(1) CFD SPRING 2012 A. PONEV

# DISCRETIZATIONS OF ADV-DIFF EQ.


$h = 1/m$ (grid spacing)

$$u_t(x_j,t) = \sum_k c_k\, u(x_{j+k},t) + O(h^q)$$

stencil coefficients local error

order of accuracy

This is a finite-difference scheme but for simple uniform discretizations it does not matter, and the distinction regards local conservation and variational structure

FINITE VOLUME FINITE ELEMENT

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$$w_j(t) \simeq u(x_j, t)$$ (Finite difference)

But could be

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

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

$$u(x,t) = F(\underline{w}, x)$$ (Finite Element, SPECTRAL)

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

$$\frac{dw}{dt} = w'(t) = \underset{\text{stencil}}{A}\, w(t)$$

Method of Lines approach

(SPLIT space and time)

(3) In finite difference methods we directly work with the PDE and replace derivatives with <u>finite-difference</u> approximations. In finite-volume methods we evaluate <u>fluxes</u> at the cell interfaces to maintain conservation. In <u>finite element</u> methods we use a weak (variational) form of the PDE, and in <u>spectral methods</u> we transform the PDE into another set of basis (Fourier) functions

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

(4) <u>Fourier Basis</u> recap

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

$$\phi_k = [\varphi_k(x_1), \dots, \varphi_k(x_m)]^T \in \mathbb{C}^m$$

(discrete Fourier modes)

$\{\phi_1, \phi_2, \dots, \phi_m\}$ is an orthonormal basis for $\mathbb{C}^m$

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

$$\Rightarrow \forall v \in \mathbb{C}^m, \quad v = \sum_k \alpha_k \phi_k$$

$k = \begin{cases} m/2 \text{ or} \\ (m-1)/2 \end{cases}$

Fourier coefficients

$$v_j = \sum_k \alpha_k e^{2\pi i k h j}$$

or $\boxed{\alpha_k = \frac{1}{m} \sum_j v_j e^{-2\pi i k j/m}}$ $\boxed{v_j = \sum_k \alpha_k e^{2\pi i k j/m}}$

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# Advection Equation

$$\begin{cases} u_t + a u_x = 0 \\ \text{Periodic} : \quad u(x \pm 1, t) = u(x,t) \end{cases}$$

← Not really a BC since there is no physical boundary!

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

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

or $$\begin{cases} w_j' = \frac{a}{h}\left(w_j - w_{j+1}\right) \\ a < 0 \end{cases}$$ ← ~~xxxxxxx~~ also upwind (downstream)

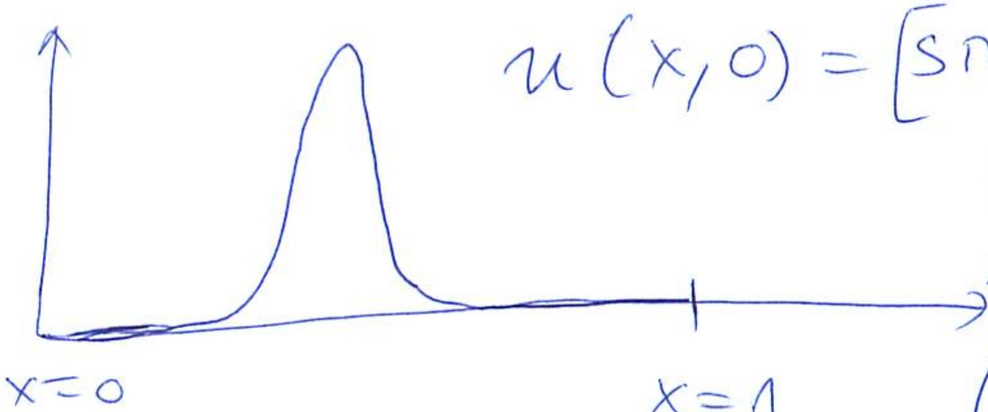
6 Or use centered difference

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

$$w_j' = \frac{a}{2h}\left[w_{j-1} - w_{j+1}\right] \leftarrow \text{central scheme}$$

<u>**Homework**</u>: Try both for $a=1$ and initial condition

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




$\left\{ h = 1/200 \text{ and } h = 1/50 \right.$

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

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# Modified Equations

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

So the upwind scheme is actually adding diffusion or artificial dissipation

$$\begin{cases} \tilde{u}_t + a\tilde{u}_x = \frac{1}{2} a h\, \tilde{u}_{xx} \leftarrow \text{modified equation} \\ d \equiv \frac{ah}{2} \quad \text{artificial dissipation} \end{cases}$$

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

$$\frac{1}{h}\left(w_{j-1} - w_j\right) = \frac{1}{2h}\left(w_{j-1} - w_{j+1}\right) + \frac{\overset{\swarrow d/a}{h/2}}{h^2}\left(w_{j-1} - 2w_j + w_{j+1}\right)$$

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

modified equation for centered scheme

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

artificial dispersion

$$\begin{cases} \tilde{u}(x,0) = e^{2\pi i k x} \Rightarrow \\ \tilde{u}(x,t) = e^{2\pi i k (x - a_k t)} \end{cases}$$

numerical phase velocity

but $a_k = a\left(1 - \frac{2}{3}\pi^2 k^2 h^2\right)$

dispersion relation

So if the solution is not smooth (has high-frequency components), it will be distorted (Gibbs phenomenon)

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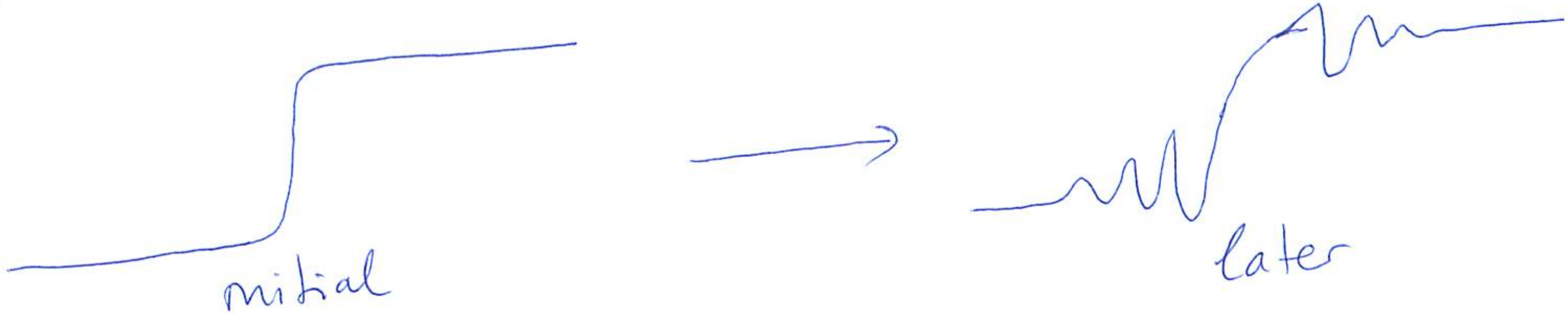



Note $k_{max} = \frac{m}{2}$ so $\frac{2}{3}\pi^2 k_{max}^2 h^2 = \frac{2}{3}\pi^2 \cdot \frac{1}{4}$

independent of $h$. So the grid must be <u>much</u> finer than the width of regions with <u>sharp gradients</u>

<u>Dilemma</u> (Central issue in adv-diff)

{ Accept low accuracy (artificial diss.)
accept low robustness (non-monotonicity)
or find a way to trade off

10 Fourier analysis

$$w_j = \sum_k \alpha_h^{(t)} e^{2\pi i k j/m}$$

$$w_j' = \sum_h \alpha_h'(t) e^{2\pi i k j/m} = \frac{a}{h}(w_{j-1} - w_j)$$

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

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

By orthogonality of Fourier basis

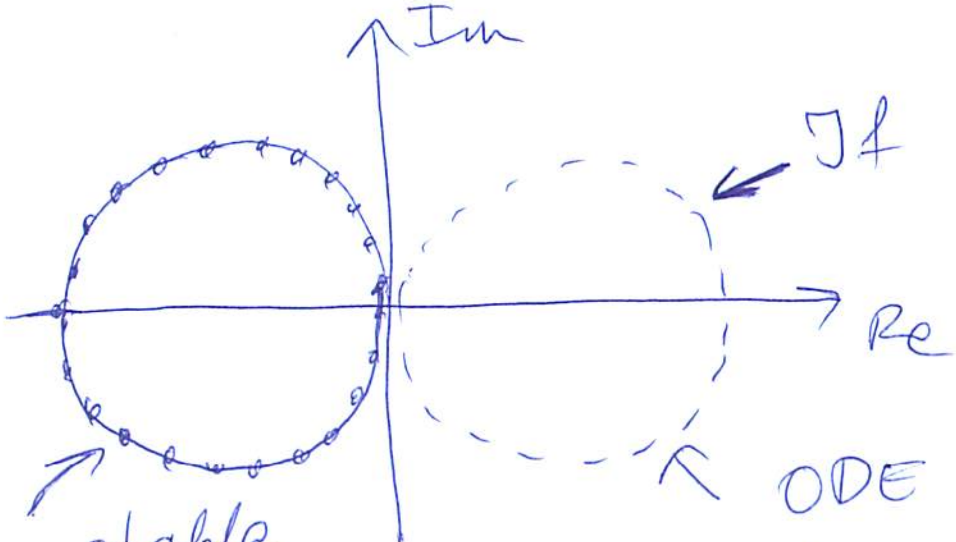
$$\alpha_h' = \alpha_h \cdot \underbrace{\frac{a}{h}\left[\left(\cos(2\pi i k/m) - 1\right) - i \sin(2\pi i k/m)\right]}$$

$\lambda_k$ - decay rate or eigenvalue of $\phi_k$

(11) Similarly, for centered discretization

$$\lambda_k = -\frac{ia}{h} \sin(2\pi k/m)$$

$a>0$
backward difference

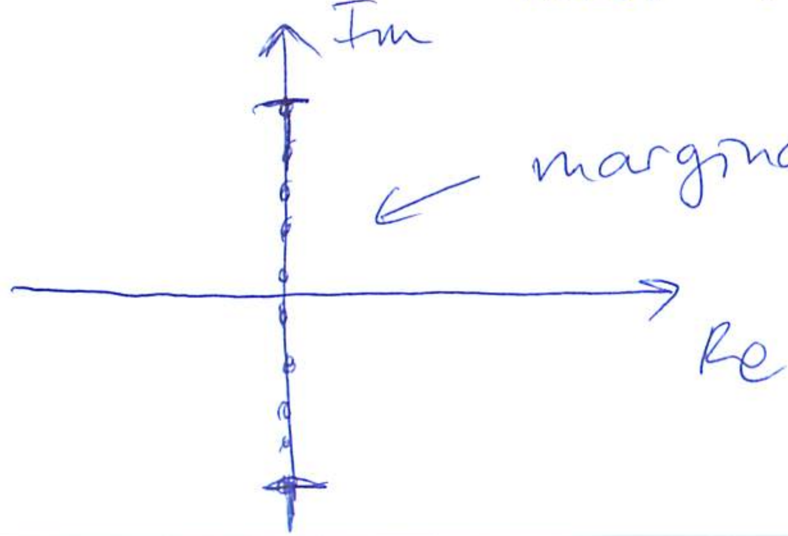



If $a<0$

ODE is stable

ODE is unstable (which is why we must look at sign of a)

centered difference




marginal stability

(12) A series expansion of the eigenvalues:

$$\begin{cases} \lambda_h = -2\pi i a k - \frac{1}{2}|a|(2\pi k)^2 h + O(h^2) & \text{for upwind} \quad \text{first-order} \\ \\ \lambda_h = \underbrace{-2\pi i a k}_{\text{correct answer (continuum PDE)}} + \frac{1}{6} i a (2\pi k)^3 h^2 + O(h^4) & \text{second-order} \end{cases}$$

$$\boxed{-a\partial_x \rightarrow -2\pi i a k \quad \text{in Fourier space}}$$

$$\begin{cases} \mathrm{Re}(\lambda_h) < 0 \rightarrow \text{dissipative scheme} \\ \mathrm{Re}(\lambda_h) = 0 \rightarrow \text{non-dissipative} \\ \mathrm{Re}(\lambda_h) > 0 \rightarrow \text{unstable} \end{cases}$$

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# Higher-Order FD schemes

$$\begin{cases} w_j' = \dfrac{a}{h} \displaystyle\sum_{k=-r}^{s} c_k \, w_{j+k} \\ \text{stencil width} = s+r+1 \end{cases}$$

Optimal-order scheme

$$q = r+s$$

**Theorem** (Iserles & Strang)

If $a>0$, the optimal-order scheme is stable for $\boxed{s \le r \le s+2}$ and unstable otherwise

(14) E.g. third-order upwind-biased method for $a>0$

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

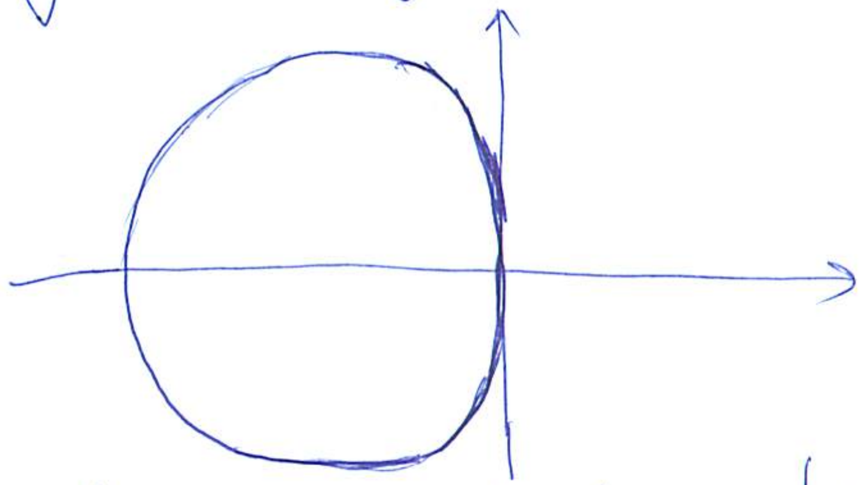
Modified eq: $\tilde{\hat{u}}_t + a\tilde{\hat{u}}_x = -\frac{|a|}{12}h^3\tilde{\hat{u}}_{xxxx}$

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

Note: $u_t = -u_{xxxx}$, $\hat{u}_t = -k^4\hat{u}$

does not satisfy a maximum principle and over/under shoots can appear

(15) While $Re(\lambda_h) < 0$ (except $\lambda_h = 0$) 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 shoots)

(16) <u>Diffusion Equation</u> $u_t = d\, u_{xx}$

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

Modified equation (<u>misleading</u>)

$$\tilde{u}_t = d\,\tilde{u}_{xx} + \underbrace{\frac{dh^2}{12}\,\tilde{u}_{xxxx}}_{\text{\underline{unstable} term}}$$

More useful to look in Fourier space:

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

<u>smoothing</u> property (desirable)

## Fourth-order

stencil

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

$j-2,\ j-1,\ j,\ j+1,\ j+2$

Always symmetric

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

Now just combine advection + diffusion for $u_t + a u_x = d u_{xx}$

Artificial diffusion $\tilde{d} = ah/2 \sim ah$

Dimensionless number <u>cell Péclet number</u>

$$\boxed{P_e = \frac{ah}{d}}$$

$P > 1$ – advection-dominated
$P < 1$ – diffusion-dominated

(18) Consider centered scheme

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

If $Pe < 2$ then

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

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

$\rightarrow$ non-oscillatory

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