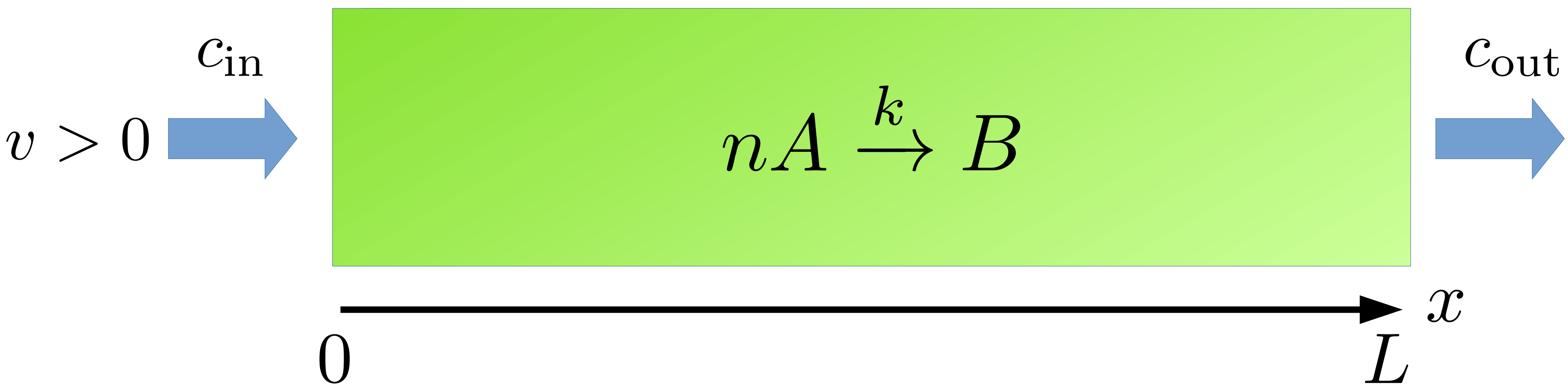
Tubular Reactor



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

Diffusion

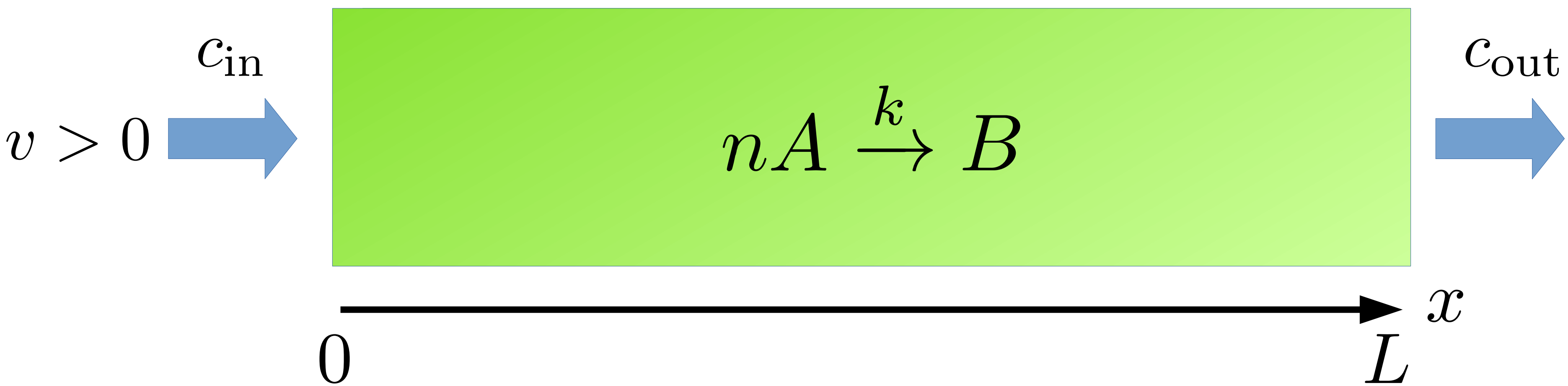
Advection/Convection

Reaction

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

(Danckwerts)

Tubular Reactor



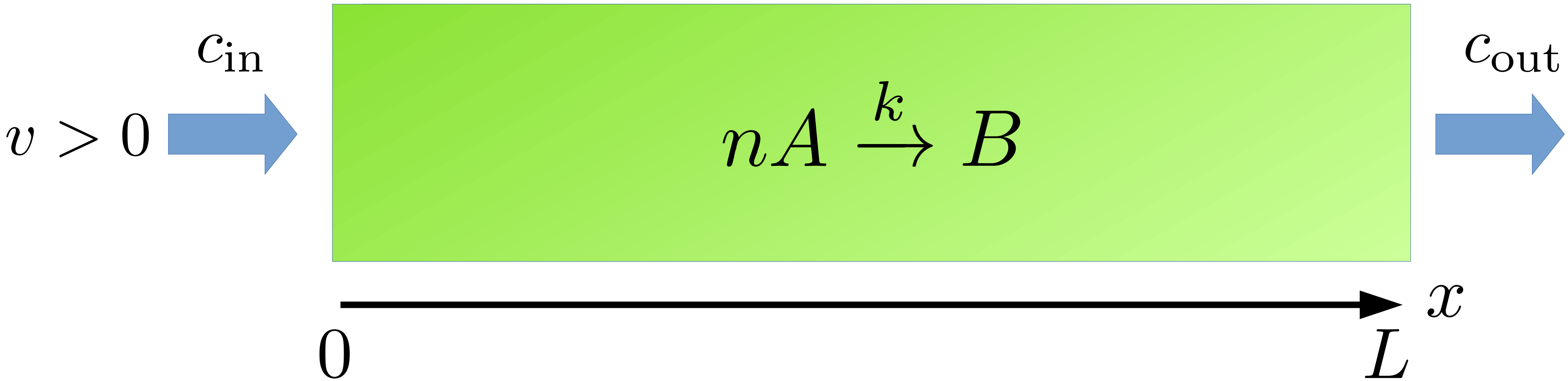
Mass balance: $$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - kc^n$$

Non-dimensionalization: $$\theta = \frac{t}{\bar{t}} = \frac{tv}{L}$$

$$z = \frac{x}{L}$$

$$u = \frac{c}{c_{\text{in}}}$$

Tubular Reactor



Mass balance: $$\frac{\partial u}{\partial \theta} = \frac{1}{Pe}\frac{\partial^2 u}{\partial z^2} - \frac{\partial u}{\partial z} - Da \cdot u^n$$

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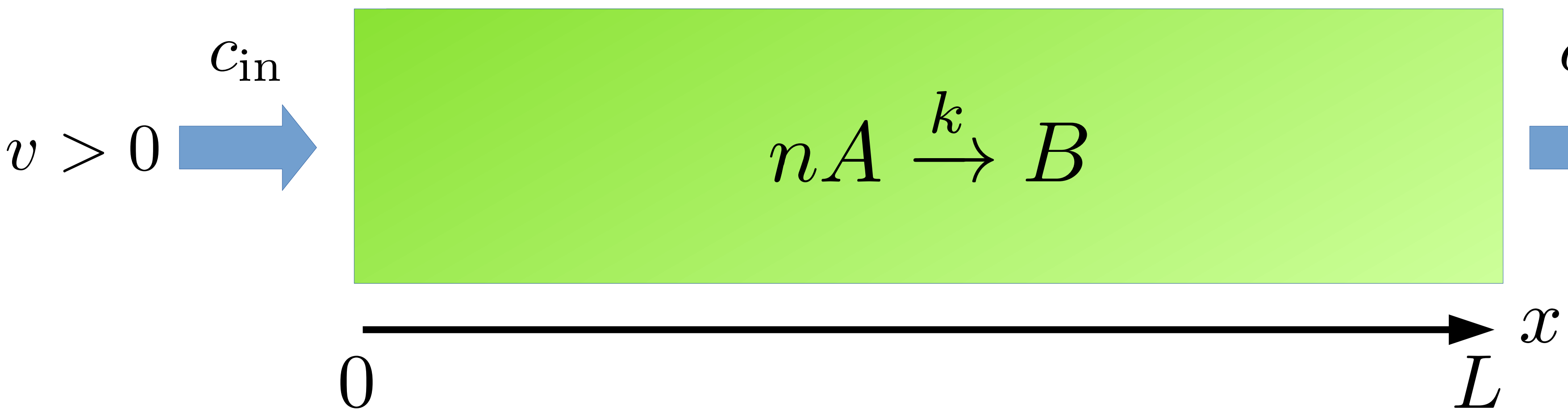
Tubular Reactor

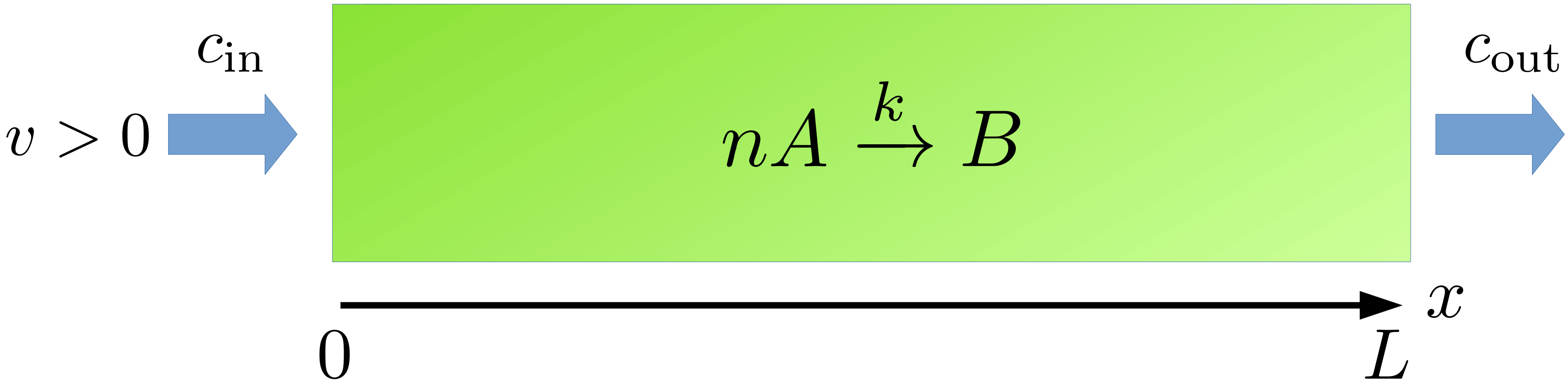


Mass balance: $$\frac{\partial u}{\partial \theta} = \frac{1}{Pe}\frac{\partial^2 u}{\partial z^2} - \frac{\partial u}{\partial z} - Da \cdot u^n$$

Peclet number: $$Pe = \frac{L^2/D}{L/v} = \frac{\tau_{Diffusion}}{\tau_{Hydrodynamics}}$$

Damköhler number: $$Da = \frac{L/v}{1/(kc_0^{n-1})} = \frac{\tau_{Hydrodynamics}}{\tau_{Reaction}}$$

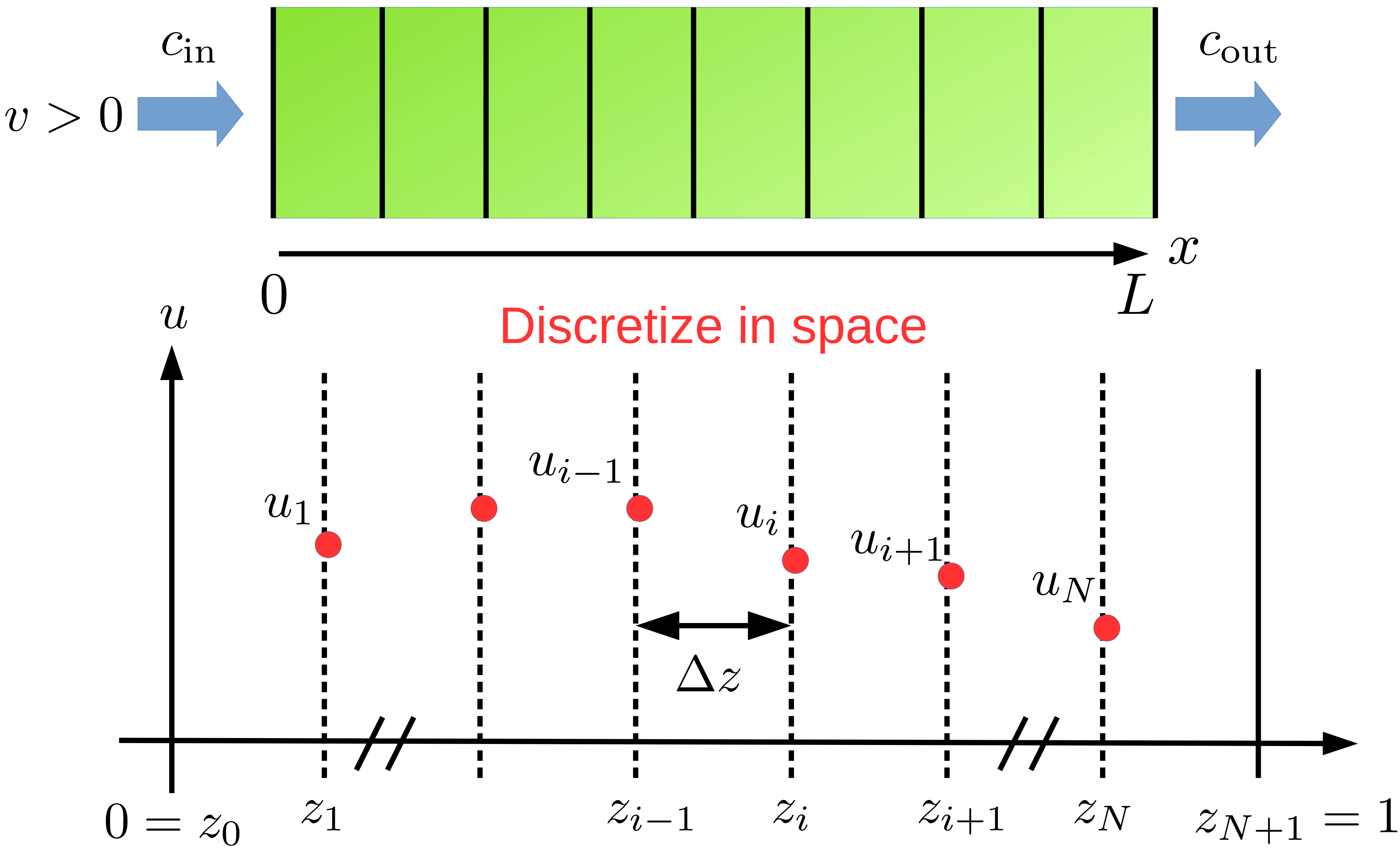
Tubular Reactor



Mass balance: $$\frac{\partial u}{\partial \theta} = \frac{1}{Pe}\frac{\partial^2 u}{\partial z^2} - \frac{\partial u}{\partial z} - Da \cdot u^n = 0$$

Steady state tubular reactor

Tubular Reactor

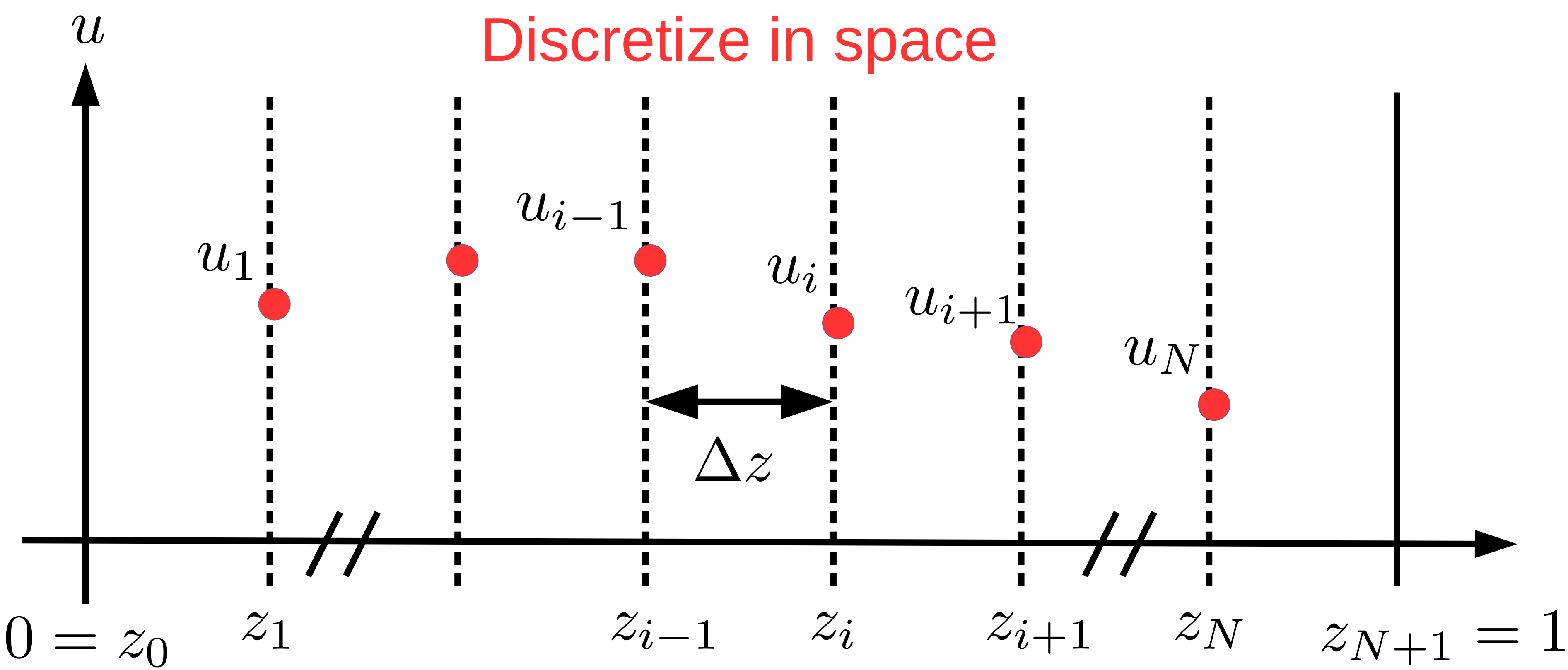


Tubular Reactor

$$\frac{1}{Pe}\frac{\partial^2 u}{\partial z^2} - \frac{\partial u}{\partial z} - Da \cdot u^n = 0$$

$$\frac{1}{Pe}\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta z^2} - \frac{u_i - u_{i-1}}{\Delta z} - Da \cdot u_i^n = 0$$

Discretize in space



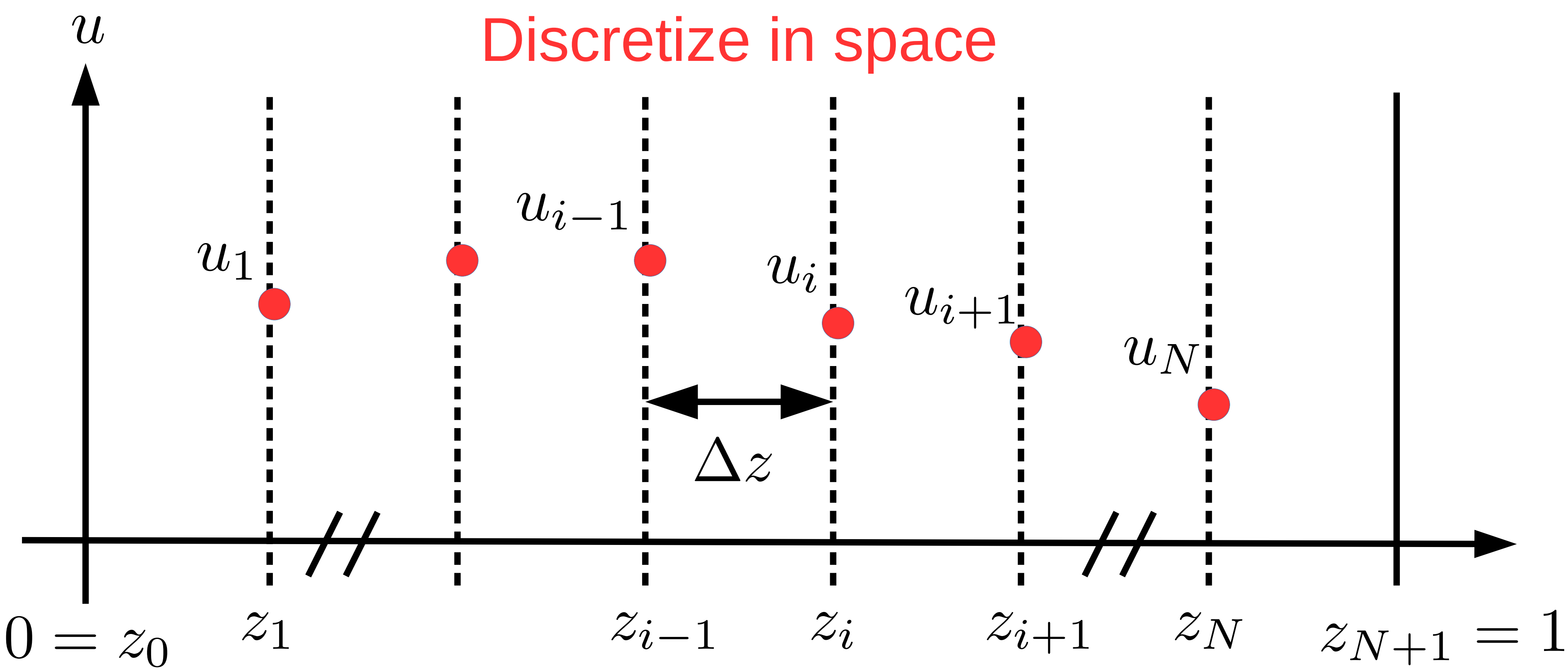
Tubular Reactor

Centered Finite Difference

Backward Finite Difference

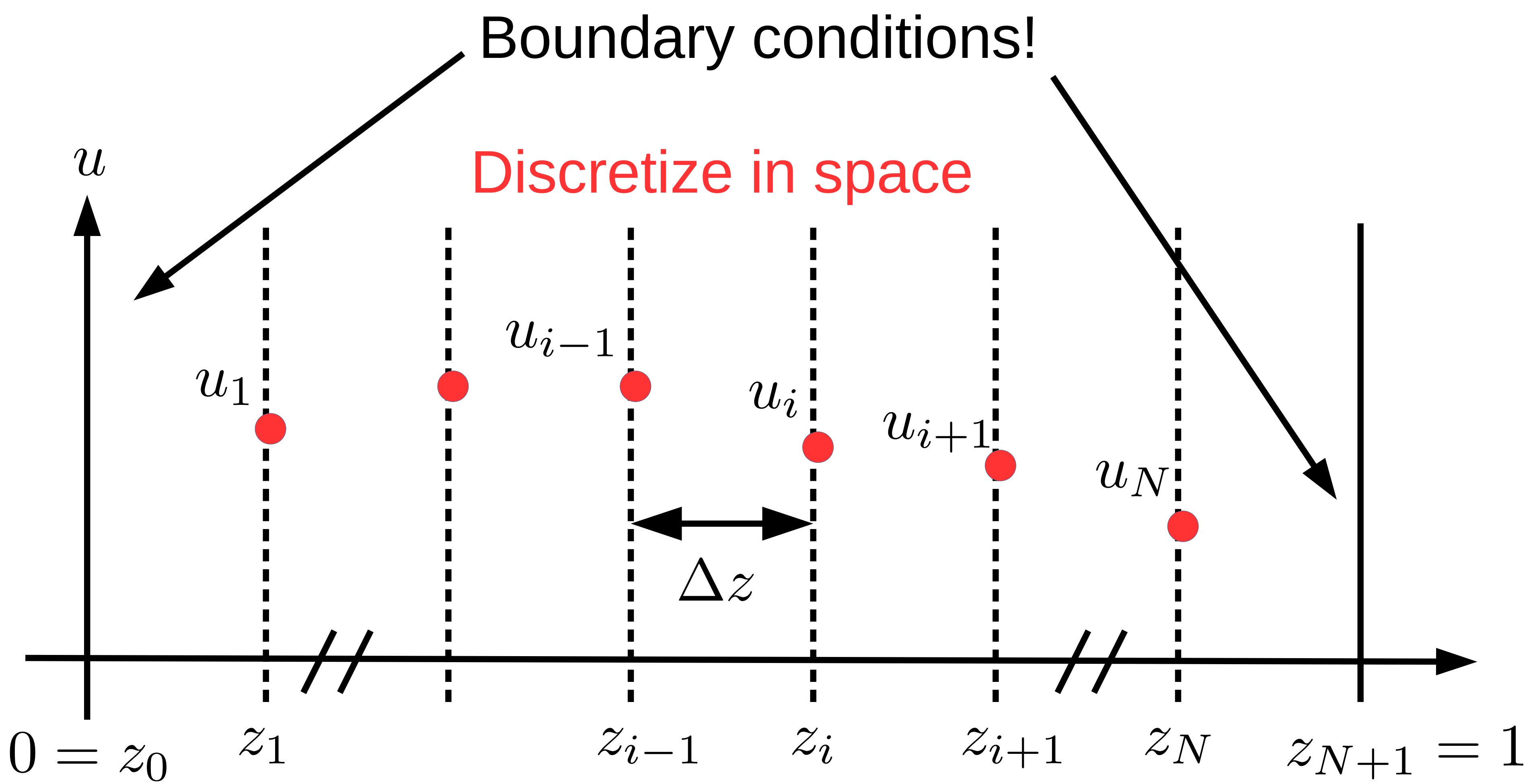
$$\frac{1}{Pe}\frac{u_{i+1}-2u_i+u_{i-1}}{\Delta z^2}-\frac{u_i-u_{i-1}}{\Delta z}-Da\cdot u_i^n=0$$

Discretize in space



Tubular Reactor

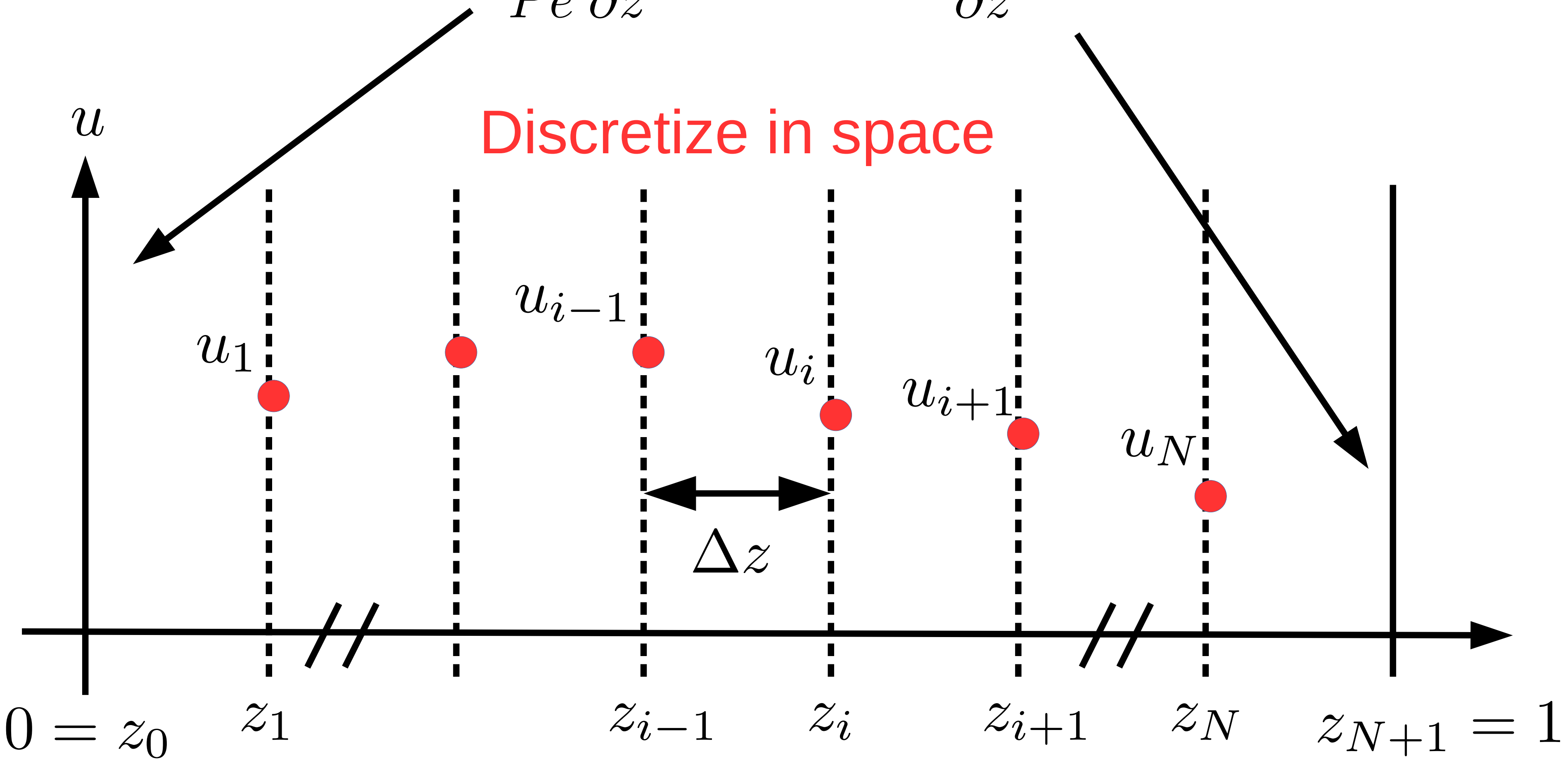
$$\frac{1}{Pe}\frac{u_{i+1}-2u_i+u_{i-1}}{\Delta z^2}-\frac{u_i-u_{i-1}}{\Delta z}-Da\cdot u_i^n=0$$



Tubular Reactor

$$\frac{1}{Pe}\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta z^2} - \frac{u_i - u_{i-1}}{\Delta z} - Da \cdot u_i^n = 0$$

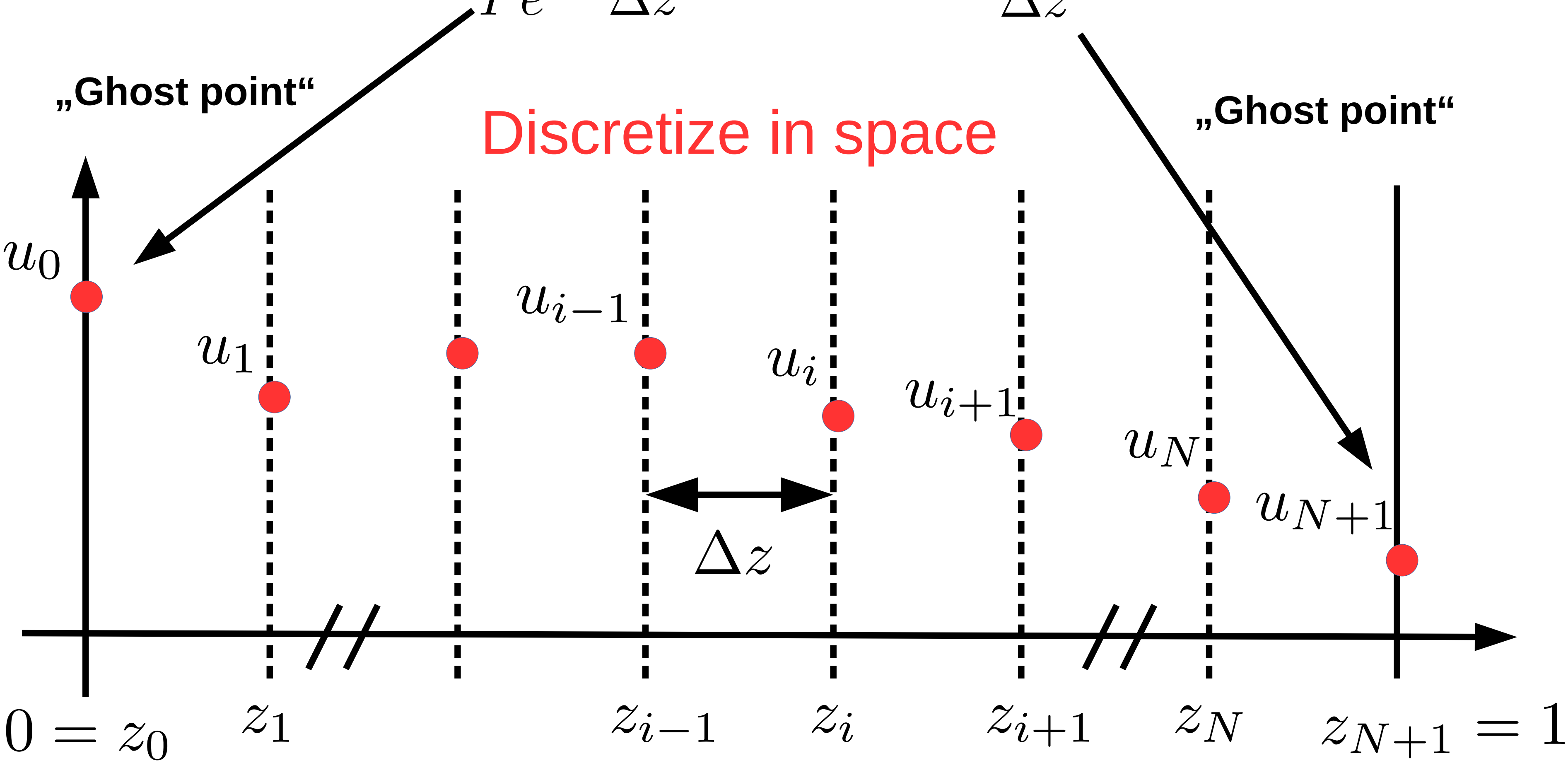
$$u(0) - \frac{1}{Pe}\frac{\partial u}{\partial z}(0) = 1 \qquad \frac{\partial u}{\partial z}(1) = 0$$



Tubular Reactor

$$\frac{1}{Pe}\frac{u_{i+1}-2u_i+u_{i-1}}{\Delta z^2}-\frac{u_i-u_{i-1}}{\Delta z}-Da\cdot u_i^n=0$$

$$u_0-\frac{1}{Pe}\frac{u_1-u_0}{\Delta z}=1 \qquad \frac{u_{N+1}-u_N}{\Delta z}=0$$



Tubular Reactor

$$\frac{1}{Pe}\frac{u_{i+1}-2u_i+u_{i-1}}{\Delta z^2}-\frac{u_i-u_{i-1}}{\Delta z}-Da\cdot u_i^n=0$$

$$u_0-\frac{1}{Pe}\frac{u_1-u_0}{\Delta z}=1 \longrightarrow u_0=\frac{1}{1+\frac{1}{Pe\Delta z}}\left(\frac{1}{Pe\Delta z}u_1+1\right)$$

$$\frac{u_{N+1}-u_N}{\Delta z}=0 \longrightarrow u_{N+1}=u_N$$

$$i=1,2,...,N$$

System of nonlinear equations!!!

Assignment 1

1. Solve the steady state tubular reactor for 20 different Peclet numbers (between 0.01 and 100) and for a first (n=1) and a second (n=2) order reaction. Use a Damköhler number of unity.
   Complete the template `rhs.m` by implementing the non-linear equations to solve.
2. Plot the conversion at the end of the reactor $1 - \frac{c_{\text{out}}}{c_{\text{in}}}$ vs. the Peclet number for both reaction orders.
   Also plot the ratio between the conversions of the first order and second order reaction
   - What is better for these reactions, a lot of back-mixing (Pe small, CSTR) or ideal plug flow (Pe large, PFR)?
   - What influence does the reaction order have overall and at low or high Peclet numbers?

Complete the template `TubReact_steady_state.m`

Assignment 1

rhs.m

```
function f = rhs(u,Pe,Da,n);

% function f = rhs(u);
%
% Purpose: compute the right-hand function of the spatially discretized
%          (non-dimensionalized) advection-diffusion-reaction equation for a
%          tubular reactor
%
%            du/dtheta = - du/dz + 1/Pe d^2u/dz^2 - Da u^n
%
%          using backward finite differences for the advection term and central
%          finite differences for the diffusion term
%
% Input: u  ... concentration
%        Pe ... Peclet number
%        Da ... Damkoehler number
%        n  ... order of reaction
%
% Output: f ... right-hand side function, i.e. du/dtheta
%
% Notes: None.
%

  % get number of grid points
  N = length(u);

  % compute grid spacing \Delta z (since non-dimensionalized 1/(N+1))
  dz = 1./(N + 1);

  % compute boundary values u_{0} and u_{N+1}
  Pedz = Pe*dz;
  u0   = 0.; % ... COMPLETE HERE ...
  uNp1 = 0.; % ... COMPLETE HERE ...

  % set up u array with boundary values, i.e. "ghost points"
  % uGH = [u_{0},u_{1},u_{2}, ... ,u_{N-1},u_{N},u_{N+1}]
  uGH = [u0; u; uNp1];

  % compute right-hand side function f
  f = zeros(size(uGH)); % ... COMPLETE HERE ...
```

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Assignment 1

rhs.m

```
function f = rhs(u,Pe,Da,n);
% ...
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  % uGH = [u_{0},u_{1},u_{2}, ... ,u_{N-1},u_{N},u_{N+1}]
  uGH = [u0; u; uNp1];

  % compute right-hand side function f
  f = zeros(size(uGH)); % ... COMPLETE HERE ...
```
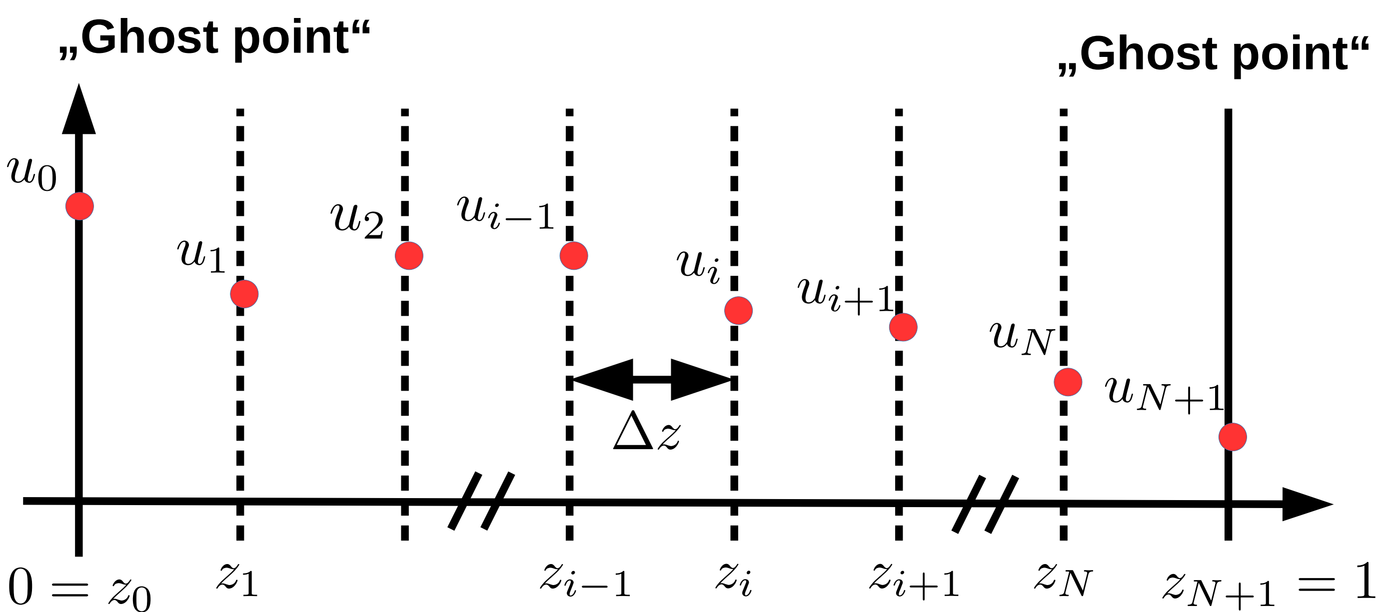

$$f_i = \frac{1}{Pe}\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta z^2} - \frac{u_i - u_{i-1}}{\Delta z} - Da \cdot u_i^n = 0$$



Assignment 1

rhs.m

```
function f = rhs(u,Pe,Da,n);
% ...
  % get number of grid points
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  % compute right-hand side function f
  f = zeros(size(uGH)); % ... COMPLETE HERE ...
```
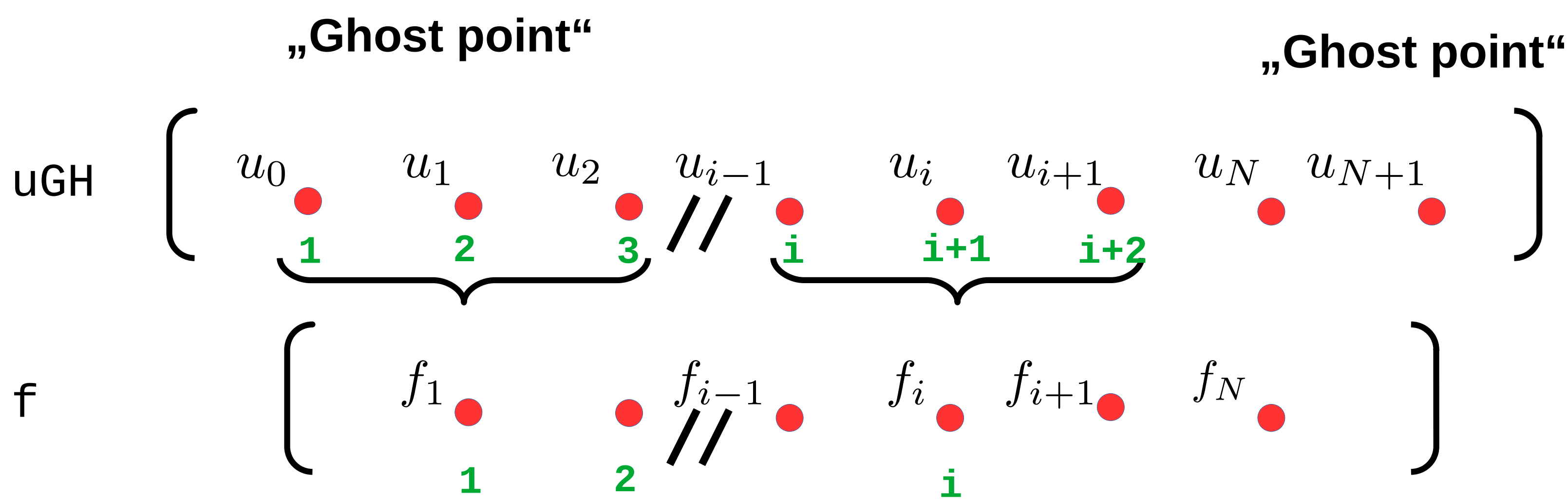

$$f_i = \frac{1}{Pe}\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta z^2} - \frac{u_i - u_{i-1}}{\Delta z} - Da \cdot u_i^n = 0$$



Array indexing (Matlab one-based indexing)

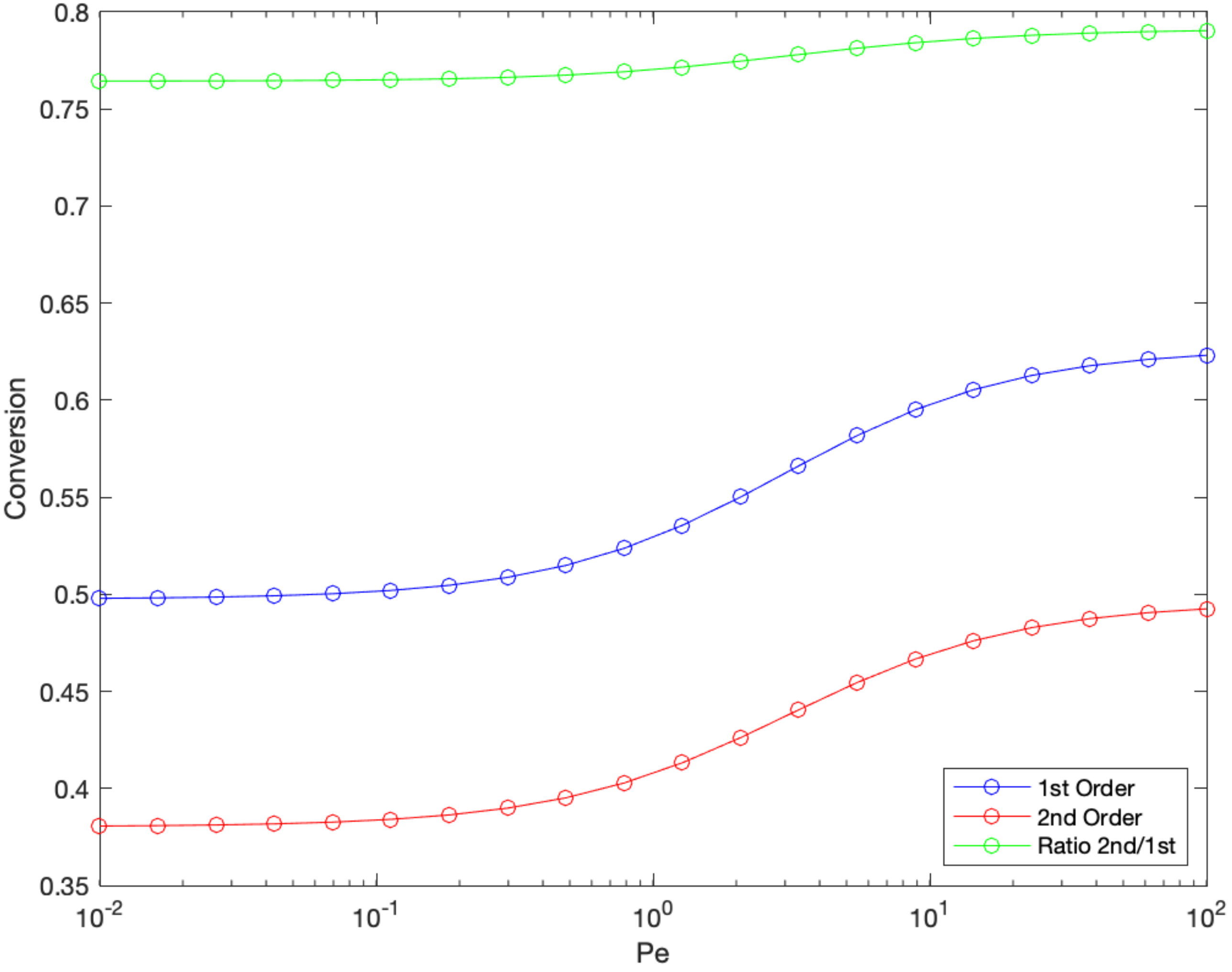
Assignment 1

TubReact_steady_state.m

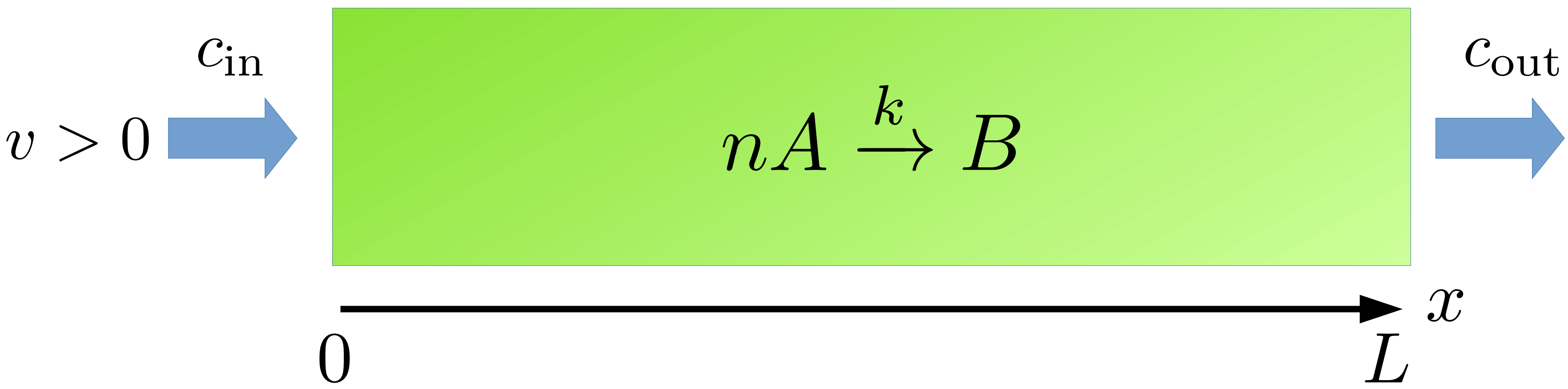
```
% set parameters
N   = 100; % number of grid points
NPe =  20; % number of Peclet numbers
Pe = logspace(-2,2,NPe); % generate NPe Peclet numbers log. spaced
                         % between 0.01 and 100
Da = 1.; % Damkoehler number

% Steady State n = 1 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
n  = 1;  % reaction order

% allocate array for concentrations
u = zeros(N,1);

% allocate array for conversion & residuum
Conversion_n1 = zeros(NPe,1);
res_n1 = zeros(NPe,1);

% solve BVP for all desired Peclet numbers
for iPe=1:NPe
  % ... COMPLETE HERE ...
  f = @(u) zeros(length(u),1);
  res_n1(iPe) = norm(f(u),Inf);
end

% ...
```

Define a function handle and use fsolve

Assignment 1



Tubular Reactor

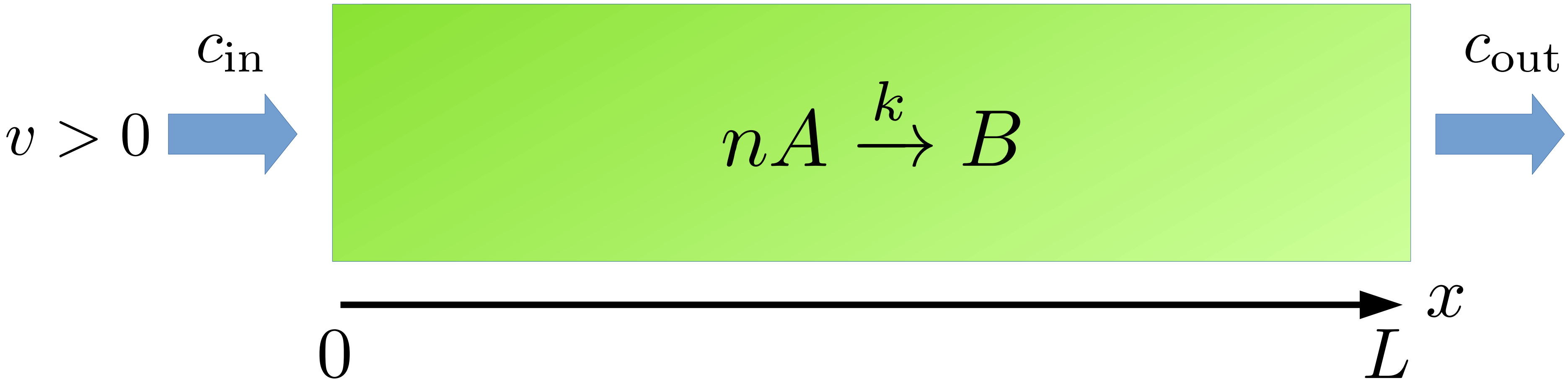


Mass balance: $$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} - v\frac{\partial c}{\partial x} - kc^n$$

Diffusion   Advection/Convection   Reaction

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

Tubular Reactor



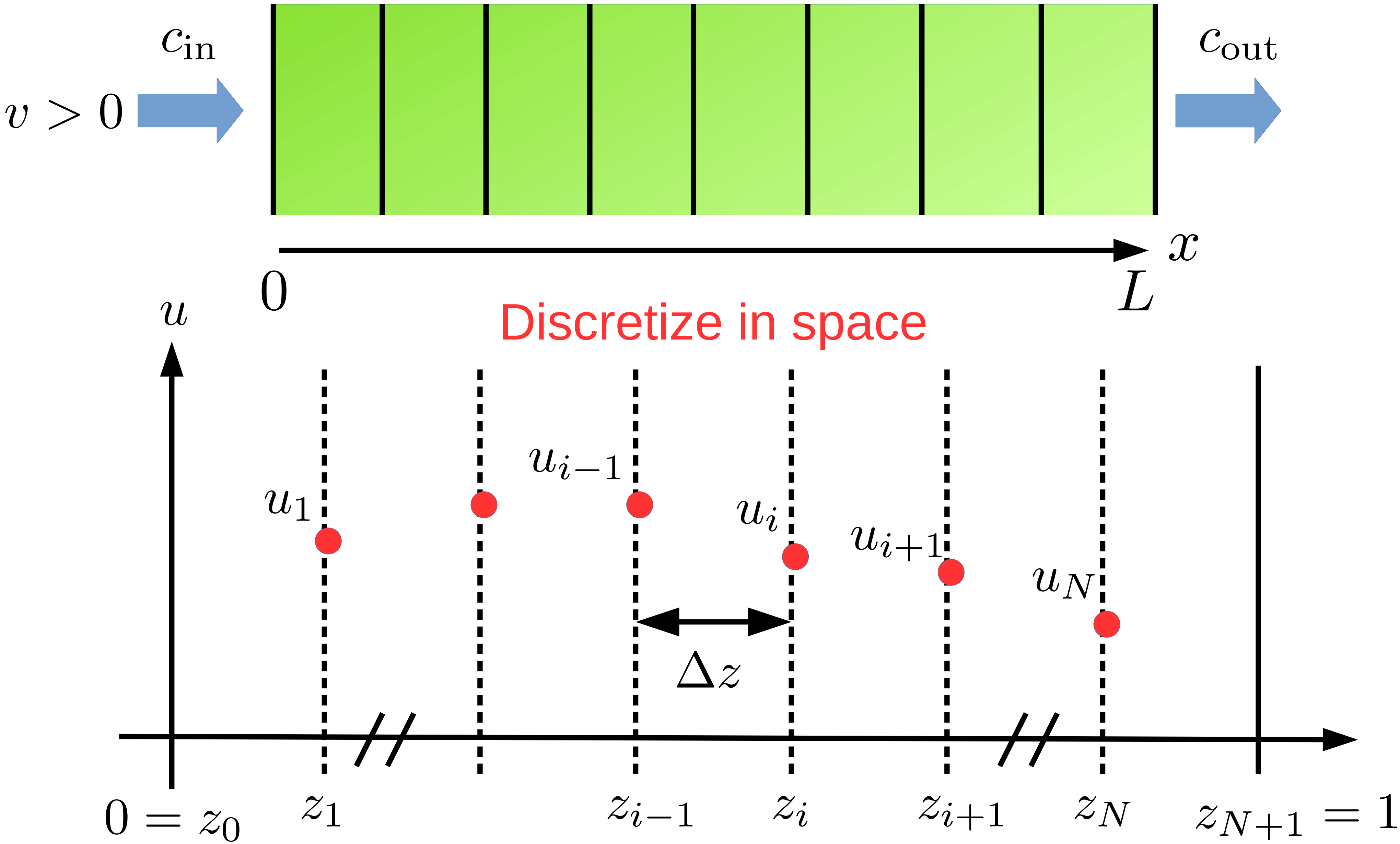
Mass balance: $$\frac{\partial u}{\partial \theta} = \frac{1}{Pe}\frac{\partial^2 u}{\partial z^2} - \frac{\partial u}{\partial z} - Da \cdot u^n$$

Dynamic tubular reactor

Boundary conditions:

$$u(0) - \frac{1}{Pe}\frac{\partial u}{\partial z}(0) = 1 \qquad \frac{\partial u}{\partial z}(1) = 0$$

Tubular Reactor

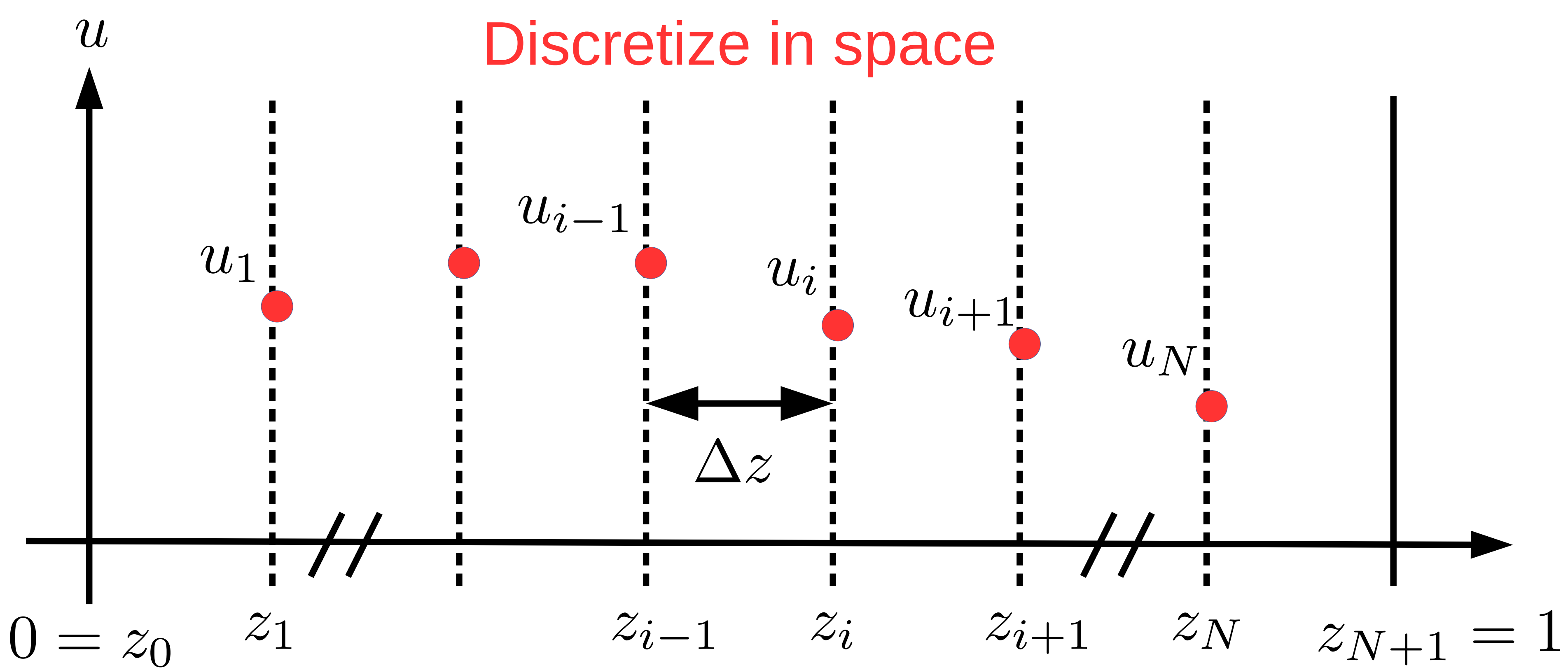


Tubular Reactor

$$\frac{\partial u}{\partial \theta} = \frac{1}{Pe}\frac{\partial^2 u}{\partial z^2} - \frac{\partial u}{\partial z} - Da \cdot u^n$$

ODEs $$\frac{\mathrm{d}u_i}{\mathrm{d}\theta} = \frac{1}{Pe}\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta z^2} - \frac{u_i - u_{i-1}}{\Delta z} - k u_i^n$$

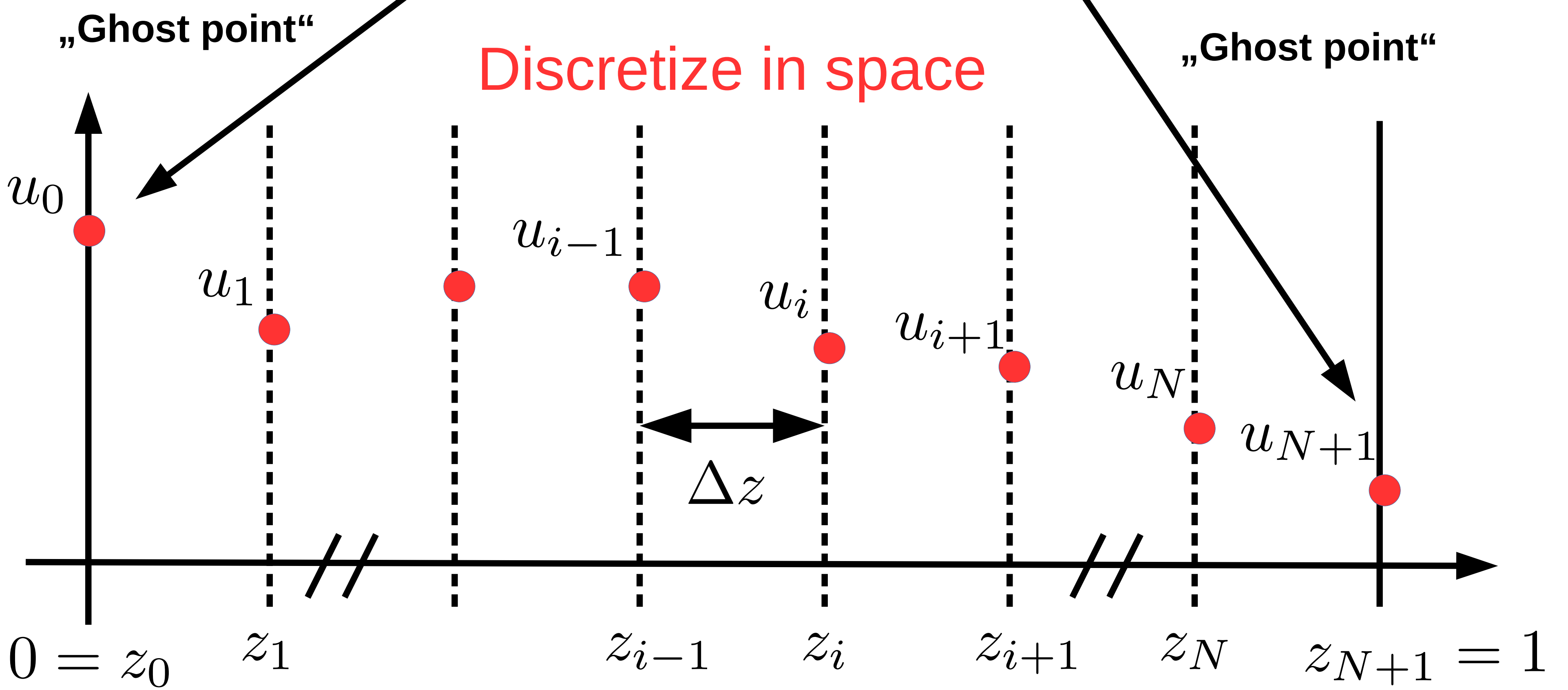
Discretize in space



Tubular Reactor

ODEs $$\frac{\mathrm{d}u_i}{\mathrm{d}\theta} = \frac{1}{Pe}\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta z^2} - \frac{u_i - u_{i-1}}{\Delta z} - k u_i^n$$

$$u_0 - \frac{1}{Pe}\frac{u_1 - u_0}{\Delta z} = 1 \qquad \frac{u_{N+1} - u_N}{\Delta z} = 0$$



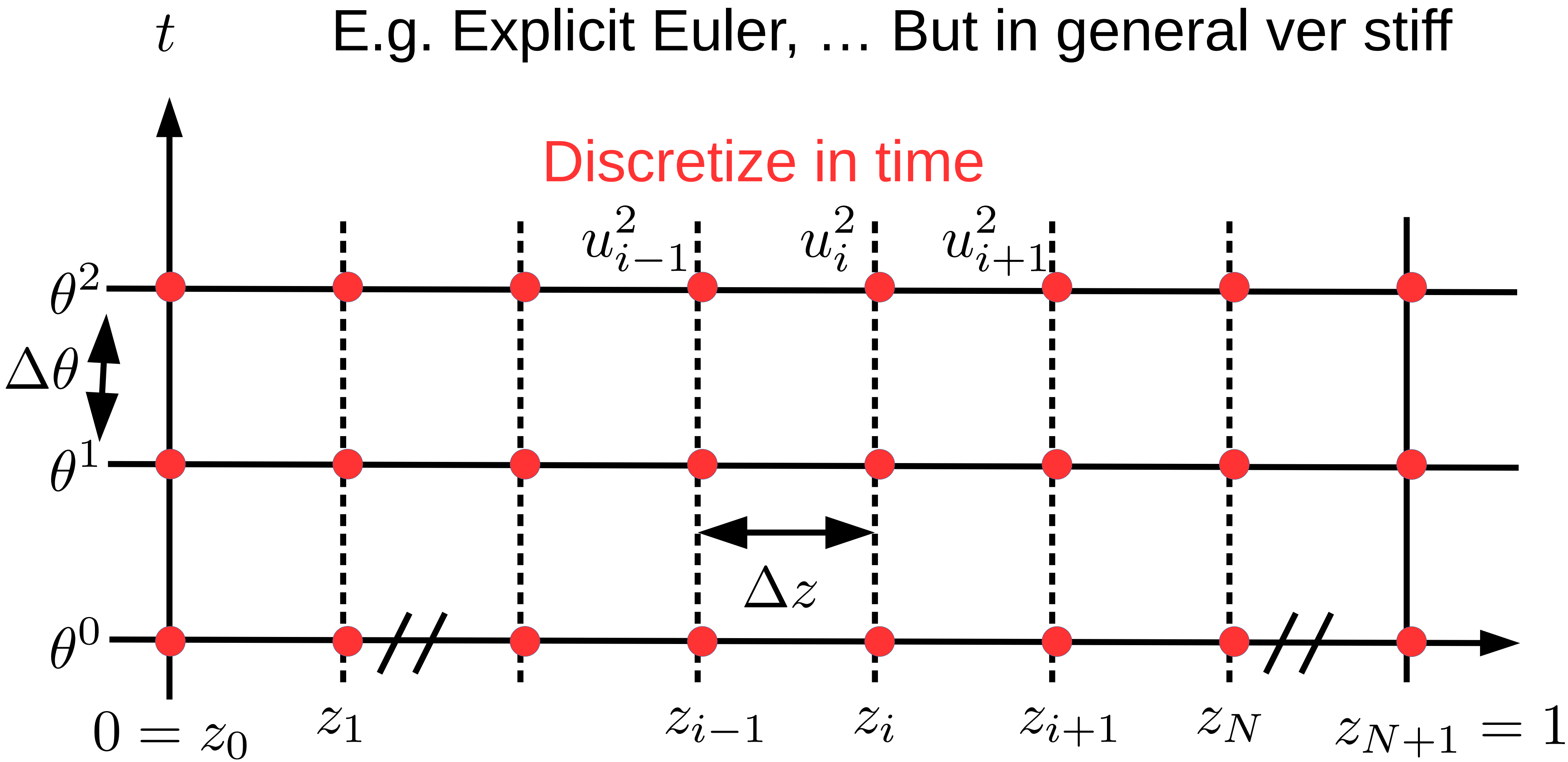
Tubular Reactor

Time index

Order of reaction

$$\frac{u_i^{n+1} - u_i^n}{\Delta\theta} = \frac{1}{Pe}\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta z^2} - \frac{u_i^n - u_{i-1}^n}{\Delta z} - k(u_i^n)^{\tilde{n}}$$

E.g. Explicit Euler, … But in general ver stiff



Tubular Reactor

$$\frac{\mathrm{d}u_i}{\mathrm{d}\theta} = \frac{1}{Pe}\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta z^2} - \frac{u_i - u_{i-1}}{\Delta z} - ku_i^n$$

$$u_0 - \frac{1}{Pe}\frac{u_1 - u_0}{\Delta z} = 1 \longrightarrow u_0 = \frac{1}{1 + \frac{1}{Pe\Delta z}}\left(\frac{1}{Pe\Delta z}u_1 + 1\right)$$

$$\frac{u_{N+1} - u_N}{\Delta z} = 0 \longrightarrow u_{N+1} = u_N$$

$$i = 1, 2, ..., N$$

System of nonlinear ODEs!!!
Stiff...

Assignment 2

1. Solve the dynamic tubular reactor from initial 0 to final time of 5 with MATLAB‘s `ode23s`

   Use the `rhs.m` from assignment 1 and the template `TubReact_dynamic.m`

   Consider only a first order reaction with Pe=100 and Da=1
2. Plot the conversion at the end of the reactor vs. dimensionless time
3. At what time does the solution reach a steady state, i.e. how many reactor volumes of solvent will you need?

Assignment 2