Computational practicum: Lecture 2

Numerical methods for partial differential equations (Part 1)

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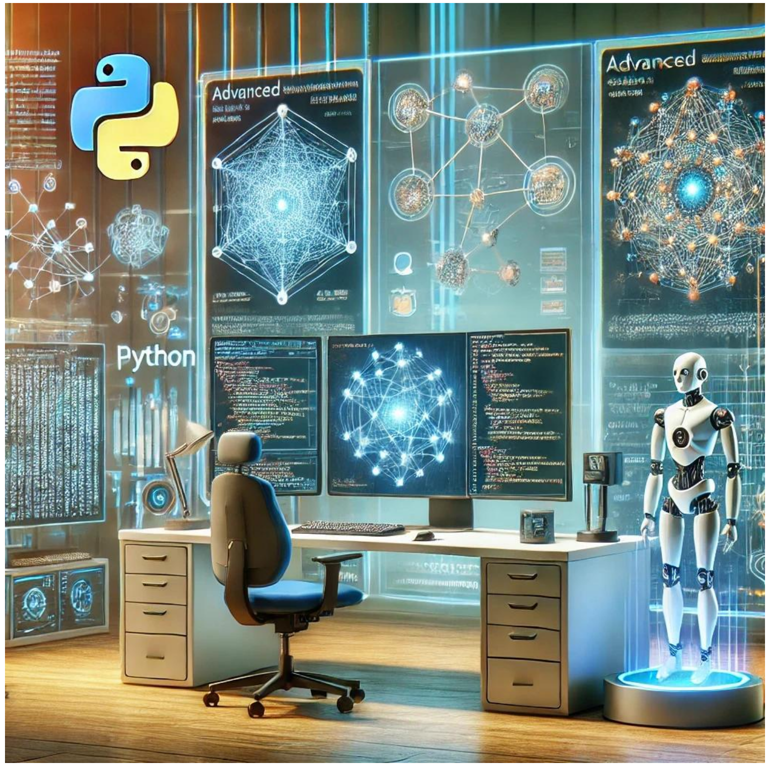
Recap last lecture

- Advanced Python programming:
  - Programming principles
  - Managing imports, packages, virtual environments
  - Managing multiple modules
  - Basic object-oriented programming (OOP)
  - Unit testing

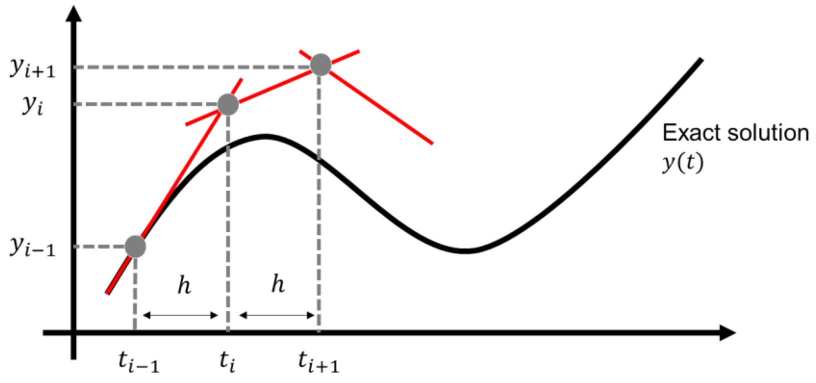


Recap from Q1: relevant concepts

Recap

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

Boundary value problems (BVPs)

- BVPs have side constraints at more than one point
- Boundary conditions define side constraints, e.g.,
  - Dirichlet boundary condition $y = f$
  - Neumann boundary condition $\frac{\mathrm{d}y}{dx} = f$
  - …

Finite difference method

- Differential equation → Finite difference equations for all nodes of a discretized domain

Learning objectives

After successfully completing this lecture, you are able to…

- Explain what a partial differential equation (PDEs) is, how it can be classified, and how it is different form ordinary differential equations (ODEs).
- Give an overview of the main techniques to solve partial differential equations in (chemical) engineering
- Implement different numerical solution approaches for parabolic PDEs from scratch
- Discuss stability of numerical solution approaches for parabolic PDEs
- Use Python libraries' built-in functions to support the solution of parabolic PDEs

Agenda

- What is a Partial Differential Equation (PDE)?
  - Classification of PDE’s (Elliptic, Parabolic, Hyperbolic)
  - Recap: Initial conditions (ICs) and boundary conditions (BCs)
- Introduction to numerical methods to solve PDEs
- Finite Difference Method for PDEs
  - Discretize the multivariate domain
  - Discretize with ghost points
- Parabolic PDE: 1D unsteady heat equation
- Semidiscrete method to solve parabolic PDEs
  - Spatial derivatives
    - Internal points
    - Handling boundary conditions
  - Time derivatives
    - Forward Euler
    - Stability
    - Backward Euler
  - Built-in IVP solvers

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Partial Differential Equations: what are?

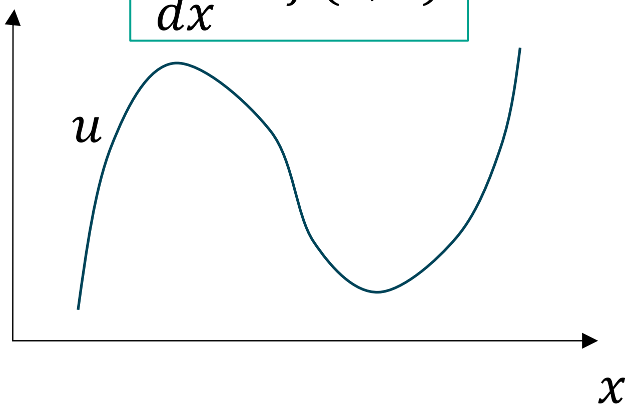
See CP Q1
Lecture 2

- Recap: Partial derivative

  Consider a function $f: D \to \mathbb{R}$, $D \subseteq \mathbb{R}^n$ with independent variables $\boldsymbol{x} = [x_1, \ldots, x_n]$. The **partial derivate** of f with respect to a variable $x_j \in \boldsymbol{x}$ is denoted by $\frac{\partial f}{\partial x_j}$.

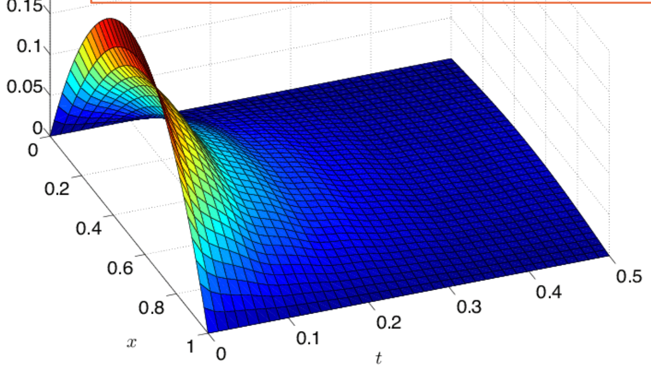
- A partial differential equation (PDE) is an equation involving partial derivatives of an unknown function with respect to more than one independent variable.

$$\boxed{\frac{du}{dx} = f(x,u)}$$



ODE vs. PDE

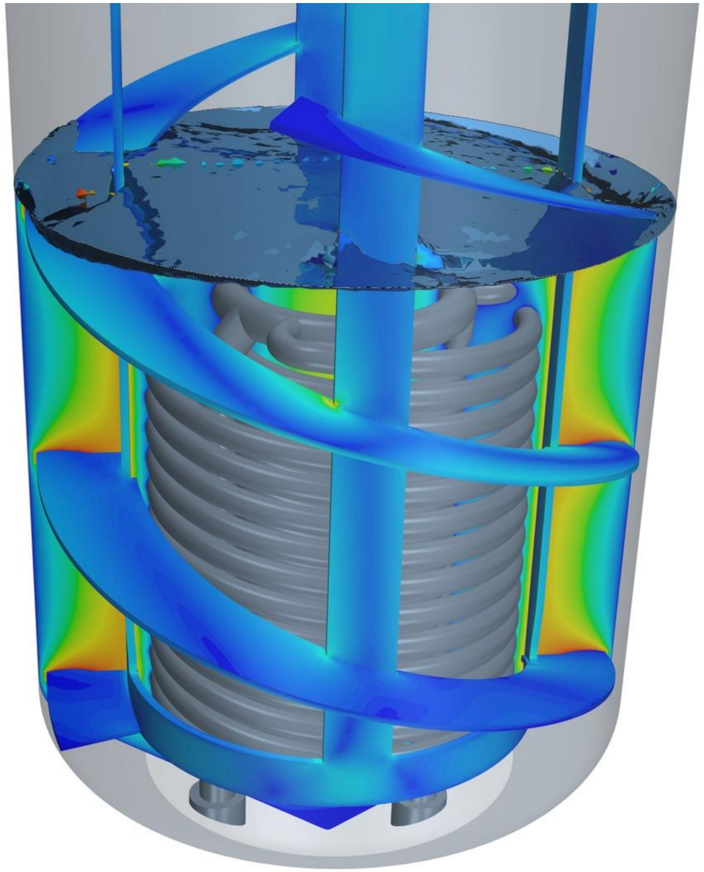
$$\boxed{\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + f(t,x,u)}$$



Partial Differential Equation: why?

- PDEs are fundamental in modeling continuous phenomena in nature and Chemical Engineering.

- Example of applications are:
  - Unsteady processes (time and space derivatives)
  - Heat/mass transfer in reactors
  - Mass transfer in separation processes
  - Navier-Stokes equations (system of PDEs)



Partial Differential Equation: scope, aim and notation

- Solving a PDE means to search for a function $u\colon \mathbb{R}^2 \to \mathbb{R}$ (or $u\colon \mathbb{R}^3 \to \mathbb{R}$) that:
  - Satisfies the relationship prescribed by a given PDE on a specified domain
  - Meets the imposed initial and/or boundary conditions
  - In case of two independent variables, the solution is a bivariate function u and can be visualized as a surface over the 2D domain (x, t) or (x, y).
- Alternative notations you may find in books and publications:

$$\frac{\partial u}{\partial x} = u_x, \frac{\partial^2 u}{\partial x^2} = u_{xx}, \frac{\partial^2 u}{\partial x \partial y} = u_{xy} = u_{yx} = \frac{\partial^2 u}{\partial y \partial x}, \frac{\partial u}{\partial t} = u_t = \dot{u}$$

Partial Differential Equation: scope, aim and notation

- We will deal with single PDEs (systems will not be analysed)
- PDE Lecture 1
  - Two independent variables: 1D space and time *(x, t)* → Parabolic PDEs
- PDE Lecture 2:
  - Two independent variables: 2D space *(x, y)* → Elliptic PDEs

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Partial Differential Equation: classification

- The *order* of a PDE is determined by the highest-order partial derivative in the PDE.
- A PDE is *linear* if the dependent variable and its partial derivatives appear only linearly (only degree one, no products/nonlinear functions), otherwise it is *non-linear*
- Given an example of PDE:

$$\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} + f(x, y) \cdot u + g(x, y, u) = 0$$

  - u is the dependent variable
  - x and y are the independent variables
  - $f(x, y) \cdot u$ is a linear function of u
  - $g(x, y, u)$ is a nonlinear function. If $g(x, y, u) = 0$, then the PDE above is linear

Partial Differential Equation: classification

A classification is available for bivariate second order PDEs:

- The general form of second order linear PDEs is:

$$a\frac{\partial^2 u}{\partial x^2} + b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + d\frac{\partial u}{\partial x} + e\frac{\partial u}{\partial y} + fu + g = 0$$

- We define the *discriminant* as the quantity $\mathrm{D} = b^2 - 4ac$, then:
  - D > 0: Hyperbolic PDE
  - D = 0: Parabolic PDE
  - D < 0: Elliptic PDE
- In this course, we cover solution methods for parabolic and elliptic PDEs.

HINT

The independent variables x and y in the definition are generic. Other can be considered (e.g., x and t).

Introduction to parabolic PDE

- Parabolic PDEs describe time-dependent, dissipative physical processes, like diffusion, which evolve toward a steady state.
  - The two independent variables are time and 1D space. Generally, we refer to as 1D parabolic PDE (referring only to spatial coordinates).
- An example is the 1D heat equation:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + S(u, x, t), \qquad 0 \leq x \leq L, \qquad t \geq 0$$

- The heat equation models the propagation of heat in a body through conduction:
  - u is the temperature (or concentration, etc.)
  - α is the thermal diffusivity $\alpha = \frac{k}{c_p \rho}$
  - $S(u, x, t)$ is the source term, potentially nonlinear

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Initial and boundary conditions

- As you may recall from Q1, differential equations are satisfied by infinitely many solutions. Additional conditions must be specified, depending on the problem, to characterize them fully.
  - Initial conditions: quantity specified for the solution of a PDE at the beginning of the time interval.
  - Boundary conditions: quantity specified for the solution of a PDE (or its derivatives) along the boundaries of the spatial domain.

- In general, you need a condition for each order of derivative appearing in the equation
  - $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 y}{\partial x^2}$ → 1 IC, 2 BC
  - $\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 y}{\partial x^2}$ → 2 IC, 2 BC

Initial and boundary conditions for parabolic PDEs

For parabolic PDEs:

- 1D parabolic PDE: $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + S(u, x, t)$
  - First order time derivative → 1 initial condition
  - 1x second order spatial derivatives → 2 boundary conditions

Recap of different boundary conditions

- There are numerous possibilities for the boundary conditions (BCs) that must be specified on the domain boundaries:
  - Dirichlet boundary conditions (*essential* BCs): the solution u is specified.

  For instance: $u(x=0)=\bar{u}$

  - Neumann boundary conditions (*natural* BCs): one of the derivatives u_x or u_y is specified.

  For instance: $\frac{\partial u}{\partial x}|_{x=L}=0$

  - Robin boundary conditions (*mixed* boundary conditions): a combination of the previous conditions is specified.

  For instance: $\alpha u(x=0)+\beta\frac{\partial u}{\partial x}|_{x=0}=q$

- We will mainly deal with Dirichlet and Neumann boundary conditions.

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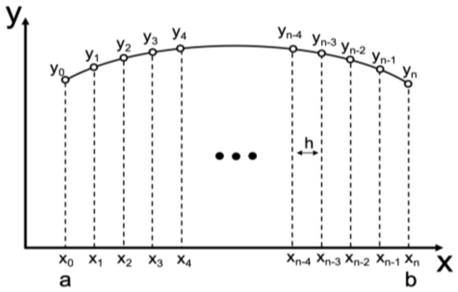
Numerical methods for solving PDEs

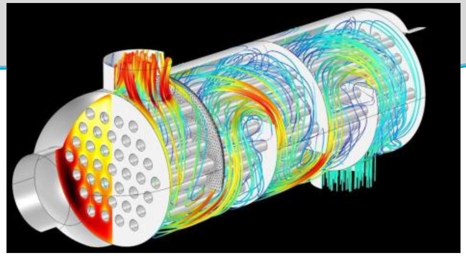
Finite Difference Method (FDM)

- The finite difference method approximates derivatives by discretizing the domain over grid points.
- Applied in mass and heat transfer problems in simple domains.



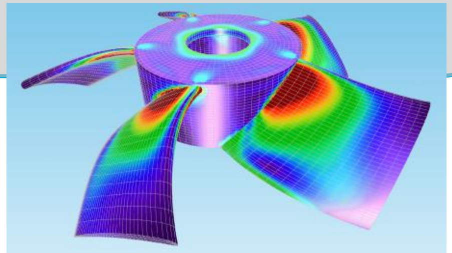
Finite Volume Method (FVM)

- The finite volume method conserves quantities by integrating over control volumes
- Widely used in computational fluid dynamics (CFD)



Finite Element Method (FEM)

- The finite element method divides the domain into elements and uses variational methods to solve.
- Ideal for structural analysis and stress distribution in materials engineering.



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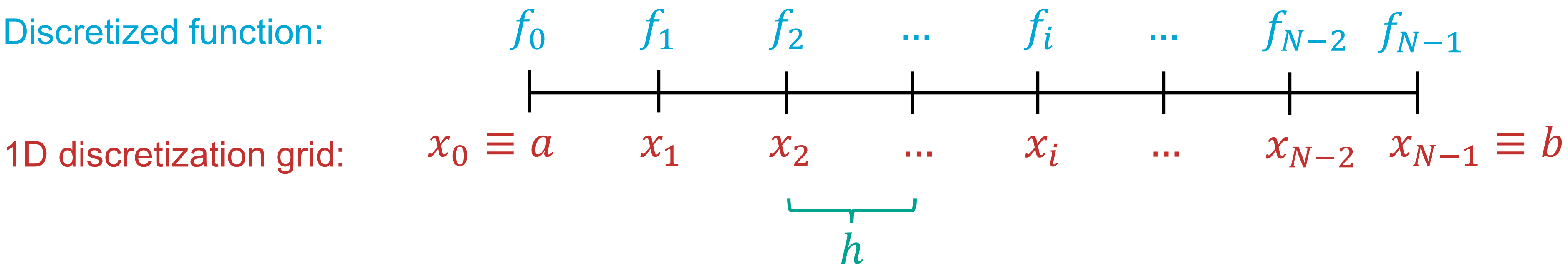
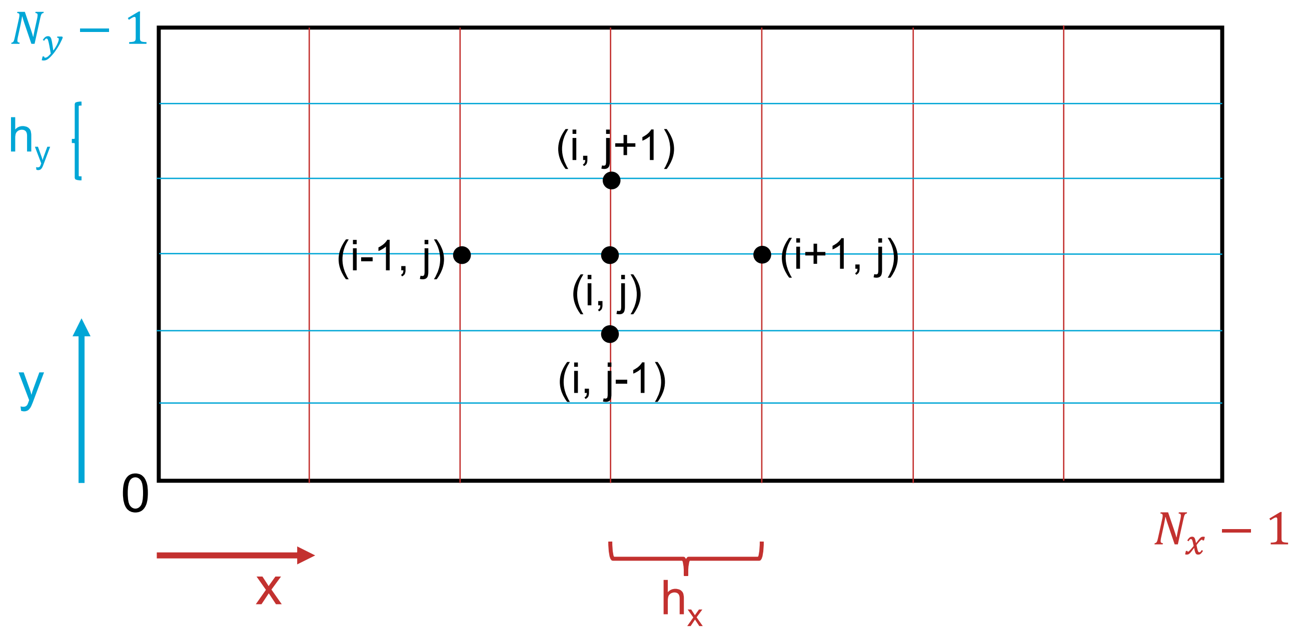
Finite difference method for PDEs: Introduction

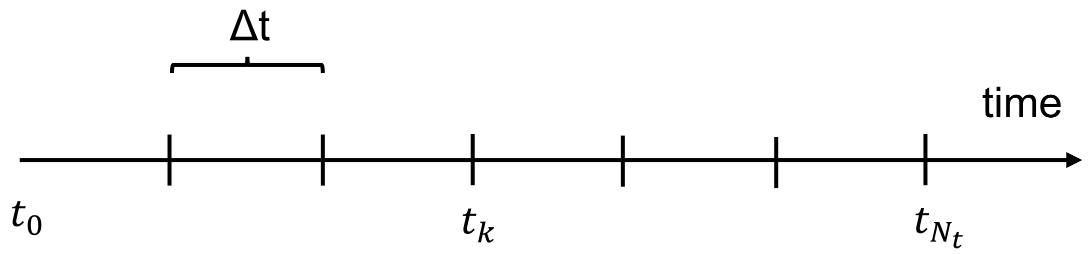
- The finite difference method (FDM) approximates derivatives in partial differential equations (PDEs) using differences between function values at discrete grid points.
  - Continuous domain → grid of discrete points
  - Partial derivatives → finite differences
  - System of algebraic equations → iterative numerical methods



Discretize multivariate domains

- By definition, PDEs involve multiple independent variables:
  - Space (x, y, z)
  - Time (t)
  - Possibly other variables
- Every variable will have its own (possibly different) discretization scheme
  - In general: $h_x \neq h_y$
  - Often: $h_x = h_y$
  - The choice of time step Δt depends on the stability of the system

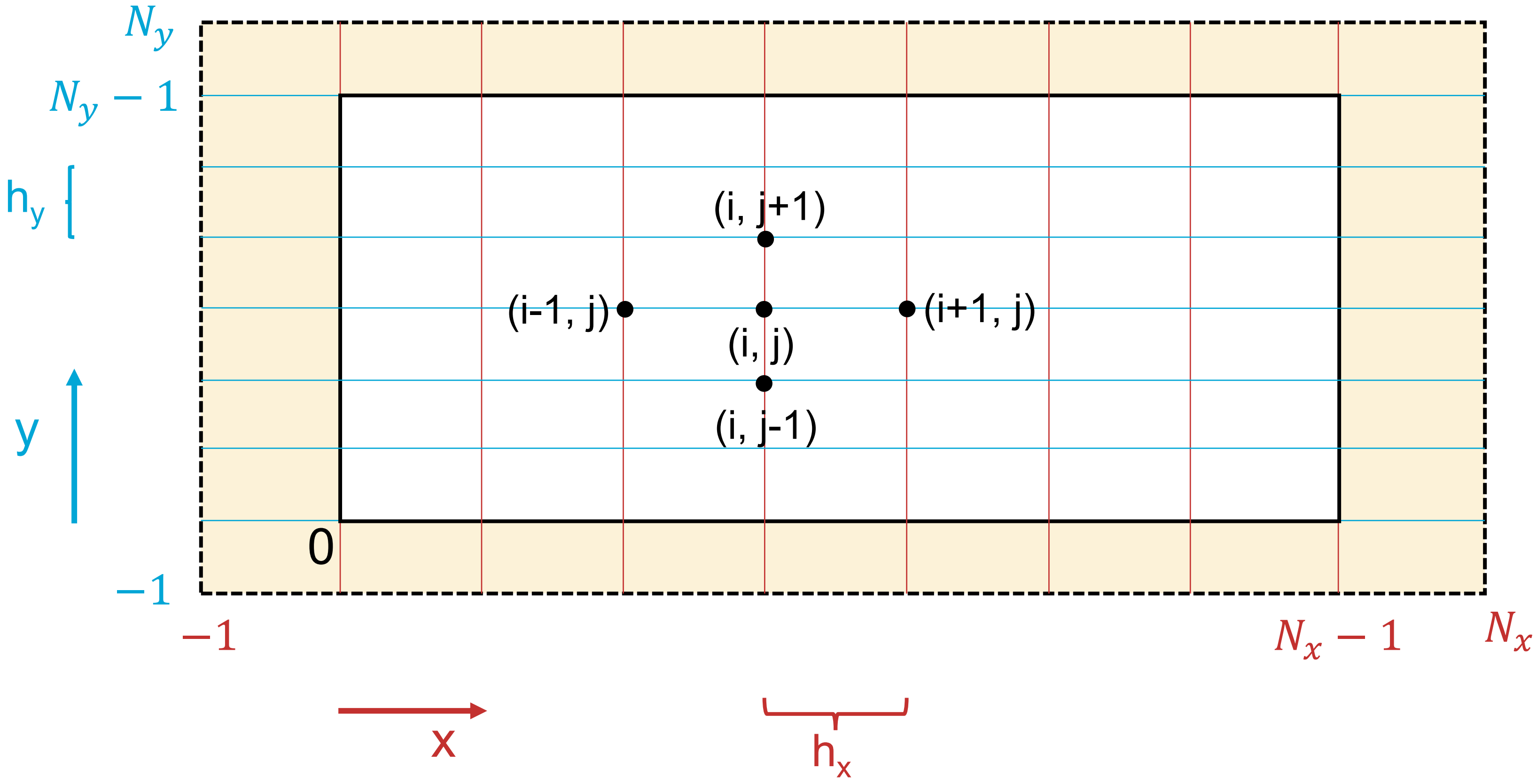




Discretization with ghost points

Recap from CP Q1L6

- Artificial (ghost) points can be added as a padding around the domain (for each coordinate: 2 points, 2 intervals)
- Useful to discretize boundary conditions with more accurate schemes



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Heat transport problem

- Microscopic governing equations for transport phenomena are typically modelled by partial differential equations, describing how quantities as concentration, velocity or temperature evolve in space and time.
- We consider the case of heat transport problem as a case study for PDEs.
- More specifically:
  - Unsteady heat transport in 1D (e.g., tube wall)
    → Parabolic PDE (this lecture)
  - Steady state heat transport in 2D (e.g., plate heat exchanger)
    → Elliptic PDE (next lecture)

Parabolic PDEs: chemical engineering applications

- We explore the solution method for parabolic PDEs, exemplified by the heat equation:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

The equation describes the transient temperature propagation along a single-dimensional space.

- Several other chemical engineering problems can be modelled as parabolic PDEs.
  - Mass diffusion equation

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

  - Concentration profiles in catalyst pellets

$$\frac{\partial C_A}{\partial t} = D \frac{\partial^2 C_A}{\partial r^2} - r_A(C_A)$$

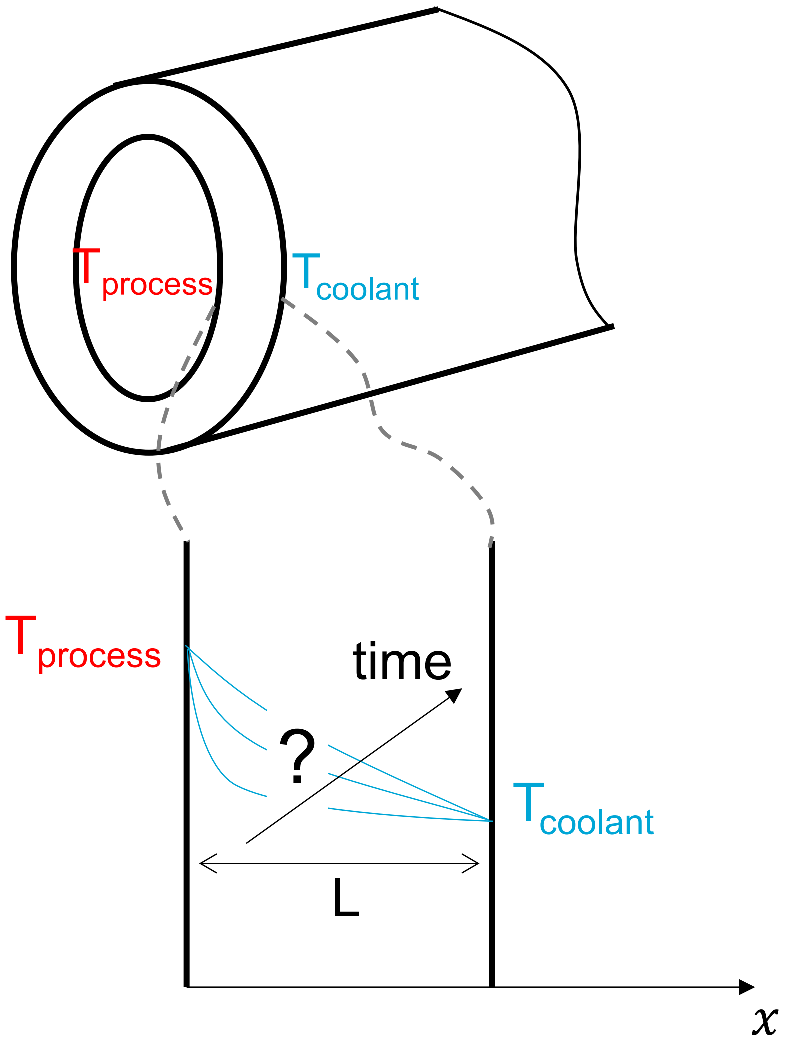
Possibly nonlinear PDE!

Case study for parabolic PDEs

- 1D Heat Equation:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

- Consider heat transfer across the wall of a tube in a shell-and-tube heat exchanger:
  - The temperatures of the process fluid (tube side) and coolant (shell side) are known.
  - Initially, the tube wall is in thermal equilibrium with the coolant.
  - How does the temperature evolve over time and across the wall?



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Semidiscrete Method: PDE to ODE system

- A way to approximate the solution of transient PDEs is to initially discretize in space and leave the time variable continuous
- Introduce spatial mesh points x_i , $i = 0, \dots, N_x - 1$, where i is the discretization index and Δx the interval
- Discretize the second order spatial derivative by finite differences (internal points):

$$\frac{d^2T}{dx^2} \approx \frac{T_{i-1} - 2T_i + T_{i+1}}{\Delta x^2}$$

Note: $T_i = T_i(t)$ is time dependent

- The equation results in a system of ODEs:

$$\frac{dT_i}{dt} = \alpha \frac{T_{i-1} - 2T_i + T_{i+1}}{\Delta x^2}, \qquad i = 1, \dots, N_x - 2$$

- With initial and boundary condition:

$$T_i(0) = T_{coolant} \quad i = 1, \dots, N_x - 2$$
$$T_0(t) = T_{process} \quad T_{N_x - 1}(t) = T_{coolant} \quad \forall t$$

Semidiscrete Method: PDE to ODE system

- In matrix form:

$$\frac{d}{dt}\boldsymbol{T} = \frac{\alpha}{\Delta x^2} A\boldsymbol{T}_{(complete)}$$

- Here, $\frac{\alpha}{\Delta x^2}$ is a scalar constant and A is a matrix
- Note that the vector $\boldsymbol{T}$ is different from the vector $\boldsymbol{T}_{(complete)}$, this is directly arising from the indices previously shown:

boundary points included

only internal points

$$\frac{d}{dt}\begin{bmatrix} T_1 \\ \vdots \\ T_{N_x-2} \end{bmatrix} = \mathrm{A}\begin{bmatrix} T_0 \\ T_1 \\ \vdots \\ T_{N_x-2} \\ T_{N_x-1} \end{bmatrix}$$

- Hence, the matrix A is rectangular ($N_x - 2 \times N_x$), thus the system is under determined.
- Two more equations are needed! → Boundary conditions!!

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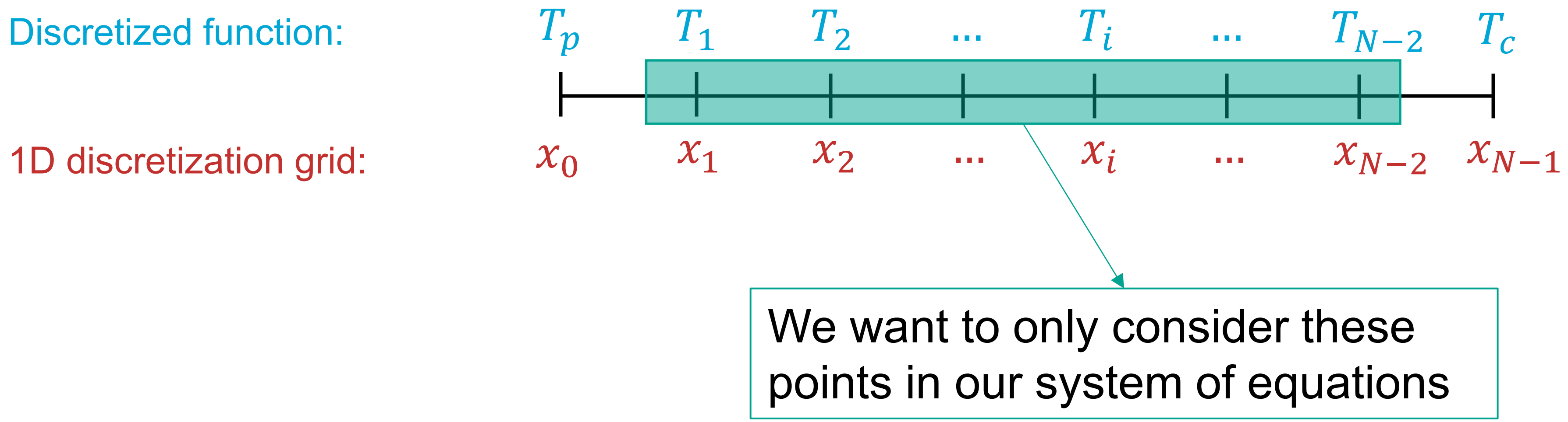
Dirichlet boundary conditions

- Remember Q1 Lecture 6 – BVP with FDM:
  We want to only use the internal points of the domain grid (vector T) to discretize the boundary conditions.
- Consider Dirichlet boundary conditions as in the stated problem: $T_0 = T_p$ and $T_{N_x-1} = T_c$



Dirichlet boundary conditions

- We can develop specialized equations for T_1 and T_{N_x-2}:

$i = 1$:

$$\frac{dT_1}{dt} = \frac{\alpha}{\Delta x^2}(T_0 - 2T_1 + T_2)$$

…but $T_0(t) = T_p \quad \forall$t, then:

$$\frac{dT_1}{dt} = \frac{\alpha}{\Delta x^2}(T_p - 2T_1 + T_2)$$

$$\frac{dT_1}{dt} = \frac{\alpha}{\Delta x^2}(-2T_1 + T_2) + \frac{\alpha}{\Delta x^2}T_p$$

Dirichlet boundary conditions

- We can develop specialized equations for T_1 and T_{N_x-2}:

$i = N_x - 2$:

$$\frac{dT_{N_x-2}}{dt} = \frac{\alpha}{\Delta x^2}\left(T_{N_x-3} - 2T_{N_x-2} + T_{N_x-1}\right)$$

…but $T_{N_x-1}(t) = T_c \quad \forall t$, then:

$$\frac{dT_{N_x-2}}{dt} = \frac{\alpha}{\Delta x^2}\left(T_{N_x-3} - 2T_{N_x-2} + T_c\right)$$

$$\frac{dT_{N_x-2}}{dt} = \frac{\alpha}{\Delta x^2}\left(T_{N_x-3} - 2T_{N_x-2}\right) + \frac{\alpha}{\Delta x^2}T_c$$

System of equations with Dirichlet boundary conditions

- The final system of ODEs given Dirichlet boundary conditions is

algebraic equations

$$\begin{cases} T_0(t) = T_p \\ \dfrac{dT_i}{dt} = \dfrac{\alpha}{\Delta x^2}(T_{i-1} - 2T_i + T_{i+1}) & \forall t \text{ and } i = 1, \dots, N_x - 2 \\ T_{N_x-1}(t) = T_c \end{cases}$$

$N_x - 2$ ordinary differential equations

- The initial condition is given by

$$T_i(0) = T_c \qquad i = 1, \dots, N_{x-2}$$

Matrix form with Dirichlet boundary conditions

- The system of ODEs given Dirichlet boundary conditions can be written in matrix form, including a vector with the initial condition

$$\frac{d}{dt}\boldsymbol{T} = \frac{\alpha}{\Delta x^2}\cdot(A\boldsymbol{T} + \boldsymbol{b}), \qquad \boldsymbol{T}(0) = \boldsymbol{T}_c,$$

$$\frac{d}{dt}\begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \end{bmatrix} = \frac{\alpha}{\Delta x^2}\begin{bmatrix} -2 & 1 & 0 & \dots & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & -2 & 1 \\ 0 & 0 & \cdots & 0 & 1 & -2 \end{bmatrix}\begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \end{bmatrix} + \frac{\alpha}{\Delta x^2}\begin{bmatrix} \mathrm{T_p} \\ 0 \\ \vdots \\ 0 \\ \mathrm{T_c} \end{bmatrix}, \qquad \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \end{bmatrix}(0) = \begin{bmatrix} T_c \\ T_c \\ \vdots \\ T_c \\ T_c \end{bmatrix}.$$

$$A \in \mathbb{R}^{N_x-2\times N_x-2} \qquad \boldsymbol{T},\boldsymbol{T}_c \in \mathbb{R}^{N_x-2} \qquad \boldsymbol{b} \in \mathbb{R}^{N_x-2}$$

Neumann boundary conditions

- For completeness, consider now the case of Neumann boundary conditions:

$$\left.\frac{\partial T}{\partial x}\right|_{x=0} = \gamma_1$$
$$\left.\frac{\partial T}{\partial x}\right|_{x=L} = \gamma_2$$

- We aim to derive an updating rule in matrix form, including Neumann boundary conditions for which the derivative is constant on the boundaries.
- We aim to use only internal discretization points ($i = 2, \dots, N_x - 3$)
- Discretization scheme:
  - First order derivative in $x = 0$ → <u>Forward</u> difference scheme
  - First order derivative in $x = \mathrm{L}$ → <u>Backward</u> difference scheme
  - Central difference scheme is possible with ghost points! (discuss this later…)

Neumann boundary conditions

- We can develop specialized equations for T_1 and T_{N_x-2}:

$i = 1$:

Forward difference scheme: $\frac{\partial T}{\partial x}|_{x=0} = \gamma_1 \quad \rightarrow \quad \frac{T_1 - T_0}{\Delta x} = \gamma_1 \rightarrow T_0 = T_1 - \gamma_1 \Delta x$

Updating equation:

$$\frac{dT_1}{dt} = \frac{\alpha}{\Delta x^2}(T_0 - 2T_1 + T_2)$$

Substituting the equation arising from the boundary condition:

$$\frac{dT_1}{dt} = \frac{\alpha}{\Delta x^2}(T_1 - \gamma_1 \Delta x - 2T_1 + T_2)$$

$$\frac{dT_1}{dt} = \frac{\alpha}{\Delta x^2}(-T_1 + T_2) - \frac{\alpha}{\Delta x}\gamma_1$$

Neumann boundary conditions

- We can develop specialized equations for T_1 and T_{N_x-2}:

$i = N_x - 2$:

Backward difference scheme: $\frac{\partial T}{\partial x}|_{x=L} = \gamma_2 \quad \rightarrow \quad \frac{T_{N_x-1} - T_{N_x-2}}{\Delta x} = \gamma_2 \rightarrow T_{N_x-1} = T_{N_x-2} + \gamma_2 \Delta x$

Updating equation:

$$\frac{dT_{N_x-2}}{dt} = \frac{\alpha}{\Delta x^2}\left(T_{N_x-3} - 2T_{N_x-2} + T_{N_x-1}\right)$$

Substituting the equation arising from the boundary condition:

$$\frac{dT_{N_x-2}}{dt} = \frac{\alpha}{\Delta x^2}\left(T_{N_x-3} - 2T_{N_x-2} + T_{N_x-2} + \gamma_2 \Delta x\right)$$

$$\frac{dT_{N_x-2}}{dt} = \frac{\alpha}{\Delta x^2}\left(T_{N_x-3} - T_{N_x-2}\right) + \frac{\alpha}{\Delta x}\gamma_2$$

System of ODEs with Neumann boundary conditions

- The Final system of equations given Neumann boundary conditions is

algebraic equations

$$\begin{cases} T_0(t) = T_1 - \gamma_1 \Delta x \\ \dfrac{dT_i}{dt} = \dfrac{\alpha}{\Delta x^2}\left(T_{i-1} - 2T_i + T_{i+1}\right) \\ T_{N_x-1}(t) = T_{N_x-2} + \gamma_2 \Delta x \end{cases} \qquad \forall t \text{ and } i = 1, \dots, N_x - 2$$

$N_x - 2$ ordinary differential equations

- The initial condition is given by

$$T_i(0) = T_c \qquad i = 1, \dots, N_{x-2}$$

Matrix form with Neumann boundary conditions

- The system of ODEs given Neumann boundary conditions can be written in matrix form, including a vector with the initial condition

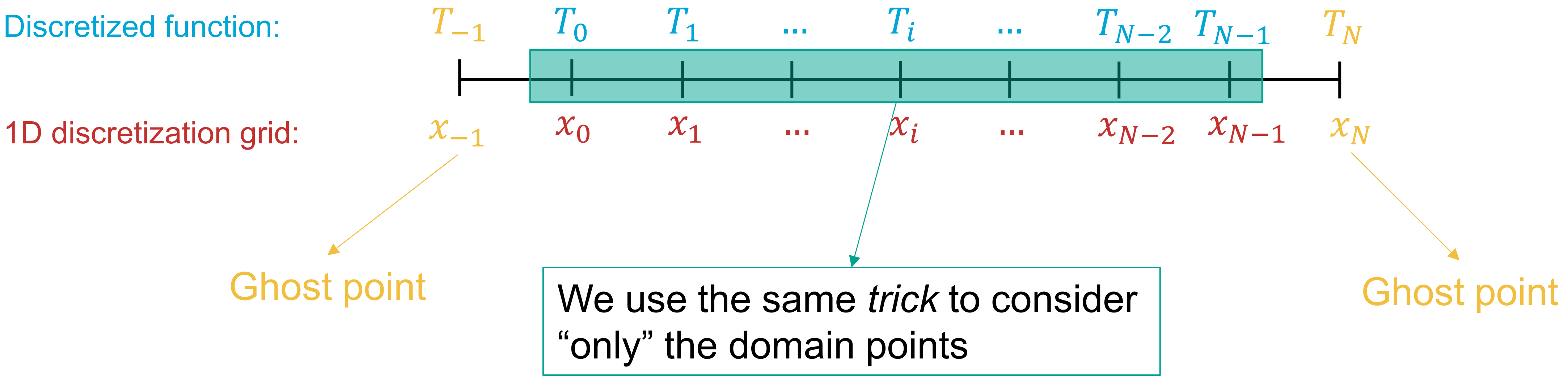
$$\frac{d}{dt}\boldsymbol{T} = \frac{\alpha}{\Delta x^2} \cdot (A\boldsymbol{T} + \boldsymbol{b}), \qquad \boldsymbol{T}(0) = \boldsymbol{T}_c,$$

$$\frac{d}{dt}\begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \end{bmatrix} = \frac{\alpha}{\Delta x^2}\begin{bmatrix} -1 & 1 & 0 & \dots & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & -2 & 1 \\ 0 & 0 & \cdots & 0 & 1 & -1 \end{bmatrix}\begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \end{bmatrix} + \frac{\alpha}{\Delta x^2}\begin{bmatrix} -\gamma_1 \Delta x \\ 0 \\ \vdots \\ 0 \\ \gamma_2 \Delta x \end{bmatrix}, \qquad \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \end{bmatrix}(0) = \begin{bmatrix} T_c \\ T_c \\ \vdots \\ T_c \\ T_c \end{bmatrix}.$$

$$A \in \mathbb{R}^{N_x-2 \times N_x-2} \qquad \boldsymbol{T}, \boldsymbol{T}_c \in \mathbb{R}^{N_x-2} \qquad \boldsymbol{b} \in \mathbb{R}^{N_x-2}$$

Neumann boundary conditions with ghost points

- The concept of ghost points can be used to unlock more <u>accurate discretization schemes</u> for Neumann boundary conditions (i.e., central difference scheme)



Neumann boundary conditions: ghost points

- We can develop specialized equations for T_0 and T_{N_x-1}: (boundary points!)

$i = 0$:

Central difference scheme: $\frac{\partial T}{\partial x}|_{x=0} = \gamma_1 \quad \rightarrow \quad \frac{T_1 - T_{-1}}{2\Delta x} = \gamma_1 \rightarrow T_{-1} = T_1 - 2\gamma_1 \Delta x$

Updating equation:

$$\frac{dT_0}{dt} = \frac{\alpha}{\Delta x^2}(T_{-1} - 2T_0 + T_1)$$

Substituting the equation arising from the boundary condition:

$$\frac{dT_0}{dt} = \frac{\alpha}{\Delta x^2}(T_1 - 2\gamma_1 \Delta x - 2T_0 + T_1)$$

$$\frac{dT_0}{dt} = \frac{\alpha}{\Delta x^2}(-2T_0 + 2T_1) - 2\frac{\alpha}{\Delta x}\gamma_1$$

Neumann boundary conditions: ghost points

- We can develop specialized equations for T_0 and T_{N_x-1}: (boundary points!)

$i = N_x - 1$:

Central difference scheme: $\frac{\partial T}{\partial x}\big|_{x=L} = \gamma_2 \quad \rightarrow \quad \frac{T_{N_x} - T_{N_x-2}}{2\Delta x} = \gamma_2 \rightarrow T_{N_x} = T_{N_x-2} + 2\gamma_2 \Delta x$

Updating equation:

$$\frac{dT_{N_x-1}}{dt} = \frac{\alpha}{\Delta x^2}\left(T_{N_x-2} - 2T_{N_x-1} + T_{N_x}\right)$$

Substituting the equation arising from the boundary condition:

$$\frac{dT_{N_x-1}}{dt} = \frac{\alpha}{\Delta x^2}\left(T_{N_x-2} - 2T_{N_x-1} + T_{N_x-2} + 2\gamma_2 \Delta x\right)$$

$$\frac{dT_{N_x-1}}{dt} = \frac{\alpha}{\Delta x^2}\left(2T_{N_x-2} - 2T_{N_x-1}\right) + 2\frac{\alpha}{\Delta x}\gamma_2$$

System of equations with Neumann bcs

- The final system of ODEs given Neumann boundary conditions with ghost points is

algebraic equations

$$\begin{cases} T_{-1}(t) = T_1 - 2\gamma_1 \Delta x \\ \dfrac{dT_i}{dt} = \dfrac{\alpha}{\Delta x^2}(T_{i-1} - 2T_i + T_{i+1}) \\ T_{N_x}(t) = T_{N_x-2} + 2\gamma_2 \Delta x \end{cases} \qquad \forall t \text{ and } i = 0, \dots, N_x - 1$$

N_x ordinary differential equations

- The initial condition is given by

$$T_i(0) = T_c \qquad i = 0, \dots, N_{x-1}$$

Matrix form with Neumann boundary conditions

- The system of ODEs given Neumann boundary conditions with ghost points can be written in matrix form, including a vector with the initial condition

$$\frac{d}{dt}\boldsymbol{T} = \frac{\alpha}{\Delta x^2} \cdot (A\boldsymbol{T} + \boldsymbol{b}), \qquad \boldsymbol{T}(0) = \boldsymbol{T}_c,$$

$$\frac{d}{dt}\begin{bmatrix} T_0 \\ T_1 \\ \vdots \\ T_{N_x-2} \\ T_{N_x-1} \end{bmatrix} = \frac{\alpha}{\Delta x^2}\begin{bmatrix} -2 & 2 & 0 & \dots & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & -2 & 1 \\ 0 & 0 & \cdots & 0 & 2 & -2 \end{bmatrix}\begin{bmatrix} T_0 \\ T_1 \\ \vdots \\ T_{N_x-2} \\ T_{N_x-1} \end{bmatrix} + \frac{\alpha}{\Delta x^2}\begin{bmatrix} -2\gamma_1\Delta x \\ 0 \\ \vdots \\ 0 \\ 2\gamma_2\Delta x \end{bmatrix}, \qquad \begin{bmatrix} T_0 \\ T_1 \\ \vdots \\ T_{N_x-2} \\ T_{N_x-1} \end{bmatrix}(0) = \begin{bmatrix} T_c \\ T_c \\ \vdots \\ T_c \\ T_c \end{bmatrix}.$$

$$A \in \mathbb{R}^{N_x-1\times N_x-1} \qquad \boldsymbol{T}, \boldsymbol{T}_c \in \mathbb{R}^{N_x-1} \qquad \boldsymbol{b} \in \mathbb{R}^{N_x-1}$$

Agenda

- What is a Partial Differential Equation (PDE)?
  - Classification of PDE's (Elliptic, Parabolic, Hyperbolic)
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    - Stability
    - Backward Euler
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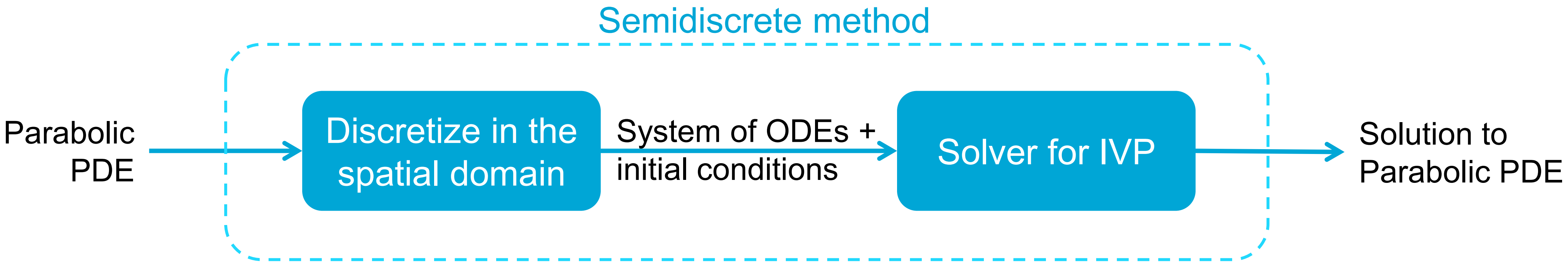
Semidiscrete Method: Solution methods

- The solution of the PDE is translated into solving a system of ODEs with given initial conditions.
- In Q1, you learnt how to solve Initial Value Problems (IVPs) in the context of ODEs:
  - Forward (explicit) Euler
  - Backward (implicit) Euler
  - More advanced schemes (Runge-Kutta)

See CP Q1 Lecture 5



Semidiscrete Method: Forward Euler

- The simplest choice for solving systems of ODEs is to use Forward (explicit) Euler method.
- Discretization of the first order time derivative:

$$\frac{dT_i}{dt} = \frac{T_i^{k+1} - T_i^k}{\Delta t}, \qquad t_k = k \cdot \Delta t$$

- The PDE can be written as:

$$\frac{T_i^{k+1} - T_i^k}{\Delta t} = \alpha \frac{T_{i-1}^k - 2T_i^k + T_{i+1}^k}{\Delta x^2}, \qquad i = 1, \dots, N_x - 2, \qquad k = 0, \dots, N_t - 2$$

- Thus, giving the updating closed form for every <u>internal</u> point: $(\mathrm{Fo} = \alpha \Delta t / \Delta x^2)$

$$T_i^{k+1} - T_i^k = Fo(T_{i-1}^k - 2T_i^k + T_{i+1}^k)$$

$$\boxed{T_i^{k+1} = T_i^k + Fo\left(T_{i-1}^k - 2T_i^k + T_{i+1}^k\right)}$$

Note: Boundary conditions determine final form of the system of equations

System of eqs with Dirichlet bcs: Forward Euler

- The final system of equations given Dirichlet boundary conditions is

$$\begin{cases} T_0^{k+1} = T_p \\ T_i^{k+1} = T_i^k + F_0\left(T_{i-1}^k - 2T_i^k + T_{i+1}^k\right) \\ T_{N_x-1}^{k+1} = T_c \end{cases} \qquad \forall k \text{ and } i = 1, \dots, N_x - 2$$

N_x algebraic equations

- The initial condition is given by

$$T_i^0 = T_c \qquad i = 1, \dots, N_{x-2}$$

- Double for-loop needed to calculate each T_i^k in the domain.

System of eqs with Neumann bcs (1): Forward Euler

- The final system of equations given Neumann boundary conditions is

$$\begin{cases} T_0^{k+1} = T_1 - \gamma_1 \Delta x \\ T_i^{k+1} = T_i^k + F_0\left(T_{i-1}^k - 2T_i^k + T_{i+1}^k\right) \\ T_{N_x-1}^{k+1} = T_{N_x-2} + \gamma_2 \Delta x \end{cases} \qquad \forall k \text{ and } i = 1, \dots, N_x - 2$$

N_x algebraic equations

- The initial condition is given by

$$T_i^0 = T_c \qquad i = 1, \dots, N_{x-2}$$

- Double for-loop needed to calculate each T_i^k in the domain.

System of eqs with Neumann bcs (2): Forward Euler

- The final system of equations given Neumann boundary conditions with **ghost points** is

$$\begin{cases} T_{\mathbf{-1}}^{k+1} = T_1 - 2\gamma_1 \Delta x \\ T_i^{k+1} = T_i^k + F_0\left(T_{i-1}^k - 2T_i^k + T_{i+1}^k\right) \\ T_{\boldsymbol{N_x}}^{k+1} = T_{N_x-2} + 2\gamma_2 \Delta \mathrm{x} \end{cases} \qquad \forall k \text{ and } i = 0, \dots, N_x - 1$$

N_x+2 algebraic equations

- The initial condition is given by

$$T_i^0 = T_c \qquad i = 1, \dots, N_{x-2}$$

- Double for-loop needed to calculate each T_i^k in the domain.

How do I avoid for-loops?

Semidiscrete Method (Matrix form): Forward Euler

- Again, the simplest choice for solving systems of ODEs is to use Forward Euler method.
- Discretization of the first order time derivative in **vector form**:

$$\frac{d\boldsymbol{T}}{dt} = \frac{\boldsymbol{T}^{k+1} - \boldsymbol{T}^{k}}{\Delta t}, \qquad t_k = k \cdot \Delta t$$

- The PDE can be written as:

Note: A and $\boldsymbol{b}$ depend on the dv and bcs

$$\frac{\boldsymbol{T}^{k+1} - \boldsymbol{T}^{k}}{\Delta t} = \frac{\alpha}{\Delta x^2}\left(A\boldsymbol{T}^{k} + \boldsymbol{b}\right), \qquad k = 0, \dots, N_t - 2$$

- Thus, giving the updating closed form: $(\mathrm{Fo} = \alpha \Delta t / \Delta x^2)$

$$\boldsymbol{T}^{k+1} - \boldsymbol{T}^{k} = Fo\left(A\boldsymbol{T}^{k} + \boldsymbol{b}\right)$$

$$\boxed{\boldsymbol{T}^{k+1} = \boldsymbol{T}^{k} + Fo\left(A\boldsymbol{T}^{k} + \boldsymbol{b}\right)}$$

It is preferable to work in matrix form for computational reasons (avoid for-loops!)

Matrix form with Dirichlet bcs: Forward Euler

- The equations can be composed in an **explicit** linear system in matrix form:

$$T^{k+1} = Fo \cdot A_{DF} T^k + Fo \cdot b_{DF}$$

$$\begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \end{bmatrix}^{k+1} = Fo \begin{bmatrix} \frac{1}{Fo} - 2 & 1 & 0 & \dots & \dots & 0 \\ 1 & \frac{1}{Fo} - 2 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & \frac{1}{Fo} - 2 & 1 \\ 0 & 0 & \cdots & 0 & 1 & \frac{1}{Fo} - 2 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \end{bmatrix}^{k} + Fo \begin{bmatrix} T_p \\ 0 \\ \vdots \\ 0 \\ T_c \end{bmatrix}$$

$A_{DF} \in \mathbb{R}^{N_x-2 \times N_x-2}$ $\quad$ $T^{k+1}, T^k \in \mathbb{R}^{N_x-2}$ $\quad$ $b_{DF} \in \mathbb{R}^{N_x-2}$

Matrix form with Neumann bcs (1): Forward Euler

- For Neumann boundary conditions the same Euler forward scheme holds. However, the matrix A and the vector $\boldsymbol{b}$ are replaced accordingly. Resulting in an **explicit** linear system in matrix form:

$$T^{k+1} = Fo \cdot A_{NF} T^k + Fo \cdot b_{NF}$$

$$\begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \end{bmatrix}^{k+1} = Fo \begin{bmatrix} \frac{1}{Fo} - 1 & 1 & 0 & \dots & \dots & 0 \\ 1 & \frac{1}{Fo} - 2 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & \frac{1}{Fo} - 2 & 1 \\ 0 & 0 & \cdots & 0 & 1 & \frac{1}{Fo} - 1 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \end{bmatrix}^{k} + Fo \begin{bmatrix} -\gamma_1 \Delta x \\ 0 \\ \vdots \\ 0 \\ \gamma_2 \Delta x \end{bmatrix}$$

$$A_{NF} \in \mathbb{R}^{N_x-2 \times N_x-2} \qquad T^{k+1}, T^k \in \mathbb{R}^{N_x-2} \qquad b_{NF} \in \mathbb{R}^{N_x-2}$$

Matrix form, Neumann bcs (2): Forward Euler

- For Neumann boundary conditions with ghost points the same Euler forward scheme holds. However, the matrix A and the vectors $\boldsymbol{b}$ and $\boldsymbol{T}$ are replaced accordingly. Resulting in an **explicit** linear system in matrix form:

$$T_G^{k+1} = Fo \cdot A_{NFG} T_G^k + Fo \cdot b_{NFG}$$

$$\begin{bmatrix} T_0 \\ T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \\ T_{N_x-1} \end{bmatrix}^{k+1} = Fo \begin{bmatrix} \frac{1}{Fo} - 2 & 2 & 0 & \dots & \dots & 0 \\ 1 & \frac{1}{Fo} - 2 & 1 & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & \frac{1}{Fo} - 2 & 1 \\ 0 & 0 & \cdots & 0 & 2 & \frac{1}{Fo} - 2 \end{bmatrix} \begin{bmatrix} T_0 \\ T_1 \\ T_2 \\ \vdots \\ T_{N_x-3} \\ T_{N_x-2} \\ T_{N_x-1} \end{bmatrix}^{k} + Fo \begin{bmatrix} -2\gamma_1 \Delta x \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 2\gamma_2 \Delta x \end{bmatrix}$$

extremes included → T_G

$A_{NFG} \in \mathbb{R}^{N_x \times N_x}$ $\quad T_G^{k+1}, T_G^k \in \mathbb{R}^{N_x}$ $\quad b_{NFG} \in \mathbb{R}^{N_x}$

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Semidiscrete Method: Forward Euler

- Considerations about Explicit Euler method are the same as discussed in Q1 Lecture 5:
- PROS:
  - simple implementation
  - explicit formula
  - efficient computation
- CONS:
  - stability issues
  - required small time steps (potential memory issues)

Stability criterion for explicit methods

- The Courant-Friedrichs-Lewy (CFL) condition is a <u>necessary</u> condition for the convergence of parabolic PDEs.
- For 1D problems parabolic PDEs, the CFL condition has the following form:

$$Fo = \frac{\alpha \Delta t}{\Delta x^2} \leq \frac{1}{2}$$

- Fo is the Fourier number (dimensionless)

- CFL condition states that, given an arbitrary space step, the time step must be <u>necessarily</u> small “enough” to converge:

$$\Delta t \leq \frac{\Delta x^2}{2\alpha}$$

Are there alternatives to explicit methods to avoid instability issues?

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Semidiscrete Method: Backward Euler

- The simplest choice for solving systems of ODEs is to use Forward (explicit) Euler method.
- Discretization of the first order time derivative:

$$\frac{\partial \boldsymbol{T}}{\partial t} = \frac{\boldsymbol{T}^{k+1} - \boldsymbol{T}^{k}}{\Delta t}, \qquad t_k = k \cdot \Delta t$$

- The PDE can be written as:

Note: A and $\boldsymbol{b}$ depend on the dv and bcs

$$\frac{\boldsymbol{T}^{k+1} - \boldsymbol{T}^{k}}{\Delta t} = \frac{\alpha}{\Delta x^2}\left(A\boldsymbol{T}^{k+1} + \boldsymbol{b}\right), \qquad k = 0, \ldots, N_t - 2$$

- Thus, giving the updating closed form: $(\mathrm{Fo} = \alpha \Delta t / \Delta x^2)$

$$\boldsymbol{T}^{k+1} - \boldsymbol{T}^{k} = Fo\left(A\boldsymbol{T}^{k+1} + \boldsymbol{b}\right)$$

$$\boxed{(I - FoA)\boldsymbol{T}^{k+1} = \boldsymbol{T}^{k} + Fo\boldsymbol{b}}$$

It is preferable to work in matrix form for computational reasons (solving systems of eq.)

Agenda

- What is a Partial Differential Equation (PDE)?
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Semidiscrete Method: ODE Solver

- Recall the method for solving parabolic PDEs:
  1. Discretize spatial derivatives with finite differences
  2. Obtain a system of ODE equations
  3. Solve the system of ODE equations
- We analysed two simple techniques for 3: Euler Forward and Backward
- More advanced schemes for ODEs can be used instead (Runge-Kutta) and built-in functions (*scipy.integrate.solve_ivp()*)

- Want to speed up your computation? Exploit the sparsity of the discretization matrices!
  - *scipy.sparse.spdiag → Define a sparse diagonal matrix*
  - *scipy.sparse.linalg.spsolve → Solve sparse linear systems efficiently*

Parabolic PDE: Live coding

- Open Colab: [Parabolic PDE - Heat Equation]

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

Learning objectives

After successfully completing this lecture, you are able to…

- Explain what a partial differential equation (PDEs) is, how it can be classified, and how it is different form ordinary differential equations (ODEs).
- Give an overview of the main techniques to solve partial differential equations in (chemical) engineering
- Implement different numerical solution approaches for parabolic PDEs from scratch
- Discuss stability of numerical solution approaches for parabolic PDEs
- Use Python libraries' built-in functions to support the solution of parabolic PDEs

Thank you very much for your attention!