CFD for Aerospace Applications

Advanced Concepts

Dr. Ziad Boutanios

Concordia University - MIAE

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Introduction

- In the previous two lectures we derived the finite volume method and applied it to the three fundamental problems of linear advection, the Burgers equation and linear diffusion.
- We also tried different schemes as required by the different problems, like the first-order upwind scheme for linear advection and the Burgers equation, and the second-order central scheme for linear diffusion.
- In general, scheme accuracy is related to stability, where stability problems can also lead to solution oscillations, especially when dealing with discontinuities like shock waves.

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- Such issues are typical of high-order advective schemes, and we will examine them in this lecture.
- We will examine a measure of solution oscillations, the so-called Total Variation (TV).
- We will examine a high-order Total Variation Diminishing (TVD) reconstruction scheme, the so-called Monotonic Upstream-centered Scheme for Conservation Laws (MUSCL).
- We will also look at consistency, stability and convergence aspects of discretization schemes.

Accuracy vs. stability

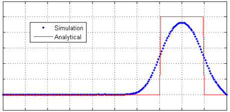

Figure 1: Solution of a step wave transport using a first-order upwind discretization of the 1D linear advection equation.

- Although stable the first-order upwind discretization of the linear advection equation is quite diffusive as can be seen for the step function in figure 1.
- In attempting to improve the accuracy of the first-order upwind discretization one naturally considers using a discretization scheme with a higher order of accuracy.

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- Here, we run into stability issues as predicted by Godunov's order barrier theorem:

  Linear numerical schemes for solving partial differential equations (PDE's), having the property of not generating new extrema (monotone scheme), can be at most first-order accurate.

- This lead to widespread efforts to develop high accuracy schemes that were not subject to Godunov's theorem by blending high-order schemes in smooth regions of the flow and first-order schemes around discontinuities.

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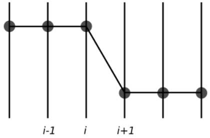

Figure 2: A 1D right running wave.

- A simple example of such issues are the oscillations encountered when using the second-order central scheme to solve the 1D linear advection problem of the right running wave of figure 2.
- The 1D linear advection transport equation with advection velocity $a > 0$ is
$$\frac{\partial q}{\partial t} + a\frac{\partial q}{\partial x} = 0,$$
and its discretization,
$$\frac{\partial q_i}{\partial t} + \frac{a}{2\Delta x}(q_{i+1} - q_{i-1}) = 0.$$
- This transient problem admits the stationary solution $q_i = (-1)^i$ when using the central scheme, which is an oscillation called odd-even mode shown in figure 3 and resulting in $\partial q_i/\partial t = 0$.

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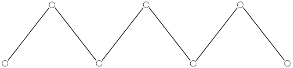

Figure 3: Odd-even mode.

- The odd-even mode oscillation can be removed by adding artificial diffusion in the form of a Laplacian or with upwinding.
- Moreover, based on figure 2 and $a > 0$ we have at point i

$$\frac{a}{2\Delta x}(q_{i+1} - q_{i-1}) < 0,$$

which requires $\dfrac{\partial q_i}{\partial t} > 0$ to satisfy the linear advection equation and produces an overshoot at point i.

- On the other hand, the upwind scheme has

$$\frac{a}{\Delta x}(q_i - q_{i-1}) = 0,$$

which produces the correct result $\dfrac{\partial q_i}{\partial t} = 0$.

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- The need to supress oscillations and overshoots in the propagation of a step discontinuity encourages the use of upwind schemes.
- However, upwind schemes are subject to the limitations of Iserles barrier theorem which states that,

  The maximum order of accuracy $O(max)$ of a stable semi-discrete advection scheme with p upwind points and d downwind points is,

$$\boxed{O(max) = \min(p + d, 2p, 2d + 2).} \tag{1}$$

- A natural conclusion of Iserles barrier theorem is that upwind biased schemes could perform better than pure upwind schemes in order to attain stable higher order accuracy since the upwinding can help stabilize the high-order part of the scheme, and in return the higher-order part can help reduce the upwinding diffusion.

Total Variation Diminishing schemes

- In order to try to reduce oscillations one naturally needs a reliable measure of them.
- One such measure of a 1D function $q(x,t)$ is the total variation TV and is defined as,

$$TV(q) = \int_a^b \left| \frac{\partial q}{\partial x} \right| dx. \tag{2}$$

- Similarly, it is defined for a discrete solution q_i^t with $i = 0, \cdots, n$ at time t as,

$$TV(q^t) = \sum_{i=1}^{n} \left| q_{i+1}^t - q_i^t \right|. \tag{3}$$

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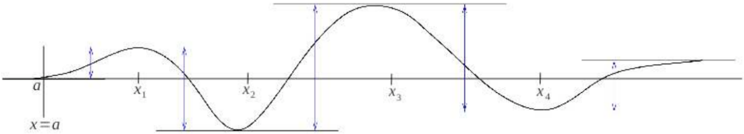

Figure 4: 1D TV calculation example.

- An example of calculation of the TV for a 1D solution function over an interval $[a, b]$ subdivided into 5 1D cells is shown in figure 4.
- The contribution to the TV of a sub-interval $[j-1, j]$ where the solution function is increasing would be $q_j - q_{j-1}$.
- Similarly, the contribution to the TV of a sub-interval $[j, j+1]$ where the solution function is decreasing would be $q_j - q_{j+1}$.
- For the entire interval the TV is then,

$$TV(q) = 2q(x_1) + 2q(x_3) + b - 2q(x_2) - 2q(x_4) - a.$$

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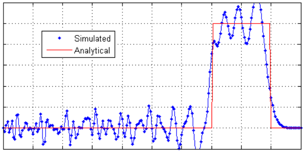

Figure 5: 1D step function solution obtained with second-order central differencing of the linear advection equation.

- Finally, for a scheme to be Total Variation Diminishing it must satisfy,

$$TV(q^{t+1}) \leq TV(q^t). \tag{4}$$

- The first-order upwind differencing scheme is TVD, and this can be verified in the step function solution profile shown in figure 1 where no spurious oscillations are present.
- The second-order central differencing scheme is not TVD and therefore introduces spurious oscillations at discontinuities.
- This can be seen in the second-order solution of a step function transported by 1D linear advection shown in figure 5.

The MUSCL scheme

- The MUSCL scheme is a finite volume method that can provide stable and highly accurate results even for flow with discontinuities.
- It is based on replacing the piecewise constant approximation of Godunov's method by reconstructed states derived from the solution at the previous time step.
- The face fluxes are reconstructed from limited left and right states at the cell faces.
- The fluxes can then be used in a Riemann solver to advance the solution in time.
- This will be demonstrated in the next slides.

Advanced Concepts

- Consider the first-order scalar linear advection equation in flux form,

$$\frac{\partial q}{\partial t} + \nabla \cdot \mathbf{f}(q) = 0, \tag{5}$$

  defined over the interval $\Omega_i \equiv [x_{i-1/2}, x_{i+1/2}]$.
- The Godunov scheme uses piecewise constant approximations for each cell leading to first-order accurate upwind discretization. The resulting semi-discrete scheme is,

$$\frac{\partial q_i}{\partial t} + \frac{\mathbf{f}(q_{i+1/2)} - \mathbf{f}(q_{i-1/2})}{\Delta x} = 0. \tag{6}$$

  Here, $q_{i-1/2} = q_{i-1}$ and $q_{i+1/2} = q_i$ and we have two such values at each interface (e.g. $q^L_{i-1/2}$ and $q^R_{i-1/2}$, $q^L_{i+1/2}$ and $q^R_{i+1/2}$) that set up a Riemann problem.
- This basic scheme is first-order accurate and smears sharp discontinuities.

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- To be able to handle sharp discontinuities Godunov's scheme can be extended with linear piecewise reconstructions of the face values which result in averages of neighbouring cells,

$$q_{i-1/2} = 0.5(q_{i-1} + q_i),$$

and

$$q_{i+1/2} = 0.5(q_i + q_{i+1}).$$

- The resulting central differencing scheme is second-order accurate but not TVD, and this can be seen in the spurious oscillations in figure 5.
- MUSCL schemes extend the idea of piecewise linear reconstructions by using slope-limited left and right extrapolated face values,

$$q^*_{i-1/2} = f\left(q^L_{i-1/2}, q^R_{i-1/2}\right),$$

and

$$q^*_{i+1/2} = f\left(q^L_{i+1/2}, q^R_{i+1/2}\right).$$

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- Such slope-limited reconstructions at the faces are designed using Taylor expansions at the cell centre. For example we can reconstruct the solution value $q^L_{i+1/2}$ with,

$$q^L_{i+1/2} = q_i + (x_{i+1/2} - x_i)\frac{\partial q_i}{\partial x} + \frac{(x_{i+1/2} - x_i)^2}{2}\frac{\partial^2 q_i}{\partial x^2} + \cdots$$

- For second-order accuracy we take,

$$q^L_{i+1/2} = q_i + (x_{i+1/2} - x_i)\frac{\partial q_i}{\partial x} \equiv q_i + \frac{1}{2}\delta_i,$$

where $\delta_i = 2(x_{i+1/2} - x_i)\dfrac{\partial q_i}{\partial x}$.

- Accordingly, we have for $q^R_{i+1/2}$ the expansion around x_{i+1},

$$q^R_{i+1/2} = q_{i+1} + (x_{i+1/2} - x_{i+1})\frac{\partial q_{i+1}}{\partial x} \equiv q_{i+1} - \frac{1}{2}\delta_{i+1},$$

where $\delta_{i+1} = 2(x_{i+1/2} - x_{i+1})\dfrac{\partial q_{i+1}}{\partial x}$.

Advanced Concepts

- The δ differences above are calculated using neighbouring cell values where we can introduce blending giving us,

$$\delta_i = \frac{1}{2}(1+b)(q_i - q_{i-1}) + \frac{1}{2}(1-b)(q_{i+1} - q_i),$$

and

$$\delta_{i+1} = \frac{1}{2}(1+b)(q_{i+1} - q_i) + \frac{1}{2}(1-b)(q_{i+2} - q_{i+1}),$$

Here, $0 \leq b \leq 1$.

- An upwind-biased approach will have $b > 0.5$ and a downwind-biased one $b < 0.5$.

Advanced Concepts

- One can also introduce limiter functions $\phi(r)$ to make the scheme TVD,

$$q^L_{i+1/2} = q_i + \phi(r_i)\delta_i,$$

and

$$q^R_{i+1/2} = q_{i+1} - \phi(r_{i+1})\delta_{i+1}.$$

Here, the r function is a solution slope between successive cells given by,

$$r_i = \frac{\delta q_{i+1/2}}{\delta q_{i-1/2}} = \frac{q_{i+1} - q_i}{q_i - q_{i-1}}$$

and

$$r_{i+1} = \frac{\delta q_{i+3/2}}{\delta q_{i+1/2}} = \frac{q_{i+2} - q_{i+1}}{q_{i+1} - q_i}.$$

Advanced Concepts

- There are several limiter functions available in the literature, with three common TVD ones provided in table 1.

Name	$\phi(r)$
minmod	max(0, min(1, r))
van Leer	$\dfrac{r+\lvert r\rvert}{1+\lvert r\rvert}$
superbee	max(0, min(2r, 1), min(r,2))

Table 1: Common limiter functions.

A MUSCL scheme second-order upwind-biased example

- Upwind fluxes at $x_{i+1/2}$ and $x_{i-1/2}$ are given by,

$$\mathbf{f}_{i+1/2} = \alpha q^L_{i+1/2} = \alpha q_i + \frac{\alpha}{2}\delta_i,$$

and

$$\mathbf{f}_{i-1/2} = \alpha q^L_{i-1/2} = \alpha q_{i-1} + \frac{\alpha}{2}\delta_{i-1}.$$

- For full upwind-bias we take $b = 1$ and get,

$$\delta_i = q_i - q_{i-1},$$

and

$$\delta_{i-1} = q_{i-1} - q_{i-2}.$$

Advanced Concepts

- The fluxes become,

$$\mathbf{f}_{i+1/2} = \alpha q_i + \frac{\alpha}{2}(q_i - q_{i-1}),$$

and

$$\mathbf{f}_{i-1/2} = \alpha q_{i-1} + \frac{\alpha}{2}(q_{i-1} - q_{i-2}).$$

- This yields the following semi-discrete second-order accurate upwind-biased scheme,

$$\frac{\partial q_i}{\partial t} = -\frac{\alpha}{2\Delta x_i}(-4q_{i-1} + 3q_i + q_{i+1}.) \tag{7}$$

- Note that this scheme will still exhibit some oscillations without a limiter function, though much less than the classical second-order central scheme.
- This will be shown in the following example simulation.

Advanced Concepts

- Consider a 1D linear advection problem with periodic boundary conditions on the interval [0, 2], with 300 cells and advection velocity $\alpha = 1$.
- The initial conditions at $t = 0$ are a succession of a smooth Gaussian profile and a step function,

$$q(x,0) = \begin{cases} e^{-20(x-0.5)^2} & \text{if } x < 1.2, \\ 1 & \text{if } 1.2 < x < 1.5, \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

- Since the linear advection equation has no diffusion operators we expect the initial conditions to be advected through the domain at the advection velocity $a = 1$ without any deformation.
- Since the boundary conditions are periodic we should have completed a full cycle at time $t = 2$ and should have $q(x,2) \approx q(x,0)$, and we will verify this for the second-order MUSCL scheme just derived with and without limiters.

Advanced Concepts

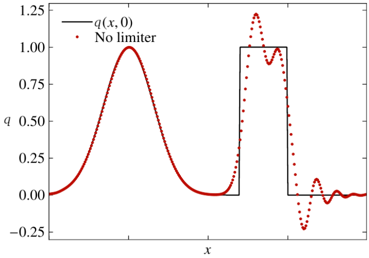

Figure 6: Second-order accurate MUSCL simulation without limiters.

- The no-limiter case matches the theoretical Gaussian curve result perfectly.
- There are still oscillations present for the step function, albeit much less than a classical second-order central differencing as seen in figure 5.

Advanced Concepts

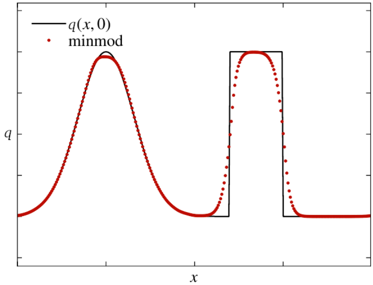

Figure 7: Second-order accurate MUSCL simulation with minmod limiter.

- The minmod limiter results in a slightly less maximum than the theoretical Gaussian curve result.
- On the other hand the oscillations of the step function result are completely gone, albeit with some diffusivity present but significantly less than the first-order upwind result of figure 1.

Advanced Concepts

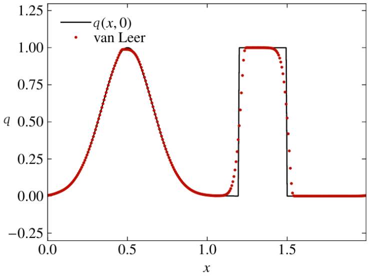

Figure 8: Second-order accurate MUSCL simulation with van Leer limiter.

- The van Leer limiter performs much better than minmod for the theoretical Gaussian curve result with minimal difference at the top of the curve.
- The step function result is also improved over minmod's with much less diffusivity, albeit still significant at the bottom left and top right of the step function.

Advanced Concepts

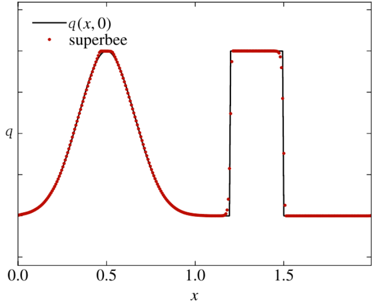

Figure 9: Second-order accurate MUSCL simulation with superbee limiter.

- The superbee limiter performs similarly to the van Leer limiter for the theoretical Gaussian curve result with minimal difference at the top of the curve.
- However, The step function superbee result is far superior to the other two limiters with minimal diffusivity, albeit still somewhat visible at the bottom left and top right of the step function.

Advanced Concepts

- In practice the van Leer limiter is often preferred since it offers good overall accuracy and its fractional r-function is computed much faster than minmod's and superbee's. These contain conditional statements in their min() and max() functions that are notoriously slow to compute.
- For example, one can run a simulation with the van Leer limiter up to a semi-converged point and then switch to the more accurate and expensive superbee for the final result, saving considerable computational resources.

Error analysis

- We have been discussing discretization error for several lectures now, strictly from the perspective of order of accuracy, which truly relates to the error between the finite difference solution and the exact one.
- There are, however, other important aspects of numerical error analysis to take into consideration.
- The quantitative ability of a *discrete operator* to represent its exact analytical counterpart is also a form of error to take into consideration.
- There is the issue of roundoff error which is due to the computer architecture itself.
- There is also the stability characteristics of the original PDE.
- We will examine all these aspects in the following slides.

The L^2 norm

- First we need to define the L^2-norm of a discretized function q denoted $||q||^2$, on a grid with cell size Δx,

$$||q||^2 = \left(\Delta x \sum_{n=-\infty}^{\infty} |q_n|^2\right)^{1/2} \tag{9}$$

- For a function f on the real line the L^2 norm is defined as,

$$||f||^2 = \left(\int_{-\infty}^{\infty} |f(x)|^2 \, dx\right)^{1/2}. \tag{10}$$

- The L^2-norm is very common in stability analysis.

Advanced Concepts

Well-posedness

- First we need to define the L^2-norm of a discretized function q, denoted $||q||^2$,

$$||q||^2 = \left(\Delta x \sum_{n=-\infty}^{\infty} |q_n|^2 \right)^{1/2} \tag{11}$$

- The L^2-norm is the most common for stability considerations.
- We start with the stability of the original PDE to be discretized and simulated with given initial values, AKA the initial value problem.
- In this context stability of the initial value problem of a PDE is called well-posedness.
- An initial value problem for a first-order PDE $Pq = 0$ is well-posed if for any time $T \geq 0$ there is a constant C_T such that any solution $q(x, t)$ satisfies

$$||q(x,t)||^2 \leq C_T ||q(x,0)||^2 \quad \text{for} \quad 0 \leq t \leq T. \tag{12}$$

Advanced Concepts

Consistency

- The next logical consideration is that of how well the chosen scheme corresponds to the PDE it is supposed to represent, AKA consistency.
- Mathematically, we say that a finite difference scheme $P_{\Delta x}^{\Delta t} q = f$ is consistent with the PDE $Pq = f$ to order (r, s) if for any smooth function $q(x, t)$,

$$Pq - P_{\Delta x}^{\Delta t} q \to O(\Delta x^r, \Delta t^s) \quad \text{as} \quad \Delta x, \Delta t \to 0. \tag{13}$$

- In layman's terms we can say that a finite difference scheme is consistent with a PDE if the error between the scheme and the PDE does not grow, or is even reduced, as we refine the time step and space intervals indefinitely.

Advanced Concepts

Consistency check example Let P be the linear advection operator with unit advection velocity,

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

Let us evaluate the consistency of the forward-time and forward-space scheme with difference operator $P_{\Delta x}^{\Delta t}$ such that,

$$P_{\Delta x}^{\Delta t} q = \frac{q_i^{n+1} - q_i^n}{\Delta t} + \frac{q_{i+1}^n - q_i^n}{\Delta x}. \tag{14}$$

- Taking a Taylor expansion in time and space around q_i^n gives us,

$$\frac{q_i^{n+1} - q_i^n}{\Delta t} = \frac{\partial q_i^n}{\partial t} + \frac{\Delta t}{2}\frac{\partial^2 q_i^n}{\partial t^2} + O(\Delta t^2).$$

$$\frac{q_{i+1}^n - q_i^n}{\Delta x} = \frac{\partial q_i^n}{\partial x} + \frac{\Delta x}{2}\frac{\partial^2 q_i^n}{\partial x^2} + O(\Delta x^2).$$

Advanced Concepts

- Using the above results in equation 14 and subtracting from Pq gives,

$$Pq - P_{\Delta x}^{\Delta t} q = \frac{\Delta t}{2} \frac{\partial^2 q_i^n}{\partial t^2} + \frac{\Delta x}{2} \frac{\partial^2 q_i^n}{\partial x^2} + O(\Delta t^2, \Delta x^2).$$

  which $\rightarrow O(\Delta t^2, \Delta x^2)$ as $(\Delta x, \Delta t) \rightarrow 0$.
- Therefore $P_{\Delta x}^{\Delta t}$ is consistent of order (2, 2) with P.

Stability

- Here we mean the stability of the finite difference scheme.
- A finite difference scheme $P_{\Delta x}^{\Delta t} q_i^n = 0$ for a first-order equation is stable in a stability region Λ if there is an integer J such that for any positive time T, there is a constant C_T such that,

$$||q^n||^2 \leq C_T \sum_{j=0}^{J} ||q^j||^2, \tag{15}$$

for $0 \leq n\Delta t \leq T$, $(\Delta t, \Delta x) \in \Lambda$.

- C_T can depend on T but not on Δx or Δt.
- Equation 15 is a relatively relaxed constraint since it allows for quite a bit of *stable* oscillation in q^n.

Advanced Concepts

- Alternatively, one can also use the following more stringent stability criterion also encountered in the literature for first-order equations,

$$||q^n||^2 \leq C_T||q^0||^2, \tag{16}$$

where C_T is still subject to the same dependencies as for equation 15.

- Althoug more stringent, this constraint may still fail in applications since it also allows for some oscillations in q^n.
- In practice, it is quite difficult to prove stability from equations 15 and 16.
- It is more convenient to use Fourier stability analysis, AKA the Neumann stability analysis, which can give quantitative estimates of the *linear growth* of errors.
- We will study it later.

Convergence

- Having discussed well-posedness of the PDE initial value problem, consistency of the finite difference scheme and its stability, we naturally come to the question of how close the numerical solution is to the exact one, which relates to convergence of the finite difference scheme.
- A one-step finite difference scheme approximating a PDE is convergent if for any solution $q(x,t)$ to the PDE, and solution q_i^n to the finite difference scheme, such that $q_i^0 \to q(x,0)$ as $i\Delta x \to x$, we have $q_i^n \to q(x,t)$ as $(i\Delta x, n\Delta t) \to (x,t)$ and $(\Delta x, \Delta t) \to 0$.
- Convergence can also be inferred by the Lax-Friedrich theorem which states that,

  A consistent finite difference scheme for a PDE for which the initial value problem is well-posed, will be convergent if and only if it is stable.

Linear stability analysis

- Stability analysis should really start with the sources of numerical error, which are the discretization error and round-off error.
- We already covered the discretization error extensively since it is the difference between the exact solution of the PDE and the numerical solution to the finite difference equation without round-off computer errors. This error is described by the scheme order of accuracy.
- The numerical round-off error is the result of the computer repetitively rounding off numbers to some significant figure, as a result of the floating point approximation. Different values of this machine error are given in table 2.
- In what follows we will use the term *error* to designate the round-off error.

Advanced Concepts

IEEE	Common name	Machine error
binary32	single precision	$2^{-24} \approx 5.96e^{-08}$
binary64	double precision	$2^{-53} \approx 1.11e^{-16}$
binary128	quadruple precision	$2^{-113} \approx 9.63e^{-35}$

Table 2: Some floating point arithmetic machine errors.

- If we call the exact solution of a finite difference equation q, and the numerical solution of a computer with finite accuracy Q, then the round-off error is $\epsilon = q - Q$.
- In turn, the exact solution can be expressed as $q = Q + \epsilon$, which means that Q is also a solution of the finite difference equation subject to machine error.
- Suppose we are dealing with the second-order accurate linear diffusion equation discretization providing q_i^{n+1},

$$q_i^{n+1} = q_i^n + \frac{\beta \Delta t}{\Delta x^2}\left(q_{i+1}^n - 2q_i^n + q_{i-1}^n\right). \tag{17}$$

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- We can replace q by $Q + \epsilon$ in equation 17 for each variable. Since Q_i^n, Q_{i+1}^n, Q_{i-1}^n and Q_i^{n+1} satisfy equation 17 to machine error (or exactly as far as the computer can tell) we are left with an equation for the discrete error variable,

$$\epsilon_i^{n+1} = \epsilon_i^n + C\left(\epsilon_{i+1}^n - 2\epsilon_i^n + \epsilon_{i-1}^n\right), \tag{18}$$

  where $C = \dfrac{\beta \Delta t}{\Delta x^2}$.

- If the error grows in time the method is unstable, and if it does not the method is stable. Therefore stability comes down to showing that the amplification factor G satisfies,

$$|G| = \left|\frac{\epsilon_i^{n+1}}{\epsilon_i^n}\right| \leq 1. \tag{19}$$

Neumann stability analysis

- The Neumann stability method is also a linear approach, which analyses the error growth by using the Fourier transform.
- This allows decomposing a normal time domain variable (e.g. $q(x, t)$, $\epsilon(x, t)$ etc.) into a frequency domain sum of terms, each with a different frequency (or waves).
- The Neumann stability analysis is especially useful when we are interested in the behaviour of the different error modes.

Advanced Concepts

- For *linear* differential equations it is possible to expand the spatial variation of error in a finite Fourier series in x over the interval L of the computational domain as,

$$\epsilon(x,t) = \sum_{m=1}^{M} E_m(t) e^{ik_m x} = \sum_{m=1}^{M} E_m(t)(\cos(k_m x) + i\sin(k_m x)), \tag{20}$$

where the wavenumber k_m is the number of waves one can fit per unit length, and the wavelength $\lambda_m = 2\pi/k_m$.

- The wavelength is defined as the distance fitting a complete wave period (see figure 10), and m is the number of waves we can fit into L.
- The real part of equation 20 represents the error and its transient nature is included by assuming its amplitude E_m is a function of time.

Advanced Concepts

- The summation over m in equation 20 represents the decomposition of the error into different frequency components, or harmonics.
- When $M \to \infty$ the summation can represent a continuous variation of ϵ as a function of x.
- In practice we consider a finite number of terms since we deal with a limited computational domain with a finite number of grid points, where the wavenumber is limited to a finite number of values as shown in figure 10.

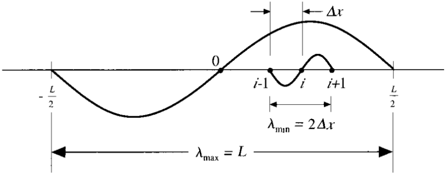

Figure 10: Maximum and minimum wavelengths of the Fourier decomposition of round-off error.

Advanced Concepts

- A full wave period requires three points, the edges and the middle.
- Therefore, the largest allowable wavelength is one wave period over the full domain length, $\lambda_{max} = L$, which corresponds to $m_{min} = L/\lambda_{max} = 1$.
- The corresponding wavenumber is $k_{min} = 2\pi/\lambda_{max} = 2\pi/L$.
- On the other hand, the smallest allowable wavelength corresponds to the smallest distance covering three grid points to fit one wave period, so $\lambda_{min} = 2\Delta x$.
- Since the total number of grid intervals is $N = L/\Delta x$, we have $\Delta x = L/N$ and $\lambda_{min} = 2L/N$.
- This gives us the maximum number of waves per L as $m_{max} = L/\lambda_{min} = N/2$.
- The corresponding wavenumber is $k_{max} = \frac{2\pi}{\lambda_{min}} = \frac{2\pi}{L/m_{max}}$.
- Both k_{min} and k_{max} show us that $k_m = \frac{2\pi m}{L}$.

Advanced Concepts

- Having figured out the wavenumber range we can now rewrite equation 20 for a grid with $N+1$ points,

$$\epsilon(x) = \sum_{m=1}^{N/2} E_m(t)e^{ik_m x}. \tag{21}$$

- Since the finite difference equation 18 is linear and each error term in the Fourier series satisfies this difference equation, the behaviour of each term in the series should be the same as the behaviour of the series itself and we only need to check a generic term for stability.
- There are two ways for doing that. The first one does not assume any specific time variation in $E_m(t)$ and the second one assumes exponential variation.
- We will look at both.

Advanced Concepts

The generic time variation

- Using a generic error term from equation 21 the individual round-off error terms in equation 18 can be written as,

$$\begin{aligned}
\epsilon_i^n &= E_m(t)e^{ik_m x},\\
\epsilon_i^{n+1} &= E_m(t+\Delta t)e^{ik_m x},\\
\epsilon_{i+1}^n &= E_m(t)e^{ik_m (x+\Delta x)},\\
\epsilon_{i-1}^n &= E_m(t)e^{ik_m (x-\Delta x)}.
\end{aligned}$$

- Plugging the terms above into equation 18 we get the amplification factor G after some manipulations,

$$\begin{aligned}
G = \frac{\epsilon_i^{n+1}}{\epsilon_i^n} &= \frac{E_m(t+\Delta t)}{E_m(t)}\\
&= 1 + C(e^{ik_m\Delta x} + e^{-ik_m\Delta x} - 2). \qquad (22)
\end{aligned}$$

Advanced Concepts

- Let us now set $\theta = k_m \Delta x \in [-\pi, \pi]$ to make the equation more readable.
- We also have the following trigonometric identities,

$$\sin\left(\frac{\theta}{2}\right) = \frac{e^{i\theta/2} - e^{-i\theta/2}}{2i}. \quad (23)$$

$$\sin^2\left(\frac{\theta}{2}\right) = -\frac{e^{i\theta} - e^{-i\theta} - 2}{4}. \quad (24)$$

- Using the above in equation 22 we get the stability condition,

$$|G| = \left|1 - 4C\sin^2\left(\frac{\theta}{2}\right)\right| \leq 1. \quad (25)$$

- This is equivalent to the two conditions $G \geq -1$ and $G \leq 1$ satisfied simultaneously.

Advanced Concepts

- The first condition $G \geq -1$ requires $C \leq 1/2\sin^2(\theta/2)$.
- Since $0 \leq \sin^2(\theta/2) \leq 1$ we get $C \leq 1/2$ the maximum limit on C without taking the wavenumber value into consideration.
- The second condition $G \leq 1$ requires $4C\sin^2(\theta/2) \geq 0$, which is true for $C \geq 0$.
- Therefore, a condition for the stability of the second-order finite difference equation for linear diffusion without taking the wavenumber into consideration is,

$$\boxed{0 \leq C \leq \frac{1}{2}.} \tag{26}$$

Advanced Concepts

The exponential time variation

- It is also reasonable to assume an exponential round-off error variation with time since it is observable in practice. We can then write,

$$\epsilon(x,t) = \sum_{m=1}^{N/2} e^{at} e^{ik_m x}, \tag{27}$$

  where a is a constant.

- Again, we look at just one term in the series, $\epsilon_m(x,t) = e^{at} e^{ik_m x}$, and the individual round-off error terms in equation 18 can be written as,

$$\begin{aligned}
\epsilon_i^n &= e^{at} e^{ik_m x}, \\
\epsilon_i^{n+1} &= e^{a(t+\Delta t)} e^{ik_m x}, \\
\epsilon_{i+1}^n &= e^{at} e^{ik_m (x+\Delta x)}, \\
\epsilon_{i-1}^n &= e^{a(t-\Delta t)} e^{ik_m (x-\Delta x)}.
\end{aligned}$$

Advanced Concepts

- Using the above in equation 18 and dividing left and right by $e^{at}e^{ik_m x}$ we get,

$$G = e^{a\Delta t} = 1 + C(e^{ik_m\Delta x} + e^{-ik_m\Delta x} - 2). \tag{28}$$

- Note that the RHS of equation 28 is identical to that of equation 22.
- Using the identity

$$\cos(k_m\Delta x) = \frac{e^{ik_m\Delta x} + e^{-ik_m\Delta x}}{2}, \tag{29}$$

we can write equation 28 as,

$$G = 1 + 2C(\cos(k_m\Delta x) - 1). \tag{30}$$

Advanced Concepts

- We note the following trigonometric identity,

$$\sin^2 \frac{k_m \Delta x}{2} = \frac{1 - \cos(k_m \Delta x)}{2}, \tag{31}$$

- Based on the previous identity and given $\theta = \dfrac{k_m \Delta x}{2}$ we can write equation 30 in its final form which is identical to equation 22,

$$G = e^{a\Delta t} = 1 - 4C\sin^2(\theta/2). \tag{32}$$

- Therefore, the stability condition for equation 32 is the same one we recovered for equation 22,

$$\boxed{0 \leq C \leq \frac{1}{2}.}$$

Advanced Concepts

- The above stability condition can be related to the wavenumber.
- For this we could take into consideration the combined effects of k_m and Δx in $\theta = k_m \Delta x$.
- This would be required for example for higher order turbulence models like LES or DNS, which are not covered in this course.
- We could also use a complex a in the exponential time dependence term $E_m(t) = e^{at}$, which sets the table for transient modes just like the wavenumbers in space and allows for even more fine-grained error analysis.
- Students interested in these topics are encouraged to consult sections 9.2 and chapter 10 in the course book by Vermeire et al.

Time stepping

- So far all the finite difference schemes we have seen consisted of first-order forward differencing in time for the transient term of the PDE, which uses the current and next time levels.
- One can also use second-order backward differencing in time which will use the previous, current and next time levels.
- Either way the current time level always appears in the transient term differencing scheme.

Explicit time stepping

- The same approach has been used for the spatial discretizations (advection and diffusion terms) except that the next time levels never appeared in them.
- In essence, all the finite difference schemes we derived took the following form for a generic vector variable $\mathbf{q}$,

$$\mathbf{q_i^{t+1}} = f(C, \mathbf{q_i^t}, \mathbf{q_{i-1}^t}, \mathbf{q_{i+1}^t}, \mathbf{q_i^{t-1}}). \tag{33}$$

- The spatial stencil in equation 33 can be further enlarged to use more of the solution values at points in the immediate vicinity of $\mathbf{q_i}$, and if the solution values are only from current and previous time levels the scheme in equation 33 is called an explicit scheme.
- Explicit schemes are simple to assemble, but are subject to Courant number limitations as far as stability is concerned.

Advanced Concepts

Implicit time stepping

- An alternative approach is to use variables from the next time level for the spatial discretizations.
- In this case the resulting finite difference scheme will take the following form for a generic vector variable $\mathbf{q}$,

$$\mathbf{q_i^{t+1}} = f(C, \mathbf{q_i^t}, \mathbf{q_{i-1}^{t+1}}, \mathbf{q_{i+1}^{t+1}}, \cdots). \tag{34}$$

- The spatial stencil in equation 34 can be further enlarged to use more of the solution values at points in the immediate vicinity of $\mathbf{q_i}$, and if we have solution values belonging to the next time level the scheme in equation 34 is called an implicit scheme.
- Implicit schemes are more difficult to assemble, but are not usually subject to Courant number limitations as far as stability is concerned.
- They also require more computer time per time step and are better suited for relatively steady-state problems.

Advanced Concepts

Meaning of the Courant number

- We have seen that the stability of an explicit finite difference scheme depends on the Courant number being less than a certain limit and obtained it for the second order accurate scheme for the linear diffusion equation.
- For linear diffusion the Courant number is given by $C = \beta\Delta t/\Delta x^2$.
- The coefficient of diffusion β has units $[m^2/s]$, so $\beta/\Delta x$ has units $[m/s]$, which is a velocity.
- We call it the diffusion transport velocity $u_d = \beta/\Delta x$.
- Let us also set a numerical grid velocity $u_g = \Delta x/\Delta t$, which is the speed at which numerical information travels crosses the entire cell.
- The Courant number for linear diffusion stability C_d can then be defined as the ratio of the diffusion velocity to grid velocity,

$$C_d = \frac{u_d}{u_g}. \tag{35}$$

Advanced Concepts

- For the linear diffusion flow to be stable we need to have $C_d = u_d/u_g < 0.5$, which means that the diffusive transport velocity cannot exceed half the the speed at which information crosses an entire cell.
- We can analyse the meaning of the Courant number further by deriving the Neumann stability condition for the forward-time backward-space finite difference scheme for the linear advection equation.
- You will carry out this exercise for your third assignment, and here we only give the final stability condition,

$$0 \leq C \leq 1, \quad \text{where} \quad C = \frac{\alpha \Delta t}{\Delta x}. \tag{36}$$

- The Courant number for linear advection stability C_a can be defined as the ratio of the advection transport velocity α to the grid velocity,

$$C_a = \frac{\alpha}{u_g}. \tag{37}$$

Advanced Concepts

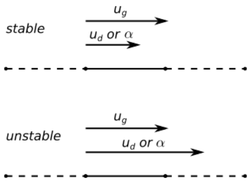

Figure 11: Stable and unstable flow configurations depending on the magnitude of the physical flow velocity compared to the numerical grid velocity u_g.

- Again, we have the requirement that the physical transport velocity cannot exceed the grid numerical transport velocity.
- This is true for all explicit schemes in general, with the stable courant number always less than one.
- If physical transport is happening faster than the scheme can transport numerical information then instability will occur.
- Both stable and unstable configurations are shown in figure 11.