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Overview

How to solve parabolic PDEs like:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x} + R$$

$$t = 0; 0 \le x \le \ell \implies c = c_0$$

with
$$t > 0; x = 0$$
 $\Rightarrow -\mathcal{D}\frac{\partial c}{\partial x} + uc = u_{in}c_{in}$

$$t > 0; x = \ell$$
 $\Rightarrow \frac{\partial c}{\partial x} = 0$

accurately and efficiently?

Today's outline

Introduction

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What is a PDE?

An equation containing a function and their derivatives to multiple independent variables.

The highest derivative appearing in the PDE

General second order ODE:

$$A\frac{\partial^2 f}{\partial x^2} + B\frac{\partial^2 f}{\partial x \partial y} + C\frac{\partial^2 f}{\partial y^2} + D\frac{\partial f}{\partial x} + E\frac{\partial f}{\partial y} + Ff = G$$

- Linear equation: Coefficients A, B, ..., G do not depend on x
- Non-linear equation: Coefficients A. B. G are a function of x and y.

Introduction

Convection

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Classification of PDE's

 $A\frac{\partial^2 f}{\partial x^2} + B\frac{\partial^2 f}{\partial x \partial y} + C\frac{\partial^2 f}{\partial y^2} + D\frac{\partial f}{\partial x} + E\frac{\partial f}{\partial y} + Ff = G$

 $A\frac{\partial}{\partial x^2} + B\frac{\partial}{\partial x\partial y} + C\frac{\partial}{\partial y^2} + D\frac{\partial}{\partial x} + E\frac{\partial}{\partial y} + Ff = G$ The discriminant Δ of a quadratic polynomial is computed as (note: only the higher order coefficients are important): $A = B^2 - AAC$

- $\Delta < 0 \Rightarrow$ Elliptic equation
- (e.g. Laplace equation for stationary diffusion in 2D)
- $\bullet \;\; \Delta = 0 \Rightarrow \mathsf{Parabolic} \; \mathsf{equation}$
- (e.g. instationary heat penetration in 1D)
- ∆ > 0 ⇒ Hyperbolic equation (e.g. wave equation)

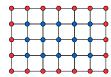






Introduction 000000000

Example elliptic PDE (boundary value problems: BVP)



- Grid point at which dependent variable has to be computed
- Grid point at which boundary condition is specified

Typical example: Poisson equation

$$\frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial y^2} = f(x, y)$$

Efficiency (memory requirements, CPU time) of the numerical method is of crucial importance.

Introduction

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Convection

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Importance of classification

Different PDE types require different solution techniques because of the difference in range of influence:

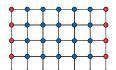
Characteristics

point P

- Curves in xy-domain along with signal propagation takes place
- Domain of dependence of point P
 points in xy-domain which influence the value of f in point P
- Range of influence of point P
 points in xv-domain which are influenced by the value of f in

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Example parabolic PDE (initial value problem: IVP)



- Grid point at which dependent variable has to be computed
- Grid point at which boundary condition is specified

Typical example: Poisson equation

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} + R$$

Stability (in numerical sense) of the numerical method is of crucial importance.

Boundary conditions

. Dirichlet or fixed condition: prescribed value of f at boundary

$$f = f_0$$
 f_0 is a known function

. Neumann condition: prescribed value of derivative of f at boundary

$$\frac{\partial f}{\partial p} = q$$
 q is a known function

 Mixed or Robin condition: relation between f and df at houndary

$$a\frac{\partial f}{\partial n} + bf = c$$
 a, b and c are known functions

Instationary diffusion equation (Fick's second law)

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$
, with $t > 0$; $x \le \ell \Rightarrow c = c_0$
 $t > 0 : x = 0 \Rightarrow c = c_1$
 $t > 0 : x = \ell \Rightarrow c = c_0$

Second derivative $\frac{\partial^2 c}{\partial v^2} \stackrel{c_{j-1}}{\bullet} \stackrel{c_j}{\bullet} \stackrel{c_{j-1}}{\bullet}$

$$c_{i+1} = c_i + \frac{\partial c}{\partial x} \left| \Delta x + \frac{1}{2} \frac{\partial^2 c}{\partial x^2} \right| \Delta x^2 + \frac{1}{6} \frac{\partial^2 c}{\partial x^3} \left| \Delta x^3 + \dots \right|$$

 $c_{i-1} = c_i - \frac{\partial c}{\partial x} \left| \Delta x + \frac{1}{2} \frac{\partial^2 c}{\partial x^2} \right| \Delta x^2 - \frac{1}{6} \frac{\partial^3 c}{\partial x^3} \left| \Delta x^3 + \dots \right|$

$$c_{i+1} + c_{i-1} = 2c_i + \frac{\partial^2 c}{\partial x^2}\Big|_i \Delta x^2 + \mathcal{O}(\Delta x^4)$$

 $\Rightarrow \frac{\partial^2 c}{\partial x^2}\Big|_i = \frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2} + \mathcal{O}(\Delta x^2)$

Due to symmetric discretization: second order (central discretization).

Numerical solution method

Finite differences (method of lines, MOL):

- Discretize spatial domain in discrete grid points
- Find suitable approximation for the spatial derivatives
- Substitute approximations in PDE, which gives a system of ODE's, one for every grid points
- Advance in time with a suitable ODE solver

Alternative methods: collocation, Galerkin or Finite Element methods

Instationary diffusion equation (Fick's second law)

An alternative discretization:

$$\frac{\partial^{2} C}{\partial x^{2}}\Big|_{i} = \frac{\frac{\partial c}{\partial x}\Big|_{i+\frac{1}{2}} - \frac{\partial c}{\partial x}\Big|_{i-\frac{1}{2}}}{\Delta x} + \mathcal{O}(\Delta x^{2}) \xrightarrow{G_{\bullet,1}} \frac{\frac{\partial c}{\partial x}\Big|_{i+\frac{1}{2}} - \frac{C}{\partial x}}{X} \xrightarrow{\frac{\partial c}{\partial x}\Big|_{i+\frac{1}{2}} - \frac{C}{\partial x}} \frac{\frac{\partial c}{\partial x}\Big|_{i+\frac{1}{2}} - C_{\bullet,1}}{X}$$

$$= \frac{C_{i+1} - C_{i} - C_{i} - C_{i-1}}{\Delta x} - \frac{C_{\bullet,1} - C_{\bullet,1}}{\Delta x} = \frac{C_{\bullet,1} - 2C_{i} + C_{\bullet,1}}{X}$$

This is convenient for the derivation of $\frac{\partial}{\partial x} \left(\mathcal{D} \frac{\partial c}{\partial x} \right)$:

$$\frac{\partial}{\partial x}\left(\mathcal{D}\frac{\partial c}{\partial x}\right) = \frac{\mathcal{D}_{1+\frac{1}{2\delta}}\frac{\partial c_{\parallel}}{|x_{\perp}|} - \mathcal{D}_{-\frac{1}{2\delta}}\frac{\partial c}{|x_{\parallel}|}}{\Delta x} = \frac{\mathcal{D}_{1+\frac{1}{2}}\frac{c_{\parallel 1} - c_{\parallel}}{\Delta x} - \mathcal{D}_{\parallel} - \frac{c_{\parallel} - c_{\parallel 1}}{\Delta x}}{\Delta x}$$

$$= \frac{\mathcal{D}_{1+\frac{1}{2}}c_{\parallel 1} - \left(\mathcal{D}_{1+\frac{1}{2}} + \mathcal{D}_{\perp}\right)c + \mathcal{D}_{\parallel} - \frac{1}{2}c_{\parallel}}{\Delta x}$$

Instationary diffusion equation (Fick's second law)

$$\begin{split} \frac{\partial^2 f}{\partial x^2} & \quad i = 1 \quad \frac{i - \frac{1}{2}}{X} \quad \frac{i}{i} \quad \frac{i + \frac{1}{2}}{X} \quad \frac{i + \frac{1}{2}}{i} \quad \frac{i + \frac{1}{2}}{4} \\ f_{i + \frac{1}{2}} & = f_i + \frac{1}{2} \Delta x \frac{\partial f}{\partial x} \Big|_i \Delta x + \frac{1}{2} \left(\frac{1}{2} \Delta x \right)^2 \frac{\partial^2 f}{\partial x^2} \Big|_i + O(\Delta x^3) \\ f_{i - \frac{1}{2}} & = f_i - \frac{1}{2} \Delta x \frac{\partial f}{\partial x} \Big|_i \Delta x + \frac{1}{2} \left(\frac{1}{2} \Delta x \right)^2 \frac{\partial^2 f}{\partial x^2} \Big|_i + O(\Delta x^3) \\ \hline f_{i + \frac{1}{2}} & = \Delta x \frac{\partial f}{\partial x} + O(\Delta x^3) \end{split}$$

$$\Rightarrow \frac{\partial f}{\partial x} = \frac{f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}}{\Delta x} + \mathcal{O}(\Delta x^2)$$

Instationary diffusion equation: Convertism Coolection Coolection

Two options:

Keep boundary conditions as additional equations

$$\begin{split} c_0 &= c_1, \frac{dc_1}{dt} = \mathcal{D}\frac{c_0 - 2c_1 + c_2}{\Delta x^2}, \frac{dc_2}{dt} = \mathcal{D}\frac{c_1 - 2c_2 + c_3}{\Delta x^2}, \\ \frac{dc_3}{dt} &= \mathcal{D}\frac{c_2 - 2c_3 + c_4}{\Delta x^2}, \frac{dc_4}{dt} = \mathcal{D}\frac{c_3 - 2c_4 + c_5}{\Delta x^2}, c_5 = c_R \end{split}$$

Substitute boundary conditions to reduce number of equations:

$$\begin{split} \frac{dc_1}{dt} &= \mathcal{D} \frac{c_1 - 2c_1 + c_2}{\Delta x^2}, \frac{dc_2}{dt} &= \mathcal{D} \frac{c_1 - 2c_2 + c_3}{\Delta x^2}, \\ \frac{dc_3}{dt} &= \mathcal{D} \frac{c_2 - 2c_3 + c_4}{\Delta x^2}, \frac{dc_4}{dt} &= \mathcal{D} \frac{c_3 - 2c_4 + c_8}{\Delta x^2} \end{split}$$

Instationary diffusion equation: spatial discretization

Substitution of spatial derivatives yields:

$$\frac{dc_i}{dt} = D \frac{c_{i-1} - 2c_i + c_{i+1}}{\Delta x^2} \quad \text{for } i = 0, \dots, N$$

For example, using 6 (ridiculously low number!) grid points:



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Instationary diffusion equation: temporal discretization

$$\frac{dc_i}{dt} = D \frac{c_{i-1} - 2c_i + c_{i+1}}{\Delta x^2}$$

Time discretization: forward Euler (explicit)

$$\begin{split} \frac{c_i^{n+1}-c_i^n}{\Delta t} &= \mathcal{D}\frac{c_{i-1}^n-2c_i^n+c_{i+1}^n}{\Delta x^2} \\ &\Rightarrow c_i^{n+1} = Foc_{i-1}^n + (1-2Fo)c_i^n + Foc_{i+1}^n \quad \text{with } Fo = \frac{\mathcal{D}\Delta t}{\Delta x^2} \end{split}$$

Straightforward updating (explicit equation), simple to implement in a program but stability constraint $Fo = \frac{\mathcal{D}\Delta t}{\lambda r^2} < \frac{1}{2}!$ Small $\Delta x \Rightarrow$ small $\Delta t \Rightarrow$ patience required \odot

Instationary diffusion equation: temporal discretization

$$\frac{c_i}{tt} = D \frac{c_{i-1} - 2c_i + c_{i+1}}{\Delta x^2}$$

$$\begin{split} & \frac{c_{j}^{n+1} - c_{i}^{n}}{\Delta t} = \mathcal{D} \frac{c_{i-1}^{n+1} - 2c_{i}^{n+1} + c_{i+1}^{n+1}}{\Delta x^{2}} \\ & \Rightarrow -Foc_{i-1}^{n+1} + (1 + 2Fo)c_{i}^{n+1} - Foc_{i+1}^{n+1} = c_{i}^{n} \quad \text{with } Fo = \frac{\mathcal{D}\Delta t}{\Delta x^{2}} \end{split}$$

Requires the solution of a system of linear equations, but no stability constraints!

Note: extension to higher order schemes (with time step adaptation) straightforward. Often second or third order optimal, because for each Euler-like step in the additional order an often large system needs to be solved (not treated in this course).

Solving the instationary diffusion equation: example

Initialise the variables and matrices

```
% Nc grid points
Nt = 40000:
                    % Nt time steps
D = 1e-8:
                    % m/s
c L = 1.0: c R = 0: % mol/m3
t end = 5000.0:
x end = 5e-3:
% Time step and grid size
dt = t end/Nt:
dx = x end/Nx:
```

% Fourier number Fo=D*dt/dx/dx

Nx = 100:

% Initial matrices for solutions (Nx times Nt) c = zeros(Nt+1.Nx+1): % All concentrations are zero c(:.1) = c L: % Concentration at left side c(:.Nx+1) = c R: % Concentration at right side

% Grid node and time step positions x = linspace(0.x end.Nx+1);

Solving the instationary diffusion equation: example

Solve the diffusion problem using explicit discretization:

$$\frac{\partial c_i}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \qquad \text{with} \qquad \frac{0 \le x \le \delta, \ \delta = 5 \cdot 10^{-3} \text{ m}}{\delta \Delta x = 100 \text{ grid cells}}$$

$$\text{with} \qquad \frac{1 \cdot 10^{-8} \text{ m}^2 \text{ s}^{-1}}{t_{\text{end}} = 5000 \text{ s}}$$

$$c_i = 1 \text{ mol m}^{-3} \text{ ag} = 0 \text{ mol m}^{-3}$$

$$c_i^{n+1} = Foc_{i-1}^n + (1 - 2Fo)c_i^n + Foc_{i+1}^n$$
 with $Fo = \frac{D\Delta t}{\Delta t^2}$

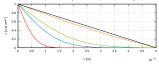
- Initialise variables
- ② Compute time step so that $Fo \le \frac{1}{2} \Rightarrow \Delta t = 0.125s!$
- Compute 40000 time steps times 100 grid nodes!
- Store solution

Solving the instationary diffusion equation: example

```
Compute the solution (nested time-and-grid loop):
for n = 1:Nt % time loop
```

and

Plotting the solution at $t = \{12.5, 62.5, 125, 625, 5000\}$ s.



Solving the diffusion equation implicitly

Linear system $Ax = \mathbf{b}$ from $-Foc_{i-1}^{n+1} + (1 + 2Fo)c_i^{n+1} - Foc_{i+1}^{n+1} = c_i^n$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -F_0 & (1+2F_0) & -F_0 & 0 & \cdots & 0 \\ 0 & -F_0 & (1+2F_0) & -F_0 & \cdots & 0 \\ 0 & 0 & -F_0 & (1+2F_0) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix}, \begin{pmatrix} c_2^{i+1} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \end{pmatrix} = \begin{pmatrix} c_2^{i} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \end{pmatrix} = \begin{pmatrix} c_2^{i+1} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \end{pmatrix} = \begin{pmatrix} c_2^{i+1} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \end{pmatrix} = \begin{pmatrix} c_2^{i+1} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \end{pmatrix} = \begin{pmatrix} c_2^{i+1} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \end{pmatrix} = \begin{pmatrix} c_2^{i+1} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \end{pmatrix} = \begin{pmatrix} c_2^{i+1} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \end{pmatrix} = \begin{pmatrix} c_2^{i+1} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \end{pmatrix} = \begin{pmatrix} c_2^{i+1} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \\ c_3^{i+1} \end{pmatrix} = \begin{pmatrix} c_2^{i+1} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \\ c_3^{i+1} \end{pmatrix} = \begin{pmatrix} c_2^{i+1} \\ c_1^{i+1} \\ c_2^{i+1} \\ c_3^{i+1} \\ c_3$$

 $1 \times c_0^{n+1} = c_0^n$ (boundary condition)

$$Foc_0^{n+1} + (1 + 2Fo)c_1^{n+1} - Foc_2^{n+1} = c_1^n$$

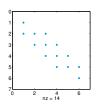
 $Foc_1^{n+1} + (1 + 2Fo)c_2^{n+1} - Foc_1^{n+1} = c_2^n$

$$Foc_i^{n+1} + (1 + 2Fo)c_i^{n+1} - Foc_i^{n+1} = c_i^n$$

 $1 \times c_{-}^{n+1} = c_{-}^{n}$ (boundary condition)

Solving the diffusion equation implicitly in Matlab

The command spy(A) shows a figure with the non-zero positions.



Solving the diffusion equation implicitly in Matlab

To solve the linear system, we need to define matrix A. It is clear that storing many zeros is not efficient in terms of memory. We use a sparse matrix format:

```
% Bands in matrix (internal cells)
A = sparse(Nx+1,Nx+1);
for i=2:Nx
    A(i.i-1) = -Fo:
    A(i,i) = (1+2*Fo);
    A(i,i+1) = -Fo;
end
% Set boundary cells, independent on neighbors:
                  % Left
A(1,1) = 1;
A(Nx+1,Nx+1) = 1; % Right
```

Solving the diffusion equation implicitly in Matlab

The concentration matrix is initialised and the boundary conditions are set as follows:

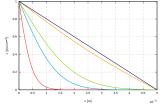
```
% Initial matrices for solutions (Nx times Nt)
c = zeros(Nt+1,Nx+1); % All concentrations are zero
                      % Concentration at left side
c(:,1) = c_L;
c(:.Nx+1) = c R:
                      % Concentration at right side
```

The right hand side vector (b) can now be set during the time-loop:

```
for n = 1:Nt-1 % time loop
   b = c(n.:)': % Set right hand side
   solX = A\b:
                     % Solve linear system
   c(n+1.:) = solX: % Store solution each time step
```

Solving the diffusion equation implicitly in Matlab





Extension with non-linear source terms

$$\frac{\partial c}{\partial t} = \mathcal{D}\frac{\partial^2 c}{\partial x^2} + R(c) \quad \text{with} \quad \begin{array}{l} t = 0; \ 0 \le x \le \ell \Rightarrow c = c_0 \\ t > 0; x = 0 \Rightarrow c = c_L \end{array}$$

Forward Euler (explicit): simply add to right-hand side

$$\begin{aligned} \frac{c_i^{n+1} - c_i^n}{\Delta t} &= \mathcal{D} \frac{c_{i-1}^n - 2c_i^n + c_{i+1}^n}{\Delta x^2} + R(c_i^n) \\ &\Rightarrow c_i^{n+1} &= Foc_{i-1}^n + (1 - 2Fo)c_i^n + Foc_{i+1}^n + R_i^n \end{aligned}$$

· Backward Euler (implicit): linearization required

$$\begin{split} &R(c_i^{n+1}) = R(c_i^n) + \frac{dR}{dc} \Big|_i^n (c_i^{n+1} - c_i^n) \\ & \frac{c_i^{n+1} - c_i^n}{\Delta t} = D \frac{c_{i-1}^{n+1} - 2c_i^{n+1} + c_{i+1}^{n+1}}{\Delta c^n} + R(c_i^{n+1}) \\ & \Rightarrow -Foc_{i-1}^{n+1} + (1 + 2Fo - \frac{dR}{dc}) \Big|_i^n c_i^{n+1} - Foc_{i+1}^{n+1} = c_i^n + R_i^n - \frac{dR}{dc} \Big|_i^n c_i^n \\ \end{split}$$

About explicit vs. implicit solutions

- Explicit solution:
 - · Easy to implement · Very small time steps required.
 - This problem took about 0.5 s.
- Implicit solution:
 - · Harder to implement, needs sparse matrix solver
 - · No stability constraint
 - This problem took about 0.05 s
- The difference will become much larger for systems with e.g. more grid nodes!

Extension with convection terms

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} - u \frac{\partial c}{\partial x} + R$$

Discretization of first derivative $\frac{dc}{dx}$ looks simple but is numerical headache!

Central discretization: $\frac{dc}{dx} = \frac{c_{i+1} - c_{i-1}}{\Delta x}$ \Rightarrow simple and easy, too bad it doesn't work: yields unstable solutions if convection dominated

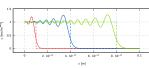
Central difference scheme of 1st derivative



Central difference for first derivative: dc $c_{i+1} - c_{i-1}$

Forward Euler discretization of temporal and spatial domain:

$$\frac{c_{i}^{n+1}-c_{i}^{n}}{\Delta t}=-u\frac{c_{i+1}-c_{i-1}}{2\Delta x}\Rightarrow c_{i}^{n+1}=c_{i}^{n}-u\frac{c_{i+1}^{n}-c_{i-1}^{n}}{2\Delta x}\Delta t$$



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First order upwind scheme of 1st derivative



Upwind scheme for first derivative:

$$-u\frac{dc}{dx}\Big|_{i} = \begin{cases}
-u\frac{c_{1}-c_{i-1}}{\Delta x} & \text{if } u \geq 0 \\
-u\frac{c_{i+1}-c_{i}}{\Delta x} & \text{if } u \geq 0
\end{cases}$$

Forward Euler discretization of temporal and spatial domain:

$$\begin{split} &\frac{c_i^{n+1}-c_i^n}{\Delta t} = -u\frac{c_{i+1}-c_{i-1}}{2\Delta x} \\ &\Rightarrow c_i^{n+1} = \left\{ \begin{array}{ll} c_i^n - u\frac{c_{i-1}-c_{i-1}}{\Delta x} & \text{if } u \geq 0 \\ c_i^n - u\frac{c_{i+1}-c_i}{\Delta x} & \text{if } u < 0 \end{array} \right. \end{split}$$

Extension with convection terms

Solution: upwind discretization. like CSTR's in series:



First order upwind:
$$-u\frac{dc}{dx}\Big|_{i} = \begin{cases} -u\frac{c_{i}-c_{i-1}}{\Delta x} & \text{if } u \geq 0 \\ -u\frac{c_{i+1}-c_{i}}{\Delta x} & \text{if } u < 0 \end{cases}$$

Stable if $Co = \frac{u\Delta t}{\Delta x} < 1$ (with Co the Courant number). However, only 1^{st} order accurate (large smearing of concentration fronts). Higher order upwind requires TVD schemes (trick of the trade)...

Upwind scheme: example

Unsteady convection through a pipe:

$$\frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x}$$
 with $u = 0.1 \text{m s}^{-1} \Rightarrow c_i^{n+1} = c_i^n - u \frac{c_i - c_{i-1}}{\Delta x} \Delta t$









Central difference and upwind in Matlab

```
The results from the previous slides were computed using this script:
Nx = 1000;
                    % No grid points
Nt = 10000;
                    % Nt time steps
u = 0.001;
c_in = 1.0;
t_end = 100.0;
x_{end} = 0.1;
% Time step and grid size
dt = t_end/Nt; dx = x_end/Nx;
% Courant number
Commadt/dx
% Initial matrices for solutions (Nx times Nt)
c1 = zeros(Nt+1,Nx+1); % All concentrations are zero
c1(:,1) = c_in;
                    % Concentration at inlet (all time steps
an = c1; c2 = c1; % Analytical and upwind solution
% Grid node and time step positions
x = linspace(0,x_end,Nx+1);
t = linspace(0,t_end,Nt+1);
```

Extension to systems of PDE's

- · Explicit methods: straightforward extension
- . Implicit methods: yields block-tridiagonal matrix (note ordering of equations: all variables per grid cell)

Central difference and upwind in Matlab

```
(continued)
for n = 1:Nt % time loop
    for i = 2:Nx % Nested loop for grid nodes
        c1(n+1.i) = c1(n.i) - u*((c1(n.i+1) - c1(n.i))
            -1))/(2*dx))*dt:
        % Upwind
        c2(n+1,i) = c2(n,i) - u*((c2(n,i) - c2(n,i-1))
            /(dx))*dt;
        % Analytical
        an(n+1.i) = (x(i) < u*t(n+1))*c in:
    end
```

Extension to 2D or 3D systems

Spatial discretization in 2 directions - different methods available:

- Explicit
 - · Fully implicit
 - 1D gives tri-diagonal matrix
 - · 2D gives penta-diagonal matrix
 - · 3D gives hepta-diagonal matrix
 - Use of dedicated matrix solvers (e.g. ICCG, multigrid, ...)
- · Alternating direction implicit (ADI)
 - Per direction implicit, but still overall unconditionally stable

Further extensions for parabolic PDEs

- · Higher order temporal discretization (multi-step) with time step adaptation
- · Non-uniform grids with automatic grid adaptation
- · Higher-order discretization methods, especially higher order TVD (flux delimited) schemes for convective fluxes (e.g. WENO schemes)
- · Higher-order finite volume schemes (Riemann solvers)

Summary

- · Several classes of PDEs were introduced · Elliptic. Parabolic. Hyperbolic PDEs
- · Diffusion equation: discretization of temporal and spatial domain was discussed
 - · Solutions of the diffusion equation using explicit and implicit
 - · How to add non-linear source terms
- · Convection: upwind vs. central difference schemes