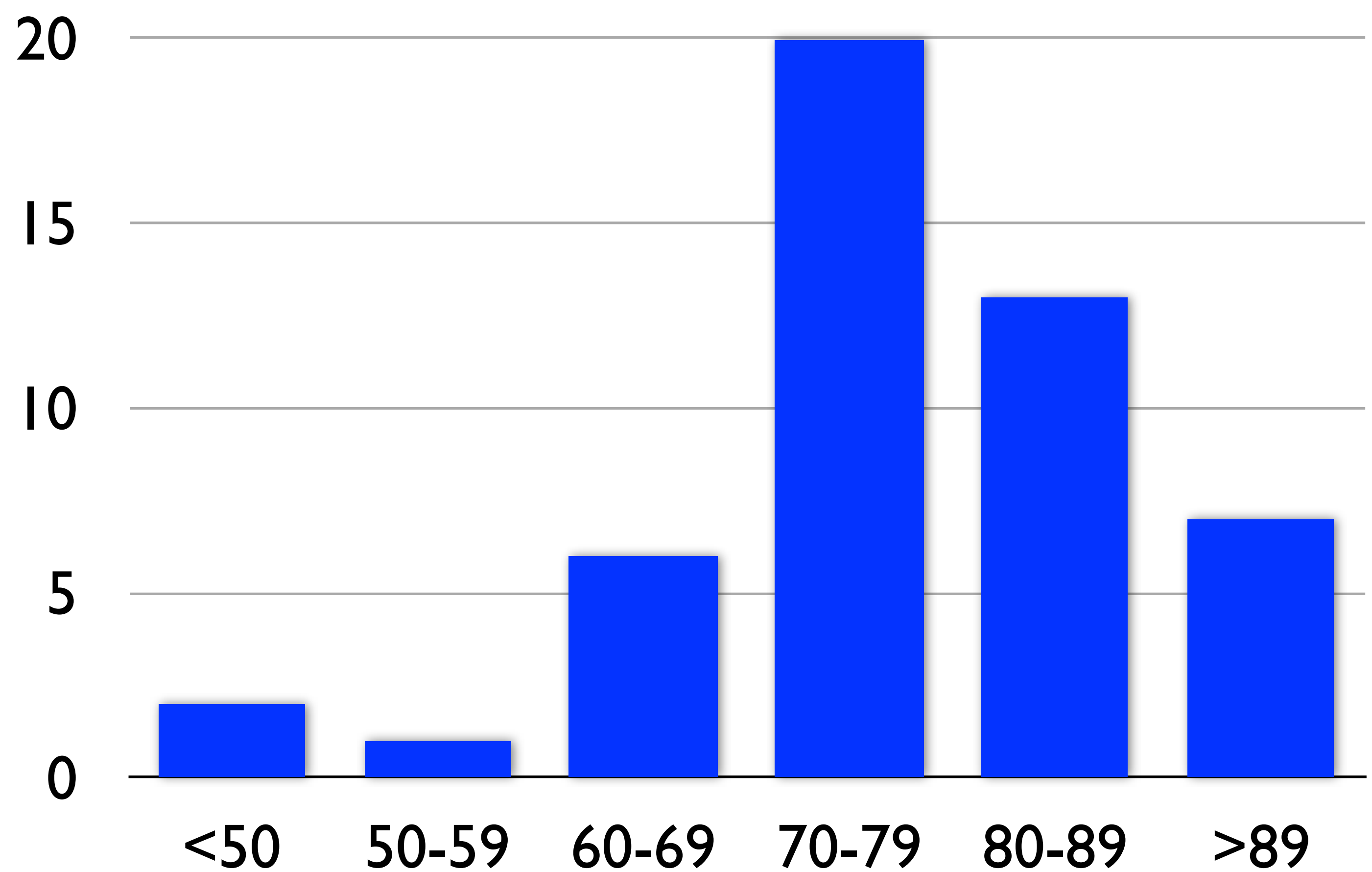
10.34: Numerical Methods Applied to Chemical Engineering

Lecture 18:
Differential Algebraic Equations

Quiz 1 Results

- Mean: 77
- Standard deviation: 12



Recap

- Numerical integration
- Implicit methods for ODE-IVPs

Recap

- Improper integrals:
  - Of the sort: $$\int_{t_0}^{\infty} \mathbf{f}(\tau) d\tau$$
  - Can be split into two domains of integration
$$\int_{t_0}^{\infty} \mathbf{f}(\tau) d\tau = \int_{t_0}^{t_f} \mathbf{f}(\tau) d\tau + \int_{t_f}^{\infty} \mathbf{f}(\tau) d\tau$$
    - The first integral can be handled with ODE-IVP methods or polynomial interpolation
    - The second must be handled separately through either:
      - transformation onto a finite domain
      - or substitution of an asymptotic approximation
  - This same idea applies to integrable singularities as well.

Recap

- Improper integrals:
  - Example:

$$\int_0^{t_f} \frac{\cos\tau}{\sqrt{\tau}} d\tau$$

$$\approx \int_0^{t_0} \frac{1-\tau^2/2}{\sqrt{\tau}} d\tau + \int_{t_0}^{t_f} \frac{\cos\tau}{\sqrt{\tau}} d\tau$$

$$\approx 2t_0^{1/2} - \frac{1}{5}t_0^{5/2} + \int_{t_0}^{t_f} \frac{\cos\tau}{\sqrt{\tau}} d\tau$$

Recap

- Example:
  - Use implicit Euler to solve:

$$\frac{dx}{dt} = \lambda x, x(0) = x_0$$

Give a closed form formula for the numerical solution

Recap

- Example:
  - Use implicit Euler to solve:

$$\frac{dx}{dt} = \lambda x, x(0) = x_0$$

  - Let: $x_k = x(k\Delta t)$

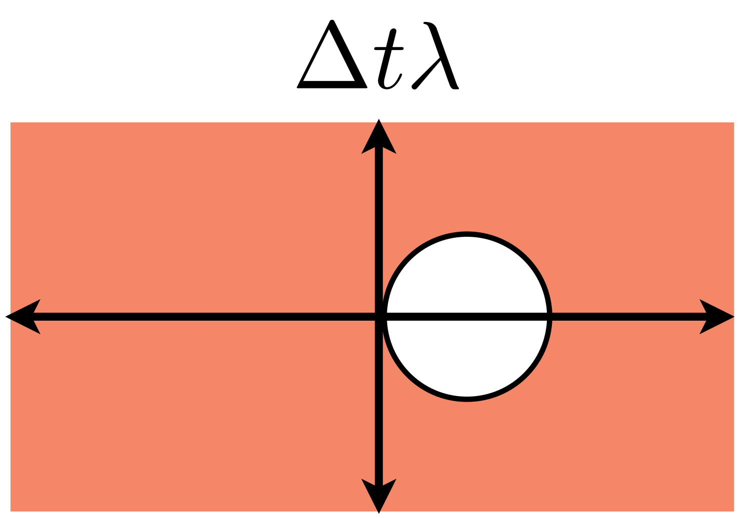
$$x_{k+1} = x_k + \Delta t \lambda x_{k+1}$$

$$x_{k+1} = \frac{1}{1 - \Delta t \lambda} x_k$$

$$x_k = \left(\frac{1}{1 - \Delta t \lambda} \right)^k x_0$$

  - Stability:

$$|1 - \Delta t \lambda| \geq 1 \Rightarrow (1 - \Delta t \mathrm{Re}\lambda)^2 + (\Delta t \mathrm{Im}\lambda)^2 \geq 1$$



Recap

- Example:
  - Use implicit Euler to solve:

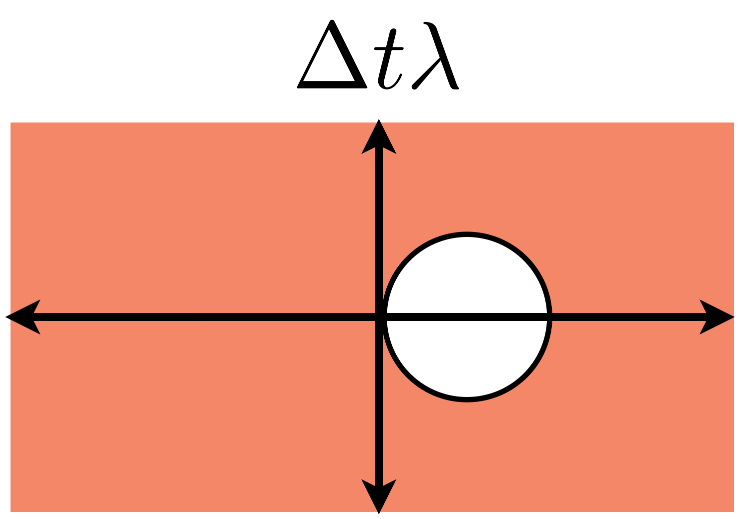
$$\frac{dx}{dt} = \lambda x, x(0) = x_0$$

  - Numerical solution:

$$x_k = \left(\frac{1}{1 - \Delta t \lambda}\right)^k x_0$$

  - Exact solution:

$$x_k = x_0 e^{k\lambda \Delta t}$$



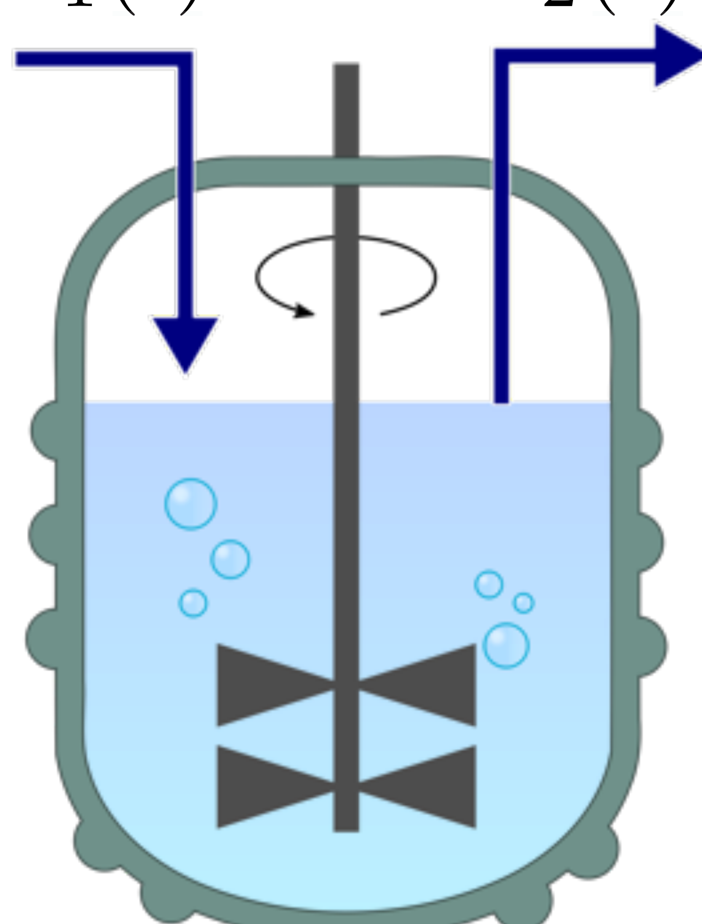
  - Stability and accuracy do not correlate!

Differential Algebraic Equations

- Problems of the sort: $\mathbf{f}\left(\mathbf{x}, \frac{d\mathbf{x}}{dt}, t\right) = 0, \;\; \mathbf{x}(0) = \mathbf{x}_0$

  - Called "well-posed" when $\mathbf{x}, \mathbf{f} \in \mathbf{R}^N$

- Example: stirred tank 1



$$\frac{dc_2}{dt} = \frac{Q}{V}\left(c_1(t) - c_2(t)\right)$$

$$c_1(t) = \gamma(t)$$

$$c_1(0) = \gamma(0), \; c_2(0) = c_0$$

Solution:

$$c_1(t) = \gamma(t)$$

$$c_2(t) = c_2(0)e^{-(Q/V)t} + \frac{Q}{V}\int_0^t \gamma(t')e^{-(Q/V)(t-t')}dt'$$

Differential Algebraic Equations

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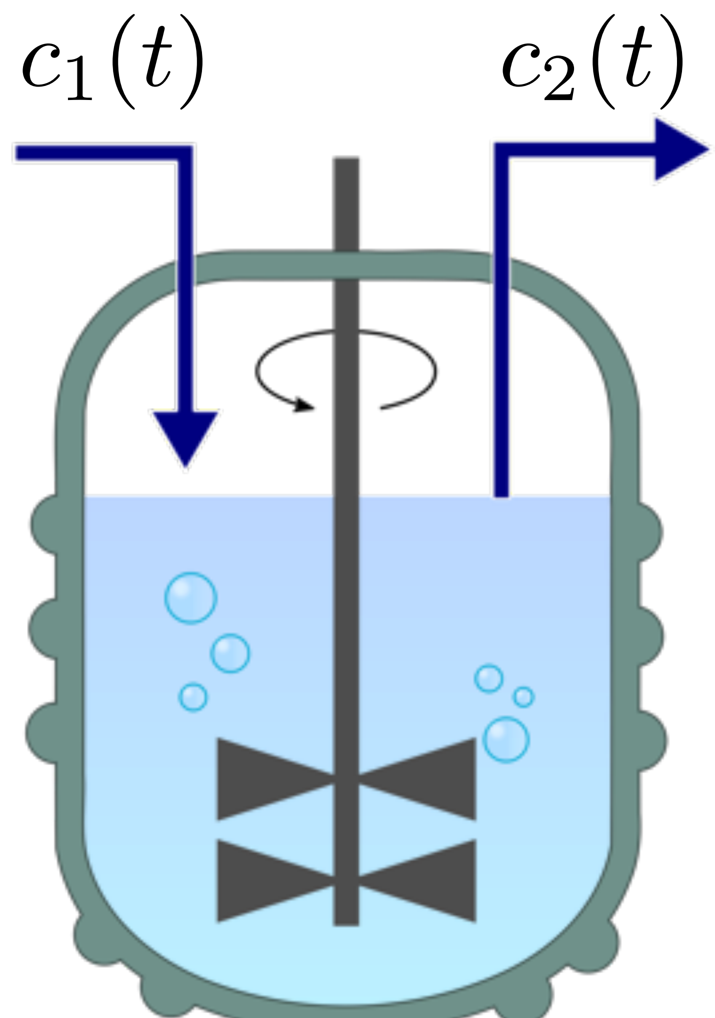
- Example: stirred tank 1



$$\left(\begin{array}{c} \frac{dc_2}{dt} - \frac{Q}{V}\left(c_1(t) - c_2(t)\right) \\ c_1(t) - \gamma(t) \end{array} \right) = 0$$

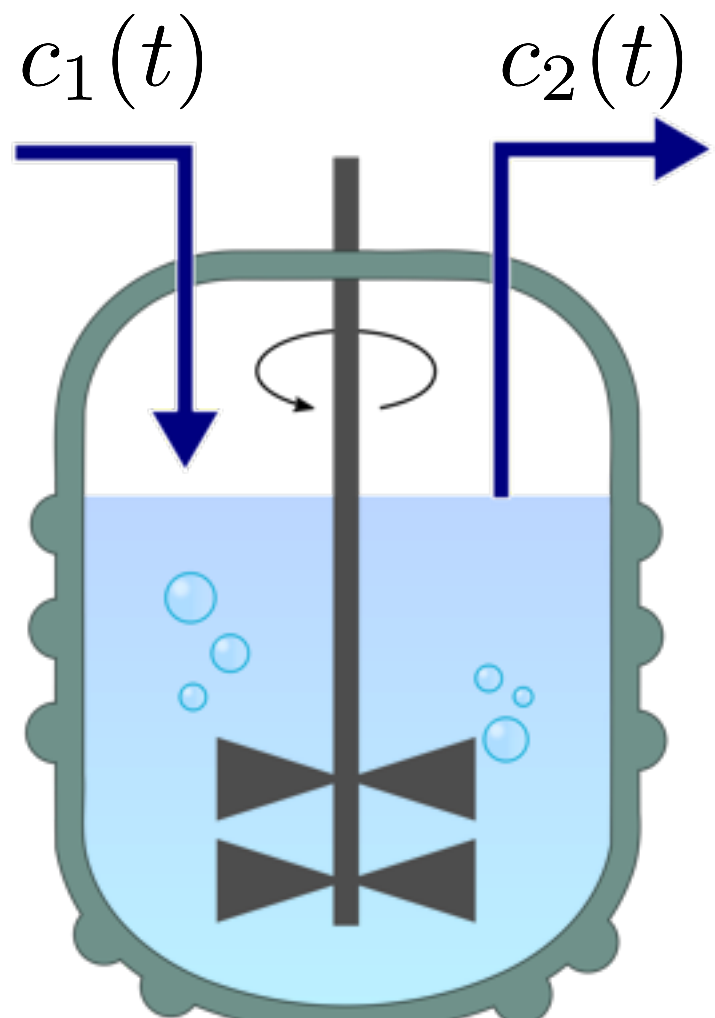
$$\left(\begin{array}{c} c_1(0) \\ c_2(0) \end{array} \right) = \left(\begin{array}{c} \gamma(0) \\ c_0 \end{array} \right)$$

Differential Algebraic Equations

- Problems of the sort: $\mathbf{f}\left(\mathbf{x}, \frac{d\mathbf{x}}{dt}, t\right) = 0, \;\; \mathbf{x}(0) = \mathbf{x}_0$

  - Called "well-posed" when $\mathbf{x}, \mathbf{f} \in \mathbf{R}^N$

- Example: stirred tank 2



$$\frac{dc_2}{dt} = \frac{Q}{V}\left(c_1(t) - c_2(t)\right)$$

$$c_2(t) = \gamma(t)$$

$$c_1(t) = c_0, \;\; c_2(0) = \gamma(0)$$

Solution:

$$c_1(t) = \gamma(t) + \frac{V}{Q}\dot{\gamma}$$

$$c_2(t) = \gamma(t)$$

Differential Algebraic Equations

- Common in dynamic simulations involving conservation, constraints, or equilibria.
  - Conservation of total:
    - energy
    - mass
    - momentum
    - particle number
    - atomic species
    - charge
  - Models of reaction networks utilizing the pseudo-steady-state approximation.
  - Models of control neglecting controller dynamics.

Semi-explicit DAEs

- Problems of the sort: $\mathbf{M}\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t), \;\; \mathbf{x}(0) = \mathbf{x}_0$
  - $\mathbf{M}$ is called the "mass matrix"
  - Stirred tank example 1:

$$\begin{pmatrix} \frac{dc_2}{dt} - \frac{Q}{V}\left(c_1(t) - c_2(t)\right) \\ c_1(t) - \gamma(t) \end{pmatrix} = 0$$

    - Semi-explicit form:

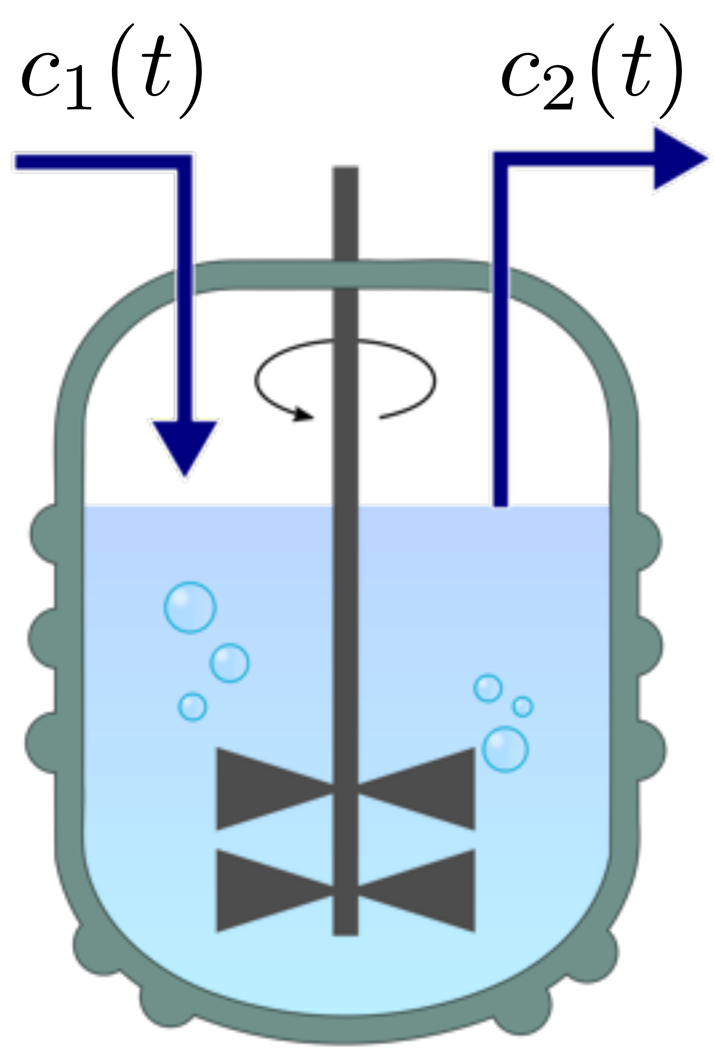
$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \frac{d}{dt}\mathbf{c} = \begin{pmatrix} \frac{Q}{V} & -\frac{Q}{V} \\ -1 & 0 \end{pmatrix} \mathbf{c} + \begin{pmatrix} 0 \\ \gamma(t) \end{pmatrix}$$

- When mass matrix is full rank these problems can be solved by applying typical ODE-IVP techniques to:

$$\frac{d\mathbf{x}}{dt} = \mathbf{M}^{-1}\mathbf{f}(\mathbf{x}, t)$$

Semi-explicit DAEs

- Write stirred tank example 2 in semi-explicit form:



$$\frac{dc_2}{dt} = \frac{Q}{V}\left(c_1(t) - c_2(t)\right)$$

$$c_2(t) = \gamma(t)$$

Semi-explicit DAEs

- Problems of the sort: $\mathrm{M}\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t), \ \mathbf{x}(0) = \mathbf{x}_0$
  - M is called the "mass matrix"
- Many semi-explicit DAEs can be written in the simplified form:

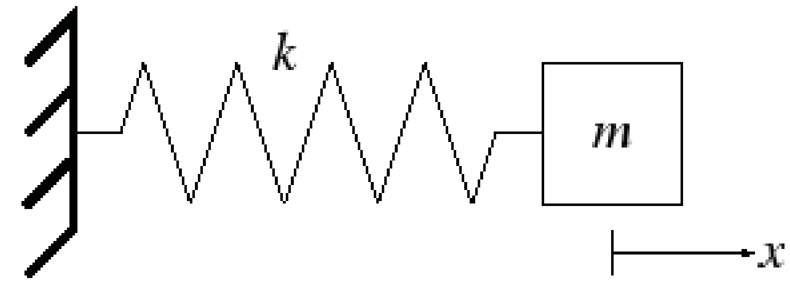
$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{y}, t) \qquad \mathbf{x}(0) = \mathbf{x}_0$$

$$0 = \mathbf{g}(\mathbf{x}, \mathbf{y}, t) \qquad 0 = \mathbf{g}(\mathbf{x}_0, \mathbf{y}(0), t)$$

  - where
    - $\mathbf{x}$ are called the differential states
    - $\mathbf{y}$ are called the algebraic states

Fully implicit DAEs

- Example: mass-spring system



- Conservation of energy: $E = \frac{1}{2}m(\dot{x})^2 + \frac{1}{2}kx^2$

$$f(x, \dot{x}, t) = \frac{1}{2}m(\dot{x})^2 + \frac{1}{2}kx^2 - E = 0$$

has a solution:

$$x = a\cos(\omega t)$$

$$\frac{1}{2}ma^2\omega^2\sin^2(\omega t) + \frac{1}{2}ka^2\cos^2(\omega t) = E$$

$$\omega = \sqrt{\frac{k}{m}},\ a = \sqrt{\frac{E}{k}}$$

Fully implicit DAEs

- Many problems contain non-linearities with respect to differentials of the state variables. $\mathbf{f}\left(\mathbf{x}, \dot{\mathbf{x}}, t\right) = 0,\ \mathbf{x}(0) = \mathbf{x}_0$

- If $\left.\frac{\partial \mathbf{f}}{\partial \dot{\mathbf{x}}}\right|_{t,\mathbf{x}}$ is full rank, then the DAE can be represented as an equivalent ODE:

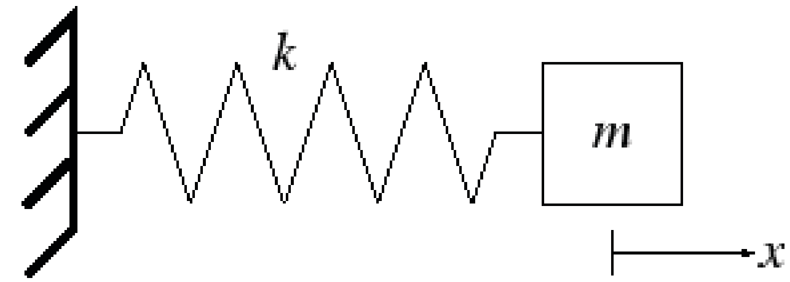
$$d\mathbf{f} = \left.\frac{\partial \mathbf{f}}{\partial \dot{\mathbf{x}}}\right|_{t,\mathbf{x}} d\dot{\mathbf{x}} + \left.\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right|_{t,\dot{\mathbf{x}}} d\mathbf{x} + \left.\frac{\partial \mathbf{f}}{\partial t}\right|_{\mathbf{x},\dot{\mathbf{x}}} dt = 0$$

↓

$$\frac{d\dot{\mathbf{x}}}{dt} = -\left(\left.\frac{\partial \mathbf{f}}{\partial \dot{\mathbf{x}}}\right|_{t,\mathbf{x}}\right)^{-1}\left(\left.\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right|_{t,\dot{\mathbf{x}}}\frac{d\mathbf{x}}{dt} + \left.\frac{\partial \mathbf{f}}{\partial t}\right|_{\mathbf{x},\dot{\mathbf{x}}}\right) = 0$$

Fully implicit DAEs

- Example: mass-spring system



- Conservation of energy: $E = \frac{1}{2}m(\dot{x})^2 + \frac{1}{2}kx^2$

$$f(x, \dot{x}, t) = \frac{1}{2}m(\dot{x})^2 + \frac{1}{2}kx^2 - E = 0$$

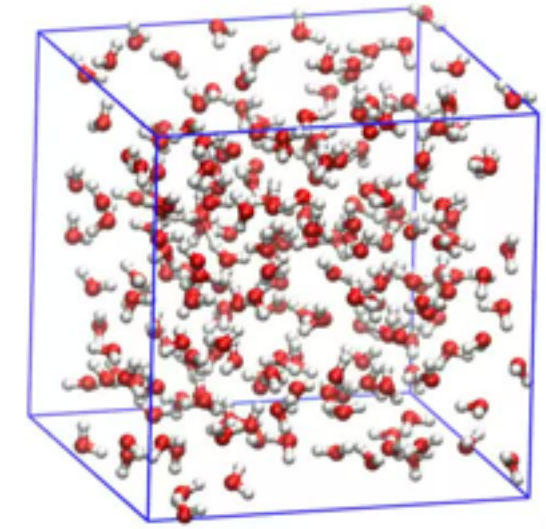
transform to ODE

$$\frac{\partial f}{\partial \dot{x}} = m\dot{x},\ \frac{\partial f}{\partial x} = kx,\ \frac{\partial f}{\partial t} = 0$$

$$\downarrow$$

$$\ddot{x} = -\frac{k}{m}x$$

Fully implicit DAEs



- Example: molecular dynamics

- Conservation of energy: $E = \frac{1}{2}m\|\dot{\mathbf{x}}\|_2^2 + V(\mathbf{x})$

$$f(\dot{\mathbf{x}}, \mathbf{x}, t) = \frac{1}{2}m\|\dot{\mathbf{x}}\|_2^2 + V(\mathbf{x}) - E$$

$$\downarrow$$

$$df = \left.\frac{\partial f}{\partial \dot{\mathbf{x}}}\right|_{t,\mathbf{x}} d\dot{\mathbf{x}} + \left.\frac{\partial f}{\partial \mathbf{x}}\right|_{t,\dot{\mathbf{x}}} d\mathbf{x} + \left.\frac{\partial f}{\partial t}\right|_{\mathbf{x},\dot{\mathbf{x}}} dt = 0$$

$$\downarrow \; \frac{\partial f}{\partial \dot{\mathbf{x}}} = m\dot{\mathbf{x}}$$

$$0 = \dot{\mathbf{x}} \cdot (m\ddot{\mathbf{x}} + \nabla V(\mathbf{x}))$$

- Simplectic integrators used to integrate equations of motion while exerting control over error in the total energy.

Numerical Simulation of DAEs

- Consider the semi-explicit DAE:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{y}, t) \qquad \mathbf{x}(0) = \mathbf{x}_0$$
$$0 = \mathbf{g}(\mathbf{x}, \mathbf{y}, t)$$

- Consider applying the forward Euler approximation:

$$\mathbf{x}(t + \Delta t) - \mathbf{x}(t) = \Delta t \mathbf{f}(\mathbf{x}(t), \mathbf{y}(t), t)$$
$$0 = \mathbf{g}(\mathbf{x}(t), \mathbf{y}(t), t)$$

- Determining the algebraic states always requires solution of a nonlinear equation.
- DAE simulation methods are inherently implicit.

Numerical Simulation of DAEs

- Consider the fully implicit DAE:

$$\mathbf{f}(\mathbf{x}, \dot{\mathbf{x}}, t) = 0, \;\; \mathbf{x}(0) = \mathbf{x}_0$$

  - No way in general to avoid solving systems of nonlinear equations.
  - Backward difference approximations for $\dot{\mathbf{x}}$ are substituted and time marching solutions determined.
    - Example, backward Euler approximation:

solve: $\mathbf{f}\left(\mathbf{x}(t_k), \dfrac{\mathbf{x}(t_k) - \mathbf{x}(t_{k-1})}{t_k - t_{k-1}}, t_k\right) = 0$ for: $\mathbf{x}(t_k)$

solve: $\mathbf{f}\left(\mathbf{x}(t_{k+1}), \dfrac{\mathbf{x}(t_{k+1}) - \mathbf{x}(t_k)}{t_{k+1} - t_k}, t_{k+1}\right) = 0$ for: $\mathbf{x}(t_{k+1})$

Numerical Simulation of DAEs

- Consider the semi-explicit DAE:

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, \mathbf{y}, t) \qquad \mathbf{x}(0) = \mathbf{x}_0$$

$$0 = \mathbf{g}(\mathbf{x}, \mathbf{y}, t)$$

- No way in general to avoid solving systems of nonlinear equations.
- Backward difference approximations for $\dot{\mathbf{x}}$ are substituted and time marching solutions determined.
    - Example, backward Euler approximation:

solve: $$0 = \frac{\mathbf{x}(t_k) - \mathbf{x}(t_{k-1})}{t_k - t_{k-1}} - \mathbf{f}(\mathbf{x}(t_k), \mathbf{y}(t_k), t_k)$$

$$0 = \mathbf{g}(\mathbf{x}(t_k), \mathbf{y}(t_k), t_k)$$

for: $\mathbf{x}(t_k)$

Numerical Simulation of DAEs

- How suitable are such approaches?
- Consider stirred tank example 1:

$$\frac{dc_2}{dt} = \frac{Q}{V}\left(c_1(t) - c_2(t)\right)$$
$$c_1(t) = \gamma(t)$$

Apply backward Euler method:

$$c_1(t_k) = \gamma(t_k)$$
$$c_2(t_k) = \frac{1}{1 + \frac{Q}{V}(t_k - t_{k-1})}\left(c_2(t_{k-1}) + \frac{Q}{V}(t_k - t_{k-1})c_1(t_k)\right)$$
$$+O((t_k - t_{k-1})^2)$$

Numerical Simulation of DAEs

- How suitable are such approaches?
- Consider stirred tank example 2:

$$\frac{dc_2}{dt} = \frac{Q}{V}\left(c_1(t) - c_2(t)\right)$$
$$c_2(t) = \gamma(t)$$

Apply backward Euler method:

$$c_2(t_k) = \gamma(t_k)$$
$$c_1(t_k) = c_2(t_k) + \frac{V}{Q}\left(\frac{c_2(t_k) - c_2(t_{k-1})}{t_k - t_{k-1}}\right) + O(t_k - t_{k-1})$$

Numerical Simulation of DAEs

- How suitable are such approaches?
- Consider the system of DAEs:

$$\begin{aligned} \dot{c}_2 &= c_1(t) \\ \dot{c}_3 &= c_2(t) \\ 0 &= c_3(t) - \gamma(t) \end{aligned}$$

What is the exact solution?
Apply backward Euler method:

$$c_3(t_k) = \gamma(t_k)$$

$$c_2(t_k) = \frac{c_3(t_k) - c_3(t_{k-1})}{t_k - t_{k-1}} \quad +O(t_k - t_{k-1})$$

$$c_1(t_k) = \frac{c_2(t_k) - c_2(t_{k-1})}{t_k - t_{k-1}} \quad +O(1)\,!$$