Computational practicum: Lecture 6 Boundary value problems (BVP): Differentiation, Finite Difference Method

Zoë J.G. Gromotka, Artur M. Schweidtmann, Ferdinand Grozema, Tanuj Karia

With support from Lukas S. Balhorn and Monica I. Lacatus

Computational Practicum
Dept. Chemical Engineering
Delft University of Technology

TU Delft
Process Intelligence Research
Delft Institute of Applied Mathematics

Wednesday, 8th October 2024

Recap last lecture

Recap

Ordinary differential equation (ODE)

- An ODE of order n is an equation of the form

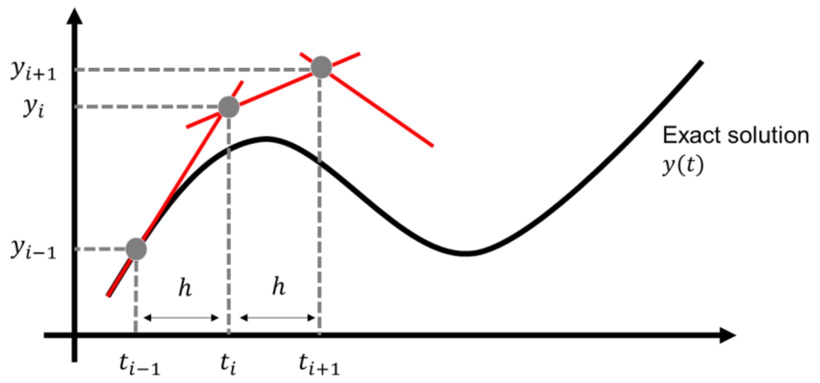
$$g\left(t, y, \frac{dy}{dt}, \dots, \frac{d^n y}{dt^n}\right) = 0,$$

or

$$\frac{d^n y}{dt^n} = f\left(t, y, \frac{dy}{dt}, \dots, \frac{d^{n-1} y}{dt^{n-1}}\right).$$

Initial value problem (IVP)

- An ODE (system) with given initial conditions is called an initial value problem (IVP).
- Numerical solution methods:
  - Forward Euler



  - Backward Euler

Learning goals of this lecture

After successfully completing this lecture, you are able to…

- categorize boundary conditions for boundary value problems (BVPs).
- implement the finite difference method for BVPs from scratch.
- discuss the principles and applications of finite volume and finite element methods.

Agenda

- **Boundary value problems (BVPs)**
  - Boundary conditions
  - Differentiation
  - Finite difference method
  - Finite volumes and finite elements

Agenda

- **Boundary value problems (BVPs)**
  - Boundary conditions
  - Differentiation
  - Finite difference method
  - Discussion on upwind/downwind discretization schemes
  - Finite volumes and finite elements

Example of a BVP

$$\frac{d^2y}{dx^2} = 4(y - x)$$

- Domain

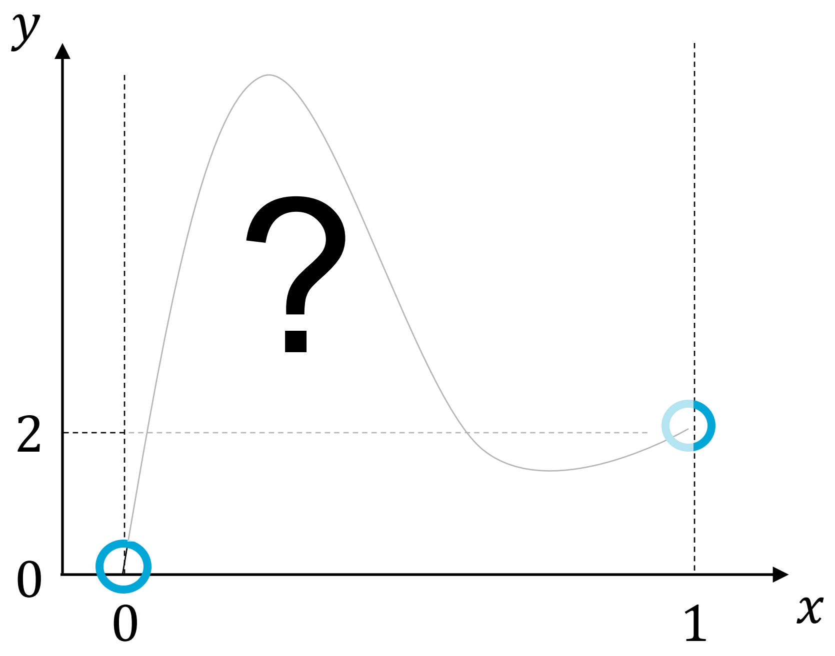
$$x \in [0,1]$$

- Boundary conditions

$$y(0) = 0, \qquad y(1) = 2$$

HINT

We need sufficient conditions for integration.
E.g., ODE 2nd order → 2 conditions,
ODE 4th order → 4 conditions.



Applicative example: plane heat conduction with known walls T; one dimensional mass diffusion with fixed I/O conditions.

Boundary value problem

Definition

An ODE does not uniquely determine a solution. Additional **side conditions** must be imposed on the solution to make it unique. These side conditions prescribe values that the solution or its derivatives must have at some specified point or points.

If all side conditions are specified at the **same point**, then we have an **initial value problem (IVP)**.

If the side conditions are specified at **more than one point**, then we have a **boundary value problem (BVP)**.
For an ODE in $\mathbb{R}$, the side conditions are typically specified at two points, namely the endpoints of some interval [a, b], which is why the side conditions are called boundary conditions or boundary values.

Heath M.T - Scientific computing: an introductory survey, SIAM (2018)

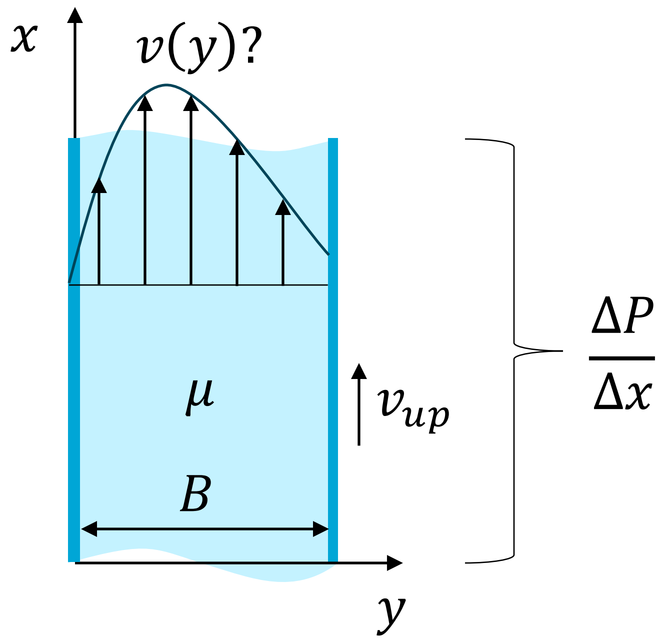
1D transport problem

- Take a Newtonian fluid undergoing laminar pressure-driven flow between two parallel and infinite plates. One plate moves with v_{up}.
- Navier-Stokes equation for v only in y direction:

$$\mu \frac{d^2 v}{dy^2} = \frac{\Delta P}{\Delta x}, \qquad y \in [0, B]$$

- Two conditions known:

$$v(y=0) = 0, \qquad v(y=B) = v_{up}$$



v: Velocity
μ: Viscosity = const.
$\frac{\Delta P}{\Delta x}$: Pressure drop = const.
B: Channel width = const.

Agenda

- **Boundary value problems (BVPs)**
  - Boundary conditions
  - Differentiation
  - Finite difference method
  - Finite volumes and finite elements

Boundary conditions

Definition

A linear ODE is **homogeneous** if $y = 0$ is a solution of the ODE. Otherwise, the ODE is **inhomogeneous.**
For example, $\frac{dy}{dx} + 3y = 2$ is inhomogeneous because $y = 0$ is not a valid solution.

A boundary condition is **homogeneous** if $y = 0$ satisfies it. Otherwise, the boundary condition is **inhomogeneous.**
For example, $y(x = 0, a) = 0 \; \forall a$ is homogeneous, but $y(x = 0, a) = 5a \; \forall a$ is not homogeneous.

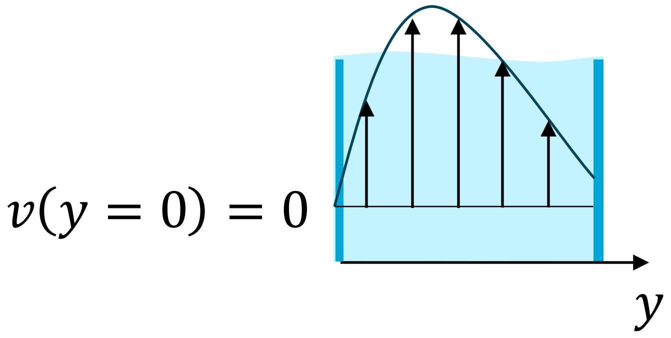
Mona Berciu (2023) - Definitions and important facts regarding ODEs and PDEs

Boundary conditions for BVPs

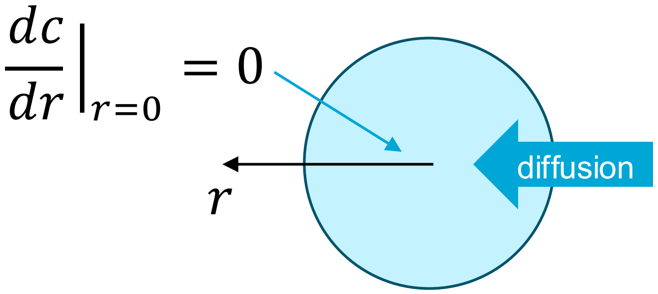
- Assume $\frac{d^2y}{dx^2} = f(x)$

- **Dirichlet** boundary condition:
  - Specifies the value of the function
  - $y = \mathrm{g}$

- **Neumann** boundary condition:
  - Specifies the value of the derivative
  - $\frac{dy}{dx} = \mathrm{g}$



Example Dirichlet: Constant velocity due to friction at wall



Example Neumann: Diffusion at catalyst pellet center is zero due to symmetry

Boundary conditions for BVPs

Mixed boundary condition

- **Robin** boundary condition
  - Specifies the combination of function and derivative value
  - $\mathrm{a}y + \mathrm{b}\frac{\mathrm{dy}}{\mathrm{dx}} = \mathrm{g}$

Mixed boundary conditions for 3rd, or higher, order BVPs

- **Cauchy** boundary condition
  - Specifies the value of the function and the derivative at different sections of the boundary
  - $y = \mathrm{g} \wedge \frac{dy}{dx} = \mathrm{p}$

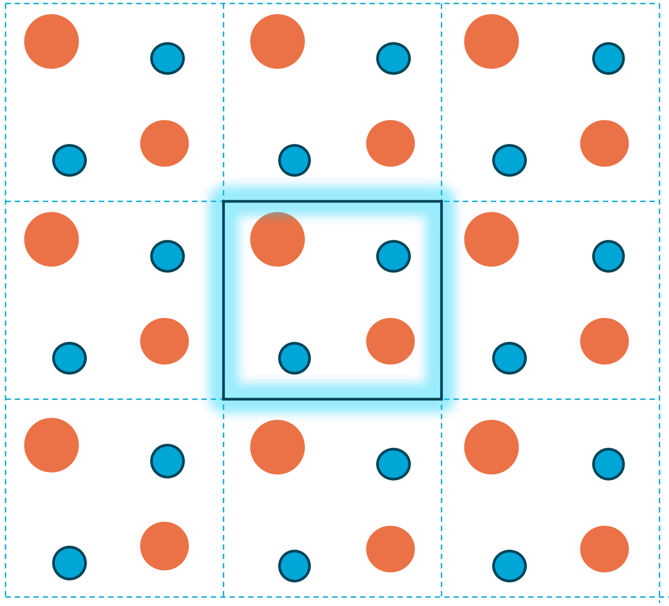
Boundary conditions

Definition

A *periodic* boundary condition states that the solution or its derivatives at two distinct points $x = x_0$ and $x = x_1$ are equal. That is,

$$y(x_0) = y(x_1) \;\; or \;\; \left.\frac{dy}{dx}\right|_{x_0} = \left.\frac{dy}{dx}\right|_{x_1}$$

In practice, these two periodic boundary conditions often occur together.

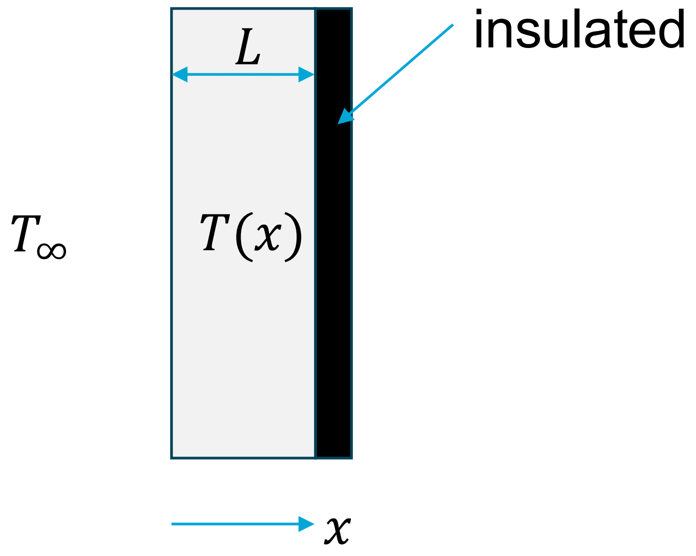


Mona Berciu (2023) - Definitions and important facts regarding ODEs and PDEs

Case study for boundary conditions

- Consider a flat metal plate of thickness L. Heat is conducted through the plate in the x-direction, and the system is at steady state.
- One side of the plate (at $x = 0$) is maintained at a fixed temperature T_∞, while the other side (at $x = L$) is insulated.
- The temperature distribution $T(x)$ in the plate is governed by the one-dimensional steady-state heat conduction equation:

$$\frac{d^2T(x)}{dx^2} = 0, x \in [0, L]$$



Agenda

- **Boundary value problems (BVPs)**
  - Boundary conditions
  - Differentiation
  - Finite difference method
  - Discussion on upwind/downwind discretization schemes
  - Finite volumes and finite elements

Recap: First order finite differences

As taught in lecture 4

Method	Formula	Error
Forward difference	$\left.\frac{df}{dx}\right\|_{x_i} \cong \frac{f(x_{i+1}) - f(x_i)}{(x_{i+1} - x_i)}$	$E = \frac{1}{(x_{i+1} - x_i)} \left.\frac{d^2 f}{dx^2}\right\|_{x_i} \frac{h^2}{2} \sim \alpha h$
Backward difference	$\left.\frac{df}{dx}\right\|_{x_i} \cong \frac{f(x_i) - f(x_{i-1})}{(x_i - x_{i-1})}$	$E = \frac{1}{(x_{i+1} - x_i)} \left.\frac{d^2 f}{dx^2}\right\|_{x_i} \frac{h^2}{2} \sim \alpha h$
Central difference	$\left.\frac{df}{dx}\right\|_{x_i} \cong \frac{f(x_{i+1}) - f(x_{i-1})}{(x_{i+1} - x_{i-1})}$	$E = \frac{1}{(x_{i+1} - x_{i-1})} \left.\frac{d^3 f}{dx^3}\right\|_{x_i} \frac{h^3}{3} \sim \alpha h^2$

Recap: Second order finite differences

As taught in lecture 4

Method	Formula	Error
Central difference	$\left.\frac{d^2f}{dx^2}\right\rvert_{x_i} \cong \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$E = \frac{1}{(x_{i+1} - x_i)^2} \left.\frac{d^4f}{dx^4}\right\rvert_{x_i} \frac{h^4}{24} \sim \alpha h^2$
Forward difference	$\left.\frac{d^2f}{dx^2}\right\rvert_{x_i} \cong \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$E \sim \alpha h$
Backward difference	$\left.\frac{d^2f}{dx^2}\right\rvert_{x_i} \cong \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	$E \sim \alpha h$

The finite difference approach

- Equation

$$\frac{d^2y}{dx^2} + \alpha\frac{dy}{dx} + \beta y = f(x) \text{ where } \alpha \text{ and } \beta \text{ are constant in this case.}$$

- Domain

$$a \leq x \leq b$$

- Boundary conditions

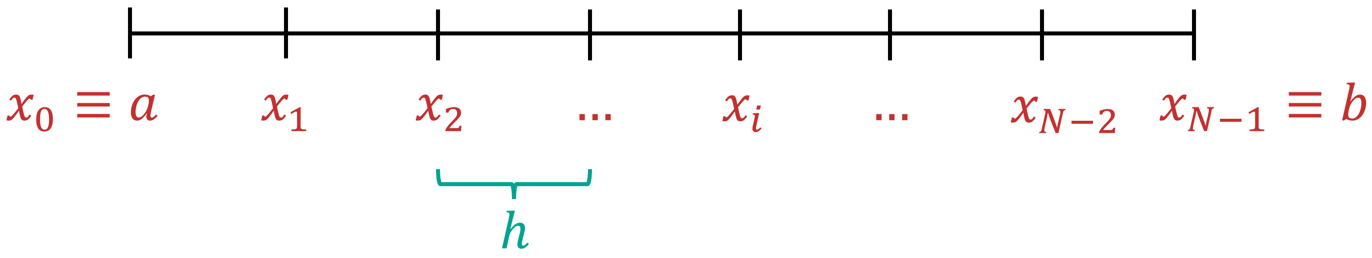
$$y(a) = y_a, \qquad y(b) = y_b$$

The finite difference approach

- Equation

$$\frac{d^2y}{dx^2} + \alpha\frac{dy}{dx} + \beta y = f(x)$$

- Discretization



- Finite differences

$$\left.\frac{dy}{dx}\right|_{x_i} = \frac{y_{i+1} - y_{i-1}}{2h}$$

$$\left.\frac{d^2y}{dx^2}\right|_{x_i} = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}$$

Agenda

- **Boundary value problems (BVPs)**
  - Boundary conditions
  - Differentiation
  - Finite difference method
  - Discussion on upwind/downwind discretization schemes
  - Finite volumes and finite elements

The finite difference approach

- Equation

$$\frac{d^2y}{dx^2} + \alpha\frac{dy}{dx} + \beta y = f(x)$$

- Finite (Central) Difference Equations

$$\frac{{\color{red}y_{i+1}} - 2{\color{cyan}y_i} + {\color{green}y_{i-1}}}{h^2} + \alpha\frac{{\color{red}y_{i+1}} - {\color{green}y_{i-1}}}{2h} + \beta {\color{cyan}y_i} = f(x_i), \qquad 1 \leq\ i \leq N-2$$

Only for internal points, would be out of range for $i = 0$ or $i = N-1$!

The finite difference approach

- Equation

$$\frac{d^2y}{dx^2} + \alpha\frac{dy}{dx} + \beta y = f(x)$$

- Finite (Central) Difference Equations

$$\Big| \cdot h^2 \qquad \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + \alpha\frac{y_{i+1} - y_{i-1}}{2h} + \beta y_i = f(x_i), \qquad 1 \le i \le N-2 \qquad \Big| \cdot h^2$$

$$(y_{i+1} - 2y_i + y_{i-1}) + \frac{h}{2}\alpha(y_{i+1} - y_{i-1}) + h^2\beta y_i = h^2 f(x_i)$$

The finite difference approach

- Equation

$$\frac{d^2y}{dx^2} + \alpha\frac{dy}{dx} + \beta y = f(x)$$

- Finite (Central) Difference Equations

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + \alpha\frac{y_{i+1} - y_{i-1}}{2h} + \beta y_i = f(x_i), \qquad 1 \le i \le N-2$$

$$rearrange \qquad (y_{i+1} - 2y_i + y_{i-1}) + \frac{h}{2}\alpha(y_{i+1} - y_{i-1}) + h^2\beta y_i = h^2 f(x_i)$$

$$y_{i-1}\left(1 - \frac{h}{2}\alpha\right) + y_i(h^2\beta - 2) + y_{i+1}\left(1 + \frac{h}{2}\alpha\right) = h^2 f(x_i)$$

The finite difference approach

- Equation

$$\frac{d^2y}{dx^2} + \alpha\frac{dy}{dx} + \beta y = f(x)$$

- Finite (Central) Difference Equations

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + \alpha\frac{y_{i+1} - y_{i-1}}{2h} + \beta y_i = f(x_i), \qquad 1 \le\ i \le N-2$$

$$(y_{i+1} - 2y_i + y_{i-1}) + \frac{h}{2}\alpha(y_{i+1} - y_{i-1}) + h^2\beta y_i = h^2 f(x_i)$$

$$y_{i-1}\left(1 - \frac{h}{2}\alpha\right) + y_i(h^2\beta - 2) + y_{i+1}\left(1 + \frac{h}{2}\alpha\right) = h^2 f(x_i)$$

$$\boxed{y_{i-1}\left(1 - \frac{h}{2}\alpha\right) + y_i(h^2\beta - 2) + y_{i+1}\left(1 + \frac{h}{2}\alpha\right) = h^2 f(x_i), \qquad \forall\ i \in [1, N-2]}$$

$$y_0 = y_a, \qquad y_{N-1} = y_b$$

The finite difference approach: Option 1

- Finite (Central) Difference Equations

$$y_{i-1}\left(1-\frac{h}{2}\alpha\right)+y_i(h^2\beta-2)+y_{i+1}\left(1+\frac{h}{2}\alpha\right)=h^2f(x_i),\qquad \forall\, i\in[1,N-2]$$

$$y_0=y_a,\qquad y_{N-1}=y_b$$

- Option 1: Assemble and solve the full system, **including** the known boundary nodes.
- **Final matrix form ($\boldsymbol{A}\boldsymbol{y}=\boldsymbol{b}$):**

$$\begin{pmatrix} 1 & 0 & . & \cdots & . & . \\ 1-\frac{h}{2}\alpha & h^2\beta-2 & 1+\frac{h}{2}\alpha & \cdots & . & . \\ . & \ddots & \ddots & \ddots & \cdots & . \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ . & \cdots & . & 1-\frac{h}{2}\alpha & h^2\beta-2 & 1+\frac{h}{2}\alpha \\ . & . & \cdots & . & 0 & 1 \end{pmatrix}\cdot\begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ \vdots \\ y_{N-2} \\ y_{N-1} \end{pmatrix}=\begin{pmatrix} y_a \\ h^2f(x_2) \\ \vdots \\ \vdots \\ h^2f(x_{N-2}) \\ y_b \end{pmatrix}$$

Known from B.C.

Known from B.C.

The finite difference approach: Option 1

- Finite (Central) Difference Equations

$$y_{i-1}\left(1-\frac{h}{2}\alpha\right)+y_i(h^2\beta-2)+y_{i+1}\left(1+\frac{h}{2}\alpha\right)=h^2 f(x_i), \qquad \forall\, i\in[1,N-2]$$

$$y_0 = y_a, \qquad y_{N-1}=y_b$$

- Option 1: Assemble and solve the full system, **including** the known boundary nodes.
- **Final matrix form ($\boldsymbol{Ay}=\boldsymbol{b}$)** defines a linear system of equations (cf. lecture 3) which can be solved using:
  - Jacobi, Gauss-Seidel
  - `np.linalg.solve(a_matrix, b_vector)`
- y_0 and y_{N-1} are known. Including them in the vector of unknowns $\boldsymbol{y}$ is **less efficient** as we are solving for already known values!

The finite difference approach: Option 2 **(preferred)**

- Finite (Central) Difference Equations

$$y_{i-1}\left(1-\frac{h}{2}\alpha\right)+y_i(h^2\beta-2)+y_{i+1}\left(1+\frac{h}{2}\alpha\right)=h^2f(x_i), \qquad \forall\ i\in[1,N-2]$$

$$y_0=y_a, \qquad y_{N-1}=y_b$$

- Option 2: Remove the **known** boundary nodes and solve a reduced system for **only** the interior nodes.
- Constructing matrix form:
  - **Start** with the finite (central) difference equation at a generic interior node i:

$$y_{i-1}\left(1-\frac{h}{2}\alpha\right)+y_i(h^2\beta-2)+y_{i+1}\left(1+\frac{h}{2}\alpha\right)=h^2f(x_i)$$

The finite difference approach: Option 2

- Constructing matrix form continued :
  - **Case** $i = 1$: here $y_{i-1} = y_0 = y_a$. Move the known term to the RHS.

$$y_1(h^2\beta - 2) + y_2\left(1 + \frac{h}{2}\alpha\right) = h^2 f(x_1) - y_a\left(1 - \frac{h}{2}\alpha\right)$$

  - **Case** $2 \leq i \leq N-3$: Neither neighbor is a boundary, so keep the standard form.

$$y_{i-1}\left(1 - \frac{h}{2}\alpha\right) + y_i(h^2\beta - 2) + y_{i+1}\left(1 + \frac{h}{2}\alpha\right) = h^2 f(x_i),\ \forall\, i \in [2, N-3]$$

  - **Case** $i = N-2$: here $y_{i+1} = y_{N-1} = y_b$. Move the known term to the RHS.

$$y_{N-3}\left(1 - \frac{h}{2}\alpha\right) + y_{N-2}(h^2\beta - 2) = h^2 f(x_{N-2}) - y_b\left(1 + \frac{h}{2}\alpha\right)$$

The finite difference approach: Option 2

- Finite (Central) Difference Equations

$$y_{i-1}\left(1-\frac{h}{2}\alpha\right)+y_i(h^2\beta-2)+y_{i+1}\left(1+\frac{h}{2}\alpha\right)=h^2f(x_i), \qquad \forall\, i\in[1,N-2]$$

$$y_0=y_a, \qquad y_{N-1}=y_b$$

- **Final matrix form ($\boldsymbol{Ay=b}$), only contains interior points**:

$$\begin{pmatrix} h^2\beta-2 & 1+\frac{h}{2}\alpha & . & \dots & . & . \\ 1-\frac{h}{2}\alpha & h^2\beta-2 & 1+\frac{h}{2}\alpha & \dots & . & . \\ . & \ddots & \ddots & \ddots & \dots & . \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ . & \dots & . & 1-\frac{h}{2}\alpha & h^2\beta-2 & 1+\frac{h}{2}\alpha \\ . & . & \dots & . & 1-\frac{h}{2}\alpha & h^2\beta-2 \end{pmatrix}\cdot\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ \vdots \\ y_{N-3} \\ y_{N-2} \end{pmatrix}=\begin{pmatrix} h^2f(x_1)-y_a\left(1-\frac{h}{2}\alpha\right) \\ h^2f(x_2) \\ \vdots \\ \vdots \\ h^2f(x_{N-3}) \\ h^2f(x_{N-2})-y_b\left(1+\frac{h}{2}\alpha\right) \end{pmatrix}$$

1D transport problem example

- Equation

$$\mu \frac{d^2 v}{dy^2} = \frac{\Delta P}{\Delta x}$$

- Domain

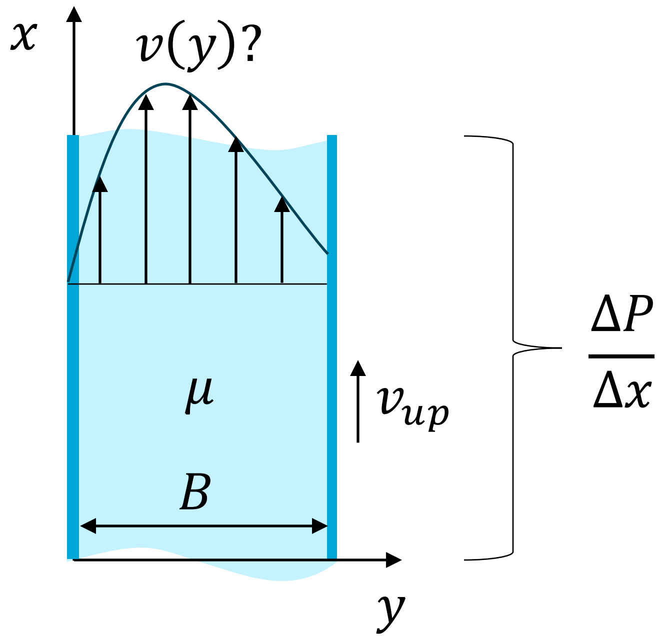
$$0 \leq y \leq B$$

- Boundary conditions

$$v(0) = 0, \qquad v(B) = v_{up}$$

- Central difference scheme:

$$\mu \frac{v_{i+1} - 2v_i + v_{i-1}}{h^2} = \frac{\Delta P}{\Delta x}$$



1D transport problem example

- Discretization

$$\mu \frac{1v_{i+1} - 2v_i + 1v_{i-1}}{h^2} = \frac{\Delta P}{\Delta x} \Rightarrow 1v_{\mathrm{i}+1} - 2v_i + 1v_{\mathrm{i}-1} = \frac{\mathrm{h}^2}{\mu}\frac{\Delta P}{\Delta x} \equiv \mathrm{c}, \qquad \forall\, i \in [1, N-2]$$

- For clarity, we write all coefficients in front of variables: $1v_{\mathrm{i}+1} - 2v_i + 1v_{\mathrm{i}-1}$
- We will focus on constructing the system matrix with option 2 (i.e. solve a reduced system for **only** the interior nodes).

1D transport problem example

- Constructing the matrix:
  - Case $i = 1$: here $v_{i-1} = v_0 = 0.$

$$1v_0 - 2v_1 + 1v_2 = c$$

$$-2v_1 + 1v_2 = c$$

  - Case $2 \leq i \leq N - 3$

$$1v_{\mathrm{i-1}} - 2v_{\mathrm{i}} + 1v_{\mathrm{i+1}} = c, \forall\, i \in [2, N-3]$$

  - Case $i = N - 2$: here $v_{N-1} = v(B) = v_{up}$

$$1v_{\mathrm{N-3}} - 2v_{\mathrm{N-2}} + v_{\mathrm{N-1}} = c$$
$$1v_{\mathrm{N-3}} - 2v_{\mathrm{N-2}} = c - v_{up}$$

- Matrix form

$$\begin{pmatrix} -2 & 1 & . & \dots & . & . \\ 1 & -2 & 1 & \dots & . & . \\ . & 1 & -2 & 1 & \dots & . \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ . & \dots & . & 1 & -2 & 1 \\ . & . & \dots & . & 1 & -2 \end{pmatrix} \cdot \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ \vdots \\ v_{N-3} \\ v_{N-2} \end{pmatrix} = \begin{pmatrix} c \\ c \\ c \\ \vdots \\ c \\ c - v_{up} \end{pmatrix}$$

Live coding: Finite difference using only interior points

- Open Colab: Interior points finite difference

- Find more in the Github repository of the course: https://github.com/process-intelligence-research/computational_practicum_lecture_coding/tree/main

Discretization with Neumann boundary condition

- Consider a rod of length L and thermal conductivity k. Suppose the rod has a constant volumetric heat source Q.The temperature distribution in the rod is governed by the steady-state heat equation:

$$-k\frac{d^2T}{dx^2} = Q$$

- Or equivalently

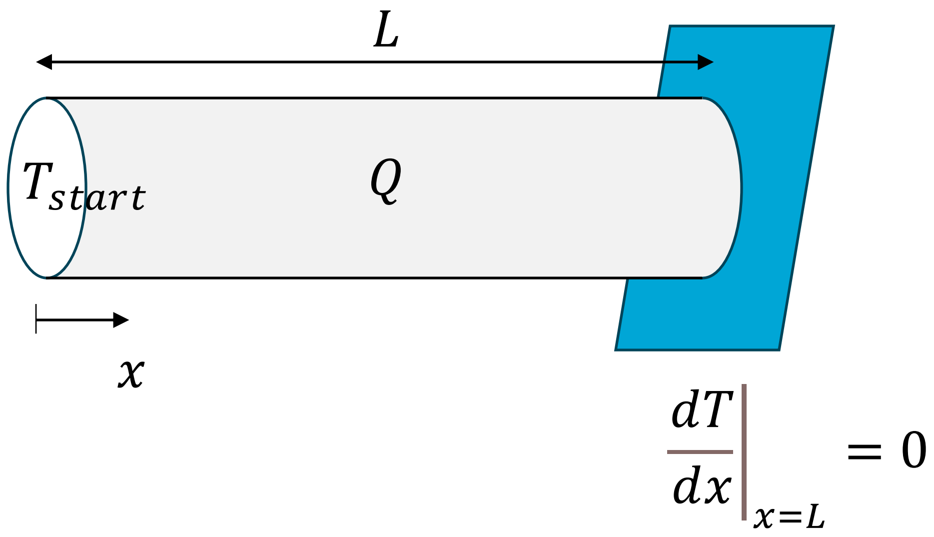
$$\frac{d^2T}{dx^2} = -\frac{Q}{k} \equiv -S \text{ with } S > 0$$

- The right side of the rod is insulated, therefore, the heat flux is zero:

$$\left.\frac{dT}{dx}\right|_{x=L} = 0$$

- The left side of the rod is in contact with a heat source, maintaining a constant temperature:

$$T(x = 0) = T_{start}$$



Discretization with Neumann boundary condition

- Discretization

$$T_{i-1} - 2T_i + T_{i+1} = -Sh^2, \qquad \forall\, i \in [1, N-2] \quad \wedge \quad T_0 = T_{start}$$

- How about the Neumann boundary condition?
- Use the backward difference scheme!

As taught in lecture 3

$$\left.\frac{dT}{dx}\right|_{x=L} \approx \frac{T_{N-1} - T_{N-2}}{h} = 0$$

HINT: connect the dots

For Neumann conditions at the beginning of the grid, use the forward difference scheme!

- This simplifies to

$$T_{N-1} = T_{N-2}$$

- Now we can construct the matrix using Option 2 (i.e. solve a reduced system for **only** the interior nodes).

Discretization with Neumann boundary condition

- Matrix construction with Option 2:
  - Case $i = 1$: here $T_{i-1} = T_0 = T_{start}$

    $$1T_0 - 2T_1 + 1T_2 = -Sh^2$$

    $$-2T_1 + 1T_2 = -T_{start} - Sh^2$$

  - Case $2 \leq i \leq N-3$

    $$1T_{i-1} - 2T_i + 1T_{i+1} = -Sh^2, \forall\, i \in [2, N-3]$$

  - Case $i = N-2$: here $T_{N-1} = T_{N-2}$

    $$1T_{N-3} - 2T_{N-2} + 1T_{N-1} = -Sh^2,$$

    $$1T_{N-3} - 1T_{N-2} = -Sh^2,$$

- Matrix form

$$\begin{pmatrix} -2 & 1 & . & \dots & . & . \\ 1 & -2 & 1 & \dots & . & . \\ . & 1 & -2 & 1 & . & . \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ . & . & . & 1 & -2 & 1 \\ . & . & . & . & 1 & -1 \end{pmatrix} \cdot \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ \vdots \\ T_{N-3} \\ T_{N-2} \end{pmatrix} = \begin{pmatrix} -T_{start} - Sh^2 \\ -Sh^2 \\ -Sh^2 \\ \vdots \\ -Sh^2 \\ -Sh^2 \end{pmatrix}$$

Accuracy of backward difference discretization

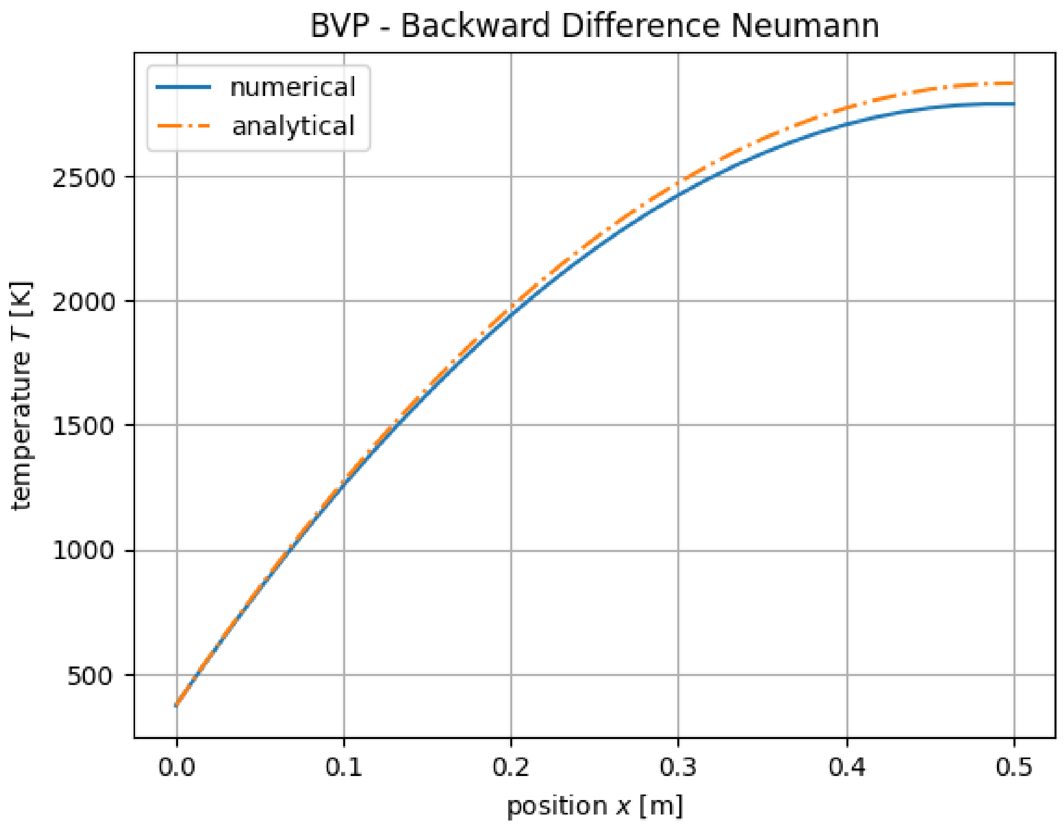
- Backward-difference is **only first order accurate!**

$$\left.\frac{dT}{dx}\right|_{x=L} \approx \frac{T_{N-1} - T_{N-2}}{h} = \mathcal{O}(h)$$

n_{steps}	$h\ [m]$	$\varepsilon\ [K]$	**Order**
21	0.025	125.0	-
41	0.0125	62.5	1.0
81	0.0062	31.3	1.0
161	0.0031	15.6	1.0

- ε : maximum absolute error between numerical and analytical solution T_{ana}

$$T_{ana} = T_{start} + S(Lx - 0.5x^2)$$

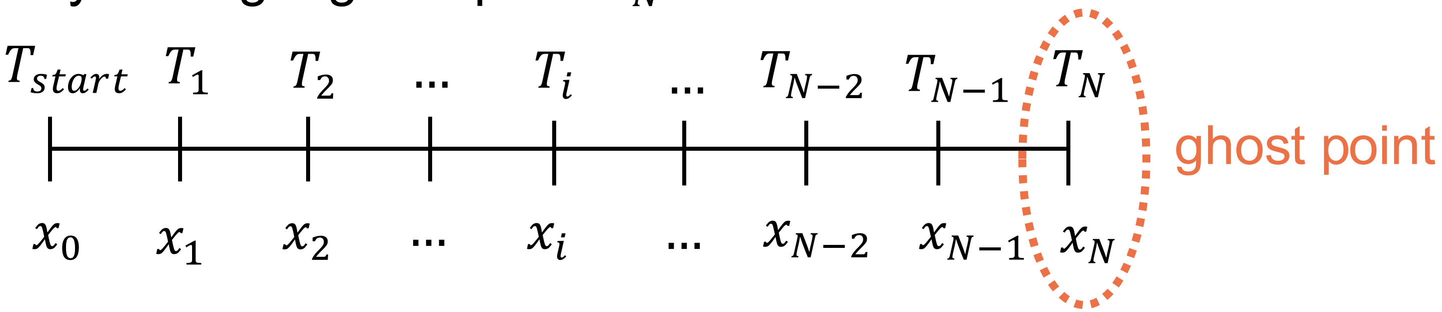


Neumann Boundary Condition: Towards 2nd Order Accuracy

- Backward-difference is **only first order accurate!**

$$\left.\frac{dT}{dx}\right|_{x=L} \approx \frac{T_{N-1} - T_{N-2}}{h} = \mathcal{O}(h)$$

- **Solution:** introduce a ghost point.
  - Extend the grid by adding a ghost point x_N.



  - Then we can use the central difference scheme to achieve **second order accuracy**!

$$\left.\frac{dT}{dx}\right|_{x=L} \approx \frac{T_N - T_{N-2}}{2h} = \mathcal{O}(\mathrm{h}^2)$$

Discretization with Neumann boundary condition

- Construct the matrix with Option 2:
  - Case $i = 1$: here $T_{i-1} = T_0 = T_{start}$

$$1T_0 - 2T_1 + 1T_2 = -Sh^2$$

$$-2T_1 + 1T_2 = -T_{start} - Sh^2$$

  - Case $2 \leq i \leq N - 2$

$$1T_{i-1} - 2T_i + 1T_{i+1} = -Sh^2, \forall\, i \in [2, N-2]$$

  - Case $i = N - 1$: here $T_N = T_{N-2}$

$$1T_{N-2} - 2T_{N-1} + 1T_N = -Sh^2,$$

$$2T_{N-2} - 2T_{N-1} = -Sh^2$$

- Matrix form

$$\begin{pmatrix} -2 & 1 & . & \cdots & . & . \\ 1 & -2 & 1 & \cdots & . & . \\ . & 1 & -2 & 1 & . & . \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ . & . & . & 1 & -2 & 1 \\ . & . & . & . & 2 & -2 \end{pmatrix} \cdot \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ \vdots \\ T_{N-2} \\ T_{N-1} \end{pmatrix} = \begin{pmatrix} -T_{start} - Sh^2 \\ -Sh^2 \\ -Sh^2 \\ \vdots \\ -Sh^2 \\ -Sh^2 \end{pmatrix}$$

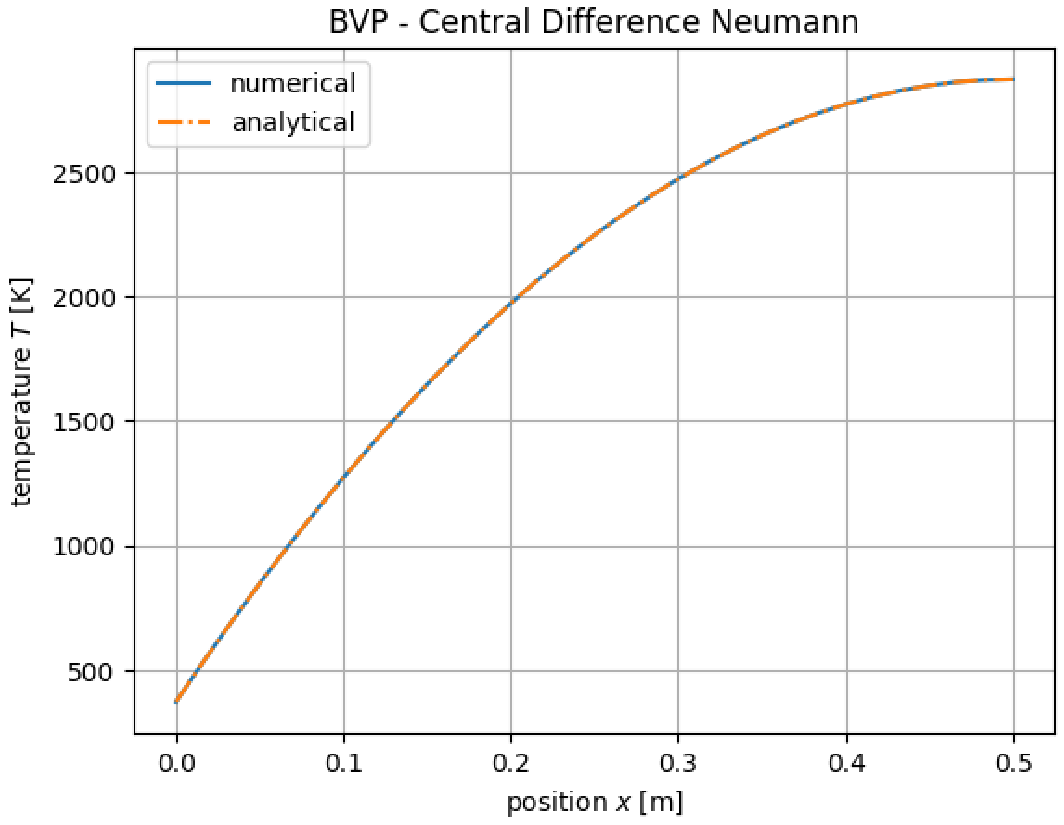
We are now solving for all interior points and the boundary point T_{N-1} whose value is unknown!

Accuracy of central difference discretization

- Central difference scheme is **second order accurate**!

$$\left.\frac{dT}{dx}\right|_{x=L} \approx \frac{T_N - T_{N-2}}{2h} = \mathcal{O}(h^2)$$

- Second-order finite-difference stencil reproduces any quadratic exactly (here the exact solution for T is quadratic in x).
- The numerical and analytic solutions coincide, resulting in **zero error**, independent of the grid resolution.



Live coding: Neumann boundary condition (ghost point)

- Open Colab: [Neumann boundary finite difference]

- Find more in the Github repository of the course: https://github.com/process-intelligence-research/computational_practicum_lecture_coding/tree/main

Agenda

- **Boundary value problems (BVPs)**
  - Boundary conditions
  - Differentiation
  - Finite difference method
  - Discussion on upwind/downwind discretization schemes
  - Finite volumes and finite elements

Are more accurate discretization schemes always a good choice?

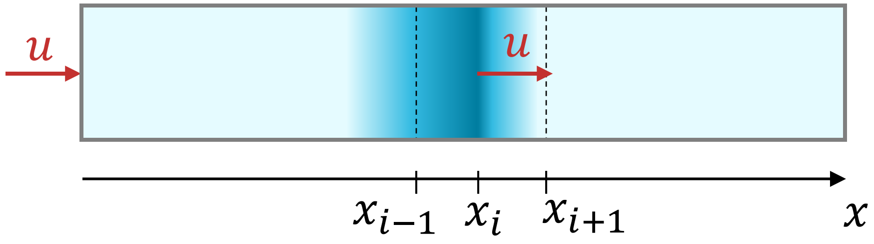
- In this section, we will discuss a specific discretization scheme to solve numerical issues in some transport phenomena problems.
- Let's consider the steady state advection-diffusion equation in 1D:

$$\frac{d}{dx}(u\phi) = \frac{d^2}{dx^2}(D\phi)$$

- With boundary conditions:

$$\phi(x = 0) = \phi_0$$
$$\phi(x = L) = \phi_L$$

- Where:
  - ϕ is some transported quantity
  - u is the velocity in x-direction in m/s
  - D is the diffusion coefficient in m^2/s



Advection-diffusion equation: discretization

- We can discretize the advection-diffusion equation using finite difference method:
  - 1st order derivative → central difference scheme
  - 2nd order derivative → central difference scheme
- Considering constant density, velocity and diffusion coefficient:

$$u\frac{u_{i+1}-u_{i-1}}{2\Delta x}=D\frac{u_{i+1}-2u_i+u_{i-1}}{\Delta x^2}$$

$$\frac{(u_{i+1}-u_{i-1})}{2}\frac{u\Delta x}{D}=(u_{i+1}-2u_i+u_{i-1})$$

- We define the nondimensional Peclet number: $Pe=\frac{u\Delta x}{D}$
- Physical meaning: Peclet number measures the ratio between convection and diffusion phenomena, in terms of characteristic time.
  - $Pe \ll 1$: diffusion is the dominating phenomena
  - $Pe \gg 1$: convection is the dominating phenomena

Upwind and Downwind schemes

- For high Peclet number ($Pe \gg 2$), the discretization scheme presented is unstable and inaccurate!
- The upwind/downwind differencing scheme takes into account the flow direction!
  - For positive velocity ($u > 0$) and $Pe \gg 2$:

$$\text{Backward Difference Scheme: } \left.\frac{d\phi}{dx}\right|_i = \frac{x_i - x_{i-1}}{\Delta x}$$

→ Upwind Scheme

  - For negative velocity ($u < 0$) and $Pe \gg 2$:

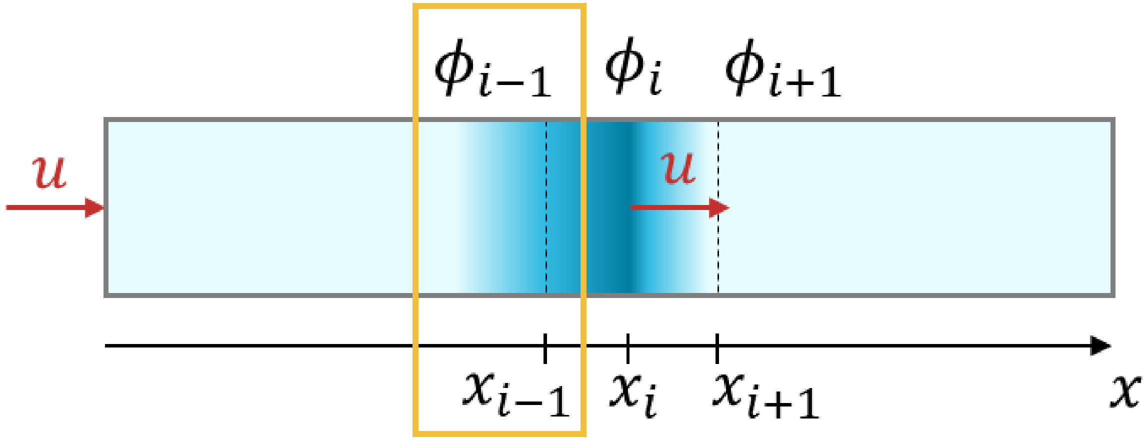
$$\text{Forward Difference Scheme: } \left.\frac{d\phi}{dx}\right|_i = \frac{x_{i+1} - x_i}{\Delta x}$$

→ Downwind Scheme

- The diffusion term can be still discretized using central difference scheme

Intuition for Upwind and Downwind schemes

- From a physical point of view, in highly convective positive flows, what happens in the point x_i is more "influenced" by point x_{i-1}, rather than x_{i+1}
- …the information flows from East to West
- Then, using central difference scheme causes numerical errors due to the overestimated importance of the West point (CDS "averages" x_{i-1} and x_{i+1})
- In this case, the Backward Difference scheme is more appropriate (and accurate), although is in principle <u>less</u> accurate than CDS.
- Then, no! More accurate discretization schemes are not always a good idea!

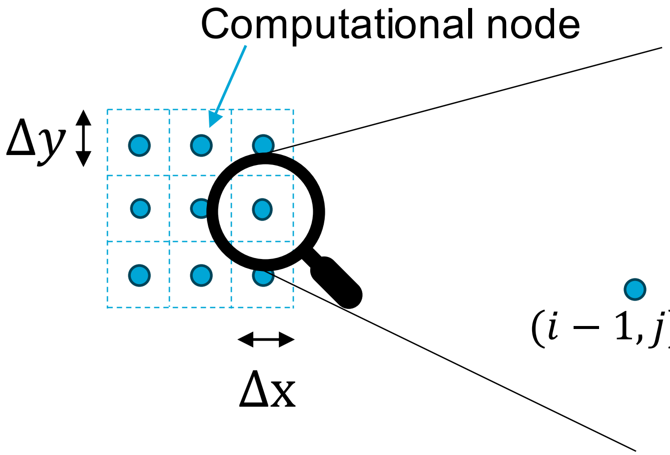


Agenda

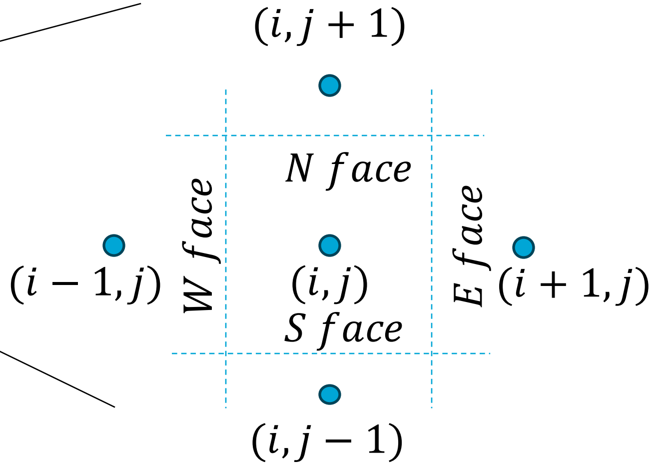
- **Boundary value problems (BVPs)**
  - Boundary conditions
  - Differentiation
  - Finite difference method
  - Discussion on upwind/downwind discretization schemes
  - Finite volumes and finite elements

Finite volumes

- Instead of defining nodes at grid points, we place nodes in the centre of volumes.
- Calculate the numerical integral over each face of the volume.
- Finite volumes enable modelling complex geometries.
- Good conservation properties.
- Applications:
  - Computational fluid dynamics (CFD).
  - Heat and mass transfer modelling.

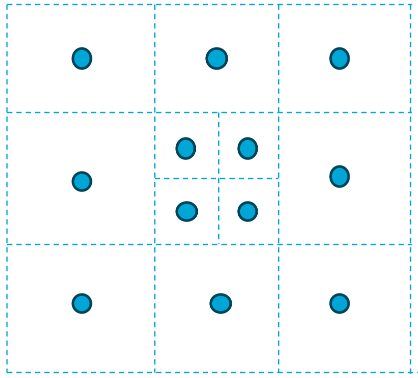


Regular 2D grid



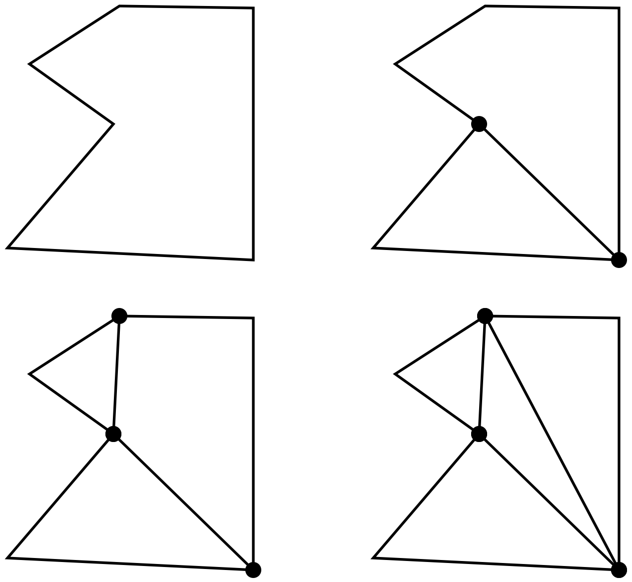
2D control volume

Irregular 2D grid



Finite elements method (FEM)

- Can automatically generate irregular grid.
- Most common method for simulations of heat and mass transfer, fluids, and mechanics.
- Steps in FEM:
  - Discretization: Generate finite elements.
  - Selection of shape functions (how variable varies inside element).
  - Formulation: Derive governing differential equations.
  - Assembly: Assemble global system of equations.
  - Solution: Apply boundary conditions and solve the system of equations.



Automatic portioning of 2-D grid

FEM is the most common method in commercial simulation software (e.g., Ansys, COMSOL).

Learning goals of this lecture

After successfully completing this lecture, you are able to…

- categorize boundary conditions for boundary value problems (BVPs).
- implement the finite difference method for BVPs from scratch.
- discuss the principles and applications of finite volume and finite element methods.

Thank you very much for your attention!