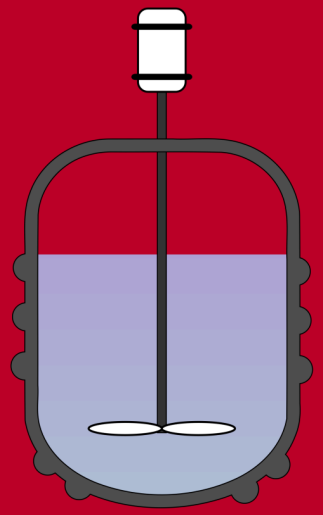
Carnegie Mellon University



Introductory Numerical Methods for Simulating Batch Reactors

Dr. Joshua Pulsipher

Learning Outcomes

1. The relative advantages/disadvantages of using **explicit Euler** methods

2. How to implement explicit Euler to **simulate ODEs** using common computation environments (e.g., Python)

3. How to **simulate batch reactors** using numerical methods

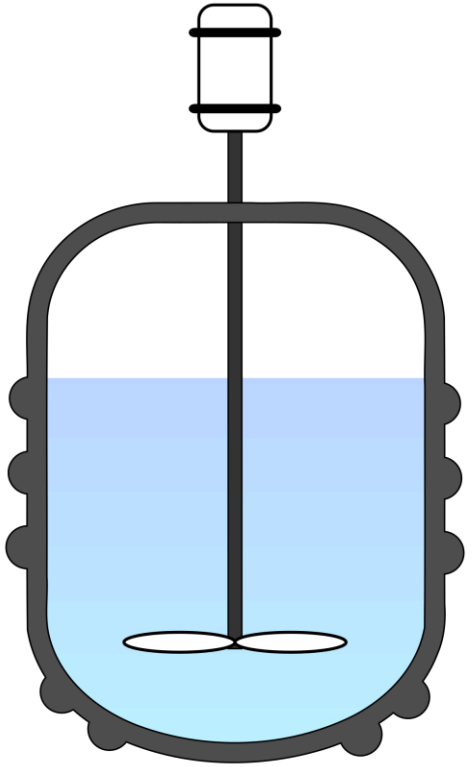
4. [Time Permitting] A familiarity of **other numerical methods/tools** for simulating batch reactors

Outline

- Overview
- Explicit Euler
- Batch Reactors
- Other Numerical Methods (If time allows)

Outline

- **Overview**
- Explicit Euler
- Batch Reactors
- Other Numerical Methods



Simulating Dynamic Systems

- Simulating dynamic systems is vital for enabling engineering applications

Curiosity Rover

Batch Reactor

- Simulate using **numerical methods to approximate dynamics** (e.g., differential equations)

- Enables us to **computationally experiment** and implement **automation**

Ordinary Differential Equations

Formulation

- General first order form

$$\frac{dy(t)}{dt} = f(y(t), t)$$
$$y(0) = y_0$$

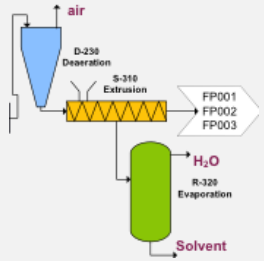
- Vectorized system

$$\frac{dy_1(t)}{dt} = f_1(y_1, y_2, \ldots, y_n)$$
$$\frac{dy_2(t)}{dt} = f_2(y_1, y_2, \ldots, y_n)$$
$$\vdots$$
$$\frac{dy_n(t)}{dt} = f_n(y_1, y_2, \ldots, y_n)$$
$$y_1(0) = y_{1,0}, y_2(0) = y_{2,0}, \ldots, y_n(0) = y_{n,0}$$

Applications

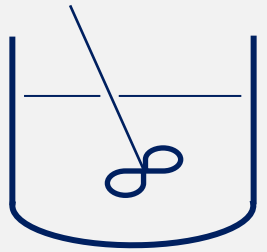
- Transient flow balance

$$\frac{df(t)}{dt} = f_{in}(t) - f_{out}(t) + f_{gen}(t)$$



- Kinetics

$$\frac{dc(t)}{dt} = kc(t)^{\alpha}$$



Analytical vs. Numerical Methods

Analytical Methods

- Separate and integrate

$$g(y)\frac{dy}{dx} = h(x) \quad \Rightarrow \quad \int g(y)dy = \int h(x)dx + C$$

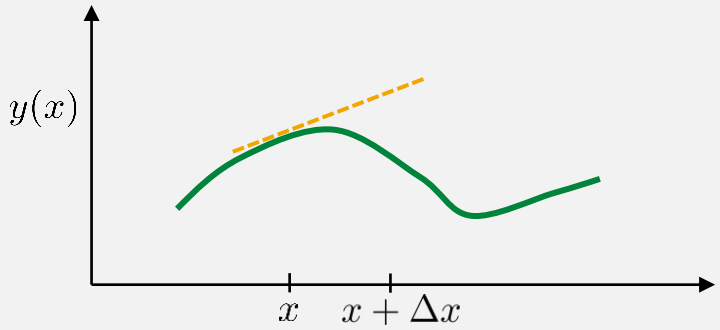
- ODEs of special forms

$$\frac{dy}{dx} = \frac{x+y}{x-y} \quad \Rightarrow \quad \frac{1}{2}\log\left(\frac{y^2}{x^2}+1\right) - \tan^{-1}\left(\frac{y}{x}\right) = C - \log(x)$$

- Solving general ODEs is often difficult or not possible

Numerical Methods

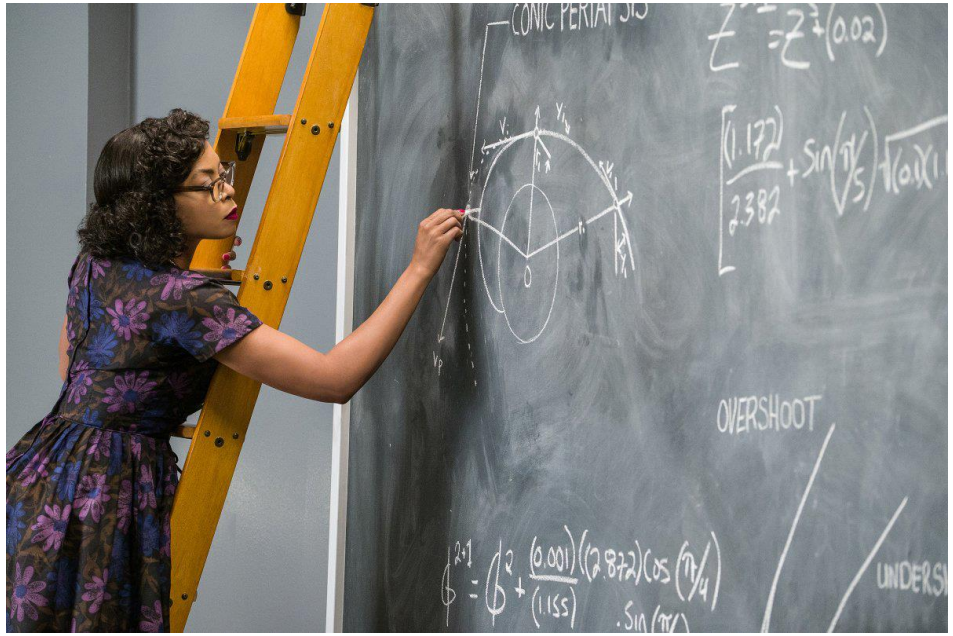
- Seek to numerically approximate the solution
- **Finite difference methods** are common



- More advanced methods are available
  - Not the focus of today

Outline

- Overview
- **Explicit Euler**
- Batch Reactors
- Other Numerical Methods



Katherine Goble

The Basics

Methodology

- Consider a 1st order ODE

$$\frac{dy(t)}{dt} = f(y(t), t)$$
$$y(0) = y_0$$

- Define time steps Δt

$$t \in [t_0, t_f] \qquad t_k = t_0 + k\Delta t$$

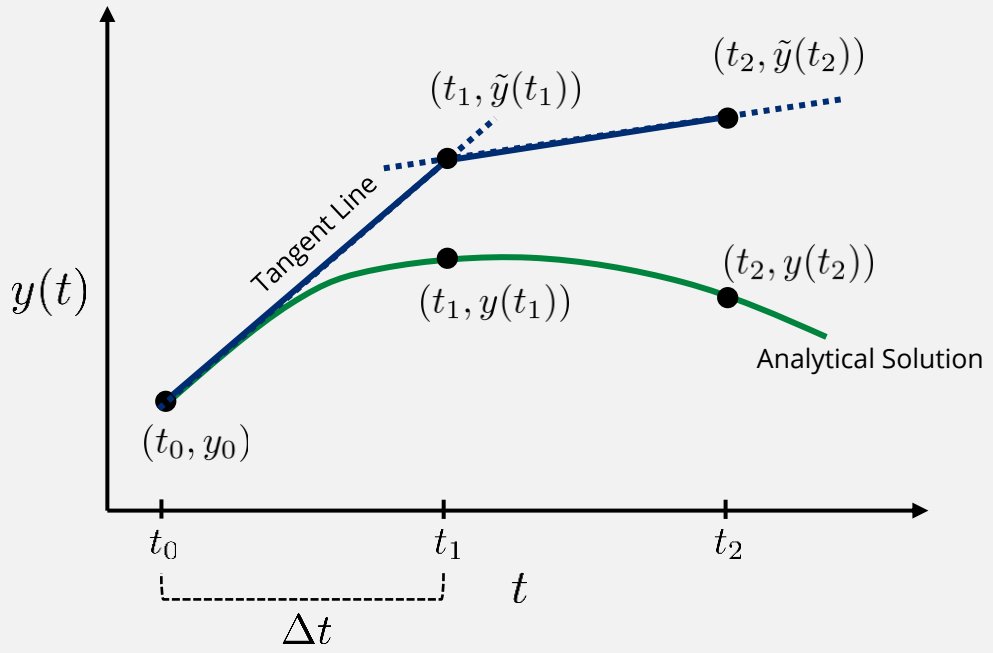
- Approximate derivative as finite difference

$$\left.\frac{dy(t)}{dt}\right|_{t_k} \approx \frac{\tilde{y}(t_{k+1}) - \tilde{y}(t_k)}{\Delta t}$$

- Define update rule

$$\tilde{y}(t_{k+1}) = \tilde{y}(t_k) + f(y(t_k), t_k)\Delta t$$

Illustration



Properties: Error

Local Truncation Error (LTE)

- Recall update rule

$$\tilde{y}(t_{k+1}) = \tilde{y}(t_k) + f(y(t_k), t_k)\Delta t$$

- Taylor series expansion of analytic solution

$$y(t_k + \Delta t) = y(t_k) + \Delta t \frac{dy(t)}{dt}\bigg|_{t_k} + O(\Delta t^2)$$

- Difference w/ explicit Euler

$$y(t_k + \Delta t) - \tilde{y}(t_{k+1}) = O(\Delta t^2)$$

- Hence, the error incurred after one step is

$$\boxed{O(\Delta t^2)}$$

Global Truncation Error (GTE)

- The number of steps

$$\frac{t - t_0}{\Delta t} \propto \frac{1}{\Delta t}$$

- Multiplying this with the LTE, we get GTE that is

$$\boxed{O(\Delta t)}$$

- Hence, explicit Euler is a **first order method**

- Higher order methods are available

Simulating a System of ODEs

System of 1st order ODEs

- General representation

$$\frac{dy_1(t)}{dt} = f_1(y_1, y_2, \ldots, y_n)$$
$$\frac{dy_2(t)}{dt} = f_2(y_1, y_2, \ldots, y_n)$$
$$\vdots$$
$$\frac{dy_n(t)}{dt} = f_n(y_1, y_2, \ldots, y_n)$$
$$y_1(0) = y_{1,0}, y_2(0) = y_{2,0}, \ldots, y_n(0) = y_{n,0}$$

- Vectorize

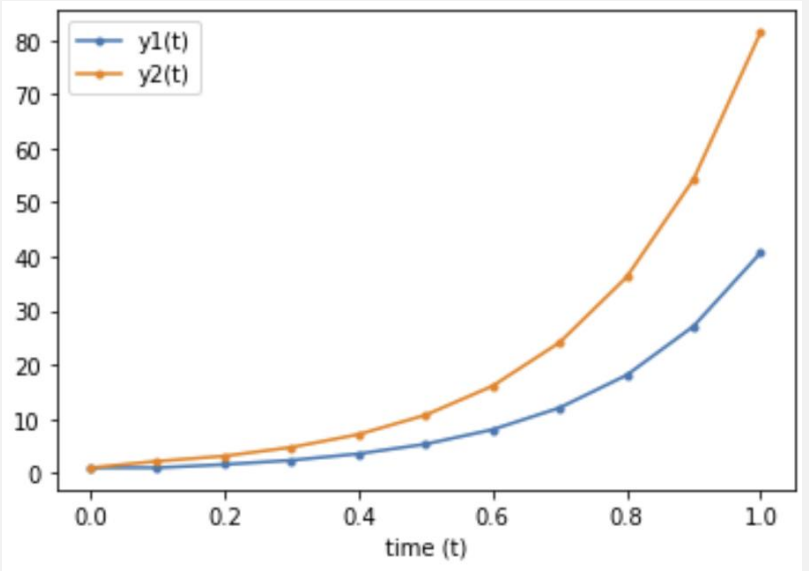
$$\frac{d\mathbf{y}(t)}{dt} = \mathbf{f}(\mathbf{y}(t), t)$$
$$\mathbf{y}(0) = \boldsymbol{y_0}$$

We can represent a higher order ODE as a 1st order system

Vectorized Explicit Euler

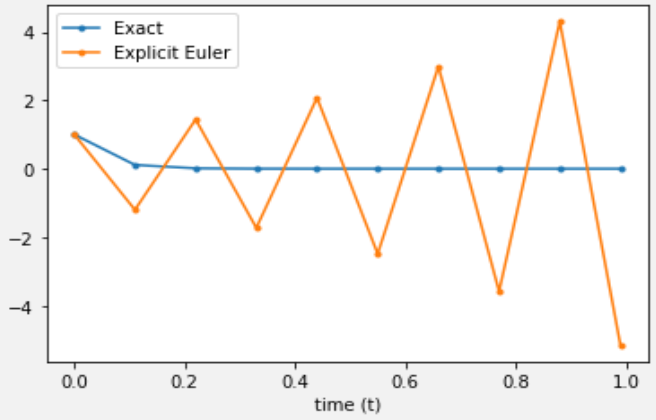
- Update rule uses vectorized representation

$$\tilde{\mathbf{y}}(t_{k+1}) = \tilde{\mathbf{y}}(t_k) + \mathbf{f}(\mathbf{y}(t_k), t_k)\Delta t$$



Properties: Stability

Example



Linear Stability

- Consider the linear ODE

$$\frac{dy(t)}{dt} = \lambda y(t)$$

- For a stable solution we must have

$$|1 + \lambda \Delta t| < 1$$

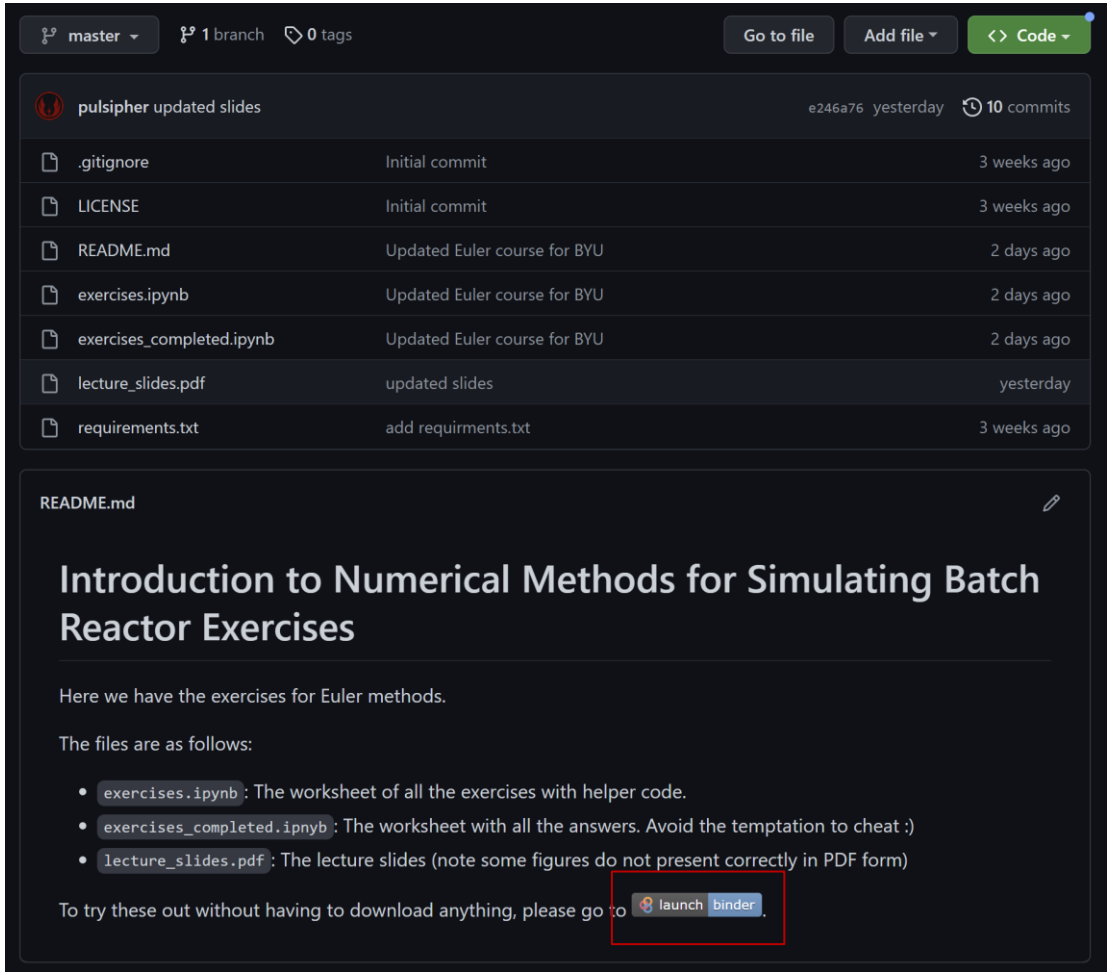
Stiff ODEs

- Systems that exhibit **numerical instability**
- Precise mathematical definition is nontrivial
- Common with **reaction systems**
  - Coexistence of small and large rate constants
- So, what can we do? → Use **implicit methods**

$$\tilde{y}(t_{k+1}) = \tilde{y}(t_k) + f(y(t_{k+1}), t_{k+1})\Delta t$$

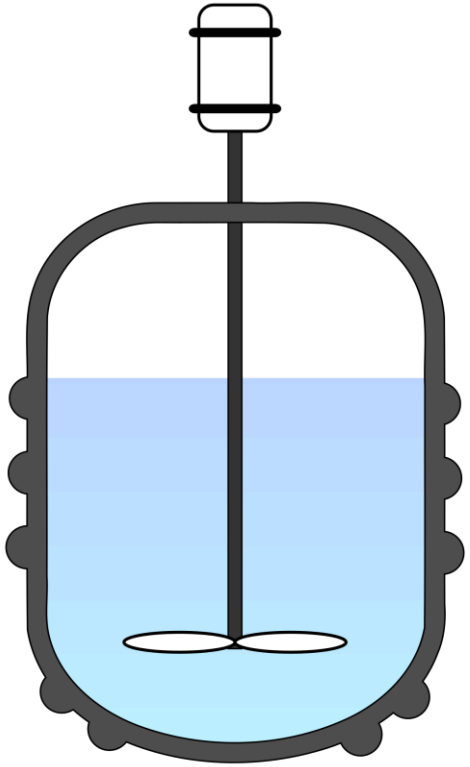
Tutorials

- Go to https://github.com/pulsipher/eulercourse
- Click on the “launch binder” button
- Open “exercise.ipynb”



Outline

- Overview
- Explicit Euler
- **Batch Reactors**
- Other Numerical Methods



Batch Reactor Modeling

Simple ODE Model

- Arrhenius equation for species i and reaction j

$$k_{ij}(t) = A_{ij} \exp\left(\frac{-E_{a,ij}}{RT(t)}\right)$$

- Reaction rates

$$r_j(\mathbf{c}, t) = \sum_{i \in I} k_{ij}(t) c_i^{\beta_{ij}}(t)$$

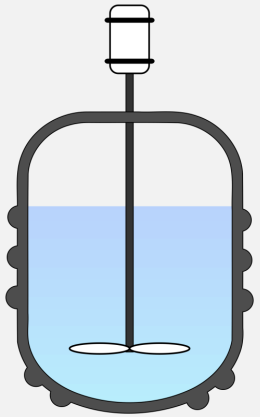
- Species generation rates

$$g_i(\mathbf{c}, t) = \sum_{j \in J} \gamma_{ij} r_j(\mathbf{c}, t)$$

- Species balances

$$\frac{dc_i(t)}{dt} = g_i(\mathbf{c}, t), \quad i \in I$$
$$c_i(0) = c_{i,0}, \quad i \in I$$

The Basics



$$\mathrm{A} \rightleftharpoons \mathrm{B}$$

- Derivation from mole balance

$$\frac{N_i(t)}{dt} = F_{i,in}(t) - F_{i,out}(t) + \int^V g_i(t) dV(t)$$

- Assume perfect mixing and constant volume

$$\frac{N_i(t)}{dt} = g_i(t)V \quad \Rightarrow \quad \frac{c_i(t)}{dt} = g_i(t)$$

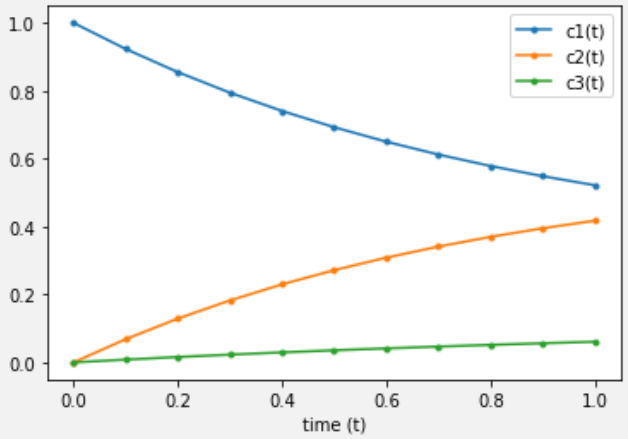
Exercise: Batch Reactor

Exercise 1

- Simulate the following reaction system using explicit Euler for $t \in [0, 1]$

$$\mathrm{A} \rightleftharpoons \mathrm{B}$$
$$\mathrm{A} \rightleftharpoons \mathrm{C}$$

- Experiment with different choices of Δt



Problem Information

$$R = 1.987$$

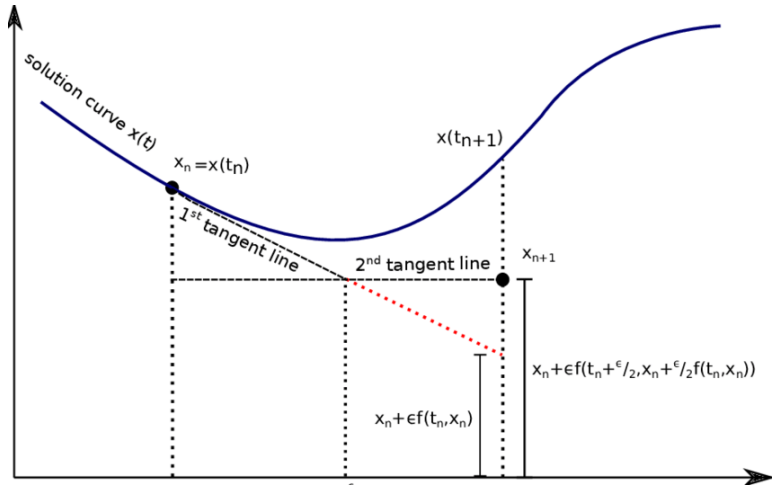
$$A = \begin{bmatrix} 3.6362e6 & 190.6879 \\ -2.5212e16 & 0 \\ 0 & -8.7409e24 \end{bmatrix}$$

$$E_a = \begin{bmatrix} 10000 & 5000 \\ 25000 & 0 \\ 0 & 40000 \end{bmatrix} \qquad \beta = 1 \qquad \gamma = \begin{bmatrix} -1 & -1 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$T(t) = \begin{cases} 333, & t < 0.5 \\ 325, & t \geq 0.5 \end{cases} \qquad \mathbf{c}_0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

Outline

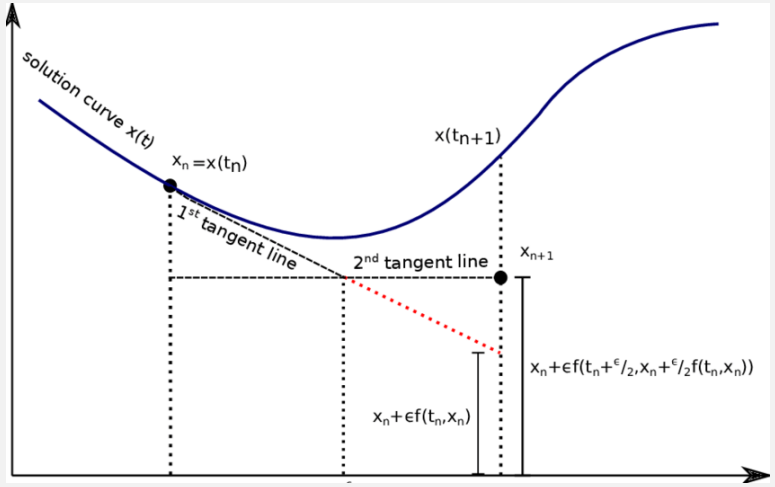
- Overview
- Explicit Euler
- Batch Reactors
- **Other Numerical Methods**



More Advanced Methods

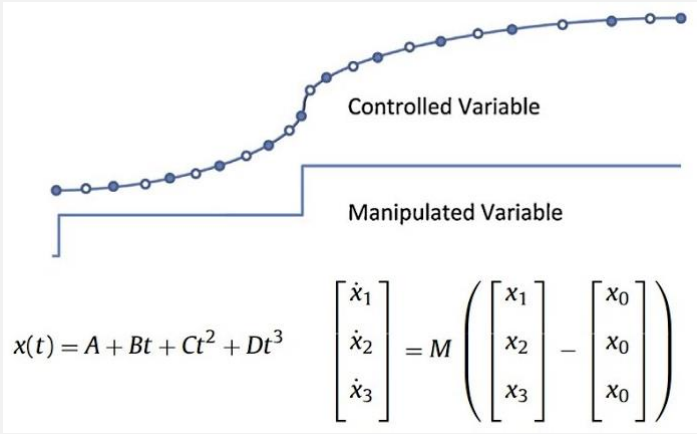
Runge-Kutta

- Family of explicit and implicit iterative methods
- Various orders based on GTE $O(h^p)$
  - 1st order methods are the Euler methods
  - 4th order methods are popular



Orthogonal Collocation over Finite Elements

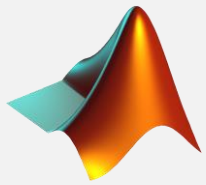
- The discretization uses finite elements
- We approximate the solution in each element as a polynomial function
- End up solving a system of linear equations



Common Simulation Tools

ODE Integrators

- Common in scripting languages
- Provide numerical solutions to ODE systems



Symbolic Solvers

- Can provide analytic solutions when possible
- Typically, not used for large problems

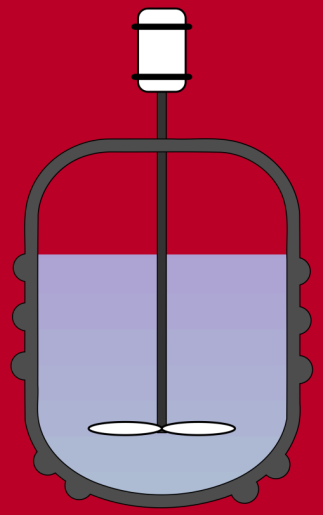
Optimization Tools

- Can incorporate differential equations when solving optimization problems

Problem Specific

- Simulate dynamics for particular systems

Carnegie Mellon University



Introductory Numerical Methods for Simulating Batch Reactors

Dr. Joshua Pulsipher