Statistical and Numerical Methods for Chemical Engineers

(401-0675-00L)

Lecture for D-CHAB Autumn Semester 2024

Dr. Roger Käppeli
Dr. Patric Müller

Statistical and Numerical Methods for Chemical Engineers

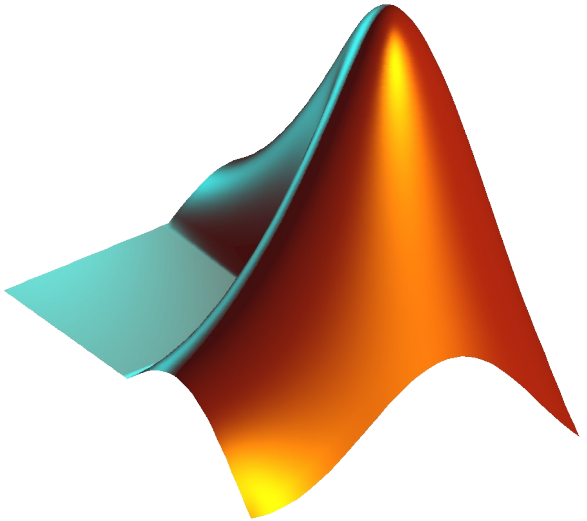
- Part one: Numerical methods (Käppeli)
  Lecture: Wednesday, 08:15-10:00, HG E 33.1
  18.09.; 25.09.; 02.10.; 09.10.; 16.10.;
  ~~23.10.~~; 30.10; 06.11.; 13.11.
- Part two: Statistical methods (Müller)
  Lecture: Wednesday, 08:15-10:00, HG E 33.1
  20.11.; 27.11.; 04.12.; 11.12.; 18.12.
- Exercises (Jiwoo Oh, Asbjörn Rasmussen)
  - Tuesday, 07:45-09:30, HCI H 8.1
    From 24.09. until 17.12.
  - Bonus (+0.25) will be explained in exercises

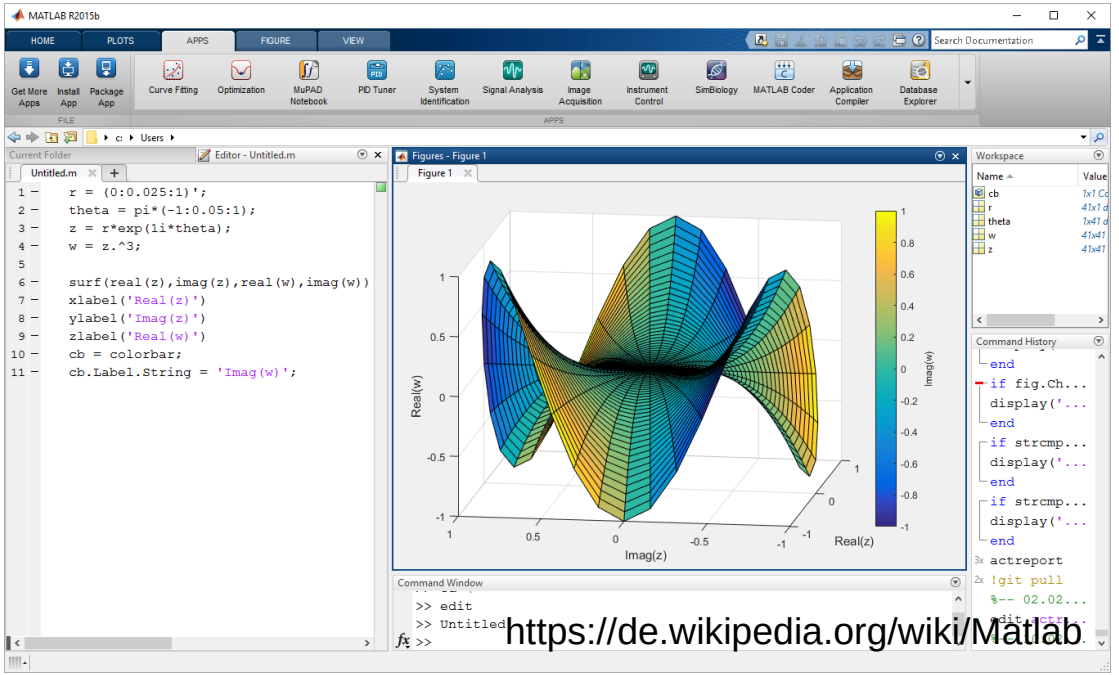
← **Start next week! This week MATLAB introduction on Thursday (see email!)**

- Case study week: 21.10.-25.10. ← **No lecture & exercise classes!**

MATLAB introduction

- Instructors: Jiwoo Oh, Asbjörn Rasmussen
- Thursday, 19.09.24
  - HCI G 174 09:00- 16:00
- See email for exact details





https://de.wikipedia.org/wiki/Matlab

Exam

- Mode of examination: Oral 20 minutes
- Language: English or German
- Two parts:
  - ~13 minutes Numerical Methods
  - ~7 minutes Statistical Methods
- “Sample” exam for Numerical Methods part in last lecture

Part one: Numerical Methods

- Lecture webpage:
  - http://www.sam.math.ethz.ch/~karoger/numci/2024/index.html
  - Lecture Notes (handwritten)
  - Script (work in progress…)
  - Slides
  - Some MATLAB codes
- Exercises webpage:
  - https://shihlab.ethz.ch/education/Snm.html

Part one: Numerical Methods

- Outline
  1. Interpolation and Numerical Calculus
  2. Non-linear Equations
  3. Ordinary Differential Equations
  4. Partial Differential Equations
  5. Linear and Non-linear Least Squares

- This is a lot...

Part one: Numerical Methods

- What are Numerical Methods?

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  - They are methods to give **approximate solutions** to hard problems (difficult or even impossible)
- Why can’t I just use a Numerical Method?

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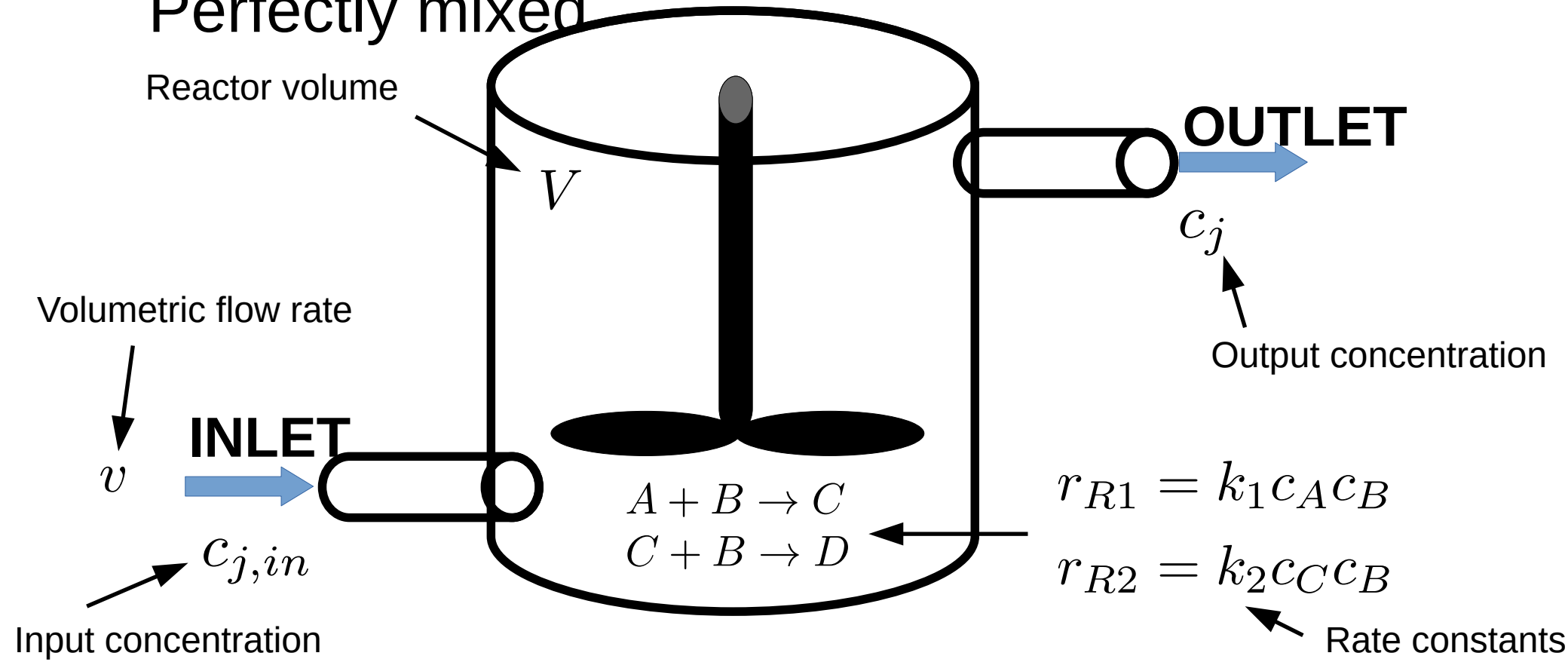
- What are Numerical Methods?
  - They are methods to give **approximate solutions** to hard problems (difficult or even impossible)
- Why can’t I just use a Numerical Method?
  - Like with any other equipment (e.g. lab apparatus) one needs to have **a basic understanding** to judge the results

Example 1: CSTR

Continuously Stirred-Tank Reactor

- CSTR operated isothermally, with negligible volume change, in inflow mode with constant fluid volume, and with two elementary reactions
  Perfectly mixed



Example 1: CSTR

Continuously Stirred-Tank Reactor

- Concentration of each species governed by set of mass balances

$$\frac{d}{dt}(Vc_A) = v(c_{A,in} - c_A) + V(-k_1 c_A c_B)$$

$$\frac{d}{dt}(Vc_B) = v(c_{B,in} - c_B) + V(-k_1 c_A c_B - k_2 c_C c_B)$$

$$\frac{d}{dt}(Vc_C) = v(c_{C,in} - c_C) + V(+k_1 c_A c_B - k_2 c_C c_B)$$

$$\frac{d}{dt}(Vc_D) = \underbrace{v(c_{D,in} - c_D)}_{\text{Inflow}} + \underbrace{V(+k_2 c_C c_B)}_{\text{Reactions}}$$

Example 1: CSTR

Continuously Stirred-Tank Reactor

- Concentration of each species governed by set of mass balances

$$\frac{d}{dt}\left(Vc_A\right) = v\left(c_{A,in} - c_A\right) \quad + V\left(-k_1 c_A c_B\right)$$

$$\frac{d}{dt}\left(Vc_B\right) = v\left(c_{B,in} - c_B\right) \quad + V\left(-k_1 c_A c_B - k_2 c_C c_B\right)$$

$$\frac{d}{dt}\left(Vc_C\right) = v\left(c_{C,in} - c_C\right) \quad + V\left(+k_1 c_A c_B - k_2 c_C c_B\right)$$

$$\frac{d}{dt}\left(Vc_D\right) = v\left(c_{D,in} - c_D\right) \quad + V\left(+k_2 c_C c_B\right)$$

Set of coupled nonlinear Ordinary Differential Equations

Solve Numerically!!! → **Chap. 3**

Example 1: CSTR

Continuously Stirred-Tank Reactor

- Concentration of each species governed by set of mass balances

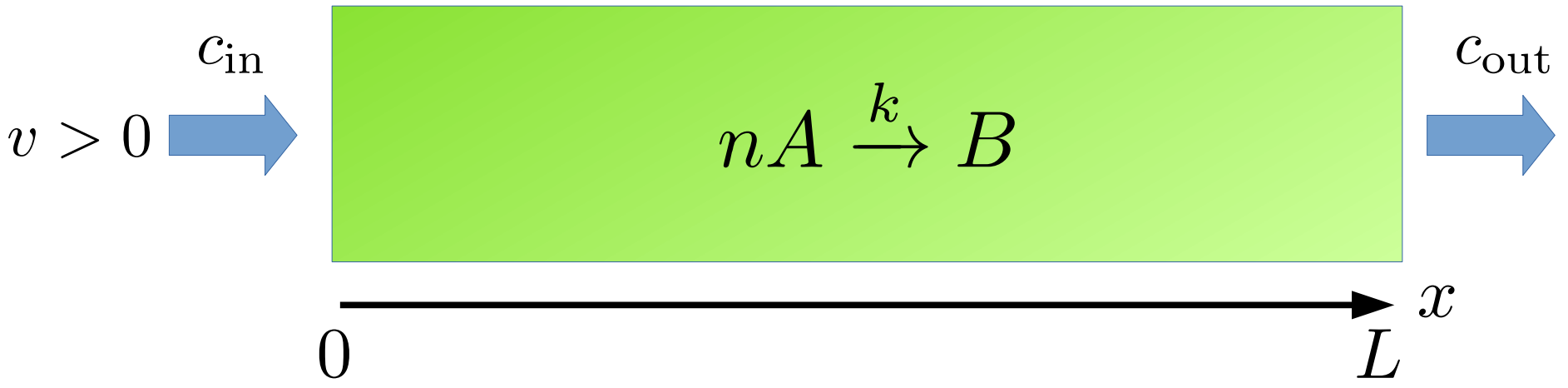
Steady state $\frac{d}{dt}(Vc_j) \rightarrow 0$

$$
\begin{aligned}
0 &= v\left(c_{A,in} - c_A\right) && + V\left(-k_1 c_A c_B\right) \\
0 &= v\left(c_{B,in} - c_B\right) && + V\left(-k_1 c_A c_B - k_2 c_C c_B\right) \\
0 &= v\left(c_{C,in} - c_C\right) && + V\left(+k_1 c_A c_B - k_2 c_C c_B\right) \\
0 &= v\left(c_{D,in} - c_D\right) && + V\left(+k_2 c_C c_B\right)
\end{aligned}
$$

Set of coupled nonlinear Equations

Solve Numerically!!! → **Chap. 2**

Example 2: Tubular Reactor



Mass balance: $$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - kc^n$$

Diffusion

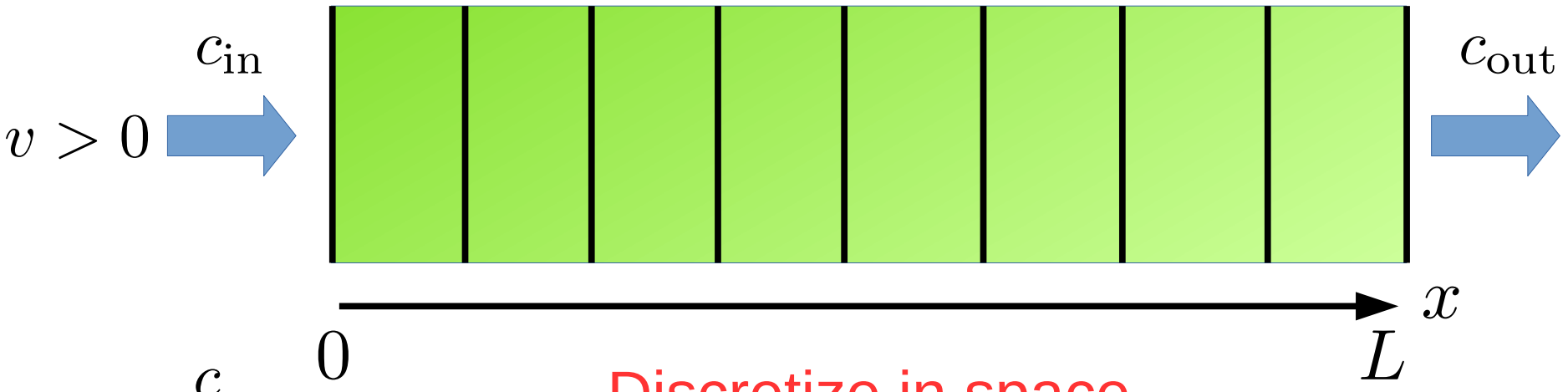
Advection/Convection

Reaction

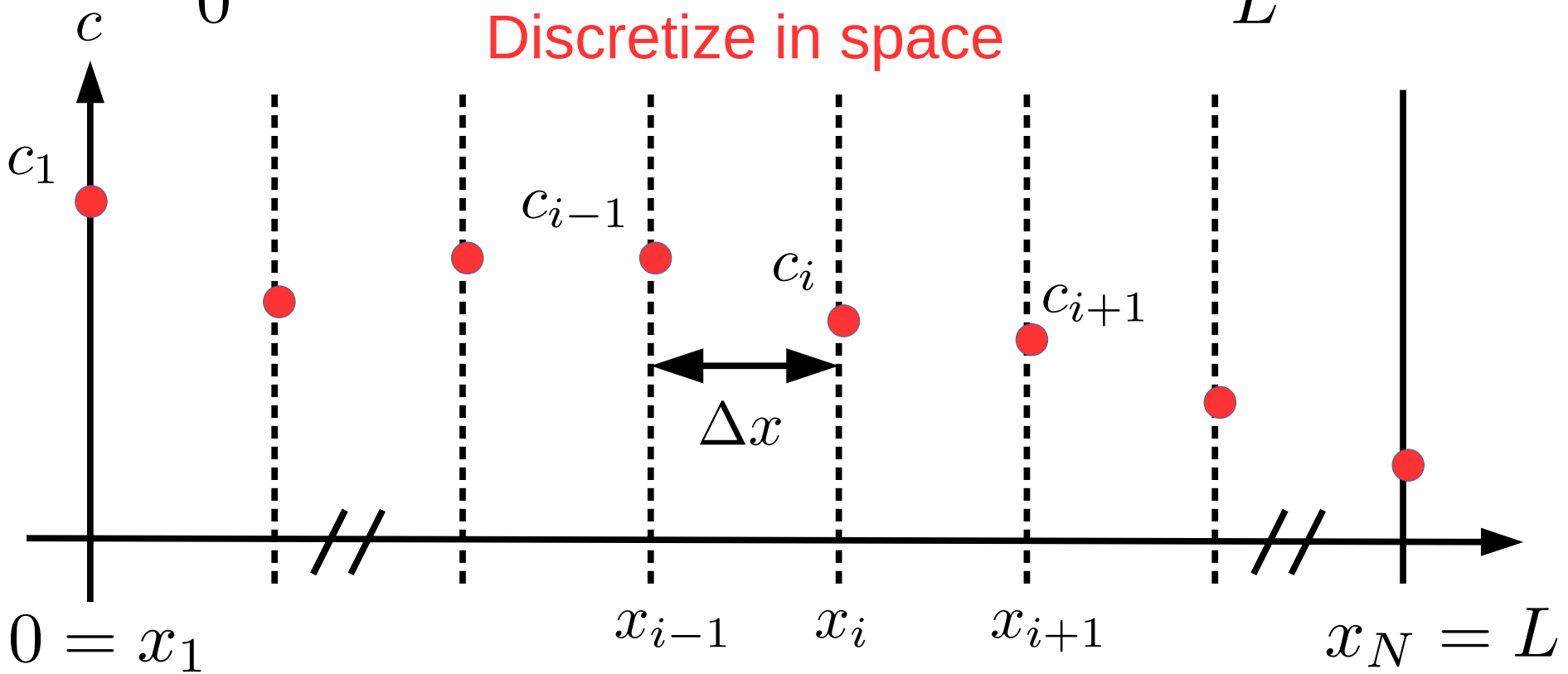
Boundary conditions: $$c(t,0) - \frac{D}{v}\frac{\partial c}{\partial x}(0) = c_{\text{in}} \qquad \frac{\partial c}{\partial x}(t,L) = 0$$

Solve Numerically!!! → **Chap. 4**

Example 2: Tubular Reactor



Discretize in space



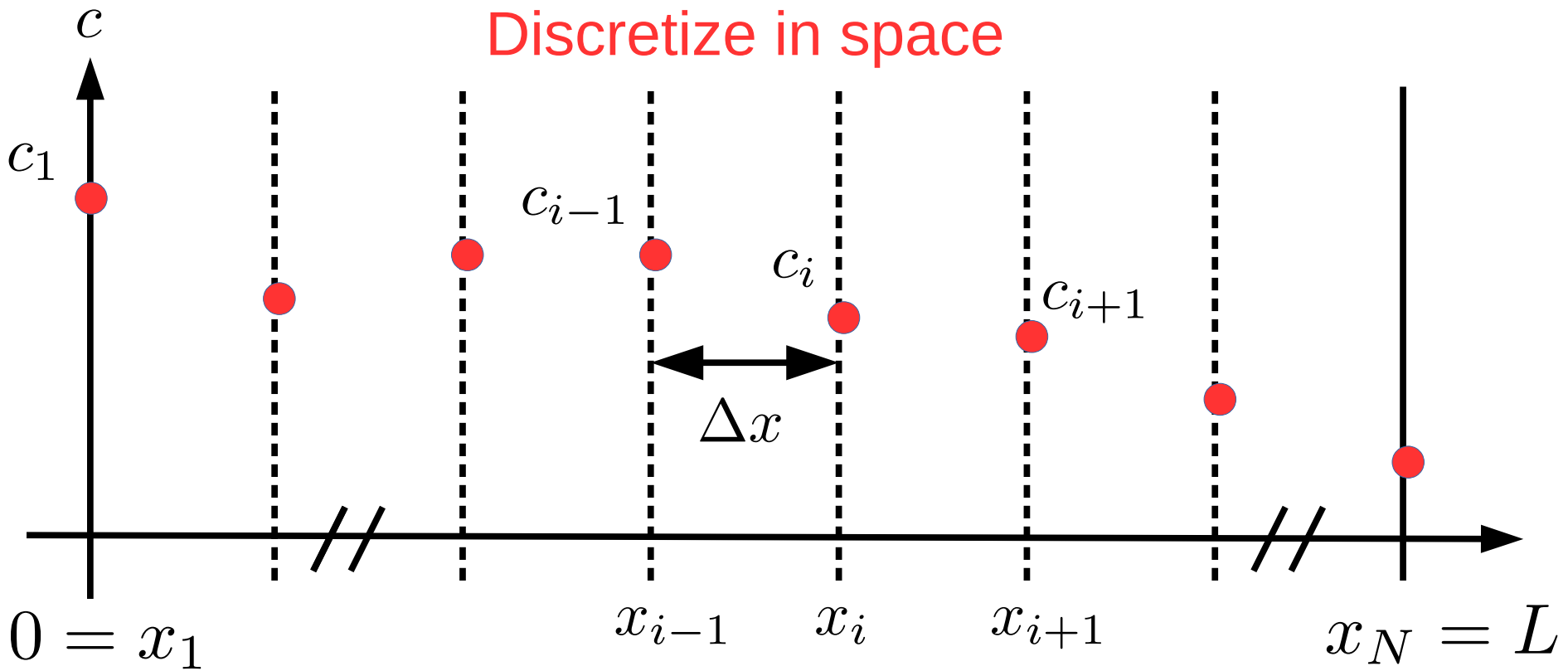
Example 2: Tubular Reactor

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - kc^n$$

Chap. 1,2,3,4

ODEs $$\frac{\mathrm{d}c_i}{\mathrm{d}t} = D\frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta x^2} - v\frac{c_i - c_{i-1}}{\Delta x} - kc_i^n$$

Discretize in space



Part one: Numerical Methods

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… “Preparation” for Statistical part

- This is a lot…

  Only an overview…

  Starter kit!

https://commons.wikimedia.org

Literature

- Not really needed to follow the course…

- But see, e.g.,
  - Press et al., “Numerical Recipes”
  - Ascher & Greif, “A First Course in Numerical Methods”
  - Beers, “Numerical Methods for Chemical Engineering”
  - ...