

Asymptotic Behavior $f(t)$ is asymptotic to t means the following:

$$f(t) \sim t^2 \text{ as } t \rightarrow 0 \text{ means } t^{-2}f(t) \rightarrow 0 \text{ as } t \rightarrow 0$$

Equivalently, we write $f(t) = t^2 + o(t^2)$. Also, it could be the case:

$$f(t) = O(t^2) \text{ means } t^{-2}f(t) \text{ is bounded as } t \rightarrow 0$$

1 Floating Point Arithmetic

A **Floating Point Number System** is a finite subset of the reals defined by $\mathbb{F}(b, K, m, M)$ where b is the base of the system, K is the number of digits, m is the smallest exponent representable and M is the largest exponent representable.

If $y \in \mathbb{F}(b, K, m, M)$, then

$$y = \pm (0.d_1d_2d_3\dots d_K)_b \times b^E, m \leq M, d_1 \neq 0 \iff y = 0$$

1.1 Round-off Error

The error in representing $z \in \mathbb{R}$ by its nearest element in $\mathbb{F}(b, K, m, M)$. If $z \in \mathbb{R}$, then

$$fl(z) = \begin{cases} \pm (0.d_1d_2\dots d_K)_b \times b^E & d_{k+1} < \frac{b}{2} \\ \pm [(0.d_1d_2\dots d_K)_b + b^{-K}] \times b^E & d_{k+1} \geq \frac{b}{2} \end{cases}$$

IEEE Double precision (Used in MATLAB) is $b = 2$ and $K = 52$. In base 10, this is approximately $K \approx 16$, $m \approx -308$, and $M \approx 308$.

1.2 Relative error in rounding

Let $y \in \mathbb{R}, y \neq 0$. $fl(y) \in \mathbb{F}(b, K, m, M)$. Assume $d_{k+1} \leq \frac{b}{2}$

$$|fl(y)| = (0.d_1d_2\dots d_K)_b \times b^E$$

The **Relative error** is

$$\text{Rel error: } \frac{|y - fl(y)|}{|y|}$$

Since $|y| = (0.d_1d_2\dots d_kd_{k+1}\dots)_b \times b^E \geq (0.1)_b \times b^E = b^{E-1}$
and $|y - fl(y)| = (0.d_{k+1}d_{k+2}\dots)_b \times b^{E-k} \leq \frac{1}{2}b^{E-k}$ thus

$$\text{Rel error: } \frac{|y - fl(y)|}{|y|} \leq \frac{1}{2}b^{1-K} =_{\text{machine}}$$

This **Machine Epsilon** is the smallest representable number In IEEE DP, $b = 2$, and $K = 52$, so $\text{machine} = 2^{-52} \approx 2.2204 \times 10^{-16}$

1.3.1 Finite Difference Operators

Recall

$$f''(x) - \frac{1}{h^2} (f(x-h) - 2f(x) + f(x+h)) = -\frac{1}{12} h^2 f^{(4)}(\xi)$$

Assume the round off error $e(x-h)$ is in the evaluation of function values $f(x-h) = \tilde{f}(x-h) + e(x-h)$.

$$f''(x) - \frac{1}{h^2} (\tilde{f}(x-h) - 2\tilde{f}(x) + \tilde{f}(x+h)) = E_h = -\frac{1}{12} h^2 f^{(4)}(\xi) + \frac{1}{h^2} (e(x-h) - 2e(x) + e(x+h))$$

$$|E_h| \leq \frac{1}{12} h^2 |f^{(4)}(\xi)| + \frac{1}{h^2} (|e(x-h)| + |2e(x)| + |e(x+h)|)$$

Assume $|f^{(4)}(\xi)| \leq M$ for $\xi \in [x-h, x+h]$ and assume $|e(x)| \leq \epsilon$ for $x \in [x-h, x+h]$.

$$|E_h| \leq \frac{1}{12} h^2 M + \frac{1}{h^2} 4\epsilon$$

The first term shrinks but the second term blows up as $h \rightarrow 0$. One hopes to find the minimum at

$$h_{\text{optimal}} = \left(\frac{48\epsilon}{M} \right)^{\frac{1}{4}}$$

We could take ϵ to be $\epsilon_{\text{machine}}$

2 Polynomial Approximations

2.1 Taylor Expansion Theorem

The Taylor series expansion for a function f centered at α evaluated at z is

$$f(z) = \sum_{k=0}^{\infty} a_k (z - \alpha)^k \quad \text{where } a_k = \frac{f^{(k)}(\alpha)}{k!}$$

A Taylor polynomial is any finite truncation of this series:

$$f(z) = \sum_{k=0}^N a_k (z - \alpha)^k \quad \text{where } a_k = \frac{f^{(k)}(\alpha)}{k!}$$

The Taylor series is the limit of the Taylor Polynomials, given that the limit exists.

Analytic Functions A function that is equal to its Taylor Series in an open interval (or open disc in the complex plane), is known as an **Analytic Function**

Maclaurin Series If the Taylor series or Polynomial is centered at the origin ($\alpha = 0$), then it is also a Maclaurin series.

2.1.1 Important Taylor Series

The Maclaurin series for $(x-1)^{-1}$ is

$$(x-1)^{-1} = 1 + x + x^2 + x^3 + \dots = \sum_{k=0}^{\infty} x^k$$

3 Numerical Linear Algebra

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4 Solving $Ax = b$

4.1 Tridiagonal Solver

For a tridiagonal system of equations

$$A\vec{u} = \vec{f}, \quad A \text{ tridiagonal}$$

take $b_1 = c_n = 0$ and

$$A = LU = \begin{pmatrix} a_1 & c_1 & & \\ b_2 & a_2 & c_2 & \\ & \ddots & \ddots & \ddots \\ & & b_n & a_n \end{pmatrix} = \begin{pmatrix} 1 & & & \\ \beta_2 & 1 & & \\ & \ddots & \ddots & \\ & & \beta_n & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 & c_1 & & \\ & \alpha_2 & c_2 & \\ & & \ddots & \ddots \\ & & & \alpha_n \end{pmatrix}$$

So to solve $LU\vec{u} = \vec{f}$

1. Solve $L\vec{v} = \vec{f}$ using Forward Substitution
2. Solve $U\vec{u} = \vec{v}$ using Backward Substitution

4.1.1 Pseudocode

INPUT: $\vec{a}, \vec{b}, \vec{c}, \vec{f}$, all length n LU decomposition:

$\alpha_1 = a_1$

for $k = 2$ to n

$\beta_k = b_k \setminus \alpha_{k-1}$

$\alpha_k = a_k - \beta_k c_{k-1}$

end

Forward Substitution:

$v_1 = f_1$

for $k = 2$ to n

$v_k = f_k - \beta_k v_{k-1}$

end

Backward Substitution:

$u_n = v_n \setminus \alpha_n$

for $k = 2$ to n

$j = (n+1) - k$

$u_j = (v_j - c_j u_{j+1}) \setminus \alpha_j$

end

Operation count: $O(n)$

4.2 Spectral Decomposition Method

If $A \in \mathbb{C}^{m \times m}$ is Hermitian, we can do the following

1. Compute the spectral decomposition (not trivial when m is large)

$$A = UDU^*$$

2. Reform equation

$$A\vec{x} = UDU^*\vec{x} = \vec{b}$$

So we see

$$\vec{x} = \alpha_1 \vec{u}_1 + \alpha_2 \vec{u}_2 + \dots + \alpha_m \vec{u}_m \implies U^* \vec{x} = \vec{\alpha}$$

and

$$\vec{b} = \beta_1 \vec{u}_1 + \beta_2 \vec{u}_2 + \dots + \beta_m \vec{u}_m \implies \beta_k = \vec{u}_k^* \vec{b}$$

so

$$U^* \vec{b} = \vec{\beta} \text{ and } D\vec{\alpha} = \vec{\beta} \implies \vec{\alpha} = D^{-1} \vec{\beta}$$

but since $D_{ii}^{-1} = \frac{1}{\lambda_i}$,

$$\alpha_k = \frac{\vec{u}_k^* \vec{b}}{\lambda_k} \implies \vec{x} = \sum_{k=1}^m \left(\frac{\vec{u}_k^* \vec{b}}{\lambda_k} \right) \vec{u}_k$$

5 Finite Differences

Finite Differences seeks to approximate an ODE or PDE over a **mesh** or **grid**. The steps involved are:

1. Discretize the PDE using a difference scheme.
2. Solve the discretized PDE by iterating and/or time stepping.

5.1 Meshes

5.1.1 Uniform Meshes

Given a closed domain $\Omega = \bar{R} \times [0, t_F]$, we divide it into a $(J+1) \times (N+1)$ grid of parallel lines. Assume $\bar{R} = [0, 1]$. Given the mesh sizes $\Delta x = \frac{1}{J}$, $\Delta t = \frac{1}{N}$, a **mesh point** is

$$(x_j, t_n) = (j\Delta x, n\Delta t) \quad j = 0, \dots, J \quad n = 0, \dots, N$$

and $x_0 = 0$, $x_n = 1$

An alternative convention uses a $(J+2) \times (N+2)$ grid with the mesh sizes $\Delta x = \frac{1}{J+1}$, $\Delta t = \frac{1}{N+1}$. $x_0 = 0$, $x_{n+1} = 1$ are the boundary points. and

$$(x_j, t_n) = (j\Delta x, n\Delta t) \quad j = 0, \dots, J+1 \quad n = 0, \dots, N+1$$

We seek approximations to the solution at these mesh points, denoted by

$$U_j^n \approx u(x_j, t_n)$$

Where initial values are exact from the initial value function $u^0(x, t) = u(x, 0)$

$$U_j^0 = u^0(x_j) \quad j = 1, \dots, J-1$$

and boundary values are exact from the boundary value functions $f(t) = u(0, t)$ and $g(t) = u(1, t)$

$$U_0^n = f(t_n) \quad U_J^n = g(t_n) \quad n = 1, 2, \dots,$$

5.2 Difference Coefficients

$$D_+, D_-$$

5.3 Explicit Scheme

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A scheme is **explicit** if the solution at the next iteration (time level t_{n+1}) can be written as a single equation involving only previous time steps. This is, if it can be written in the form

$$U_j^{n+1} = \sum_i \sum_{k \leq n} a_{i,k} U_i^k + b_{i,k} f_i^k$$

Example For the Heat Equation $u_t = u_{xx}$, using a forward difference in time and a centered difference in space, we get

$$U_j^{n+1} = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n) \quad \mu := \frac{\Delta t}{(\Delta x)^2}$$

Pseudocode :

```
At  $n = 0$ ,  $U_j^0 = u^0(x_j, 0)$ 
for  $n = 1 : N$ 
   $U_0^n = 0, U_J^n = 0$ 
  for  $j = 1 : (J - 1)$ 
     $U_j^{n+1} = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n)$ 
  end
end
```

The **stability** of the problem depends on μ .

5.4 Truncation Error

Example For our model problem (the Heat Equation), the truncation error is

$$T(x, t) := \frac{D_{+t}u(x, t)}{\Delta t} - \frac{D_x^2 u(x, t)}{(\Delta x)^2}$$

So we see that since $u_t - u_{xx} = 0$,

$$T(x, t) = (u_t - u_{xx}) + \left(\frac{1}{2} u_{tt} \Delta t - \frac{1}{12} u_{xxxx} (\Delta x)^2 \right) + \dots = \left(\frac{1}{2} u_{tt} \Delta t - \frac{1}{12} u_{xxxx} (\Delta x)^2 \right) + \dots$$

If we truncate this Infinite Taylor series using $\eta \in (t, t + t\Delta t)$ and $\xi \in (x - \Delta x, x + \Delta x)$ and assume the boundry and initial data are consistent at the corners and are both sufficientl smooth, we can then estimate $|u_{tt}(x, \eta)| \leq M_{tt}$ and $|u_{xxxx}(\xi, n)| \leq M_{xxxx}$, so it follows that

$$|T(x, t)| \leq \frac{1}{2} \Delta t \left(M_{tt} - \frac{1}{6\mu} M_{xxxx} \right)$$

We can assume these bounds will hold uniformly over the domain. We see that

$$|T(x, t)| \rightarrow 0 \text{ as } \Delta t, \Delta x \rightarrow 0 \quad \forall (x, t) \in \Omega$$

and this result is independent of any relaton between the two mesh sizes. Thus this scheme is **unconditionally consistent** with the differential equation.

Since $|T(x, t)|$ will behave asymptotically like $O(\Delta t)$ as $\Delta t \rightarrow 0$, this scheme is said to have **first order accuracy**

Since $u_t = u_{xx}$, $u_{tt} = u_{xxxx}$ and so for $\mu = \frac{1}{6}$,

$$T(x, t) = \frac{1}{2} \Delta t \left(u_{tt} - \frac{1}{6\mu} u_{xxxx} \right) + O((\Delta t)^2) = O((\Delta t)^2)$$

and so the scheme is **second order accurate** for $\mu = \frac{1}{6}$

We can define notation: $T_j^n = T(x_j, t_n)$

5.5 Consistency

Does the difference scheme approximate the PDE as $\Delta x, \Delta t \rightarrow 0$?

A scheme is consistent if

$$T(x, t) \rightarrow 0 \text{ as } \Delta x, \Delta t \rightarrow 0$$

- A scheme is **unconditionally consistent** if the scheme is consistent for any relationship between Δx and Δt
- A scheme is **conditionally consistent** if the scheme is consistent only for certain relationships between Δx and Δt

5.6 Accuracy

Take μ finite, so $(\Delta t)^{\frac{a}{b}} = \mu(\Delta x)^{\frac{c}{d}}$, so $(\Delta t)^\alpha = (\Delta t)^{ad} = \mu^{bd}(\Delta x)^{cb}$ and we have

$$|T(x, t)| = O(\Delta t^\alpha)$$

- If $\alpha = 1$, the scheme is **first order accurate**.
- If $\alpha = 2$, the scheme is **second order accurate**.
- etc...
- The scheme is **α -order accurate**.

5.7 Convergence

A scheme is **convergent** if as $\Delta t, \Delta x \rightarrow 0$ for any fixed point (x^*, t^*) in the domain,

$$x_j \rightarrow x^*, t_n \rightarrow t^* \implies U_j^n \rightarrow u(x^*, t^*)$$

It suffices to show this for mesh points for sufficiently refined meshes, as convergence at all other points will follow from continuity of $u(x, t)$. We suppose that we can find a bound for the error \bar{T} :

$$|T_j^n| \leq \bar{T} < \infty$$

We denote the **error**

$$e_j^n := U_j^n - u(x_j, t_n)$$

Taking the difference between the scheme and $u(x_j, t^{n+1})$ in terms the truncation error and the exact solution at previous time steps yields the error at e_j^{n+1} . If the RHS of our difference scheme is represented by D , then

$$e_j^{n+1} = DU_j^n - (Du(x_j, t_n) + T(x_j, t_n)\Delta t) = De_j^n - T_j^n \Delta t$$

Choose μ such that the coefficients of the RHS are positive so that you may estimate $E^n := \max\{|e_j^n|, j = 0, \dots, J\}$ and so

$$E^{n+1} \leq E^n + \bar{T}\Delta t \text{ s.t. } E^0 = 0$$

and thus

$$E^n \leq n\bar{T}\Delta t \quad n = 0, 1, 2, \dots$$

and considering the domain

$$E^n \leq \bar{T}t_F \quad n = 0, 1, 2, \dots, N$$

and since $\bar{T} \rightarrow 0$ as $\Delta t, dx \rightarrow 0$, $E^n \rightarrow 0$

Example For Fourier Analysis with $u(x_j, t_n)$ in the definition of T_j^n we obtain

$$e_j^{n+1} = e_j^n + \mu D_x^2 e_j^n - T_j^n \Delta t$$

which is

$$e_j^{n+1} = (1 - 2\mu)e_j^n + \mu e_{j+1}^n + \mu e_{j-1}^n - T_j^n \Delta t$$

For $\mu \leq \frac{1}{2}$, define $E^n := \max \{|e_j^n|, j = 0, \dots, J\}$ and so

$$|e_j^{n+1}| \leq E^n + \bar{T} \Delta t \implies E^{n+1} \leq E^n + \bar{T} \Delta t$$

Since $E^0 = 0$ (the initial values are exact), we have

$$E^n \leq n \bar{T} \Delta t = \frac{1}{2} \Delta t \left(M_{tt} - \frac{1}{6\mu} M_{xxxx} \right) t_F \rightarrow 0 \text{ as } t \rightarrow 0$$

5.7.1 Refinement Path

A **refinement path** is a sequence of pairs of mesh sizes each which tends to zero

$$\text{refinement path} := \{((\Delta x)_i, (\Delta t)_i), i = 0, 1, 2, \dots; (\Delta x)_i, (\Delta t)_i \rightarrow 0\}$$

We can specify particular paths by requiring certain relationships between the mesh sizes.

Examples $(\Delta t)_i \sim (\Delta x)_i$ or $(\Delta t)_i \sim (\Delta x)_i^2$

Theorem For the heat equation, $\mu_i = \frac{(\Delta t)_i}{(\Delta x)_i^2}$ and if $\mu_i \leq \frac{1}{2} \forall i$ and if for all sufficiently large values of i and the positive numbers n_i, j_i are such that

$$n_i(\Delta t)_i \rightarrow t > 0, j_i(\Delta x)_i \rightarrow x \in [0, 1]$$

and if $|u_{xxxx}| \leq M_{xxxx}$ uniformly on Ω , then the approximations $U_{j_i}^{n_i}$ generated by the explicit scheme for $i = 0, 1, \dots$ converge to the solution $u(x, t)$ of the differential equation uniformly in the region.

This means that arbitrarily good accuracy can be attained by use of a sufficiently fine mesh.

5.8 Error: Fourier Analysis

Let

$$U_j^n = (\lambda)^n e^{ik(j\Delta x)}$$

where $\lambda(k)$ is known as the **amplification factor** of the **Fourier Node** U_j^n . Place this into the difference equation of your scheme and solve for λ . We then have another numerical approximation

$$U_j^n = \sum_{-\infty}^{\infty} A_m e^{-im\pi(j\Delta x)} (\lambda(k))^n$$

which can be compared to the Fourier expansion approximating the exact solution.

Example For $U_j^n = U_j^n + \mu(U_{j+1}^n - 2U_j^n + U_{j-1}^n)$, we see

$$\lambda(k) = 1 + \mu(e^{ik\Delta x} - 2 + e^{-ik\Delta x}) = 1 - 4\mu \sin^2\left(\frac{1}{2}k\Delta x\right)$$

So now

$$e^{-k^2\Delta t} - \lambda(k) = \left(1 - k^2\Delta t + \frac{1}{2}k^4\Delta t(\Delta t)^2 - \dots\right) - \left(1 - k^2\Delta t + \frac{1}{12}k^4\Delta t(\Delta x)^2 - \dots\right) = \left(\frac{(\Delta t)^2}{2} - \frac{\Delta t(\Delta x)^2}{12}\right)k^4 - \dots$$

Thus we have first order accuracy in general but second order accuracy if $(\Delta x)^2 = 6\Delta t$.

5.9 Stability

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A scheme is **stable** if there exists a constant K such that

$$|(\lambda)|^n \leq K, \quad n\Delta t \leq t_F, \quad \forall k$$

That is, if the difference in the solutions of the DE and the numerical DE is bounded uniformly in the domain for any amount of time less than t_F . Thus

$$|\lambda(k)| \leq 1 + K'\Delta t$$

This is necessary and sufficient.

5.10 Implicit Scheme

If the scheme cannot be written in a form that has U_j^{n+1} explicitly computed given values $U_j^n, j = 0, 1, \dots, J$, it is implicit. Implicit schemes involve more work but often have higher accuracy and/or stability, and thus much larger time steps allow us to reach the solution much more quickly.

Example

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j+1}^{n+1} - 2U_j^{n+1} + U_{j-1}^{n+1}}{(\Delta x)^2}$$

which can be written as

$$\Delta_t U_j^{n+1} = \mu \delta_x^2 U_j^{n+1} \quad \mu = \frac{\Delta t}{(\Delta x)^2}$$

This involves solving a system of linear equations. However, Fourier analysis for the stability shows

$$\lambda = \frac{1}{1 + 4 \sin^2 \left(\frac{1}{2} k \Delta t \right)}$$

Since $\lambda < 1$ for any positive μ , this scheme is **unconditionally stable**

5.11 Other Conditions

If an equation obeys extra conditions such as a Maximum Principle, uniqueness condition, or a physical constraint, the numerical scheme must also obey such conditions else it may not converge.

6 Methods

6.1 Weighted Average θ method

Given two schemes, you can weight one θ and the other with $(1 - \theta)$ and add them together. Then stability, coverage, and accuracy may depend on θ , and it can be chosen to

Example For the explicit and implicit first order accurate schemes for the heat equation are averaged, we have

$$U_j^{n+1} - U^n = \mu (\theta \delta_x^2 U_j^{n+1} + (1 - \theta) \delta_x^2 U_j^n)$$

$\theta = 0$ yields the explicit scheme and $\theta = 1$ yields the implicit scheme.

7 General Boundary Conditions

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Boundary conditions like

$$u_x = \alpha(t)u + g(t) \quad x = 0$$

Can be handled like

$$\frac{U_1^n - U_0^n}{\Delta x} = \alpha^n U_0^n + g^n \implies U_0^n = \beta^n U_1^n - \beta^n g^n \Delta t \quad \beta^n = \frac{1}{1 + \alpha^n \Delta x}$$

Dirichlet conditions are trivial

$$u(0, t) = 0 \implies U_0^n = 0$$

$$D_x^2 y_i = D_+ D_- y_i = \frac{1}{h^2} (y_{i+1} - 2y_i + y_{i-1})$$

$$y_{i\pm 1} = y_i \pm hy'_i + \frac{1}{2}h^2 y''_i \pm \frac{1}{6}h^3 y'''_i + \frac{1}{24}h^4 y''''_i \dots$$

$$D_x^2 y_i = \frac{1}{h^2} \left(y_i + hy'_i + h^2 y''_i + \frac{1}{6}h^3 y'''_i + \frac{1}{24}h^4 y''''_i - 2y_i + y_i - hy'_i + h^2 y''_i - \frac{1}{6}h^3 y'''_i + \frac{1}{24}h^4 y''''_i + \dots \right)$$

which simplifies to

$$D_x^2 y_i = y''_i + O(h^2)$$

Let $u_i \approx y_i = y(x_i)$

$$u_{xx} + q(x)u = f(x)$$

with $u(0) = \alpha$ and $u(1) = \beta$ becomes

$$\frac{-1}{h^2} (u_{i+1} - 2u_i + u_{i-1}) + q_i u_i = f_i$$

or

$$\begin{cases} -u_2 + (2 + h^2 q_1)u_1 = h^2 f_1 + \alpha & i = 1 \\ -u_{i+1} + (2 + h^2 q_i)u_i - u_{i-1} = h^2 f_i & 2 \leq i \leq n \\ (2 + h^2 q_n)u_n - u_{n-1} = h^2 f_n + \beta & i = n \end{cases}$$

where $u_0 = \alpha$ and $u_{n+1} = \beta$ we must solve

$$A_n \vec{u}_n = \begin{pmatrix} 2 + h^2 q_1 & -1 & & \\ -1 & 2 + h^2 q_2 & -1 & \\ & \ddots & \ddots & \ddots \\ & & -1 & 2 + h^2 q_n \end{pmatrix} \begin{pmatrix} u_1 \\ \vdots \\ \vdots \\ u_n \end{pmatrix} = \begin{pmatrix} h^2 f_1 + \alpha \\ h^2 f_2 \\ \vdots \\ h^2 f_n + \beta \end{pmatrix} = \vec{f}_n$$

Note: A_n is tridiagonal and symmetric. We can solve this by using $A_n = LU$

$$L\vec{v}_n = \vec{f}_n \quad U\vec{u}_n = \vec{v}_n$$

8 New Notes

9 Finite Difference Coefficients

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9.1 Centered Differences

For the difference scheme for the α derivative of f ,

$$f^{(\alpha)}(x_i) \approx D_h^\alpha f = \frac{1}{d} \frac{a_{i-4}f(x_{i-4}) + \dots + a_i f(x_i) + \dots + a_{i+4}f(x_{i+4})}{h^\alpha}$$

where d is the denominator to make the coefficients a_i integers. If we want the scheme to have accuracy β ,

$$f^{(\alpha)}(x_i) = D_h^\alpha f + Oh^\beta$$

Then the difference coefficients are given by

α	β	d	a_{i-4}	a_{i-3}	a_{i-2}	a_{i-1}	a_i	a_{i+1}	a_{i+2}	a_{i+3}	a_{i+4}
1	2	2				-1	0	1			
	4	12			1	-8	0	8	-1		
	6	60		-1	9	-45	0	45	-9	1	
	8	840	3	-32	168	-672	0	672	-168	32	-3
2	2	1				1	-2	1			
	4	12			-1	16	-30	16	-1		
	6	180		2	-27	270	-490	270	-27	2	
	8	5040	-9	128	-1008	8064	-14350	8064	-1008	128	-9
3	2	2			-1	2	0	-2	1		
	4	8		1	-8	13	0	-13	8	-1	
	6	240	-7	72	-338	488	0	-488	338	-72	7
4	2	1			1	-4	6	-4	1		
	4	6		-1	12	-39	56	-39	12	-1	
	6	240	7	-96	676	-1952	2730	-1952	676	-96	7

9.2 Forward/Backwards Differences

For the difference scheme for the α derivative of f ,

$$f^{(\alpha)}(x_i) \approx D_{\pm}^\alpha f = \frac{1}{d} \frac{a_i f(x_i) + \dots + a_{i\pm 4} f(x_{i\pm 4}) + \dots + a_{i\pm 8} f(x_{i\pm 8})}{h^\alpha}$$

where d is the denominator to make the coefficients a_i integers. If we want the scheme to have accuracy β ,

$$f^{(\alpha)}(x_i) = D_{\pm}^\alpha f + Oh^\beta$$

9.2 Forward/Backwards Differences

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When the difference coefficients are given by

α	β	d	a_i	a_{i+1}	a_{i+2}	a_{i+3}	a_{i+4}	a_{i+5}	a_{i+6}	a_{i+7}	a_{i+8}
1	1	1	∓ 1	± 1							
	2	2	∓ 3	± 4	∓ 1						
	3	6	∓ 11	± 18	∓ 9	± 2					
	4	12	∓ 25	± 48	∓ 36	± 16	∓ 3				
	5	60	∓ 137	± 300	∓ 300	± 200	∓ 75	± 12			
	6	60	∓ 147	± 360	∓ 450	± 400	∓ 225	± 72	∓ 10		
2	1	1	1	-2	1						
	2	1	2	-5	4	-1					
	3	12	35	-104	114	-56	11				
	4	12	45	-154	214	-156	61	-10			
	5	180	812	-3132	5265	-5080	2970	-972	137		
	6	180	938	-4014	7911	-9490	7389	-3616	1019	-126	
3	1	1	∓ 1	± 3	∓ 3	1					
	2	2	∓ 5	± 18	∓ 24	± 14	∓ 3				
	3	4	∓ 17	± 71	∓ 118	± 98	∓ 41	± 7			
	4	8	∓ 49	± 232	∓ 461	± 496	∓ 307	± 104	∓ 15		
	5	120	∓ 967	± 5104	∓ 11787	± 15560	∓ 12725	± 6432	∓ 1849	± 232	
	6	240	∓ 2403	± 13960	∓ 36706	± 57384	∓ 58280	± 39128	∓ 16830	± 4216	∓ 469
4	1	1	1	-4	6	-4	1				
	2	1	3	-14	26	-24	11	-2			
	3	6	35	-186	411	-484	321	-114	17		
	4	6	56	-333	852	-1219	1056	-555	164	-21	
	5	240	3207	-21056	61156	-102912	109930	-76352	33636	-8576	967

New Notes

10 Two Dimensional Problems

Given a problem

$$u_t = b(u_{xx} + u_{yy}) \quad \Omega = [0, X] \times [0, Y]$$

With initial conditions on Ω for $t = 0$ and boundary conditions on $\partial\Omega$

So for a uniform grid mesh

$$U_{i,j}^N \approx u(x_i, y_j, t_n) = u(i\Delta x, j\Delta y, n\Delta t), i = 0, 1, \dots, I, j = 0, 1, \dots, J, n = 0, 1, \dots, N$$

Explicit Scheme

$$\frac{U_{i,j}^{n+1} - U_{i,j}^n}{\Delta t} = b \left(\frac{\delta_x^2 U_{i,j}^n}{\Delta x^2} + \frac{\delta_y^2 U_{i,j}^n}{\Delta y^2} \right)$$

Consistency

$$T_{ij}^n = \left(\frac{1}{2} \Delta t u_{tt} - \frac{1}{12} b (\Delta x^2 u_{xxxx} + \Delta y^2 u_{yyyy}) \right)_{ij}^n + \dots$$

$$T_{ij}^n \approx O(\Delta t + \Delta x^2 + \Delta y^2)$$

Stability

$$U_{ij}^n \approx (\lambda)^n e^{i(k_x i \Delta x + k_y j \Delta y)}$$

????

Convergence The error estimate

$$e_{ij}^n = U_{ij}^n - u_{ij}^n$$

$$U_{ij}^n = U_{ij}^n + b (\mu_x \delta_x^2 U_{ij}^n + \mu_y \delta_y^2 U_{ij}^n)$$

$$e_y^{n+1} = e_y^n + b (\mu_x \delta_x^2 e_{ij}^n + \mu_y \delta_y^2 e_{ij}^n) - \Delta t T_{ij}^n$$

$$\mu_x = b \frac{\Delta t}{\Delta x^2}, \mu_y = b \frac{\Delta t}{\Delta y^2}$$

10.0.1 θ Scheme

Accuracy is $O(\Delta t + \Delta x^2 + \Delta y^2)$, but if $\theta = \frac{1}{2}$ we have the Crank-Nicholson Scheme with accuracy $O(\Delta t^2 + \Delta x^2 + \Delta y^2)$.

This requires to solve a system

$$A \vec{U}^{n+1} = \vec{b}^n$$

Where U_{ij}^n is reshaped into a vector.

10.1 Alternating Direction Implicit (ADI) Methods

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We see to modify the 2D problem so that we solve several 1D problems. We approximate the 2D Crank-Nicholson scheme

$$\left(1 - \frac{1}{2}\mu_x\delta_x^2\right)\left(1 - \frac{1}{2}\mu_y\delta_y^2\right)U_{ij}^{n+1} = \left(1 - \frac{1}{2}\mu_x\delta_x^2\right)\left(1 - \frac{1}{2}\mu_y\delta_y^2\right)U_{ij}^n \quad (1)$$

Note that

$$\left(1 - \frac{1}{2}\mu_x\delta_x^2\right)\left(1 - \frac{1}{2}\mu_y\delta_y^2\right) = 1 - \frac{1}{2}\mu_x\delta_x^2 - \frac{1}{2}\mu_y\delta_y^2 + \frac{1}{4}\mu_x\mu_y\delta_x^2\delta_y^2 \approx O(\Delta t T_{ij}^{n+\frac{1}{2}})$$

We solve for the intermediate solution

$$\left(1 - \frac{1}{2}\mu_x\delta_x^2\right)U_{ij}^{n+\frac{1}{2}} = \left(1 + \frac{1}{2}\mu_y\delta_y^2\right)U_{ij}^n \text{ using a system of equations. Then for the solution at the next step we must solve another system.}$$

Stability is based on Fourier Analysis on equation (??) and shows that this scheme is unconditionally stable.

Maximum principle on (??) yields that we require $\mu_x \leq 1$. The same analysis on (??) yields that we require $\mu_y \leq 1$. Thus we require $\max\{\mu_x, \mu_y\} \leq 1$.

Consistency

$$T_{ij}^{n+\frac{1}{2}} = \left(\frac{1}{24}\Delta t^2 u_{ttt} - \frac{1}{12}u_{xxxx} - \frac{1}{12}\Delta y^2 u_{yyyy} - \frac{1}{8}\Delta t^2 u_{xtt} - \frac{1}{8}\Delta t^2 u_{yzt} + \frac{1}{4}\Delta t^2 u_{xyzt}\right)_{ij}^{n+\frac{1}{2}} + \dots \approx O(\Delta t^2 + \Delta x^2 + \Delta y^2)$$

10.2 Locally One Dimensional (LOD) Scheme

We can expand this to 3D

$$u_t = b(u_{xx} + u_{yy} + u_{zz})$$

$$\begin{cases} \left(1 - \frac{1}{2}\mu_x\delta_x^2\right)U_{ij}^{n+*} = \left(1 + \frac{1}{2}\mu_x\delta_x^2\right)U_{ij}^n \\ \left(1 - \frac{1}{2}\mu_y\delta_y^2\right)U_{ij}^{n+**} = \left(1 + \frac{1}{2}\mu_y\delta_y^2\right)U_{ij}^{n+*} \\ \left(1 - \frac{1}{2}\mu_z\delta_z^2\right)U_{ij}^{n+1} = \left(1 + \frac{1}{2}\mu_z\delta_z^2\right)U_{ij}^{n+**} \end{cases}$$

11 First Order Problems

$$F(Du, u, x) = 0$$

In general there is no classical solution globally. Weak solutions may exist.

11.1 Method of Characteristics

$$\begin{aligned} z(s)u(x(s)), \vec{p}(s) &= Du(x(s)) \\ \begin{cases} \dot{x}(s) = D_{\vec{p}}F(\vec{p}(s), z(s), x(s)) \\ \dot{z}(s) = D_{\vec{p}}F(\vec{p}(s), z(s), x(s)) \cdot \vec{p}(s) \\ \dot{\vec{p}}(s) = -D_x F - D_z F \cdot \vec{p}(s) \end{cases} \end{aligned}$$

Model problem: Transport equation/advection equation

$$u_t + a(x, t)u_x \quad u(x, t=0) = u^0(x)$$

If a constant:
Upwind Scheme

$$\text{If } (a) = \pm 1, \frac{U_j^{n+1} - U_j^n}{\Delta t} + a \frac{\pm U_j^n \mp U_{j\mp 1}^n}{\Delta x} = 0$$

11.2 Schemes for Parabolic Equations

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Courant Friedrich Lowry (CFL) Condition for convergence

$$|v| \leq 1 \quad v = \frac{a\Delta t}{\Delta x} \text{ (CFL number)}$$

- The CFL is necessary but not sufficient for convergence.
- This ensures the domain of dependence of the scheme is a subset of the domain of dependence of the equation.

Characteristic Ray Tracing Method (Semi-Lagrangian Method)

11.2.1 Euler Schemes

Upwind Differencing Interpolate $U(x^*, t_n)$ with $\{U_j^n\}_{j=0}^J$

Forward Time - Backward Difference Scheme

....?

Higher Dimensions

$$u_t + au_x + bu_y = 0, \quad a, b > 0$$

Let $v_x = a \frac{\Delta t}{\Delta x}$, $v_y = b \frac{\Delta t}{\Delta y}$

$$\frac{U_{i,j}^{n+1} - U_{i,j}^n}{\Delta t} + a \frac{U_{i,j}^n - U_{i-1,j}^n}{\Delta x} + b \frac{U_{i,j}^n - U_{i,j-1}^n}{\Delta x} = 0$$

- CFL conditions: $|\nu_x| \leq 1$, $|\nu_y| \leq 1$
- We find that we require $\nu_x + \nu_y \leq 1$

Backward Time - Forward Difference Scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + a \frac{U_j^{n+1} - U_{j-1}^{n+1}}{\Delta x} = 0$$

Since the computational domain of dependence is a rectangle, CFL will be satisfied.

- Unconditionally stable

Forward Time - Central Difference Scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + a \frac{U_{j-1}^{n+1} - U_{j+1}^{n+1}}{2\Delta x} = 0$$

- Unconditionally unstable

Backward Time - Central Difference Scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + a \frac{U_{j-1}^{n+1} - U_{j+1}^{n+1}}{2\Delta x} = 0$$

- Unconditionally stable
- Accuracy is $O((\Delta x)^2)$

Lax-Wendroff

$$\left(-\frac{\nu^2}{2} - \frac{\nu}{2}\right) U_{j-1}^{n+1} + (1 + \nu^2) U_j^{n+1} + \left(-\frac{\nu^2}{2} - \frac{\nu}{2}\right) U_{j+1}^{n+1} = U_j^n$$

- Unconditionally Stable
- Accuracy $O((\Delta x)^2 + (\Delta t)^2)$

Crank-Nicolson

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + a \frac{1}{2} \left(\frac{U_{j-1}^{n+1} - U_{j-1}^n}{2\Delta x} + \frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x} \right) = 0$$

- Unconditionally Stable with $|\lambda| = 1$, so may become unstable due to roundoff error
- Accuracy $O((\Delta x)^2 + (\Delta t)^2)$

Lax Friedrichs Higher Dimensions

$$U_{i,j}^{n+1} = \frac{1}{4} (U_{i+1,j}^n + U_{i-1,j}^n + U_{i,j+1}^n + U_{i,j-1}^n) - \frac{1}{2} \nu_x (U_{i+1,j}^n - U_{i-1,j}^n) - \frac{1}{2} \nu_y (U_{i,j+1}^n - U_{i,j-1}^n)$$

- $\lambda = \frac{1}{2}(\cos(\xi) + \cos(\eta)) - i(\nu_x \sin(\xi) + \nu_y \sin(\eta))$
- $\nu_x^2 + \nu_y^2 \leq 1$

Euler Scheme

$$U_{ij}^{n+\frac{1}{2}} = U_{ij}^{n-\nu_x \Delta x_0} U_{ij}^n + \frac{1}{2} \nu_x^2 \delta_x^2 U_{ij}^n$$

$$U_{ij}^{n+1} = U_{ij}^{n+\frac{1}{2}} - \nu_y \Delta y_0 U_{ij}^{n+\frac{1}{2}} + \frac{1}{2} \nu_y^2 \delta_y^2 U_{ij}^{n+1}$$

- Accuracy $O((\Delta t)^2 + (\Delta x)^2 + (\Delta y)^2)$
- $\max\{|\nu_x|, |\nu_y|\} \leq 1$

Leap Frog

Beam Wamming?

12 2.20.2014

$$u_t + au_x + bu_y = 0$$

Method of Characteristics tells us

$$u(x, y, t) = u^0(x - at, y - bt),$$

Forward Time Upwind Scheme

$$U_{i,j}^{n+1} = U_{i,j}^{n-\frac{1}{2}\nu_x} (U_{i,j}^n - U_{i-1,j}^n) - \frac{1}{2}\nu_y (U_{i,j}^n - U_{i,j-1}^n)$$

- CFL condition: $\max\{|\nu_x|, |\nu_y|\} \leq 1$
- Stability (Fourier analysis) $|\nu_x| + |\nu_y| \leq 1$

- Truncation error: $O(\Delta t + \Delta x + \Delta y)$

Law Wendroff Scheme

$$U_{i,j}^{n+\frac{1}{2}} = U_{i,j} - \frac{1}{2}\nu\Delta x_0 U_{i,j}^n + \frac{1}{2}\nu_x^2\delta_x^2 U_{i,j}^n$$

$$U_{i,j}^{n+1} = U_{i,j}^{n+\frac{1}{2}} - \nu_y\Delta y_0 U_{i,j}^n + \frac{1}{2}\nu_y^2\delta_y^2 U_{i,j}^n$$

- CFL condition: $\max\{|\nu_x|, |\nu_y|\} \leq 1$
- Stability (Fourier analysis) $|\nu_x| + |\nu_y| \leq 1$
- Truncation error: $O((\Delta t)^2 + (\Delta x)^2 + (\Delta y)^2)$

13 ADI Schemes

13.1 Locally One Dimensional Scheme

$$(1 + \nu_x\Delta x_0)U_{i,j}^{n+\frac{1}{2}} = U_{i,j}^n$$

$$(1 + \nu_y\Delta y_0)U_{i,j}^{n+1} = U_{i,j}^{n+\frac{1}{2}}$$

- CFL condition: ?
- Stability: Unconditionally Stable. Fourier Analysis: we find $|\lambda| \leq 1$.
- Truncation error: $O(\Delta t + (\Delta x)^2 + (\Delta y)^2)$

13.2 Crank Nicolson Scheme

$$\frac{U_{i,j}^{n+1} - U_{i,j}^n}{\Delta t} + \frac{1}{2}\nu_x\Delta x_0(U_{i,j}^n + U_{i,j}^{n+1}) + \frac{1}{2}\nu_y\Delta y_0(U_{i,j}^n + U_{i,j}^{n+1}) = 0$$

- CFL condition: ?
- Stability: Unconditionally Stable. Unproven
- Truncation error: $O((\Delta t)^2 + (\Delta x)^2 + (\Delta y)^2)$

Beam Warming

$$\left(1 + \frac{1}{2}\nu_x\Delta x_0\right)U_{i,j}^* = \left(1 - \frac{1}{2}\nu_x\Delta x_0\right)\left(1 - \frac{1}{2}\nu_y\Delta y_0\right)U_{i,j}^n$$

$$\left(1 + \frac{1}{2}\nu_y\Delta y_0\right)U_{i,j}^{n+1} = U_{i,j}^*$$

- CFL condition: ?
- Stability: $|\lambda| = 1$
- Truncation error: ?

Consistency, convergence, stability, and Lax Equivalence Theorem.
Consider the problem in the general form.

$$\begin{cases} \frac{\partial u}{\partial t} = Lu & \Omega \times [0, t_F] \\ g(u) = g_0 & u \in \partial\Omega \\ u(x, 0) = u^0(x) & x \in \Omega, t = 0 \end{cases}$$

We assume that Ω is bounded, and L represents a differential operator such that $\frac{\partial u}{\partial t} = Lu$ is **well posed**:

- **Existence of solutions:** A solution exists for all data u^0 for which $\|u^0\|$ is bounded.
- **Continuous dependence on data:** There exists a constant K such that for any pair of solutions u and v , $\|u - v\| \leq K\|u^0 - v^0\|$ for all $t \leq t_F$.

Schemes for solutions

$$B_1 \vec{U}^{n+1} = B_0 \vec{U}^n + \vec{F}^n$$

Assume B_1 exists. Then a solution to the difference scheme exists:

$$\vec{U}^{n+1} = B_1^{-1} (B_0 \vec{U}^n + \vec{F}^n)$$

The truncation error is defined by the equation

$$B_1 \vec{u}^{n+1} = B_0 \vec{u}^n + \vec{F}^n + \vec{T}^n$$

Thus subtracting the discrete PDE scheme by the continuous PDE scheme we get

$$\vec{U}^{n+1} - \vec{u}^{n+1} = B_1^{-1} (B_0 (\vec{U}^n - \vec{u}^n) - \vec{T}^n)$$

Using the implied recursive relationship,

$$\vec{U}^{n+1} - \vec{u}^{n+1} = B_1^{-1} \vec{T}^{n-1} + B_1^{-1} B_0 \vec{U}^{n-1} - \vec{u}^{n-1} + \dots + (B_1^{-1} B_0)^{n-1} B_1^{-1} \vec{T}^0$$

So if $\|(B_1^{-1} B_0)^n\| \leq K \forall n \Delta t \leq t_F$ and $\|B_1^{-1}\| \leq K_1 \Delta t$, then $\|(B_1^{-1} B_0)^m B_0\| \leq K_1 K \Delta t \forall m \leq n$ so $\|\vec{U}^n - \vec{u}^n\| \leq K_1 K \Delta t \sum_{m=0}^{n-1} \|\vec{T}^m\|$

- **Consistency:** $T_{i,j}^n \rightarrow 0$ as $\Delta t, \Delta x, \Delta y, \dots \rightarrow 0$ for all i, j which implies $B_1 \vec{u}^{n+1} - (B_0 \vec{u}^n + \vec{F}^n) \rightarrow \frac{\partial u}{\partial t} - Lu$
- **Accuracy:** If p, q are the largest positive numbers for which $T_{i,j}^n \leq O((\Delta t)^p + h^q)$ as $\Delta t \rightarrow 0$ and $h \rightarrow 0$ for sufficiently smooth u , where $h = \max \Delta x, \Delta y, \dots$, the scheme is said to have **order of accuracy** p in Δt and q in h .
- **Stability:** The scheme is said to be **stable** if two solutions \vec{U}^n and \vec{V}^n of the scheme which have the same inhomogeneous terms \vec{F}^n but start from different initial data \vec{U}^0 and \vec{V}^0 satisfy

$$\|\vec{U}^n - \vec{V}^n\| \leq K \|\vec{U}^0 - \vec{V}^0\| \quad \forall n \Delta t \leq t_F$$

for some constant K independent of the initial data and mesh sizes. Equivalently,

$$\|(B_1^{-1} B_0)^n\| \leq K \quad \forall n \Delta t \leq t_F$$

14.1 Dissipation and Dispersion

– A maximum principle is sometimes necessary for Parabolic

- **Convergence:** The scheme provides **convergent approximations** to the problem if $\|\vec{U}^n - \vec{u}^n\| \rightarrow 0$ as $\Delta t, h \rightarrow 0, n\Delta t \rightarrow t \in [0, t_F]$ for every u^0 for which the problem is well posed.

Lax Equivalence Theorem For a consistent difference approximation to a well posed linear evolutionary problem which is uniformly stable in the sense that $\|B\| \leq K\Delta t$ for some constant K , the stability of the scheme is necessary and sufficient for convergence.

14.1 Dissipation and Dispersion

The **Dissipation** of solutions of PDEs is when the Fourier modes do not grow with time and at least one mode decays. The PDE is **Non-dissipative** if the Fourier modes neither decay nor grow.

The **Dispersion** of solutions of PDEs is when the Fourier modes of differing wave lengthd (or wave numbers) propagate at different speeds.

Von Neumann Condition A necessary condition for stability is that there exists a constant K such that

$$|\lambda(\vec{k})| \leq 1 + K\Delta t, \forall \vec{k}, n\Delta t \leq t_F$$

or as $\Delta t \rightarrow 0$ and $h \rightarrow 0$

$$|\lambda(\vec{k})|^n \leq K$$

or

$$|\lambda(\vec{k})|^n \leq (1 + K\Delta t)^n \approx (1 + K\Delta tn) + O((\Delta t)^2)$$