

## Partial differential equations

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Introduction  
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Stationary diffusion equation  
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Convection  
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Conclusions  
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### Today's outline

#### 1 Introduction

#### 2 Stationary diffusion equation

Discretization  
Solving the diffusion equation  
Non-linear source terms

#### 3 Convection

Discretization  
Central difference scheme  
Upwind scheme

#### 4 Conclusions

Other methods  
Summary

Introduction  
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Stationary diffusion equation  
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Convection  
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Conclusions  
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### 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

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

### Overview

#### Main question

How to solve parabolic PDEs like:

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

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

accurately and efficiently?

## Classification of PDE's

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

The discriminant  $\Delta$  of a quadratic polynomial is computed as (note: only the higher order coefficients are important):

$$\Delta = B^2 - 4AC$$

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

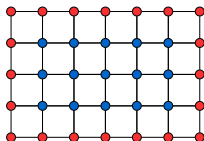


## Importance of classification

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  $P$**   
points in  $xy$ -domain which are influenced by the value of  $f$  in point  $P$

## Example elliptic PDE (boundary value problems: BVP)



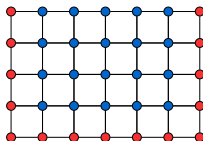
- Grid point at which dependent variable has to be computed
- Grid point at which boundary condition is specified

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)



- 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.





## Instantaneous diffusion equation: temporal discretization

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

Time discretization: backward Euler (implicit)

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

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

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 instantaneous diffusion equation: example

Initialise the variables and matrices:

```
Nx = 100;           % Nc grid points
Nt = 40000;         % Nt time steps
D = 1e-8;           % m^2/s
c_L = 1.0; c_R = 0; % mol/m^3
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^2;

% Initial matrices for solutions (Nx times Nt)
c = zeros(Nt+1, Nx+1); % All concentrations are zero
c(1,1) = 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 instantaneous diffusion equation: example

Solve the diffusion problem using explicit discretization:

$$\frac{\partial c_i}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \quad \text{with}$$

$$0 \leq x \leq \delta, \quad \delta = 5 \cdot 10^{-3} \text{ m}$$

$$\delta/\Delta x = 100 \text{ grid cells}$$

$$D = 1 \cdot 10^{-8} \text{ m}^2 \text{ s}^{-1}$$

$$t_{\text{end}} = 5000 \text{ s}$$

$$c_L = 1 \text{ mol m}^{-3} \quad c_R = 0 \text{ mol m}^{-3}$$

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

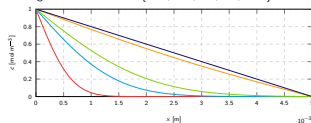
- 1 Initialise variables
- 2 Compute time step so that  $Fo \leq \frac{1}{2} \Rightarrow \Delta t = 0.125 \text{ s}$
- 3 Compute 40000 time steps times 100 grid nodes!
- 4 Store solution

## Solving the instantaneous 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  $t = \{12.5, 62.5, 125, 625, 5000\} \text{ s}$ .







## Central difference scheme of 1st derivative

Unsteady convection:

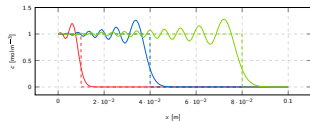
$$\frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x}$$

Central difference for first derivative:

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

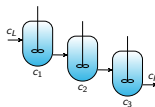
Forward Euler discretization of temporal and spatial domain:

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



## Extension with convection terms

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



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

Stable if  $Co = \frac{u\Delta t}{\Delta x} < 1$  (with  $Co$  the Courant number). However, only 1<sup>st</sup> 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:

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

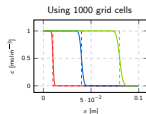
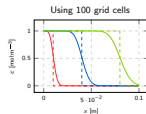
Forward Euler discretization of temporal and spatial domain:

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

## Upwind scheme: example

Unsteady convection through a pipe:

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





## Central difference and upwind in Matlab

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

```
Nx = 1000;           % Nx 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);
```

## 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
        % 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 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