Statistical and Numerical Methods for Chemical Engineers

(401-0675-00L)

Lecture for D-CHAB Autumn Semester 2023

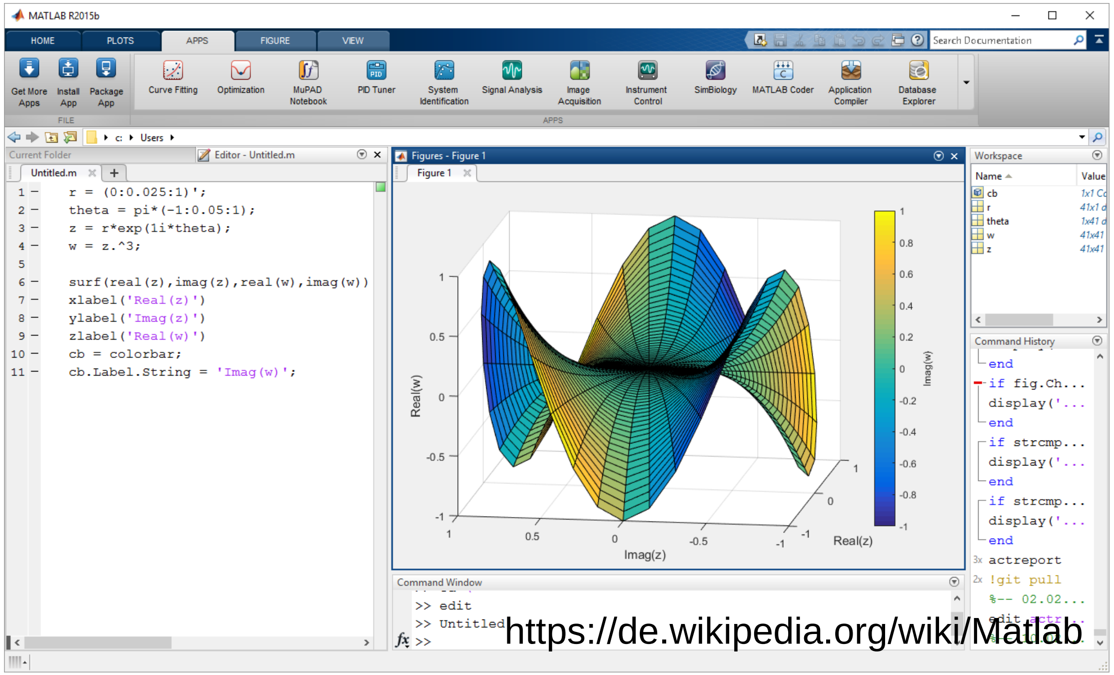
Dr. Roger Käppeli
Dr. Patric Müller

Statistical and Numerical Methods for Chemical Engineers

- Part one: Numerical methods (Käppeli)
  Lecture: Wednesday, 08:15-10:00, HG E 33.1
  20.09.; 27.09.; 04.10.; 11.10.; 18.10.;
  ~~25.10.~~; 01.11; 08.11.; 15.11.
- Part two: Statistical methods (Müller)
  Lecture: Wednesday, 08:15-10:00, HG E 33.1
  22.11.; 29.11.; 06.12.; 13.12.; 20.12.
- Exercises (Jiwoo Oh, Sarah Duclos Ivetich)
  - Tuesday, 07:45-09:30, HCI H 8.1
    From 26.09. until 19.12. ← **Start next week! This week MATLAB introduction on Thursday (email!)**
- Case study week: 23.10.-27.10. ← **No lecture & exercise classes!**

MATLAB introduction

- Instructors: Jiwoo Oh, Sarah Duclos Ivetich
- Thursday, 21.09.23
  - HCI J 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/2023/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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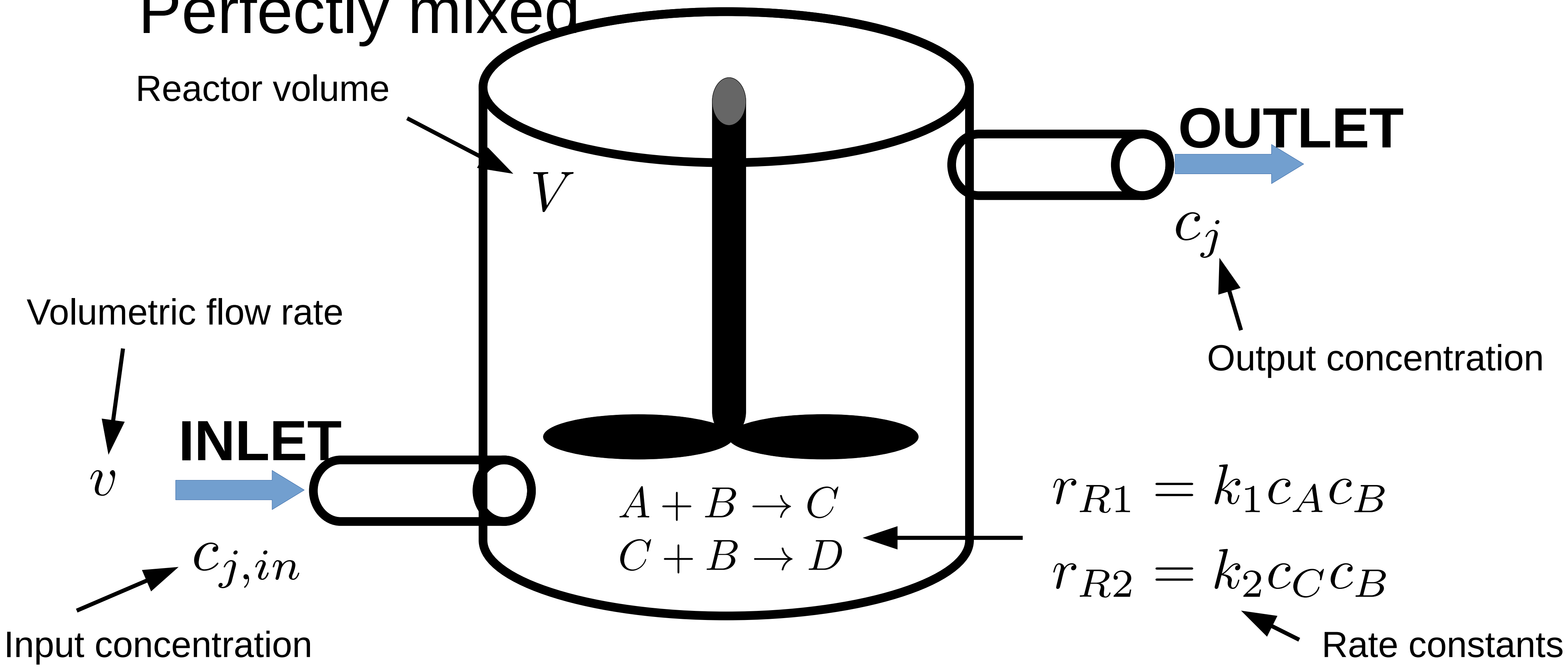
- What are Numerical Methods?
  - They are methods to give **approximate solutions** to hard problems (difficult or even impossible)
- Why can’t I just use a Numerical Method?
  - Like with any other equipment (e.g. lab apparatus) one needs to have **a basic understanding** to judge the results

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

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

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

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

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

Inflow

Reactions

Example 1: CSTR

Continuously Stirred-Tank Reactor

- Concentration of each species governed by set of mass balances

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

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

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

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

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

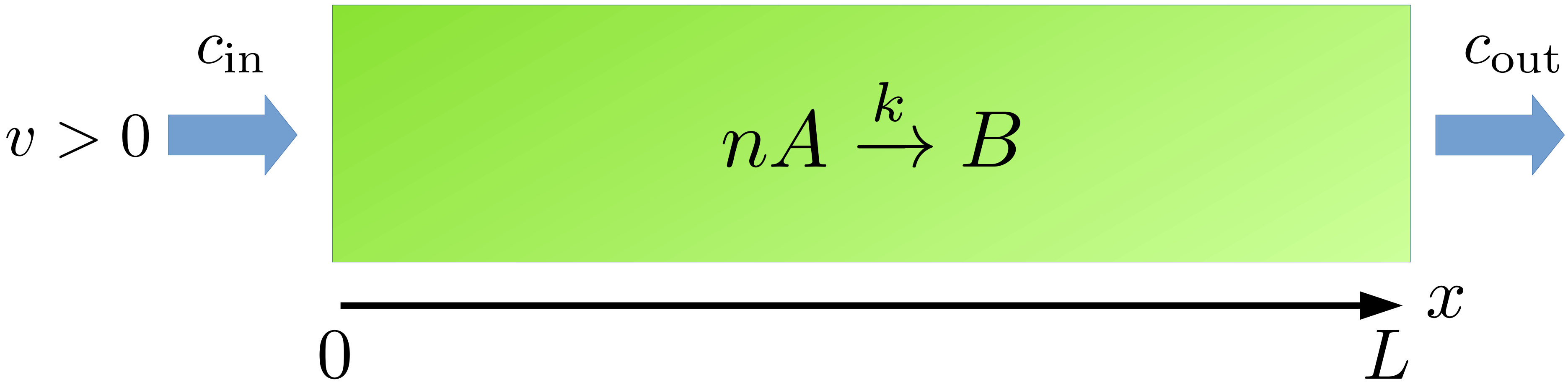
Steady state $\frac{d}{dt}(Vc_j) \rightarrow 0$

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

Set of coupled nonlinear Equations

Solve Numerically!!! → **Chap. 2**

Example 2: Tubular Reactor



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

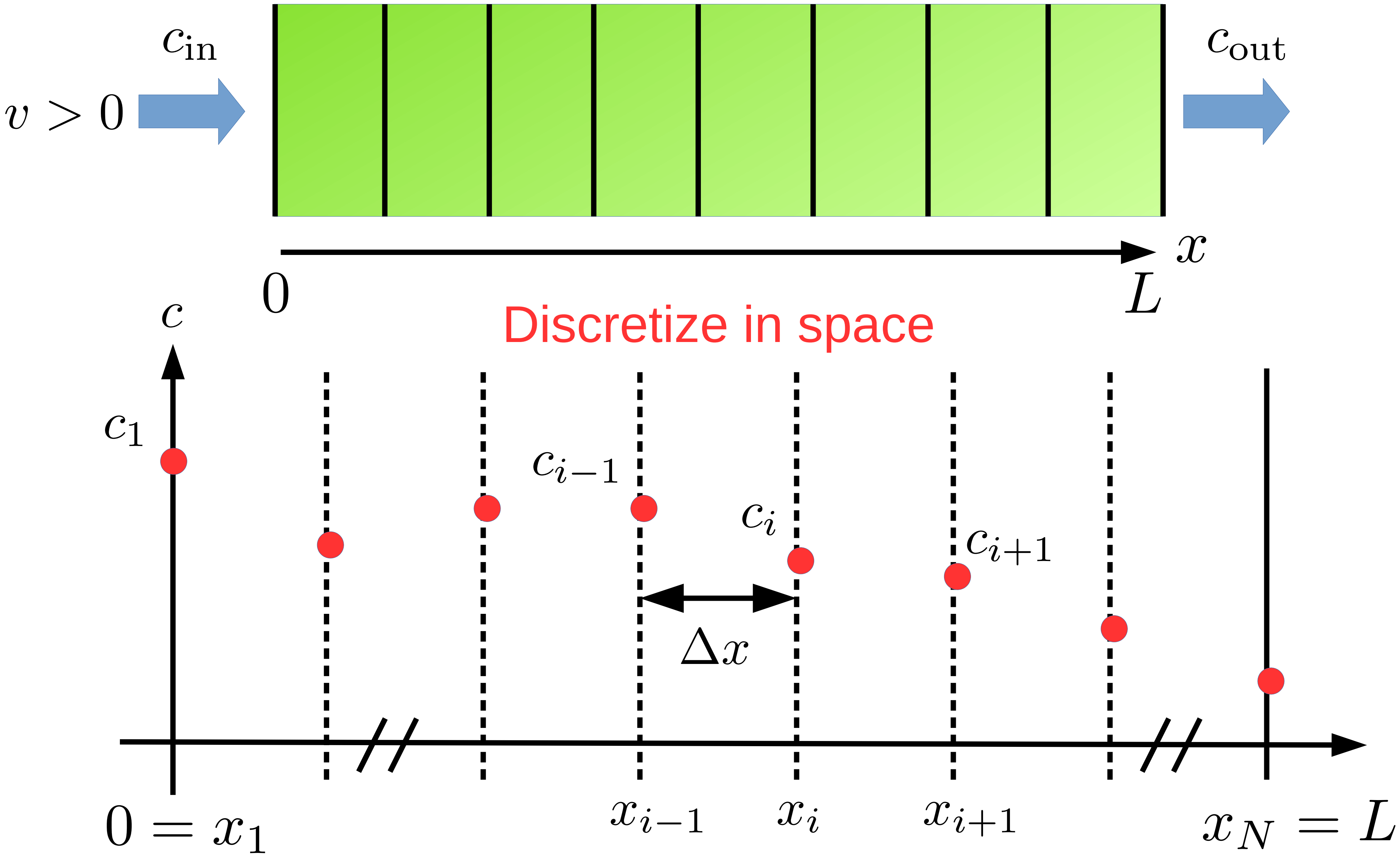
Reaction

Diffusion   Advection/Convection

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



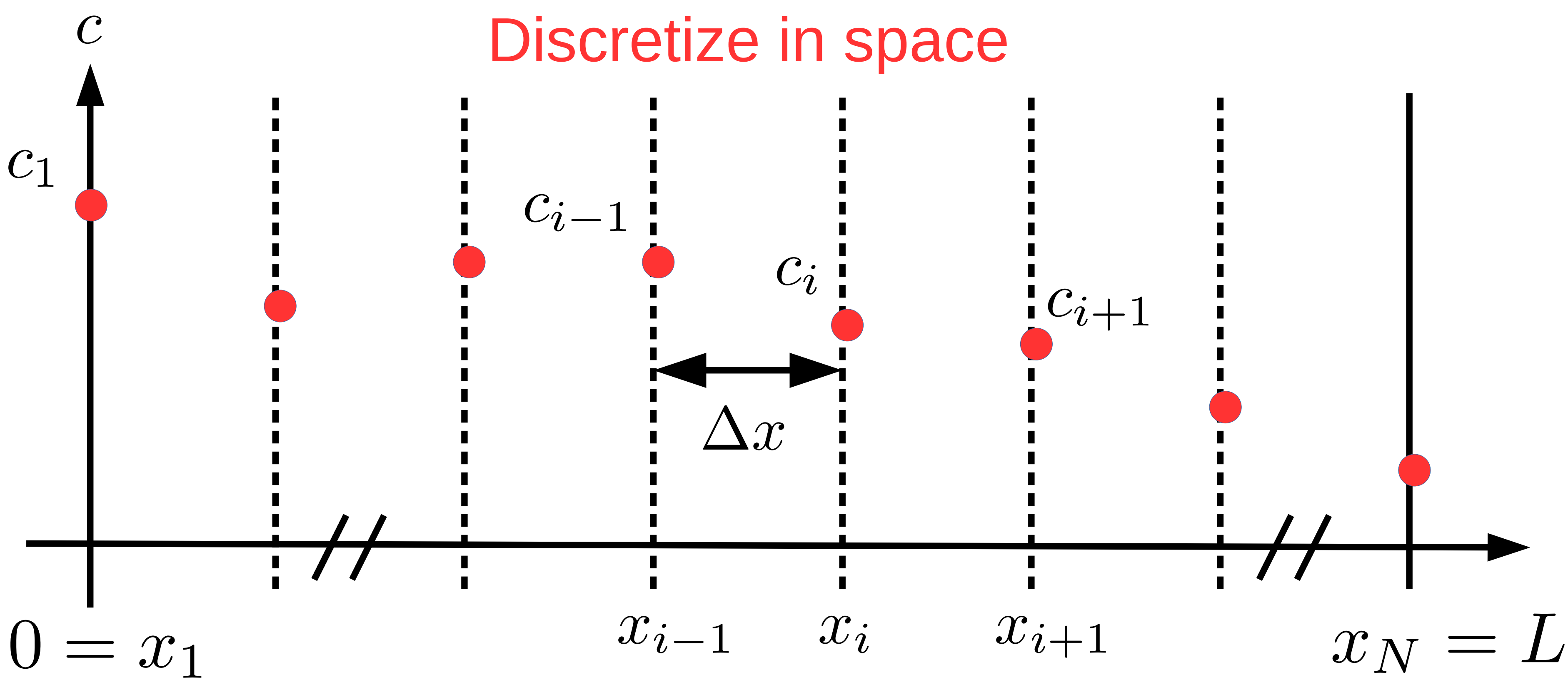
Example 2: Tubular Reactor

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

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



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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”
  - ...