Partial differential equations

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Today's outline

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Overview

Main question

How to solve parabolic PDEs like:

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

with

$$\begin{aligned} t &= 0; 0 \leq x \leq \ell & &\Rightarrow c = c_0 \\ t &> 0; x = 0 & &\Rightarrow -\mathcal{D}\frac{\partial c}{\partial x} + uc = u_{\text{in}} c_{\text{in}} \\ t &> 0; x = \ell & &\Rightarrow \frac{\partial c}{\partial x} = 0 \end{aligned}$$

accurately and efficiently?

What is a PDE?

Partial differential equation

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

Order of PDE

The highest derivative appearing in the PDE

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

Classification of PDE's

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

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$\Delta = B^2 - 4AC$

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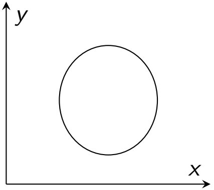
- $\Delta < 0 \Rightarrow$ Elliptic equation
  (e.g. Laplace equation for stationary diffusion in 2D)
- $\Delta = 0 \Rightarrow$ Parabolic equation
  (e.g. instationary heat penetration in 1D)
- $\Delta > 0 \Rightarrow$ Hyperbolic equation
  (e.g. wave equation)



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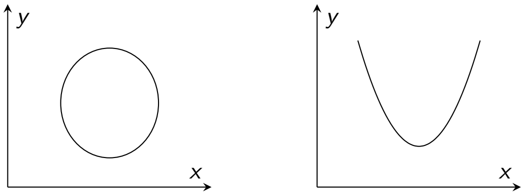

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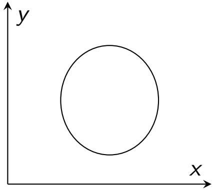

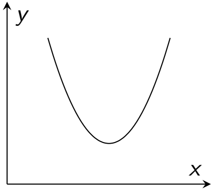

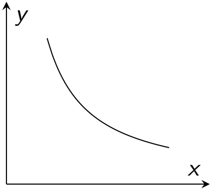

Importance of classification

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

- *Characteristics*
  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*
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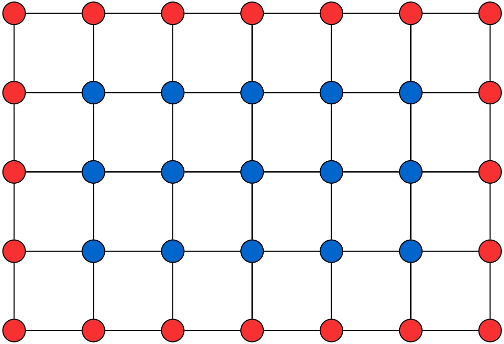
Example elliptic PDE (boundary value problems: BVP)



● Grid point at which dependent variable has to be computed

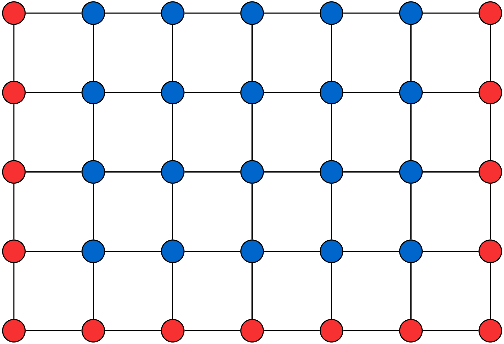
● Grid point at which boundary condition is specified

Typical example: Poisson equation

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

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

Example parabolic PDE (initial value problem: IVP)



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Grid point at which boundary condition is specified

Typical example: Poisson equation

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

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

Boundary conditions

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

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

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

  $\dfrac{\partial f}{\partial n} = q$ $\qquad$ q is a known function

- Mixed or Robin condition: relation between f and $\frac{\partial f}{\partial n}$ at boundary

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

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Numerical solution method

Finite differences (method of lines, MOL):

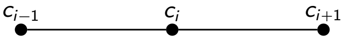
1. Discretize spatial domain in discrete grid points
2. Find suitable approximation for the spatial derivatives
3. Substitute approximations in PDE, which gives a system of ODE's, one for every grid points
4. Advance in time with a suitable ODE solver

Alternative methods: collocation, Galerkin or Finite Element methods

Instationary diffusion equation (Fick's second law)

$$\frac{\partial c}{\partial t} = \mathcal{D}\frac{\partial^2 c}{\partial x^2}, \quad \text{with} \quad \begin{array}{l} t = 0; 0 \leq x \leq \ell \Rightarrow c = c_0 \\ t > 0; x = 0 \Rightarrow c = c_L \\ t > 0; x = \ell \Rightarrow c = c_R \end{array}$$

Second derivative $\dfrac{\partial^2 c}{\partial x^2}$



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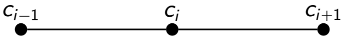

$$c_{i+1} = c_i + \left.\frac{\partial c}{\partial x}\right|_i \Delta x + \frac{1}{2}\left.\frac{\partial^2 c}{\partial x^2}\right|_i \Delta x^2 + \frac{1}{6}\left.\frac{\partial^3 c}{\partial x^3}\right|_i \Delta x^3 + \ldots$$

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

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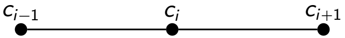

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$$c_{i+1} + c_{i-1} = 2c_i + \left.\frac{\partial^2 c}{\partial x^2}\right|_i \Delta x^2 + \mathcal{O}(\Delta x^4)$$

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

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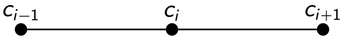

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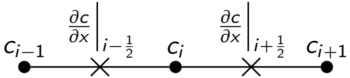
Due to symmetric discretization: second order (central discretization).

Instationary diffusion equation (Fick's second law)

An alternative discretization:

$$\left.\frac{\partial^2 c}{\partial x^2}\right|_i = \frac{\left.\frac{\partial c}{\partial x}\right|_{i+\frac{1}{2}} - \left.\frac{\partial c}{\partial x}\right|_{i-\frac{1}{2}}}{\Delta x} + \mathcal{O}(\Delta x^2)$$



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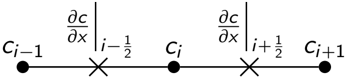

$$= \frac{\frac{c_{i+1} - c_i}{\Delta x} - \frac{c_i - c_{i-1}}{\Delta x}}{\Delta x} = \frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2}$$

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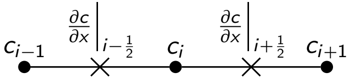

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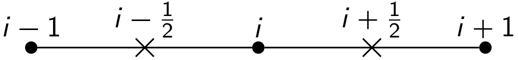
This is convenient for the derivation of $\frac{\partial}{\partial x}\left(\mathcal{D}\frac{\partial c}{\partial x}\right)$:

$$\frac{\partial}{\partial x}\left(\mathcal{D}\frac{\partial c}{\partial x}\right) = \frac{\mathcal{D}_{i+\frac{1}{2}}\left.\frac{\partial c}{\partial x}\right|_{i+\frac{1}{2}} - \mathcal{D}_{i-\frac{1}{2}}\left.\frac{\partial c}{\partial x}\right|_{i-\frac{1}{2}}}{\Delta x} = \frac{\mathcal{D}_{i+\frac{1}{2}}\frac{c_{i+1} - c_i}{\Delta x} - \mathcal{D}_{i-\frac{1}{2}}\frac{c_i - c_{i-1}}{\Delta x}}{\Delta x}$$

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

Instationary diffusion equation (Fick's second law)

$$\frac{\partial^2 f}{\partial x^2}$$



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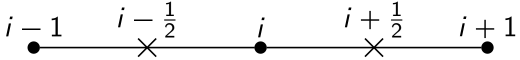

$$f_{i+\frac{1}{2}} = f_i + \frac{1}{2}\Delta x \left.\frac{\partial f}{\partial x}\right|_i \Delta x + \frac{1}{2}\left(\frac{1}{2}\Delta x\right)^2 \left.\frac{\partial^2 f}{\partial x^2}\right|_i + \mathcal{O}(\Delta x^3)$$

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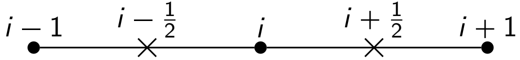

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$$\Rightarrow \left.\frac{\partial f}{\partial x}\right|_i = \frac{f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}}}{\Delta x} + \mathcal{O}(\Delta x^2)$$

Symmetric discretization yields second order!

Instationary diffusion equation: spatial discretization

Substitution of spatial derivatives yields:

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

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

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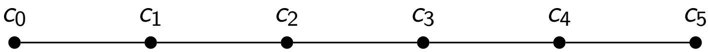

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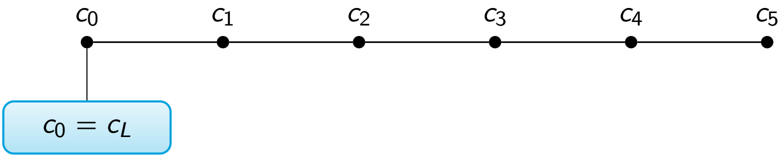

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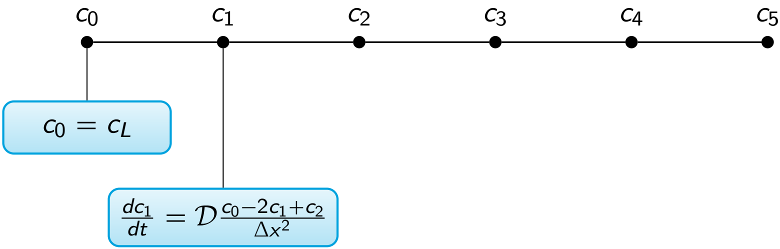

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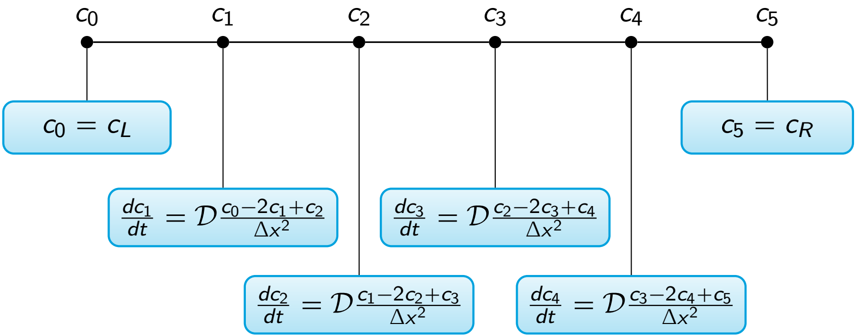

Instationary diffusion equation: boundary conditions

Two options:

1. Keep boundary conditions as additional equations:

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

2. Substitute boundary conditions to reduce number of equations:

$$\frac{dc_1}{dt} = \mathcal{D}\frac{c_L - 2c_1 + c_2}{\Delta x^2}, \frac{dc_2}{dt} = \mathcal{D}\frac{c_1 - 2c_2 + c_3}{\Delta x^2},$$
$$\frac{dc_3}{dt} = \mathcal{D}\frac{c_2 - 2c_3 + c_4}{\Delta x^2}, \frac{dc_4}{dt} = \mathcal{D}\frac{c_3 - 2c_4 + c_R}{\Delta x^2}$$

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1. Keep boundary conditions as additional equations:

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

2. Substitute boundary conditions to reduce number of equations:

$$\frac{dc_1}{dt} = \mathcal{D}\frac{c_L - 2c_1 + c_2}{\Delta x^2}, \frac{dc_2}{dt} = \mathcal{D}\frac{c_1 - 2c_2 + c_3}{\Delta x^2},$$
$$\frac{dc_3}{dt} = \mathcal{D}\frac{c_2 - 2c_3 + c_4}{\Delta x^2}, \frac{dc_4}{dt} = \mathcal{D}\frac{c_3 - 2c_4 + c_R}{\Delta x^2}$$

Instationary diffusion equation: temporal discretization

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

Time discretization: forward Euler (explicit)

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

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

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

Small $\Delta x \Rightarrow$ small $\Delta t \Rightarrow$ patience required ☹

Instationary diffusion equation: temporal discretization

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

Time discretization: backward Euler (implicit)

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

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

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

Solve the diffusion problem using explicit discretization:

$$\frac{\partial c_i}{\partial t} = \mathcal{D}\frac{\partial^2 c}{\partial x^2} \quad \text{with} \quad \begin{aligned} &0 \leq x \leq \delta,\ \delta = 5 \cdot 10^{-3}\ \mathrm{m} \\ &\delta/\Delta x = 100 \text{ grid cells} \\ &\mathcal{D} = 1 \cdot 10^{-8}\ \mathrm{m^2\,s^{-1}} \\ &t_{\mathrm{end}} = 5000\ \mathrm{s} \\ &c_{\mathrm{L}} = 1\ \mathrm{mol\,m^{-3}}\ c_{\mathrm{R}} = 0\ \mathrm{mol\,m^{-3}} \end{aligned}$$

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

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

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

Solving the instationary diffusion equation: example

Initialise the variables and matrices:

```
Nx = 100;                % 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;          % s
x_end = 5e-3;            % m

% Time step and grid size
dt = t_end/Nt;
dx = x_end/Nx;

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

% 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

Compute the solution (nested time-and-grid loop):

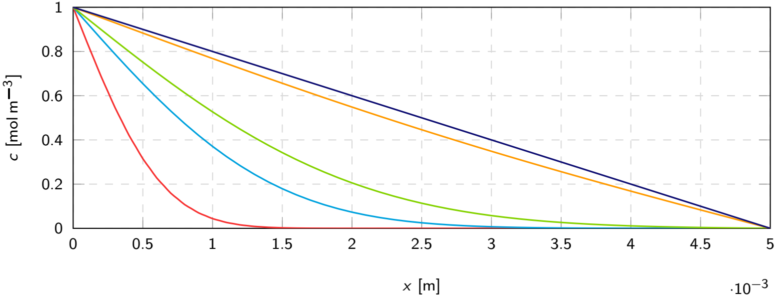
```
for n = 1:Nt % time loop
    for i = 2:Nx % Nested loop for grid nodes
        c(n+1,i) = Fo*c(n,i-1) + (1-2*Fo)*c(n,i) + Fo*
            c(n,i+1);
    end
end
```

Solving the instationary diffusion equation: example

Compute the solution (nested time-and-grid loop):

```
for n = 1:Nt % time loop
    for i = 2:Nx % Nested loop for grid nodes
        c(n+1,i) = Fo*c(n,i-1) + (1-2*Fo)*c(n,i) + Fo*
            c(n,i+1);
    end
end
```

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



Solving the diffusion equation implicitly

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

$$\begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -Fo & (1+2Fo) & -Fo & 0 & \cdots & 0 \\ 0 & -Fo & (1+2Fo) & -Fo & \cdots & 0 \\ 0 & 0 & -Fo & (1+2Fo) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix} \cdot \begin{pmatrix} c_0^{n+1} \\ c_1^{n+1} \\ c_2^{n+1} \\ c_3^{n+1} \\ \vdots \\ c_m^{n+1} \end{pmatrix} = \begin{pmatrix} c_0^n \\ c_1^n \\ c_2^n \\ c_3^n \\ \vdots \\ c_m^n \end{pmatrix}$$

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

Solving the diffusion equation implicitly

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$$
\begin{pmatrix}
1 & 0 & 0 & 0 & \cdots & 0 \\
-Fo & (1+2Fo) & -Fo & 0 & \cdots & 0 \\
0 & -Fo & (1+2Fo) & -Fo & \cdots & 0 \\
0 & 0 & -Fo & (1+2Fo) & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 1
\end{pmatrix}
\cdot
\begin{pmatrix}
c_0^{n+1} \\ c_1^{n+1} \\ c_2^{n+1} \\ c_3^{n+1} \\ \vdots \\ c_m^{n+1}
\end{pmatrix}
=
\begin{pmatrix}
c_0^n \\ c_1^n \\ c_2^n \\ c_3^n \\ \vdots \\ c_m^n
\end{pmatrix}
$$

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

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Solving the diffusion equation implicitly

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

$$\begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -Fo & (1+2Fo) & -Fo & 0 & \cdots & 0 \\ 0 & -Fo & (1+2Fo) & -Fo & \cdots & 0 \\ 0 & 0 & -Fo & (1+2Fo) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix} \cdot \begin{pmatrix} c_0^{n+1} \\ c_1^{n+1} \\ c_2^{n+1} \\ c_3^{n+1} \\ \vdots \\ c_m^{n+1} \end{pmatrix} = \begin{pmatrix} c_0^n \\ c_1^n \\ c_2^n \\ c_3^n \\ \vdots \\ c_m^n \end{pmatrix}$$

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Solving the diffusion equation implicitly

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$$\begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -Fo & (1+2Fo) & -Fo & 0 & \cdots & 0 \\ 0 & -Fo & (1+2Fo) & -Fo & \cdots & 0 \\ 0 & 0 & -Fo & (1+2Fo) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix} \cdot \begin{pmatrix} c_0^{n+1} \\ c_1^{n+1} \\ c_2^{n+1} \\ c_3^{n+1} \\ \vdots \\ c_m^{n+1} \end{pmatrix} = \begin{pmatrix} c_0^n \\ c_1^n \\ c_2^n \\ c_3^n \\ \vdots \\ c_m^n \end{pmatrix}$$

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Solving the diffusion equation implicitly

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

$$\begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -Fo & (1+2Fo) & -Fo & 0 & \cdots & 0 \\ 0 & -Fo & (1+2Fo) & -Fo & \cdots & 0 \\ 0 & 0 & -Fo & (1+2Fo) & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix} \cdot \begin{pmatrix} c_0^{n+1} \\ c_1^{n+1} \\ c_2^{n+1} \\ c_3^{n+1} \\ \vdots \\ c_m^{n+1} \end{pmatrix} = \begin{pmatrix} c_0^n \\ c_1^n \\ c_2^n \\ c_3^n \\ \vdots \\ c_m^n \end{pmatrix}$$

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

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

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$Foc_2^{n+1} + (1+2Fo)c_3^{n+1} - Foc_4^{n+1} = c_3^n$

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

Solving the diffusion equation implicitly in Matlab

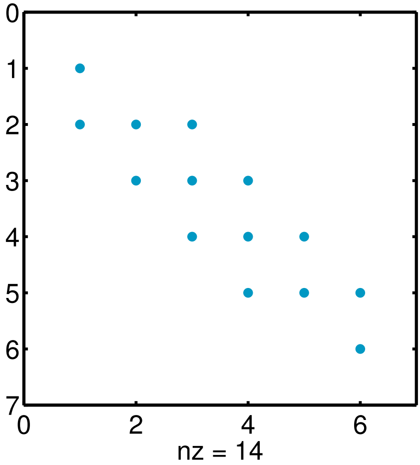
To solve the linear system, we need to define matrix A. It is clear that storing many zeros is not efficient in terms of memory. We use a *sparse matrix* format:

```
% 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:
A(1,1 ) = 1;          % Left
A(Nx+1,Nx+1) = 1;    % Right
```

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

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

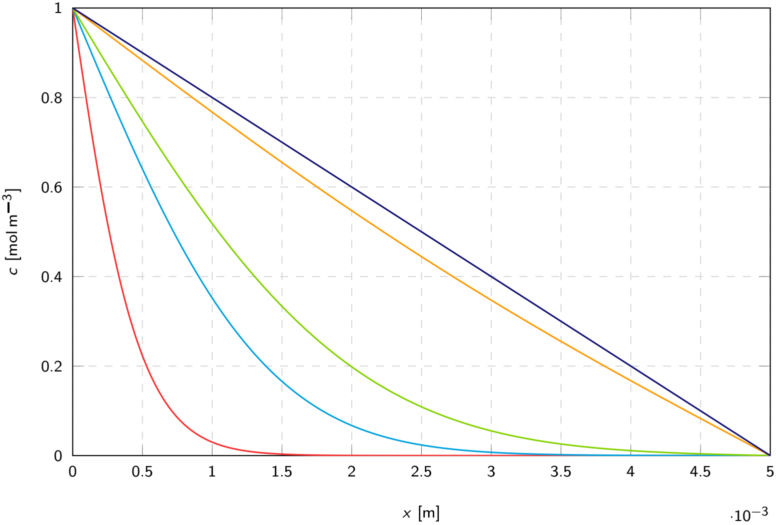
```
% Initial matrices for solutions (Nx times Nt)
c = zeros(Nt+1,Nx+1);  % All concentrations are zero
c(:,1)    = c_L;       % Concentration at left side
c(:,Nx+1) = c_R;       % Concentration at right side
```

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
end
```

Solving the diffusion equation implicitly in Matlab

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



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 non-linear source terms

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

Extension with non-linear source terms

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

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = \mathcal{D}\frac{c_{i-1}^{n} - 2c_i^{n} + c_{i+1}^{n}}{\Delta x^2} + R(c_i^{n})$$

$$\Rightarrow c_i^{n+1} = Foc_{i-1}^n + (1 - 2Fo)c_i^n + Foc_{i+1}^n + R_i^n$$

Extension with non-linear source terms

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$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = \mathcal{D}\frac{c_{i-1}^{n} - 2c_i^{n} + c_{i+1}^{n}}{\Delta x^2} + R(c_i^{n})$$

$$\Rightarrow c_i^{n+1} = Foc_{i-1}^n + (1 - 2Fo)c_i^n + Foc_{i+1}^n + R_i^n$$

- Backward Euler (implicit): linearization required

$$R(c_i^{n+1}) = R(c_i^n) + \left.\frac{dR}{dc}\right|_i^n (c_i^{n+1} - c_i^n)$$

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = \mathcal{D}\frac{c_{i-1}^{n+1} - 2c_i^{n+1} + c_{i+1}^{n+1}}{\Delta x^2} + R(c_i^{n+1})$$

$$\Rightarrow -Foc_{i-1}^{n+1} + (1 + 2Fo - \left.\frac{dR}{dc}\right|_i^n)c_i^{n+1} - Foc_{i+1}^{n+1} = c_i^n + R_i^n - \left.\frac{dR}{dc}\right|_i^n c_i^n$$

Extension with convection terms

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

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

Unsteady convection:

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x}$$

Central difference for first derivative:

$$\frac{dc}{dx} = \frac{c_{i+1} - c_{i-1}}{2\Delta x}$$

Central difference scheme of 1st derivative

Unsteady convection:

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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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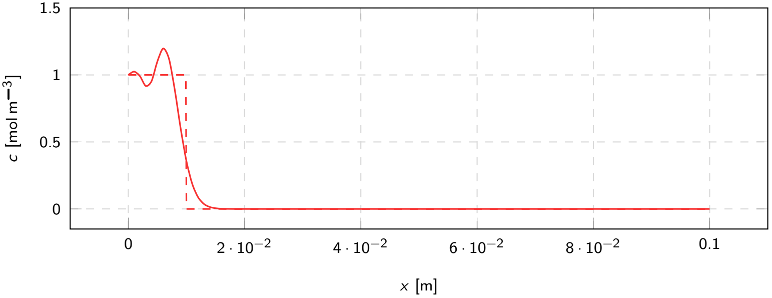

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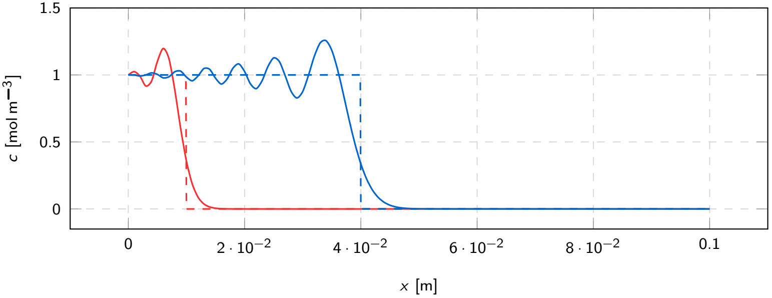

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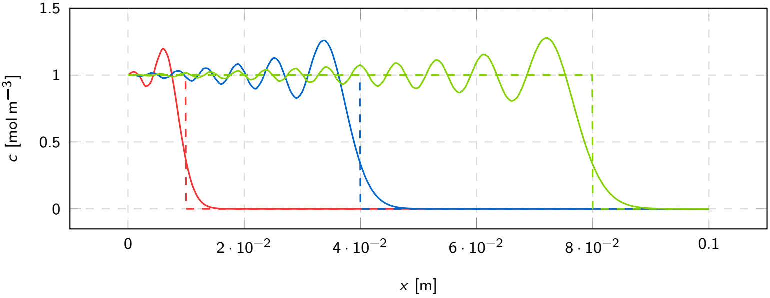
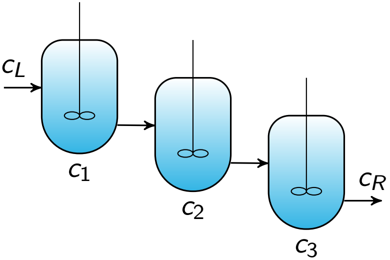


Extension with convection terms

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



First order upwind: $$-u\frac{dc}{dx}\bigg|_i = \begin{cases} -u\dfrac{c_i - c_{i-1}}{\Delta x} & \text{if } u \geq 0 \\[2ex] -u\dfrac{c_{i+1} - c_i}{\Delta x} & \text{if } u < 0 \end{cases}$$

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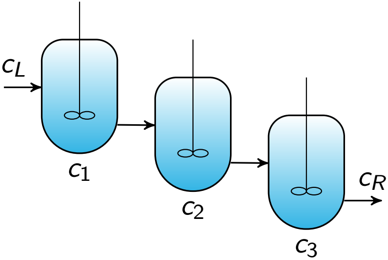

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Stable if $Co = \frac{u\Delta t}{\Delta x} < 1$ (with Co the Courant number). However, only 1$^{\text{st}}$ order accurate (large smearing of concentration fronts). Higher order upwind requires TVD schemes (trick of the trade)...

First order upwind scheme of 1st derivative

Unsteady convection:

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x}$$

Upwind scheme for first derivative:

$$-u\left.\frac{dc}{dx}\right|_i = \begin{cases} -u\dfrac{c_i - c_{i-1}}{\Delta x} & \text{if } u \geq 0 \\ -u\dfrac{c_{i+1} - c_i}{\Delta x} & \text{if } u < 0 \end{cases}$$

First order upwind scheme of 1st derivative

Unsteady convection:

$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x}$$

Upwind scheme for first derivative:

$$-u\frac{dc}{dx}\bigg|_i = \begin{cases} -u\dfrac{c_i - c_{i-1}}{\Delta x} & \text{if } u \geq 0 \\ -u\dfrac{c_{i+1} - c_i}{\Delta x} & \text{if } u < 0 \end{cases}$$

Forward Euler discretization of temporal and spatial domain:

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

$$\Rightarrow c_i^{n+1} = \begin{cases} c_i^n - u\dfrac{c_i - c_{i-1}}{\Delta x} & \text{if } u \geq 0 \\ c_i^n - u\dfrac{c_{i+1} - c_i}{\Delta x} & \text{if } u < 0 \end{cases}$$

Upwind scheme: example

Unsteady convection through a pipe:

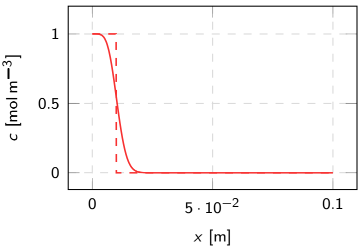
$$\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} \quad \text{with} \quad u = 0.1\,\mathrm{m\,s^{-1}} \Rightarrow c_i^{n+1} = c_i^n - u\frac{c_i - c_{i-1}}{\Delta x}\Delta t$$

Upwind scheme: example

Unsteady convection through a pipe:

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

Using 100 grid cells

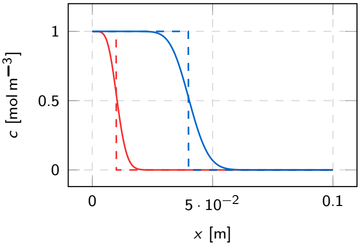


Upwind scheme: example

Unsteady convection through a pipe:

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

Using 100 grid cells

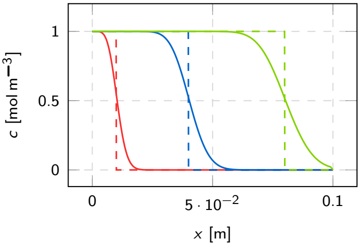


Upwind scheme: example

Unsteady convection through a pipe:

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

Using 100 grid cells

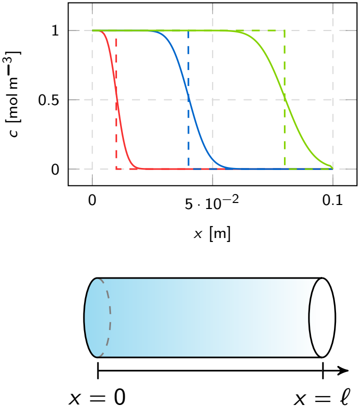


Upwind scheme: example

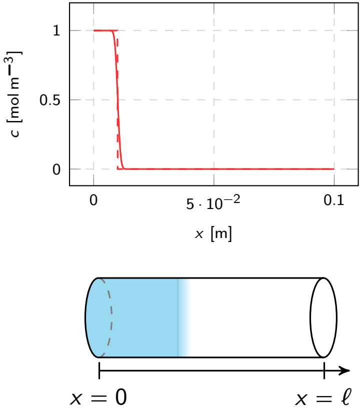
Unsteady convection through a pipe:

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

Using 100 grid cells



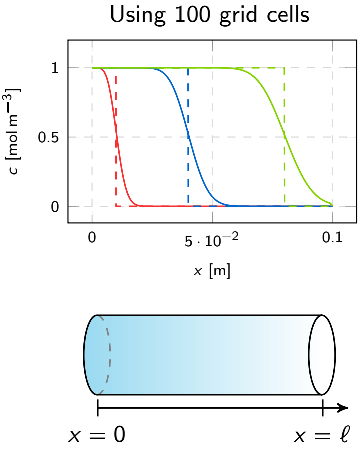
Using 1000 grid cells

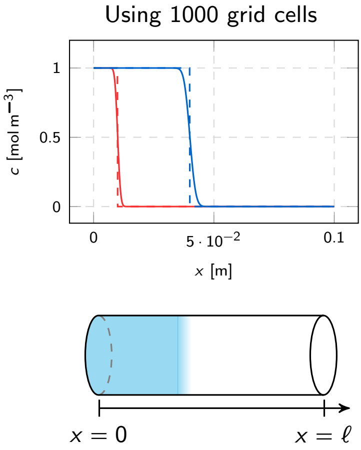


Upwind scheme: example

Unsteady convection through a pipe:

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

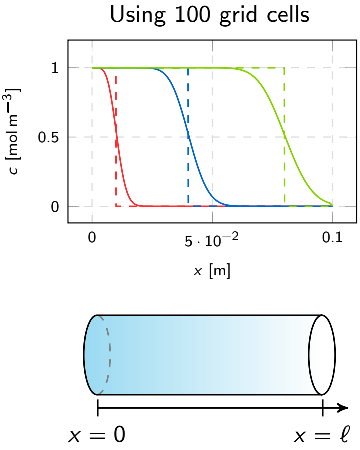


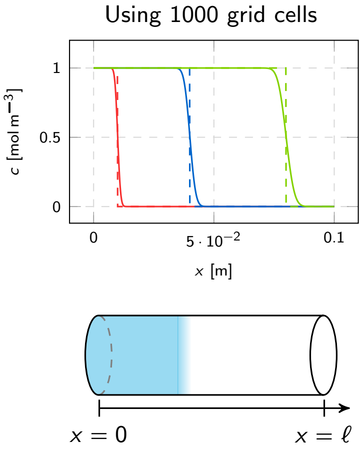


Upwind scheme: example

Unsteady convection through a pipe:

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





Central difference and upwind in Matlab

The results from the previous slides were computed using this script:

```
Nx = 1000;              % Nc grid points
Nt = 10000;             % Nt time steps
u = 0.001;              % m/s
c_in = 1.0;             % mol/m3
t_end = 100.0;          % s
x_end = 0.1;            % m

% Time step and grid size
dt = t_end/Nt; dx = x_end/Nx;

% Courant number
Co=u*dt/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);
```

Central difference and upwind in Matlab

(continued)

```
for n = 1:Nt % time loop
    for i = 2:Nx % Nested loop for grid nodes
        % Central difference
        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
end
```

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)

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 methods
  - How to add non-linear source terms
- Convection: upwind vs. central difference schemes