because of this, the initial conditions become boundary conditions, i.e., the value of the function along the boundaries is completely specified.

1.2 Fourier domain

One can Fourier-transform the quantities \( u(x) = \int_{-\infty}^{\infty} \hat{u}(\xi)e^{i\xi x}d\xi \) of a linear PDE to arrive at an ODE, which can then be solved and transformed back to arrive at the solution of the initial PDE.

- hyperbolic - advection-equation: \( u_t + cu_x = 0 \) \( \rightarrow \hat{u}(\xi, t) + ci\xi \hat{u}(\xi, t) \rightarrow \hat{u}(\xi, t) = \hat{u}(\xi, 0)e^{-i\xi ct} \rightarrow u(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(\xi, 0)e^{i\xi (x-ct)}d\xi \). The solution moves to right without changing shape, only the phase of modes is modified
- parabolic - heat equation: \( u_t = \kappa u_{xx} = 0 \) \( \rightarrow \hat{u}(\xi, t) = -\kappa \xi^2 \hat{u}(\xi, t) \) showing exponential decay, with the highest decay rate for the highest frequencies

1.3 Method of undetermined coefficients

In this method derivatives are approximated by a linear combination of function values and the coefficients are chosen such that the result is exact for certain simple functions (linear, quadratic, etc). Expanding in Taylor series around \( x = x_0 \)

\[ u_{i+1} = u_i + hu_{x,i} + h^2u_{xx,i} + .. \] (2)
\[ u_i = u_i \] (3)
\[ u_{i-1} = u_i - hu_{x,i} + h^2u_{xx,i} + .. \] (4)
such that \( u_{xx,i} \approx Au_{i+1} + Bu_i + Cu_{i-1} = A(u_i + hu_{x,i} + h^2u_{xx,i} + ..) + Bu_i + Cu_i - hu_{x,i} + h^2u_{xx,i} + .. >. \) Collecting coefficients by their order in \( h \):
\[ A + B + C = 0, Ah + 0 - Ch = 0 \text{ and } Ah^2/2 + 0 + Ch^2/2 = 1 \text{ such that} \]
\[ u_{xx|1} \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} \quad (5) \]

The error term or local truncation error (LTE) \( \tau = Ah^4/24 + Ch^4/24 \) \( u_{xxxx,i} = h^2/12u_{xxxx,i} + \ldots \). This finite difference (FD) scheme is said to be of order two in space, or \( \mathcal{O}(\Delta x^2) \). Here

\[ f(s) = \mathcal{O}(\phi(s)) \text{ if } \exists \text{ a constant } A \text{ such that } |f(s)| \leq A |\phi(s)| \quad \forall s \in S \quad (6) \]

Note that \( A \) can be very large, especially in problems where the solutions change rapidly in time. A scheme is said to be consistent if in the limit \( \Delta x \to 0 \) the finite difference operators converge to the continuous operators.

### 1.4 Equivalence theorem

- The Lax Equivalence theorem for linear PDEs: consistency (local error) + stability ⇔ convergence (global error)

- Lax-Richtmeyer Equivalence theorem: given a well-posed linear hyperbolic PDE and its FD approximation which satisfies the consistence condition, then stability is the necessary and sufficient condition for convergence

### 1.5 Method of lines

In this method one discretizes in space first and then integrates in the time direction to obtain the solution. It is easy to implement, just use your favourite time integration method, it is transparent for understanding stability aspects but it is not as efficient as specially designed methods that discretize in space and time simultaneously. As an illustration of this method, the FTCS scheme for the heat equation (see Ch. 2) can be written

\[ \frac{u(t + \Delta t) - u(t)}{\Delta t} = Au(t) \quad (7) \]

### 1.6 Stability

#### 1.6.1 Eigenvalue method

Consider the eigenvalue problem \( \hat{u}(t) = \lambda u(t) \) with \( u(0) = u_0 \) with the exact solution consisting of oscillations or exponential growth/decay depending on \( \lambda \in \mathbb{C} \). Discretizing using EF gives at a time \( t = n\Delta t \) the solution \( u^n = u_0(1 + \lambda\Delta t)^n \). This solution by EF is stable for \( |1 + \lambda \Delta t| \leq 1 \) constituting a circular stability region centred around \( z = \lambda \Delta t = 1 \). After discretizing a particular equation in space one generally obtains a matrix analogue of the discussed 1D-example: \( \hat{u} = Au \). In this case a similar stability analysis can be made, but now using the eigenvalues of the matrix \( A \):

- A method is stable of \( \lambda \Delta t \in S \), where \( \lambda \) is any eigenvalue of \( A \) and \( S \) = stability region of the ODE method.
The eigenvalues of the matrix A depend on the equation you are solving and the scheme that is used. For the Forward in Time Central in Space (FTCS) discretization of the heat equation the eigenvalues are 

\[ \lambda_p = \frac{4}{\Delta x^2} \sin^2 \frac{p \Delta x}{2} \]

along the negative real axis. The method using EF is therefore stable for \( -\frac{\Delta t}{\Delta x^2} \leq \frac{1}{2} \), constituting a severe restriction.

The following examples are discussed further in Ch. 2. Here we just note the stability region of the time integration with \( z \equiv \Delta t \):

- **FTCS:** 
  \[ S = \{ z \in \mathbb{C} | |1 + z| \leq 1 \} \]

- **Crank-Nicolson:** 
  \[ S = \{ z \in \mathbb{C} | \Re\{z\} \leq 0 \} \]

- **BTCS:** 
  \[ S = \{ z \in \mathbb{C} | \frac{1}{1 - z} \leq 1 \} \]

### 1.6.2 Von Neumann stability analysis

Assume the distribution of errors along the coordinate \( x \) at time level \( n \) is given by a Fourier series in \( x \):

\[ \varepsilon^n(x) = e^{at} \sum_{m \geq 0} e^{i\xi_m x} \quad (8) \]

When the finite difference equations are linear, the behaviour of each separate term of the series \( \sim \) behaviour of the whole series. Just dealing with one term of the series, one inserts \( \varepsilon^n_m = e^{at} e^{i\xi_m x} \) in the FD equation. We have

\[ g \equiv \left| \frac{\varepsilon_{n+1}^m}{\varepsilon^n_m} \right| = e^{at} \quad (9) \]

where the amplification factor should be \( g \leq 1 \) for stability. As an example we consider the FTCS discretization of the heat equation. We assume \( u^n_j = U^n_j + \varepsilon^n_j \) with \( U \) the exact solution of the discretized equation and \( \varepsilon^n_j \) the round-off error. Inserting \( u_j \) into the discretized equations and subtracting the same equation, only now with the exact solution \( U^n_j \) inserted, yields by linearity only the difference

\[ \frac{\varepsilon^{n+1}_j - \varepsilon^n_j}{\Delta t} = \kappa \frac{\varepsilon^{n+1}_j - 2\varepsilon^n_j + \varepsilon^{n-1}_j}{(\Delta x)^2} \quad (10) \]

Inserting \( \varepsilon^n_j = e^{at} e^{i\xi_m x} \) and dividing by \( e^{at} e^{i\xi_m x} \) gives

\[ \frac{e^{a\Delta t} - 1}{\Delta t} = \kappa \frac{e^{i\xi_m \Delta x} - 2 + e^{-i\xi_m \Delta x}}{(\Delta x)^2} \quad (11) \]

The growth factor is thus \( e^{at} = 1 - \frac{4\kappa \Delta t}{(\Delta x)^2} \sin (\xi_m \Delta x/2)^2 \), thereby yielding the same result for stability as the eigenvalue method. The criterion \( g \leq 1 \) yields \( \kappa \Delta t/(\Delta x)^2 \leq 1/2 \), the familiar result.

### 1.7 Numerical diffusion

Several FD schemes that are consistent with the equation they are intended to solve actually solve a ‘modified’ equation with an extra diffusion-like term. For positive diffusion constant this enhances the stability properties of the scheme.
When this “numerical diffusion constant” however becomes negative, the scheme is rendered unconditionally unstable. Some examples of occurring numerical diffusion constants $\epsilon$ are in the Lax-Friedrichs scheme (LF), the Lax-Wendroff scheme (LW) and the upwind scheme (upw)

$$\varepsilon_{LF} = \frac{(\Delta x)^2}{2\Delta t}, \varepsilon_{LW} = \frac{c^2 \Delta t}{2}, \varepsilon_{upw} = \frac{c \Delta x}{2}$$

1.8 CFL condition

Courant-Friedrichs-Lewy (1928) stated that for stability: the CFL number $\sigma = c \Delta t / \Delta x$ has to be chosen such that the “domain of dependence” of the PDE, the characteristic lines has to be within the “domain of dependence” of the FD-scheme. This implies that the FD-scheme must include all physical information which influences the system at $x_j, t^{n+1}$. The collection of points in (x,t)-space needed in the evaluation of one new value of the solution is called the “stencil” of the scheme. By the CFL criterion the width of the stencil in the x-direction at a time $t - \Delta t$, cannot be larger than $c \Delta t$

This criterion is necessary, not sufficient for stability. It is however sufficient for LF and upwind. Usually it overlaps with the stability criterion resulting from a von Neumann analysis.
2 Various schemes

2.1 Heat equation

\[ u_t = \kappa u_{xx} \]  

- Forward Time Centred Space (FTCS):

\[ \frac{u_i^{n+1} - u_i^n}{\Delta t} = \kappa \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2} \]  

\[ \tau = O(\Delta t, \Delta x^2) \]

- Backward Time Centred Space (BTCS):

\[ \frac{u_i^{n+1} - u_i^n}{\Delta t} = \kappa \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2} \]  

This is an implicit method. It is unconditionally stable, as is easily obtained using a von Neumann stability analysis. Each time step the matrix equation \( Au_{n+1} = u_n \) has to be solved, where \( A \) is a tridiagonal matrix with non-zero elements \(-\mu, 1 + 2\mu\) and \(-\mu\), where \( \mu = \kappa \Delta t / (\Delta x)^2 \)

- Leapfrog:

\[ \frac{u_i^{n+1} - u_i^n}{2\Delta t} = \kappa \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2} \]  

\[ \tau = O(\Delta t^2, \Delta x^2) \]  

For this three-level scheme extra starting values are needed. It can be shown to be unconditionally unstable for the heat equation. It is however still occasionally used by some people, and it might work for small times.

- Dufort-Frankel:

\[ \frac{u_i^{n+1} - u_i^n}{2\Delta t} = \kappa \frac{u_{i+1}^{n+1} - u_i^{n+1} - u_{i-1}^{n+1} + u_{i-2}^{n+1}}{\Delta x^2} \]  

This scheme is inconsistent for \( \Delta t / \Delta x \equiv \beta = \text{constant} \). It actually solves \( u_t + \beta^2 u_{tt} = \kappa u_{xx} \). \( \tau = O(\Delta t^2, \Delta x^2) - u_{tt} \mid_n^{n+1} \)

- Crank-Nicolson (or trapezoidal):

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

\[ \tau = O(\Delta t^2, \Delta x^2) \]  

This scheme is implicit, one needs to solve a tridiagonal linear system for \( u_i^{n+1} \).

In two dimensions one just uses the same second derivative discretization as one would use in one dimension to evaluate \( \nabla^2 u \), keeping the \( y \)-index \( j \) fixed in evaluating \( u_{xj} \) and keeping the \( x \)-index \( i \) fixed in evaluating \( u_{yj} \) to obtain a FD equation for \( u_{ij}^n \). Using EF on a rectangular grid with grid size \( h \) yields a stability criterion of \( \kappa \Delta t / h^2 \leq 1/4 \), i.e. two times as strict as in one dimension. A better choice would be a trapezoidal (CN) time integration, which is unconditionally stable and second order accurate in time. This requires, however, an expensive matrix inversion with a sparse matrix which is no longer tridiagonal, but consists of three non-zero element ‘bands’. Perhaps a better option is
Alternative direction scheme. This is an example of a splitting method which uses two half-time steps

\[
\frac{u_{j,k}^{n+1/2} - u_{j,k}^n}{\Delta t/2} = \frac{\kappa}{(\Delta x)^2} \delta_x^2 u_{j,k}^{n+1/2} + \frac{\kappa}{(\Delta y)^2} \delta_y^2 u_{j,k}^n
\]  

(19)

\[
\frac{u_{j,k}^{n+1} - u_{j,k}^{n+1/2}}{\Delta t/2} = \frac{\kappa}{(\Delta x)^2} \delta_x^2 u_{j,k}^{n+1/2} + \frac{\kappa}{(\Delta y)^2} \delta_y^2 u_{j,k}^{n+1}
\]  

(20)

where in the first step \(u_{j,k}^{n+1/2}\) has to be found implicitly, but can then be directly used in the second half-time step where \(u_{j,k}^{n+1}\) is obtained implicitly. One thus has to solve a tridiagonal matrix equation twice. Although both steps separately have their own stability criterion, the combined method for a full time step is unconditionally stable.

2.2 Linear Advection equation

\[
\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0
\]  

(21)

When the advection speed \(c\) is a function of \(x\), discontinuities can arise. Take e.g. \(c(x) = \sin x\). The solution then has characteristics \(X(t) = t \sin x + X(0)\) because, using the chain rule, \(u(X(t), t)\) is constant in time. Take e.g. two characteristics with \(X(0) = \pi\) and \(X(0) = \pi - \varepsilon\) such that for \(t = \varepsilon/(\sin \pi - \varepsilon)\) the two characteristics “meet”. I.e. starting from different initial conditions, the two solutions converge to the same point leading to a discontinuity.

- Forward Time Centred Space (FTCS):

\[
\frac{u_{j,k}^{n+1} - u_{j,k}^n}{\Delta t} = \frac{c}{2\Delta x} (u_{i+1}^n - u_{i-1}^n)
\]  

(22)

Although consistent, this scheme is unconditionally unstable. This can be understood from evaluating the LTE = \(-\frac{\Delta t}{2} u_{tt}^n + \ldots\), which, with from the advection equation itself \(u_{tt} = c^2 u_{xx}\), implies some numerical diffusion with a negative sign, i.e. trouble.

- Lax-Friedrichs:

\[
u_{i,j}^{n+1} = \frac{1}{2} (u_{i,j-1}^n + u_{i,j+1}^n) - \frac{c\Delta t}{2\Delta x} (u_{i+1}^n - u_{i-1}^n)
\]  

(23)

This scheme is obtained by replacing \(u_i^n\) with an average value \(u_{i,j}^{n+1} = \frac{1}{2} (u_{i,j-1}^n + u_{i,j+1}^n)\) in the FTCS method. Because \(\frac{1}{2} (u_{i,j-1}^n + u_{i,j+1}^n) = u_{i,j}^n + \frac{1}{2} (u_{i,j-1}^n - 2u_i^n + u_{i,j+1}^n)\) some artificial diffusion is added and one actually solves the advection-diffusion equation with diffusion constant \(\varepsilon = (\Delta x)^2/2\Delta t\). The method can be written as \(\dot{u}(t) = Bu(t)\) with \(B\) a matrix consisting of \(-c^2/2\Delta x\) times the skew-symmetric tridiagonal (-1,0,1) matrix plus \(\varepsilon/(\Delta x)^2\) times the symmetric (1,-2,1) matrix, yielding eigenvalues \(\lambda_p = \frac{c^2}{2\Delta x} \sin 2\pi p \Delta x - \frac{2\varepsilon}{(\Delta x)^2} (1 - \cos 2\pi p \Delta x)\). The eigenvalues no longer lie along the imaginary axis in the \(z = \lambda\Delta t\)-plane, but form an ellipse with centre and radius given by \(\frac{2c\Delta t}{(\Delta x)^2}\) such that for \(c\Delta t/\Delta x \leq 1\) they all lie within the EF stability region, rendering the method conditionally stable.
Some second order in space and time options

- Crank Nicolson trapezoidal method for \( \dot{\mathbf{u}} = A\mathbf{u} \)

- Two-level explicit:

\[
  u_{j}^{n+1} = u_{j}^{n} - \frac{c\Delta t}{2\Delta x} (u_{j+1}^{n} - u_{j-1}^{n}) + \frac{c^{2}(\Delta t)^{2}}{8(\Delta x)^{2}} (u_{j+2}^{n} - 2u_{j}^{n} + u_{j-2}^{n}) \tag{24}
\]

This scheme has a five-point stencil and requires additional boundary conditions. The method is obtained from taking another time derivative of the system \( \dot{\mathbf{u}} = A\mathbf{u} \) yielding \( \ddot{\mathbf{u}} = A^{2}\mathbf{u}(t) \) which gives a second order method

\[
  \mathbf{u}_{n}^{n+1} = \mathbf{u}_{n}^{n} + \Delta t \mathbf{A}\mathbf{u}_{n}^{n} + \frac{1}{2}(\Delta t)^{2}A^{2}\mathbf{u}(t) \tag{25}
\]

- Lax-Wendroff

\[
  u_{j}^{n+1} = u_{j}^{n} - \frac{c\Delta t}{2\Delta x} (u_{j+1}^{n} - u_{j-1}^{n}) + \frac{c^{2}(\Delta t)^{2}}{2(\Delta x)^{2}} (\frac{u_{j+1}^{n+1} - 2u_{j}^{n+1} + u_{j-1}^{n+1}}{\Delta x}) \tag{25}
\]

This scheme can be obtained by Taylor expanding the advection equation, replacing \( u_{t} \) by \(-cu_{x}\) and \( u_{tt} \) by \( c^{2}u_{xx} \) using central FDs and in the time direction EF. This scheme actually solves the equation \( u_{t} + cu_{x} = -(1/6)c(\Delta x)^{2}(1 - (c\Delta t/\Delta x)^{2})u_{xxx} \) to third order, thereby showing some artificial numerical dispersion due to the non-zero right hand side. The resulting oscillations lag behind the solution due to the negative sign, and are damped by a term proportional to \( u_{xxx} \) in the modified equation.

Upwind methods use different spatial discretizations depending on the (local) sign of \( c \).

- First order upwind. For \( c > 0 \) it is just FTFS

\[
  u_{j}^{n+1} = u_{j}^{n} - \frac{c\Delta t}{\Delta x} (u_{j}^{n} - u_{j-1}^{n}) \tag{26}
\]

When \( c > 0 \), FTBS is used. The scheme is only first order accurate in both space and time. Note that the right hand side can be written as

\[
  u_{j}^{n} - \frac{c\Delta t}{2\Delta x} (u_{j+1}^{n} - u_{j-1}^{n}) + \frac{c^{2}(\Delta t)^{2}}{2(\Delta x)^{2}} (u_{j+1}^{n+1} - 2u_{j}^{n+1} - u_{j-1}^{n+1})
\]

so that a numerical diffusion term with diffusion coefficient \( \varepsilon_{upw} = c\Delta x/2 \) is introduced. One can even show that upwind schemes for the advection equation, to first order, actually solve a modified advection-diffusion equation to second order accuracy. Note that for \( c < 0 \) this becomes negative diffusion, showing that the displayed FTBS can only stably be used for \( c > 0 \).

- Beam-Warming method: second order upwind. Again, for \( c > 0 \)

\[
  u_{j}^{n+1} = u_{j}^{n} - \frac{c\Delta t}{2\Delta x} (3u_{j}^{n} - 4u_{j-1}^{n} + u_{j-2}^{n}) + \frac{1}{2}c^{2} (\frac{\Delta t}{\Delta x})^{2} (u_{j-1}^{n} - 2u_{j-2}^{n} + u_{j-3}^{n}) \tag{27}
\]

The derivation goes analogously to that of the Lax-Wendroff scheme, using a one-sided approximation for spatial derivatives. It is stable for \( 0 \leq c\Delta t/\Delta x \leq 2 \). The modified equation for this equation is \( u_{t} + cu_{x} = \frac{1}{2}c(\Delta x)^{2}(2 - \frac{3c\Delta t}{\Delta x} + (\frac{c\Delta t}{\Delta x})^{2})u_{xxx} \)

Note that it can be proven that there exist no explicit unconditionally stable FD schemes for solving hyperbolic PDEs.
2.3 Non-linear advection equation

\[ u_t + F(u)_x = 0 \] (28)

An example is the conservative form of the Burger’s equation in which
\[ F(u) = \frac{1}{2} u^2. \]
Performing the differentiation, the non-conservative form \( u_t + uu_x = 0 \) is obtained. The characteristics satisfy \( x(t)' = u(x(t), t) \).

• Two “natural” discretizations are

\[ u_j^{n+1} = u_j^n - \frac{\Delta t}{\Delta x} u_j^n (u_j^n - u_{j-1}^n) \] (29)

With \( k = j \) this gives a wrong solution. With \( k = j - 1 \) it gives a better solution, but with the wrong wave speed.

• Lax-Friedrichs

\[ u_j^{n+1} = \frac{1}{2} (u_{j+1}^n + u_{j-1}^n) - \frac{\Delta t}{4\Delta x} ((u_{j+1}^n)^2 - (u_{j-1}^n)^2) \] (30)

which yields the correct speed.

• Non-linear Lax-Wendroff

\[ u_j^{n+1} = u_j^n - \Delta t \frac{F_{j+1}^n - F_{j-1}^n}{2\Delta x} + \frac{(\Delta t)^2(\Delta x)^2}{2} \left[ F'(u_{j+\frac{1}{2}}) (F_{j+1}^n - F_{j}^n) - F'(u_{j-\frac{1}{2}}) (F_{j}^n - F_{j-1}^n) \right] \] (31)

This scheme is obtained using a second order Taylor expansion and substituting \( u_{tt} = \partial_t (-F(u)_x) = - \partial_x (F(u)_t) = .. = \partial_x Q \) with \( Q \equiv F'(u) \partial_x F(u) \). Furthermore one uses central differences (CD), a whole step for \( \partial_x F \) and half step for \( \partial_x Q \), using \( Q_{j+\frac{1}{2}} = F'(u_{j+\frac{1}{2}}) (F_{j+1}^n - F_{j}^n) / \Delta x \). Note that for \( F(u) = cu \) the linear Lax-Wendroff result is obtained.

2.4 Wave equation

\[ \frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \] (32)

The general solution in terms of initial shape and time-derivative of wave \( u(x, 0) = f(x) \) and \( u_t(x, u) = g(x) \) is obtained from solving for d’Alembert’s solution \( G(x - ct) + F(x + ct) \) to yield \( u(x, t) = \frac{1}{2} (f(x - ct) + f(x + ct)) + \frac{1}{c} \int_{x-ct}^{x+ct} g(s) \, ds \).

Using central differences for both second derivatives yields

\[ u_j^{n+1} = \sigma^2 u_{j+1}^n + 2(1 - \sigma^2) u_j^n + \sigma^2 u_{j-1}^n - u_j^{n-1} \] (33)

To get this scheme started, however, one needs \( u_1^1 \) which, if calculated using \( u_j = f_j + \Delta t \), renders the whole scheme first order accurate in time. It is
therefore better to use 
\[ u_j^1 = f_j + \Delta t g_j + \frac{\sigma^2}{2(\Delta x)^2} (f_{j+1} - 2f_j + f_{j-1}) = \frac{1}{2}\sigma^2f_{j+1} + (1 - \sigma^2)f_j + \frac{1}{2}\sigma^2f_{j-1} + \Delta t g_j \]

preserving the \( O(\delta x^2) + O(\Delta t^2) \) accuracy of the central difference scheme.

### 2.5 Advection-diffusion equation

\[ u_t + cu_x - \varepsilon u_{xx} = 0 \quad (34) \]

For the standard CD discretization it can be proven that a sufficient criterion for which \( u_{j}^n \) remains positive is \( \Delta t \leq \frac{(\Delta x)^2}{2\varepsilon} \) and the mesh Peclet number \( Pe_m \equiv \frac{|c|\Delta x}{\varepsilon} \leq 2 \).

The steady state version has, with \( u(0) = 0 \) and \( u(1) = 1 \), as exact solution 
\[ u(x) = (e^{c\xi} - 1)/(e^{\xi} - 1) \] yielding a ‘boundary layer’ of \( O(\xi/\varepsilon) \). The corresponding FD scheme using central differences has the exact solution 
\[ u_j = P_j - 1/(P_{N}-1) \]
with \( P_j = (1 + Pe^j_m)/(1 - Pe^j_m) \). For \( Pe^j_m > 1 \) one has \( P_j < 0 \) so that the numerical solution shows oscillations or wiggles, which can be shown to be associated with the combination of first and second derivatives in the original equation. The solution, circumventing the use of very small grid sizes, is using an upwind scheme with the same exact solution but with \( P_j = 1 + Pe^j_m \).

The wiggles are then absent, but at the cost of introducing some numerical diffusion.
3 Higher order methods

3.1 Finite Differences

Using Taylor expansions, higher order approximations can be found. As an example, an approximation of \( u_{xx} \) using the five values \( u_{j-2} \) to \( u_{j+2} \) has an error term of \( \mathcal{O}(\Delta x^6) \). At the boundaries one now needs additional values, which over determines the system rendering it ill-posed. Another downside is that the matrix becomes less sparse, making it computationally more expensive to invert.

3.2 Spectral methods

Finite element methods or spectral methods can also be used to obtain higher order accuracy. Spectral methods can be used when the function to be obtained is periodic over a certain interval, allowing a Fourier expansion to be inserted into the DE. Differentiating the expansion analytically yields an extra prefactor \( 2\pi ik/L \) while performing the differentiation by a central FD yields \((iN/L)\sin 2\pi k/N\) showing that a sufficient number of terms should be included for these two expressions to match. Applying the method to the heat equation yields for the coefficients \( a_k(t) = e^{-k^2t}a_k(0) \) where the initial coefficients can be obtained from an inverse FT. One can show that

\[
|u(x, t) - u^N(x, t)| = \sum_{k=N}^{\infty} a_k(0)e^{ikx}e^{-k^2t} \leq \max_{0 \leq x \leq 2\pi} |a_k(0)| \int_N^\infty e^{-tx^2} \, dx \quad (35)
\]

The convergence is thus determined by the complimentary error function.

3.3 Non-uniform grids

Using Taylor expansions to find a FD approximation to a first derivative yields a two point stencil \( u_i' = (u_{i+1} - u_{i-1})/(h_{i+1} + h_i) \) where, with \( h_i \equiv x_i - x_{i-1} \), the denominator is \( x_{i+1} - x_{i-1} \). The local truncation error is \( h_i^3/6(h_{i+1} + h_i) - h_i^3/6(h_{i+1} + h_i) + .. \) allowing one to choose the \( h_i \) such that the lowest order error term vanishes. This technique makes the error of higher order, which is called supra convergence.
4 Adaptive Mesh Refinement

Several types of Adaptive Mesh Refinement (AMR) variants exist

- H-refinement - specific cells are split up into smaller cells
- p-refinement - using finite elements, the degree of piecewise polynomials is varied per element
- r-refinement - nodes are moved around, while keeping the number of nodes constant

4.1 Mapping method

The idea considered here is to devise a mapping based on the numerical solution, which maps a non-uniform mesh in the physical space to a uniform grid on which the FD discretization is performed. Consider e.g. the advection-diffusion equation

\[ u_x = \varepsilon u_{xx} \] (36)

with \( u(0) = 0 \) and \( u(1) = 1 \). Define a transformation \( x \rightarrow \xi \in [0, 1] \) with \( v(\xi) \equiv u(x(\xi)) \) such that

\[ \frac{v_{\xi}}{x_{\xi}} = \frac{\xi}{x_{\xi}} \left[ \frac{v_{\xi \xi} x_{\xi} - v_{\xi} x_{\xi \xi}^2}{x_{\xi}} \right] \] (37)

Now when one chooses \( v(\xi) = \xi \), such that a uniform distribution of \( \xi \) yields a uniform distribution in \( v(\xi) = u(x(\xi)) \), the equation becomes \( \varepsilon x_{\xi \xi} + x_{\xi}^2 = 0 \) and \( x(0) = 0 \) and \( x(1) = 1 \). One has in general \( v_{\xi} = u_{\xi} x_{\xi} \) such that the particular mapping \( v(\xi) = \xi \) satisfies \( x_{\xi} u_{\xi} = 1 \). I.e. \( x_{\xi} \) is inversely proportional to the grid point concentration, where \( u_{\xi} \) is large as \( x_{\xi} \) is small as is desirable.

This example leads to a principle that could be used for other equations as well:

\[ x_{\xi} \omega = 1 \text{ or } (\omega x_{\xi})_{\xi} = 0 \] (38)

with \( \omega > 0 \) a ‘monitor function’ that is ideally some measure of the numerical error.

Using \( dx/d\xi = (d\xi/dx)^{-1} \) one obtains \( d\xi/dx = \omega \) or, with \( \xi(x_R) - \xi(x_L) = 1 \), after integrating \( c = 1/\int \omega dx \) or \( \frac{dx}{dx} = \frac{\omega(x)}{\int x L \omega dx} \), from which the inverse transformation is obtained

\[ \xi(x) = \frac{\int_{x_L}^{x} \omega(x')dx'}{\int_{x_L}^{x U} \omega(x')dx'} \] (39)

The Jacobian of the transformation \( dx/d\xi > 0 \) such that the transformation is regular, or non-singular. Note that the principle \( (\omega x_{\xi})_{\xi} = 0 \) is equivalent to minimization of the functional \( F = \int_{x_L}^{x U} \omega x_{\xi}^2 d\xi \), which can easily be derived from the Euler-Lagrange equations. The discussed principle is therefore analogous to the minimization of the energy of a spring system between the mesh points.
4.2 Equidistribution principle

In discrete terms the application of such a transformation \( d\xi/dx = \omega \) implies for the mesh size \( \Delta x_i = c/\omega_i \). Because \( \int_{x_i}^{x_{i+1}} \omega \, dx = c \) independent of \( i \)

\[
\int_{x_i}^{x_{i+1}} \omega \, dx = \frac{1}{N} \int_{x_1}^{x_N} \omega \, dx
\]

(40)

showing that \( \omega \) is equally distributed over all subintervals, a principle called the equidistribution principle. The equidistribution of the monitor function ensures \( \Delta x_i \) is small where \( \omega_i \) is large.

4.3 Choices of Monitor functions

- \( \omega = u_x \) In this case \( x \xi \omega = x \xi (v_\xi/x_\xi) = v_\xi \) such that the same change in the solution \( u \) occurs over each mesh interval. The downside is that the mesh elements become infinitely large when there is no variation in the solution.

- \( \omega = \sqrt{1 + u_x^2} \) From \( ds^2 = dx^2 + du^2 = dx^2(1 + u_x^2) \) this can be seen to be the arc length of the solution curve, thereby circumventing the problem of diverging mesh element sizes.

4.4 Possible Problems

- Big jumps in mesh size can deteriorate the accuracy of the scheme. The LTE of \( u_{x,i} \) \( \approx (u_{i+1} - u_{i-1})/((\Delta x_i + \Delta x_{i-1}) \), for example, is given by

\[
-\frac{1}{2} u_{xx,i}(1 - r \Delta x_i) - \frac{1}{2} u_{xx,i}(1 + r^2) \Delta x_i^2 + \ldots \] such that, when the ‘grid size ratio’ or ‘local stretching factor’ \( r \equiv \Delta x_{i-1}/\Delta x_i \), is \( r = 1 + O(\Delta x_i) \) the method is of second order. When \( r \) becomes too large, however, the method becomes first order. Now \( r = (x_i - x_{i-1})/(x_{i+1} - x_i) = (x_\xi \Delta \xi - \frac{1}{2} \Delta \xi^2 x_{\xi,i})/(x_\xi \Delta \xi + \frac{1}{2} \Delta \xi^2 x_{\xi,i}) + \ldots = 1 - \Delta x_i x_{\xi,i}/x_{\xi,i}^2 + \ldots \) such that \( \Delta x_i x_{\xi,i}/x_{\xi,i}^2 \) should be of order one to maintain the uniform-grid accuracy of the scheme. The grid is said to be ‘quasi uniform’.

- Taking the time-derivative of the following form of the equidistribution principle \( \int_{x_i}^{x_{i+1}(t)} \omega \, dx = (\frac{1}{N}) \omega \) gives \( \omega \dot{x}_i + \int_{x_i}^{x_{i+1}(t)} \partial_t \omega \, dx = (i/N) \dot{\omega}(t) \). Introducing small perturbations \( \delta x_i \) on the grid points \( x_i \) yields, up to first order, \( \omega \delta \dot{x}_i + (\partial_\omega \omega) \delta x_i \dot{\omega} \delta x_i + (\partial_t \omega) \delta x_i = 0 \), equivalent with \( (d/dt)[\omega \delta x_i] = 0 \), or

\[
\delta x_i(t) = \frac{\omega(x_i(0), 0)}{\omega(x_i(t), t)} \delta x_i(0)
\]

(41)

From this we see that \( \omega(x_i(0), 0)/\omega(x_i(t), t) \) should be smaller than one to ensure stability. A possibly resulting instability may be prevented by adding a small ‘delay’-term to the equidistribution principle.

The solution to these problems is to apply some type of ‘smoothing’ of the mesh in both space, to ensure quasi-uniformity, and time, to ensure stability. This is exemplified by the following numerical implementation involving spatial and temporal smoothing parameters \( \sigma \) and \( \tau_t \). Consider a 1D linear time
dependent advection-diffusion equation plus source term for the function $u(x)$. Let the transformation be the solution of

$$[(S(x_\xi + \tau_s x_\xi)|\omega]_\xi \quad \text{with}$$

$$\omega = \sqrt{1 + \sum_k \alpha_k (u_{x,k})^2} \quad \text{and} \quad S = 1 - \sigma (\sigma + 1)(\Delta \xi)^2 \frac{\partial^2}{\partial \xi^2}$$

Some properties of this choice include

- The Jacobian $J = x_\xi > 0$ such that no node crossing is possible
- $|x_\xi| \leq 1/\sqrt{\sigma (\sigma + 1)\Delta \xi}$ ensuring quasi-uniformity for $\sigma = O(1)$
- For $\tau_s = \sigma = 0$ the method equidistributes the arc length

One should choose ($0 \leq \tau_s \leq 10^{-3} \times$) physical time-scale, $\sigma = O(1)$ ($\sigma = 2$ usually suffices) and, $\alpha_k = O(1)$ depending on $x$ and $u_k$ scales. A semi-discretization of Eq. 42 is given by

$$\left[\Delta x_{i+1} + \tau_s \frac{d\Delta x_{i+1}}{d\theta}\right] \omega_{i+1} - \left[\Delta x_i + \tau_s \frac{d\Delta x_i}{d\theta}\right] \omega_{i+1} = 0$$

where $\Delta x_i = \Delta x_i - \sigma (\sigma + 1)(\Delta x_{i+1} - 2\Delta x_f + \Delta x_{i-1})$