Discretizations of Adv-Diff Eq.

\[ u_t (x, t) = \sum_{k} C_k u(x, j+k, t) + O(h^2) \]

This is a finite-difference scheme, but for simple uniform discretizations it does not matter, and the distinction regards local conservation and variational structure.
$w_j(t) \approx u(x_j, t)$ (Finite difference)

But could be:

$$w_j(t) = \frac{1}{h} \int_{x-h/2}^{x+h/2} u(x, t) \, dx \quad \text{(Finite Volume)}$$

Or the relation could be expressed the other way, e.g., interpolation:

$$u(x_1, t) = F(w, x) \quad \text{(Finite Element Spectral)}$$

From here, we convert the PDE into a system of ODEs for $w$

$$\frac{dw}{dt} = w'(t) = A \, w(t) \quad \text{Method of Lines approach (Split space and time)}$$
In finite difference methods we directly work with the PDE and replace derivatives with finite-difference approximations. In finite-volume methods we evaluate fluxes at the cell interfaces to maintain conservation. In finite element methods we use the weak (variational) form of the PDE, and in spectral methods we transform the PDE into another basis (Fourier) set of functions.

For low-order (second-order) typically in the end all discretizations look the same and the main task is to analyze them!
Fourier Basis

\[ \Phi_k(x) = e^{2\pi i k x}, \quad k \in \mathbb{Z} \text{ (wavenumber)} \]

\[ \Phi_k = [\Phi_k(x_1), \ldots, \Phi_k(x_m)]^T \in \mathbb{C}^m \]

(discrete Fourier modes)

\{\phi_1, \phi_2, \ldots, \phi_m\} is an orthonormal basis for \( \mathbb{C}^m \)

or better use \{\phi_{-k}, \ldots, \phi_0, \ldots, \phi_{m-k-1}\}

\[ \forall \mathbf{u} \in \mathbb{C}^m, \quad \mathbf{u} = \sum_{k} \alpha_k \phi_k \]

Fourier coefficients

or \[ \alpha_k = \frac{1}{m} \sum_j u_j e^{-2\pi i k j / m} \]

\[ v_j = \sum_{k} \alpha_k e^{2\pi i k j / m} \]
Advection Equation

\[ u_t + a u_x = 0 \]

Periodic: \( u(x \pm 1, t) = u(x, t) \)

not really a BC since there is no physical boundary!

\[ u_x(x) \approx \frac{1}{h} \left[ u(x) - u(x-h) \right] \]

\[ \Rightarrow \begin{cases} \frac{\partial w_j}{\partial x} = \frac{a}{h} \left[ w_{j-1} - w_j \right] \leq \text{upwind scheme} \\ a > 0 \ (\text{use information downstream}) \end{cases} \]

or \[ \begin{cases} \frac{\partial w_j}{\partial x} = \frac{a}{h} \left( w_j - w_{j+1} \right) \leq \text{upwind also} \\ a < 0 \ (\text{downstream}) \end{cases} \]
Or use centered difference

\[ u_x = \frac{1}{2h} \left[ u(x+h) - u(x-h) \right] \]

\[ w'_j = \frac{a}{2h} \left[ w_{j-1} - w_{j+1} \right] \quad \text{central scheme} \]

Homework: Try both for \( a = 1 \) and initial condition

\[ u(x, 0) = \left[ \sin \left( \frac{\pi x}{100} \right) \right] \]

Use MATLAB's ODE solvers to solve the system of ODEs to high temporal accuracy.

\[ x = 0 \quad \text{and} \quad x = 1 \]

\[ h = \frac{1}{200} \quad \text{and} \quad h = \frac{1}{50} \]
Modified Equations

\[ \frac{1}{h} [u(x-h) - u(x)] = -u_x(x) + \frac{1}{2} h u_{xx}(x) + O(h^2) \]

So the upwind scheme is actually adding diffusion or artificial dissipation

\[ \tilde{u}_t + a \tilde{u}_x = \frac{1}{2} ah \tilde{u}_{xx} \text{ equation} \]
\[ d = \frac{ah}{2} \text{ artificial dissipation} \]

The upwind scheme is a second-order approximation to the modified and not the original equation.

\[ \frac{1}{h} (w_{j-1} - w_j) = \frac{1}{2} \left( w_{j-1} - w_{j+1} \right) + \frac{h/2}{h^2} (w_{j-1} - 2w_j + w_{j+1}) \]
\( \frac{1}{2h} [u(x-h) - u(x+h)] = -u_x(x) - \frac{h^2}{6} u_{xxx}(x) + O(h^4) \)

modified equation for centered scheme

\( \tilde{u}_t + a \tilde{u}_x = -\frac{ah^2}{6} \tilde{u}_{xxx} \)

artificial dispersion

\[
\begin{align*}
\tilde{u}(x,0) &= e^{2\pi ikx} \\
\tilde{u}(x,t) &= e^{2\pi ik(x - \alpha_k t)}
\end{align*}
\]

 numerical phase velocity

But \( \alpha_k = a \left( 1 - \frac{2}{3} \pi^2 \ell^2 k^2 h^2 \right) \)

dispersion relation

So if the solution is not smooth (has high-frequency components), it will be distorted (Gibbs phenomenon)
Note \( k_{\text{max}} = \frac{m}{2} \) so \( \frac{2}{3} \pi^2 k_{\text{max}}^2 h^2 = \frac{2}{3} \pi^2 \cdot \frac{1}{4} \) independent of \( h \). So the grid must be much finer than the width of regions with sharp gradients.

Dilemma (Central issue in ade-diff)

- Accept low accuracy (artificial diss.)
- Accept low robustness (non-monotonicity)

or find a way to trade off
Fourier analysis

\[ w_j = \sum_k \chi_k(t) e^{2\pi i k j / m} \]

\[ w_j' = \sum_k \chi_k'(t) e^{2\pi i k j / m} = \frac{a}{h} (w_{j-1} - w_j) \]

\[ = \sum_k \frac{a}{h} \left[ \chi_k e^{2\pi i k (j-1) / m} - \chi_k e^{2\pi i k j / m} \right] \]

\[ = \sum_k \frac{a}{h} (e^{-2\pi i k / m} - 1) \chi_k e^{2\pi i k j / m} \]

By orthogonality of Fourier basis

\[ \chi_k' = \chi_k \cdot \frac{a}{h} \left[ (\cos(2\pi i k / m) - 1) - i \sin(2\pi i k / m) \right] \]

\[ \lambda_k - \text{decay rate or eigenvalue of } \phi_k \]
Similarly, for centered discretization

$$\lambda_k = -ie_k \sin\left(2\pi k/m\right)$$

If $a > 0$

ODE is unstable

If $a < 0$

ODE is stable

(Which is why we must look at sign of $a$)

Centered difference

Marginal stability
A series expansion of the eigenvalues:

\[ \lambda_h = -2\pi i a k - \frac{1}{2} |a| (2\pi k)^2 h + O(h^2) \]

for upwind first-order correct answer (continuum PDE)

\[ \lambda_h = -2\pi i a k + \frac{1}{6} i a (2\pi k)^3 h^2 + O(h^4) \]

second-order

\[ -a^2 \chi_x \rightarrow -2\pi i a k \text{ in Fourier space} \]

\[ \left\{ \begin{array}{ll}
\text{Re} (\lambda h) < 0 & \text{dissipative scheme} \\
\text{Re} (\lambda h) = 0 & \text{non-dissipative} \\
\text{Re} (\lambda h) > 0 & \text{unstable}
\end{array} \right. \]
Higher-Order FD schemes

\[ w'_j = \frac{a}{h} \sum_{k=1}^{S} C_k w_{j+k} \]

stencil width = \( s + r + 1 \)

Optimal-order scheme

\[ q = r + s \]

Theorem (Iserles & Strang)

If \( a > 0 \), the optimal-order scheme

is stable for \( s \leq r \leq s + 2 \)

and unstable otherwise
E.g. third-order upwind-biased method for $a > 0$

$$w_j' = \frac{a}{h} \left[ -\frac{1}{6} w_{j-2} + w_{j-1} - \frac{1}{2} w_j - \frac{1}{3} w_{j+1} \right]$$

Modified eq: $\tilde{u}_t + a \tilde{u}_x = -\frac{|a|}{12} h^3 \tilde{u}^{xxxx}$

So now the dissipative term is $O(h^3)$ and also fourth-order, not second-order diffusive.

Note: \[ \begin{align*}
\hat{u}_t &= -U^{xxxx}, & \hat{u}_t &= -k^4 \hat{u} \\
\text{does not satisfy a maximum principle and over/under shoots can appear}
\end{align*} \]
While $\text{Re}(\lambda n) < 0$ (except $\lambda n = 0$), there are many nearly imaginary eigenvalues.

The fourth-order central advection

$$w_j' = \frac{a}{h} \left[ -\frac{1}{12} w_{j-2} + \frac{2}{3} w_{j-1} - \frac{2}{3} w_{j+1} + \frac{1}{12} w_{j+2} \right]$$

has the same dispersive error as the upwind-biased scheme, but no artificial dissipation to damp oscillations (over/under shots).
Diffusion Equation \[ \frac{\partial u}{\partial t} = d \frac{\partial^2 u}{\partial x^2} \]

\[ w_j' = \frac{1}{h^2} \left[ w_{j-1} - 2w_j + w_{j+1} \right] \]

Modified equation (misleading)

\[ \tilde{u}_t = d \tilde{u}_{xx} + \frac{h^2}{12} \tilde{u}_{xxxx} \]

Unstable term

More useful to look in Fourier space:

\[ \left\{ \begin{array}{l}
\lambda_k = -\frac{4d}{h^2} \sin^2(kh) = -4d \pi^2 k^2 + O(h^2) \\
\lambda_k < 0 \text{ for all } k
\end{array} \right. \]

Smoothing property (desirable)
Fourth-order stencil

\[ w_j = \frac{1}{h^2} \left[ -\frac{1}{12}, \frac{4}{3}, -\frac{5}{2}, \frac{4}{3}, -\frac{1}{12} \right] \]

\[ j-2, j-1, j, j+1, j+2 \]

Always symmetric

Is marginally better but a lot more expensive in higher dimensions!

Now just combine advection + diffusion

\[ u_t + a u_x = d u_{xx} \]

Artificial diffusion \[ T = ah/2 \sim ah \]

Dimensionless number: cell Péclet number

\[ Pe = \frac{ah}{d} \]

\[ P > 1 \quad \text{advection-dominated} \]

\[ P < 1 \quad \text{diffusion-dominated} \]
Consider centered scheme

\[ w_j' = \left( \frac{1}{h^2} + \frac{a}{2h} \right) w_{j-1} - \frac{2d}{h^2} w_j + \left( \frac{1}{h^2} - \frac{a}{2h} \right) w_{j+1} \]

If \( Pe < 2 \) then

\[ \frac{1}{h^2} - \frac{a}{2h} = \frac{1}{h^2} \left( 1 - \frac{Pe}{2} \right) > 0 \]

and this makes the oscillations go away (we get monotonicity)

\[ \rightarrow \text{non-oscillatory} \]

But for \( Pe \gg 1 \) we need to add artificial dissipation in regions of steep gradients (e.g., third-order upwind biased)