Introduction to Simulation - Lecture 12

Methods for Ordinary Differential Equations

Jacob White

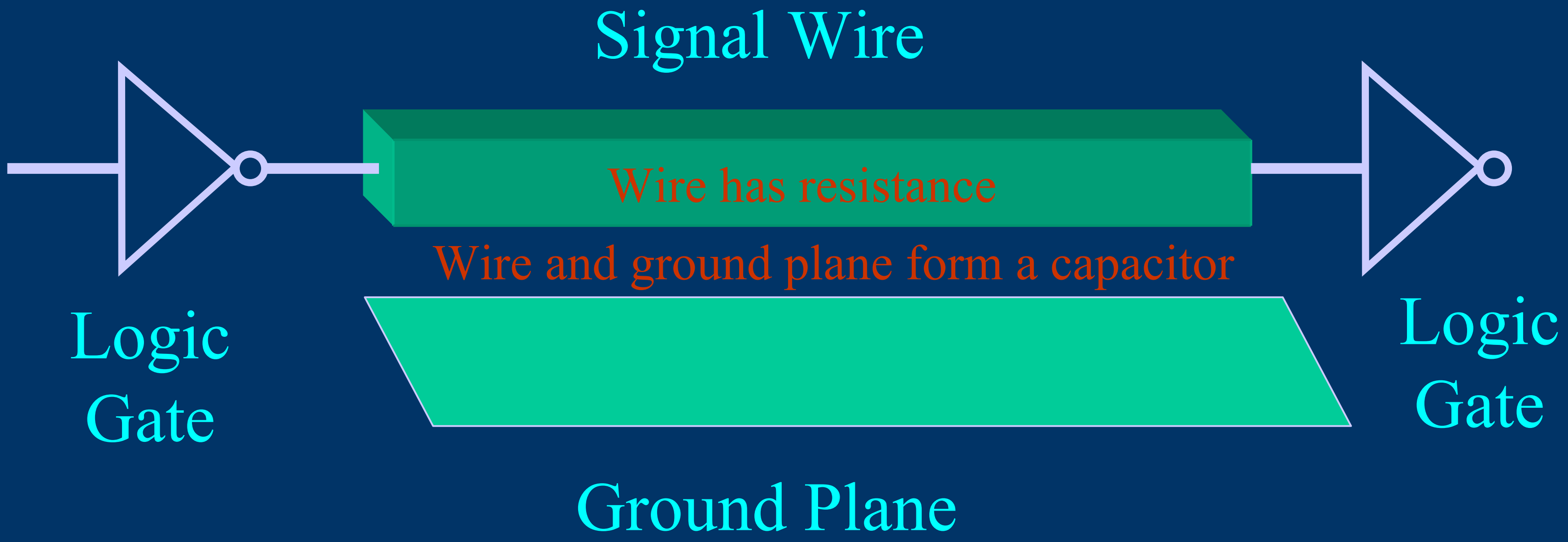
Thanks to Deepak Ramaswamy, Jaime Peraire, Michal Rewienski, and Karen Veroy

Outline

- Initial Value problem examples
  - Signal propagation (circuits with capacitors).
  - Space frame dynamics (struts and masses).
  - Chemical reaction dynamics.
- Investigate the simple finite-difference methods
  - Forward-Euler, Backward-Euler, Trap Rule.
  - Look at the approximations and algorithms
  - Examine properties experimentally.
- Analyze Convergence for Forward-Euler

Application Problems

Signal Transmission in an Integrated Circuit

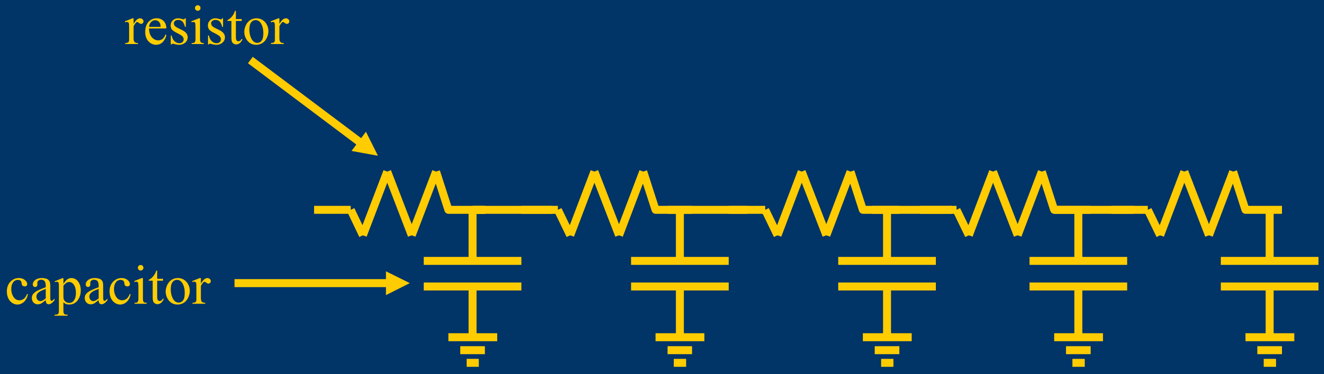


- Metal Wires carry signals from gate to gate.
- How long is the signal delayed?

Application Problems

Signal Transmission in an Integrated Circuit

Circuit Model

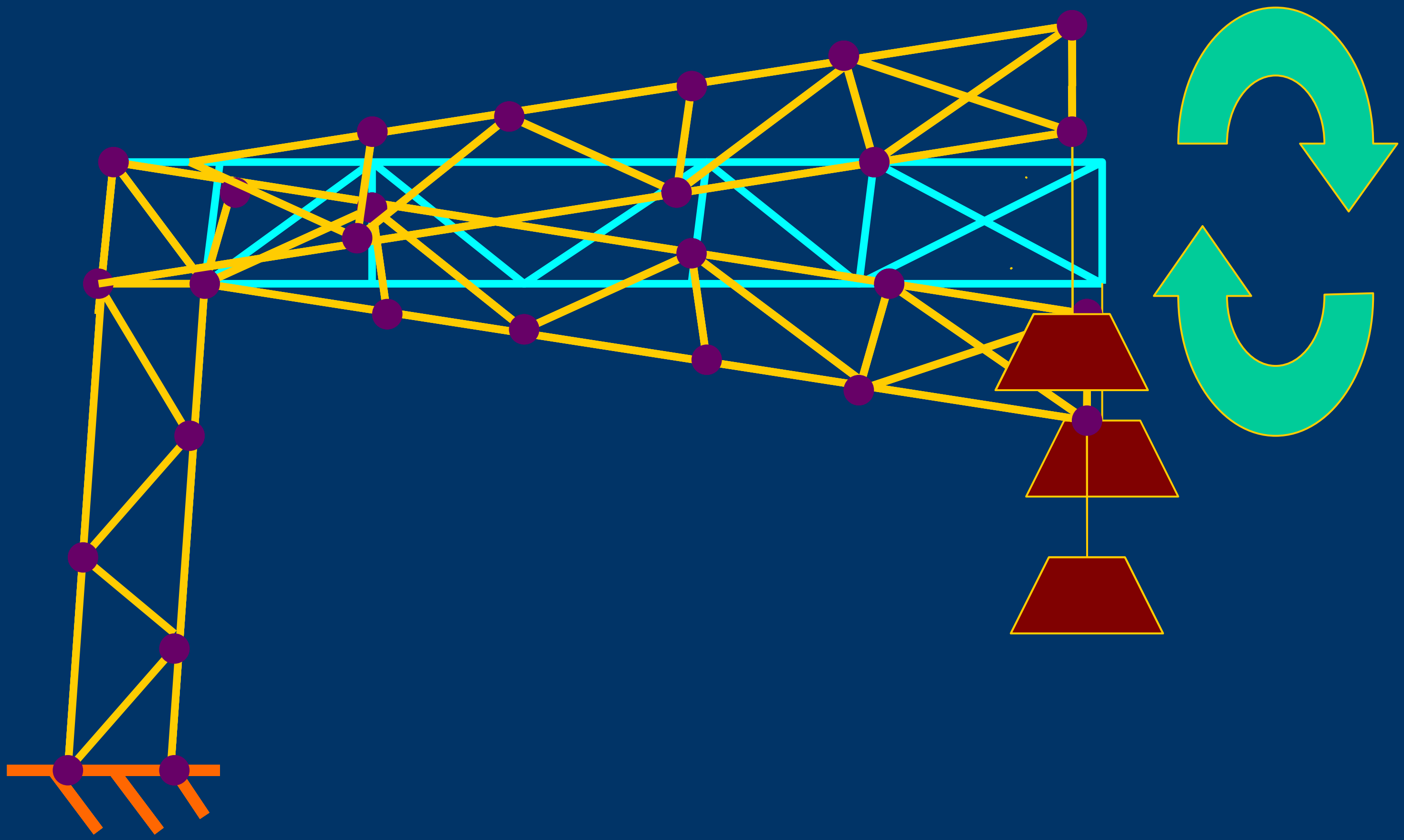


Constructing the Model

- Cut the wire into sections.
- Model wire resistance with resistors.
- Model wire-plane capacitance with capacitors.

Application Problems

Oscillations in a Space Frame

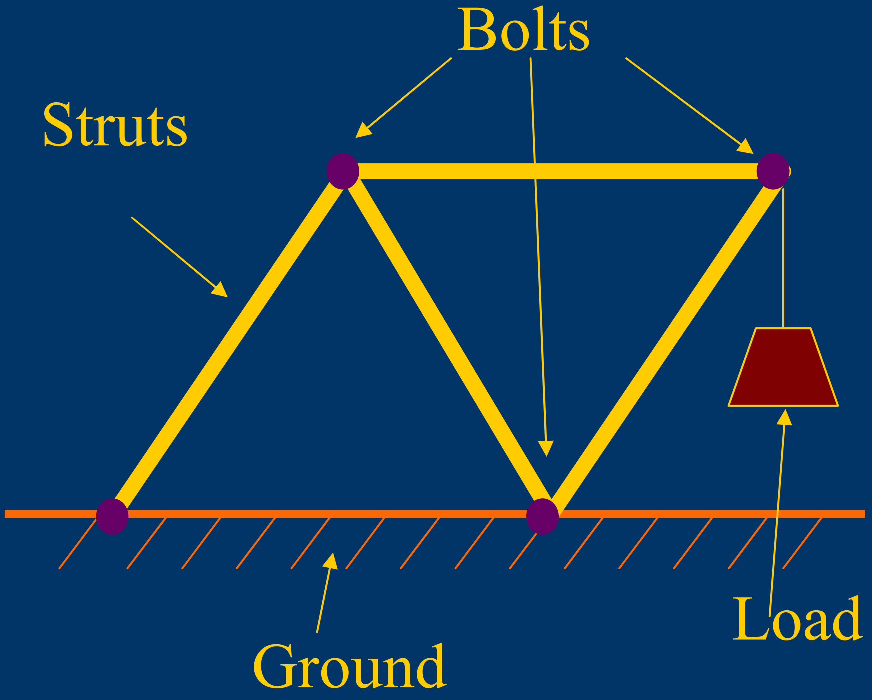


- What is the oscillation amplitude?

Application Problems

Oscillations in a Space Frame

Simplified Structure

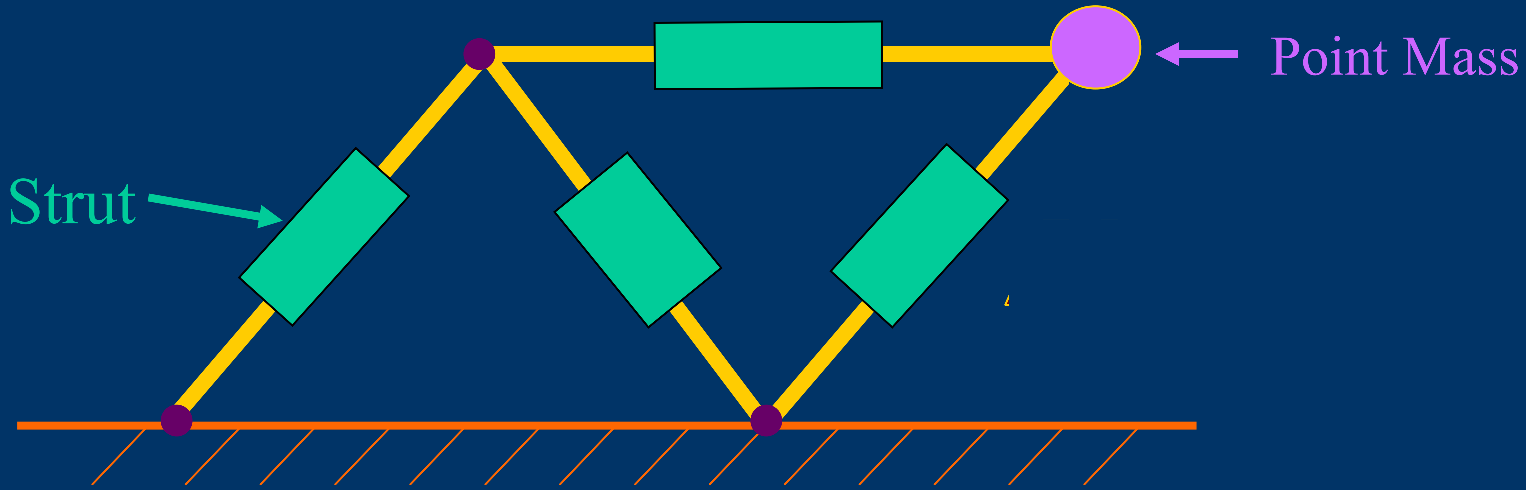


Example Simplified for Illustration

Application Problems

Oscillations in a Space Frame

Modeling with Struts, Joints and Point Masses

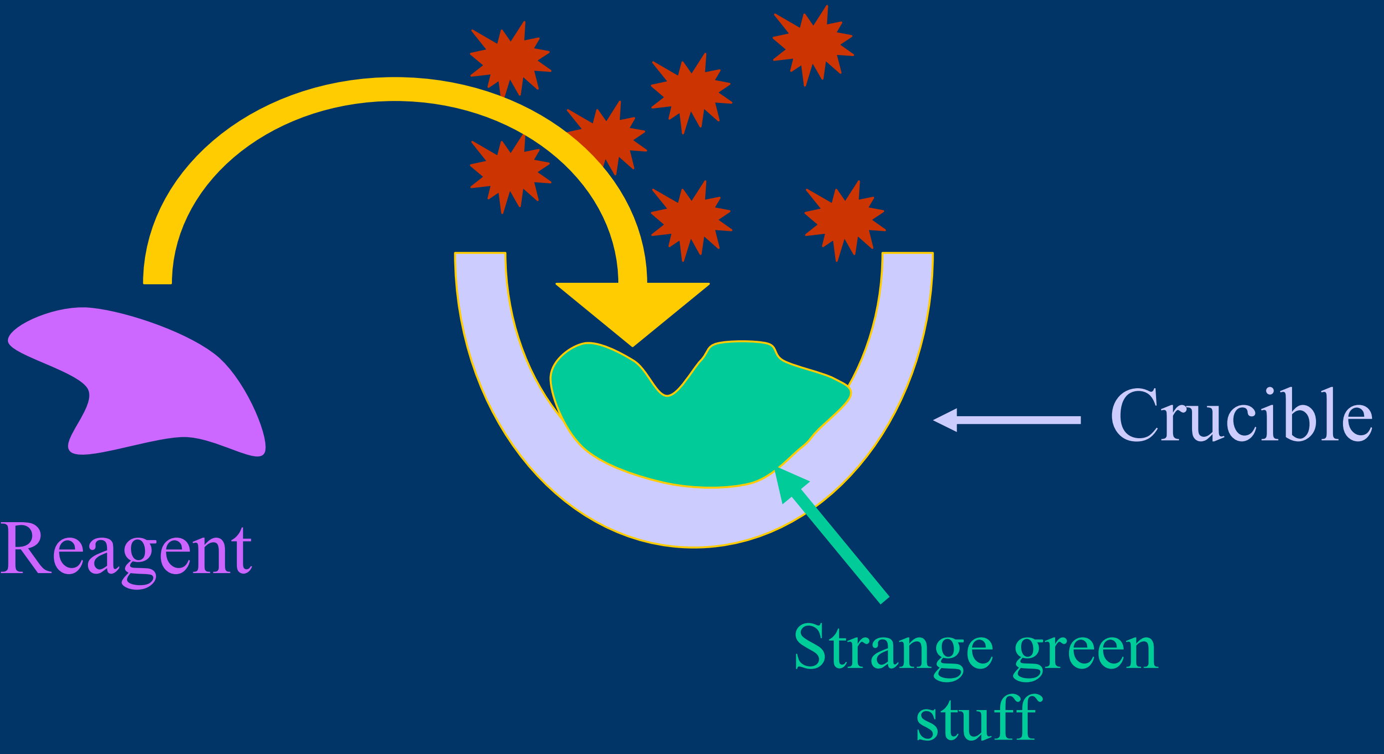


Constructing the Model

- Replace Metal Beams with Struts.
- Replace cargo with point mass.

Application Problems

Chemical Reaction Dynamics

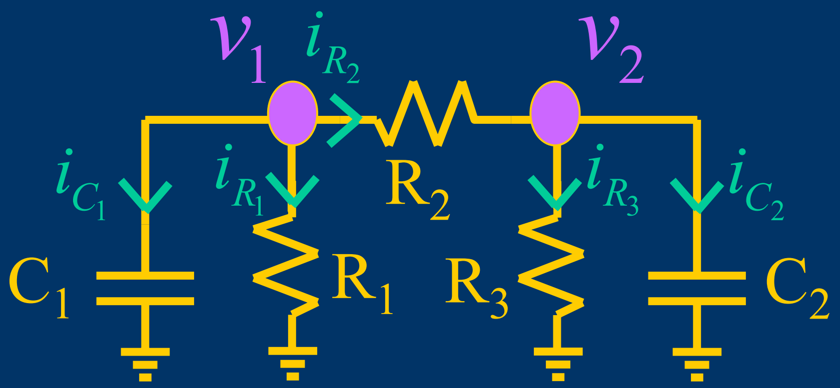


- How fast is product produced?
- Does it explode?

Application Problems

Signal Transmission in an Integrated Circuit

A 2x2 Example



Constitutive Equations

$$i_c = C\frac{dv_c}{dt}$$

$$i_R = \frac{1}{R}v_R$$

Conservation Laws

$$i_{C_1} + i_{R_1} + i_{R_2} = 0$$

$$i_{C_2} + i_{R_3} - i_{R_2} = 0$$

Nodal Equations Yields 2x2 System

$$\begin{bmatrix} C_1 & 0 \\ 0 & C_2 \end{bmatrix} \begin{bmatrix} \frac{dv_1}{dt} \\ \frac{dv_2}{dt} \end{bmatrix} = - \begin{bmatrix} \frac{1}{R_1} + \frac{1}{R_2} & -\frac{1}{R_2} \\ -\frac{1}{R_2} & \frac{1}{R_3} + \frac{1}{R_2} \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix}$$

Application Problems

Signal Transmission in an Integrated Circuit

A 2x2 Example

Let $C_1 = C_2 = 1,\ R_1 = R_3 = 10,\ R_2 = 1$

$$\begin{bmatrix} C_1 & 0 \\ 0 & C_2 \end{bmatrix}\begin{bmatrix}\frac{dv_1}{dt}\\ \frac{dv_2}{dt}\end{bmatrix} = -\begin{bmatrix}\frac{1}{R_1}+\frac{1}{R_2} & -\frac{1}{R_2} \\ -\frac{1}{R_2} & \frac{1}{R_3}+\frac{1}{R_2}\end{bmatrix}\begin{bmatrix}v_1\\ v_2\end{bmatrix} \Longrightarrow \frac{dx}{dt} = \underbrace{\begin{bmatrix}-1.1 & 1.0\\ 1.0 & -1.1\end{bmatrix}}_{A} x$$

Eigenvalues and Eigenvectors

$$A = \begin{bmatrix}\boxed{\begin{matrix}1\\ 1\end{matrix}} & \boxed{\begin{matrix}-1\\ 1\end{matrix}}\end{bmatrix}\begin{bmatrix}-0.1 & 0\\ 0 & -2.1\end{bmatrix}\left(\begin{bmatrix}1 & -1\\ 1 & 1\end{bmatrix}\right)^{-1}$$

eigenvectors

Eigenvalues

An Aside on Eigenanalysis

Consider an ODE: $\frac{dx(t)}{dt} = Ax(t), \quad x(0) = x_0$

Eigendecomposition: $A = \underbrace{\begin{bmatrix} \vdots & \vdots & \vdots \\ E_1 & E_2 & E_n \\ \vdots & \vdots & \vdots \end{bmatrix}}_{E} \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n \end{bmatrix} \begin{bmatrix} \vdots & \vdots & \vdots \\ E_1 & E_2 & E_n \\ \vdots & \vdots & \vdots \end{bmatrix}^{-1}$

Change of variables: $Ey(t) = x(t) \Leftrightarrow y(t) = E^{-1}x(t)$

Substituting: $\frac{dEy(t)}{dt} = AEy(t), \quad Ey(0) = x_0$

Multiply by E^{-1}: $\frac{dy(t)}{dt} = E^{-1}AEy(t) = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n \end{bmatrix} y(t)$

An Aside on Eigenanalysis Continued

From last slide: $$\frac{dy(t)}{dt} = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_n \end{bmatrix} y(t)$$ Decoupled Equations!

Decoupling: $$\frac{dy_i(t)}{dt} = \lambda_i y_i(t) \Rightarrow y_i(t) = e^{\lambda_i t} y(0)$$

Steps for solving $\frac{dx(t)}{dt} = Ax(t), \quad x(0) = x_0$

1) Determine E, λ

2) Compute $y(0) = E^{-1} x_0$

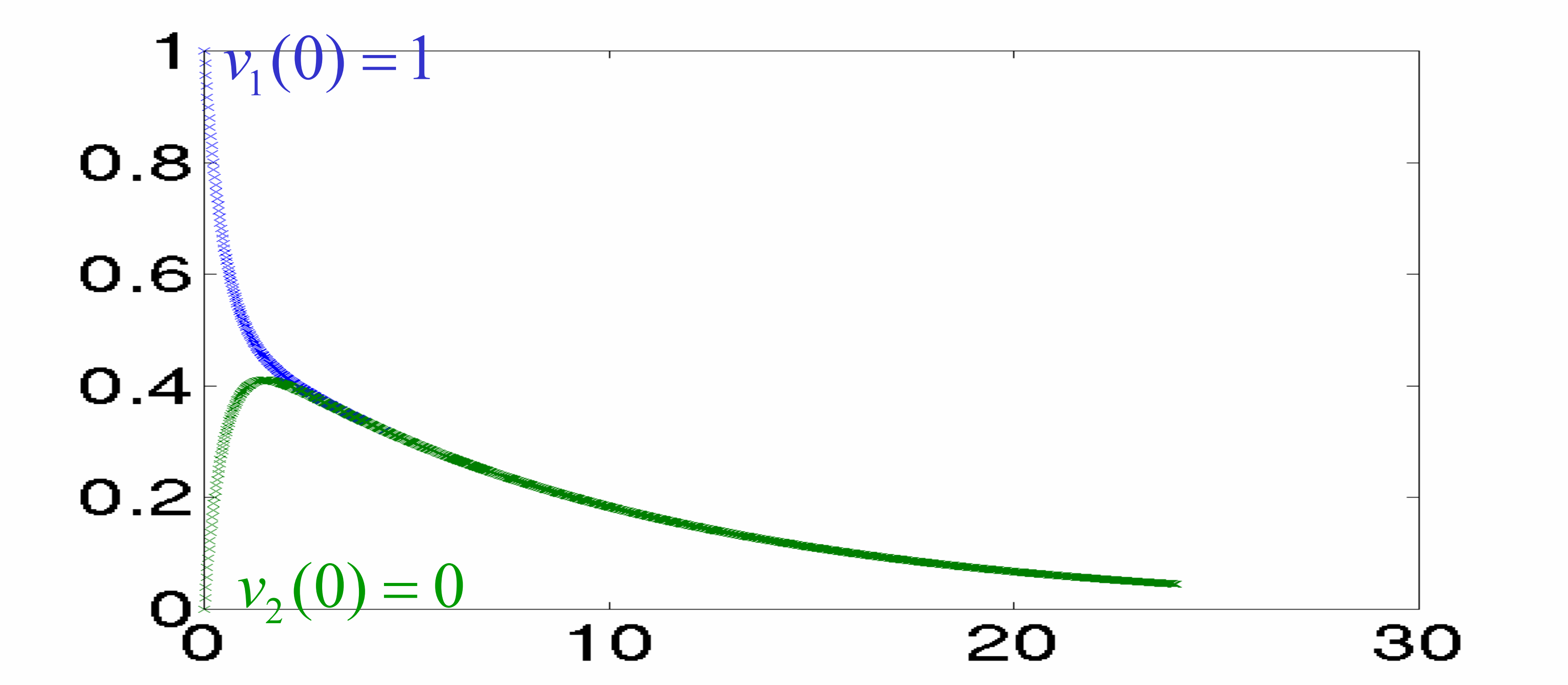
3) Compute $$y(t) = \begin{bmatrix} e^{\lambda_1 t} & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & e^{\lambda_n t} \end{bmatrix} y(0)$$

4) $x(t) = Ey(t)$

Application Problems

Signal Transmission in an Integrated Circuit

A 2x2 Example



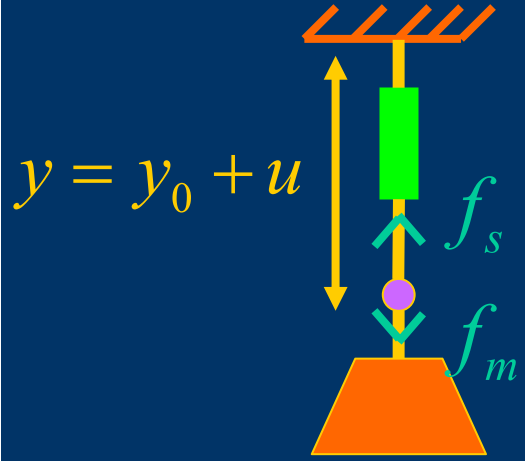
Notice two time scale behavior

- v_1 and v_2 come together quickly (fast eigenmode).
- v_1 and v_2 decay to zero slowly (slow eigenmode).

Application Problems

Struts, Joints and point mass example

A 2x2 Example



Constitutive Equations

$$f_m = M \frac{d^2u}{dt^2}$$

$$f_s = EA_c * \frac{y - y_0}{y_0} = \frac{EA_c}{y_0} u$$

Conservation Law

$$f_s + f_m = 0$$

Define v as velocity (du/dt) to yield a 2x2 System

$$\begin{bmatrix} M & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{dv}{dt} \\ \frac{du}{dt} \end{bmatrix} = \begin{bmatrix} 0 & -\frac{EA_c}{y_0} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} v \\ u \end{bmatrix}$$

Application Problems

Struts, Joints and point mass example

A 2x2 Example

Let $M = 1, \quad \dfrac{EA_c}{y_0} = 1$

$$\begin{bmatrix} M & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \dfrac{dv}{dt} \\ \dfrac{du}{dt} \end{bmatrix} = \begin{bmatrix} 0 & -\dfrac{EA_c}{y_0} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} v \\ u \end{bmatrix} \Longrightarrow \frac{dx}{dt} = \underbrace{\begin{bmatrix} 0 & -1.0 \\ 1.0 & 0 \end{bmatrix}}_{A} x$$

Eigenvalues and Eigenvectors

$$A = \begin{bmatrix} -1 & -1 \\ i & -i \end{bmatrix} \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} \left(\begin{bmatrix} -1 & -1 \\ i & -i \end{bmatrix} \right)^{-1}$$

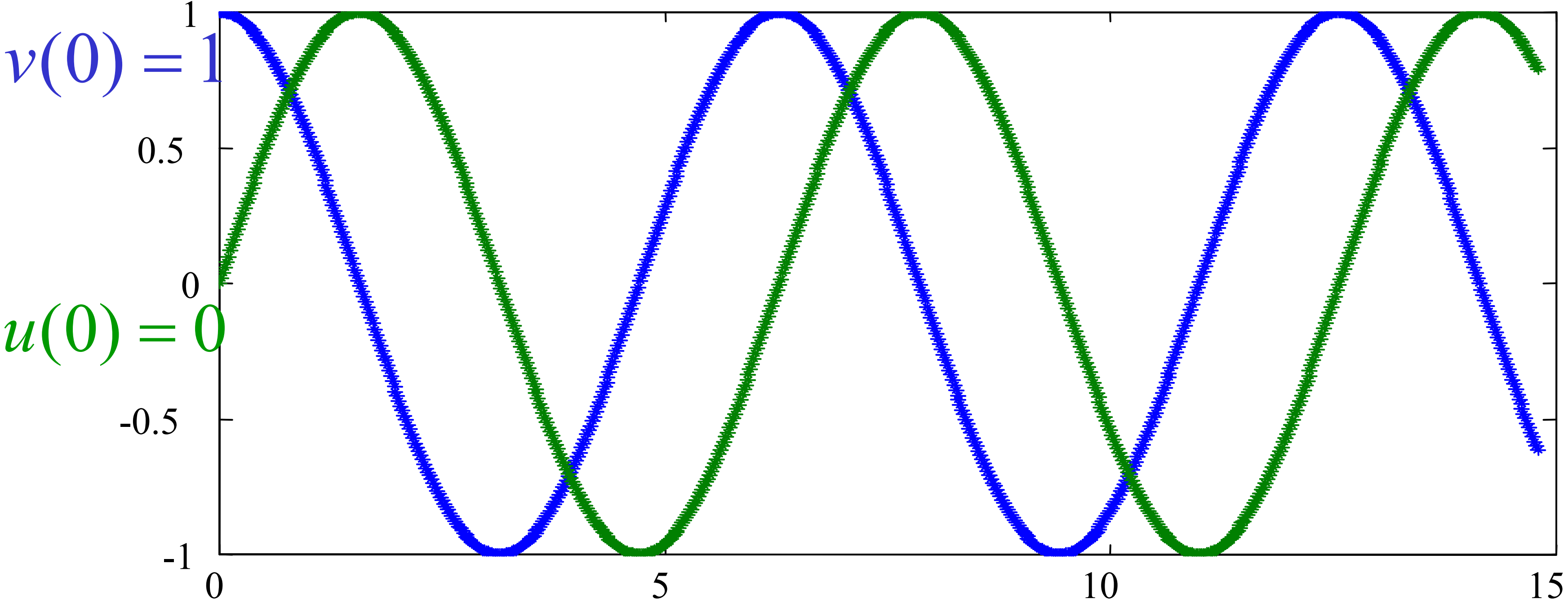
eigenvectors

Eigenvalues

Application Problems

Struts, Joints and point mass example

A 2x2 Example



Note the system has imaginary eigenvalues

- Persistent Oscillation
- Velocity, v, peaks when displacement, u, is zero.

Application Problems

Chemical Reaction Example

A 2x2 Example

Amount of reactant $= R$, the temperature $= T$

$$\frac{dT}{dt} = -T + R$$

More reactant causes temperature to rise, higher temperatures increases heat dissipation causing temperature to fall

$$\frac{dR}{dt} = -R + 4T$$

Higher temperatures raises reaction rates, increased reactant interferes with reaction and slows rate.

Application Problems

Chemical Reaction Example

A 2x2 Example

$$\begin{bmatrix} \dfrac{dT}{dt} \\ \dfrac{dR}{dt} \end{bmatrix} = \begin{bmatrix} -1 & 1 \\ 4 & -1 \end{bmatrix} \begin{bmatrix} T \\ R \end{bmatrix} \quad \Longrightarrow \quad \frac{dx}{dt} = \underbrace{\begin{bmatrix} -1 & 1 \\ 4 & -1 \end{bmatrix}}_{A} x$$

Eigenvalues and Eigenvectors

$$A = \begin{bmatrix} \boxed{\begin{matrix} 1 \\ 2 \end{matrix}} & \boxed{\begin{matrix} -1 \\ 2 \end{matrix}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -3 \end{bmatrix} \left(\begin{bmatrix} 1 & -1 \\ 2 & 2 \end{bmatrix} \right)^{-1}$$

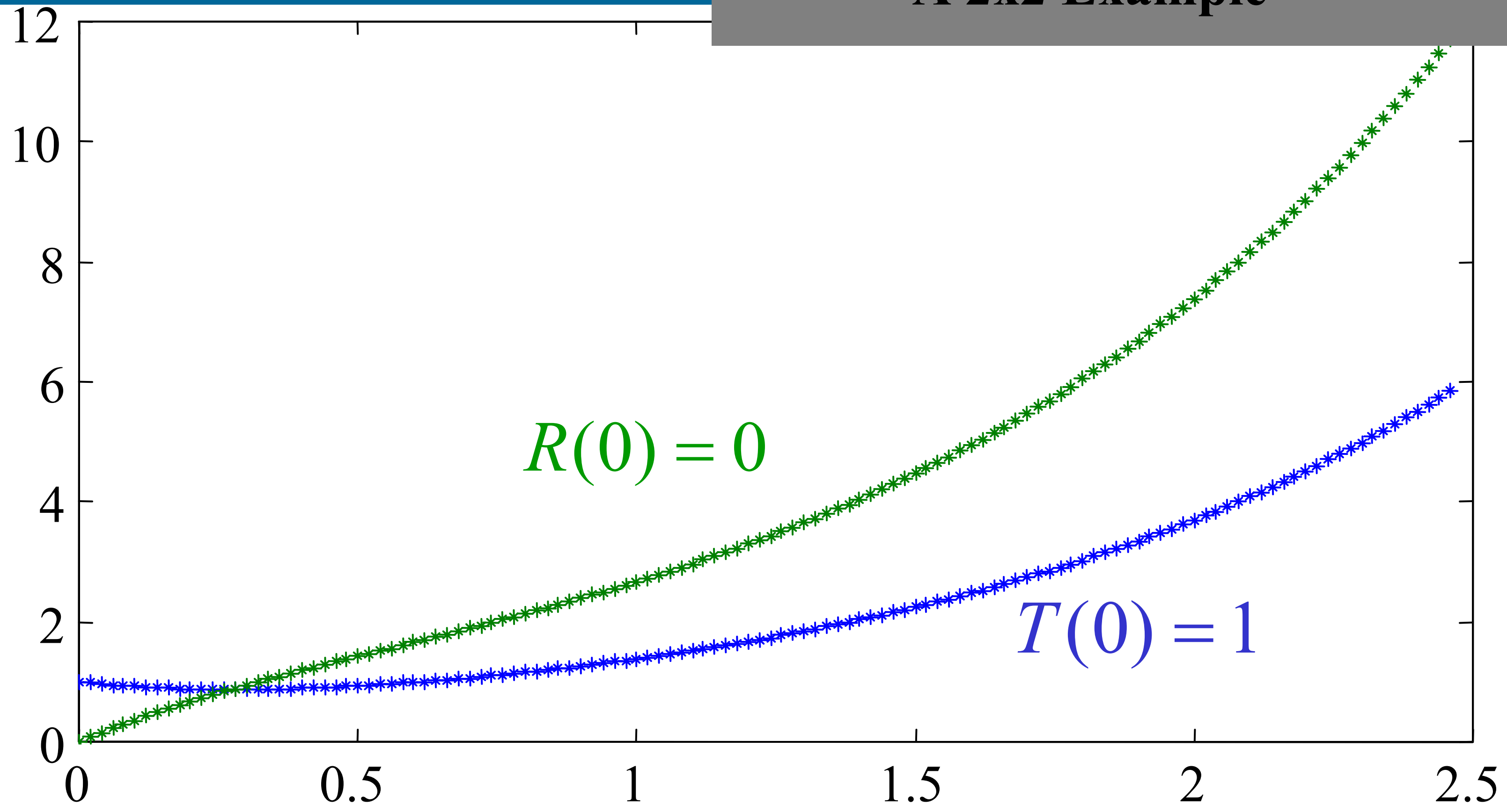
eigenvectors

Eigenvalues

Application Problems

Chemical Reaction Example

A 2x2 Example



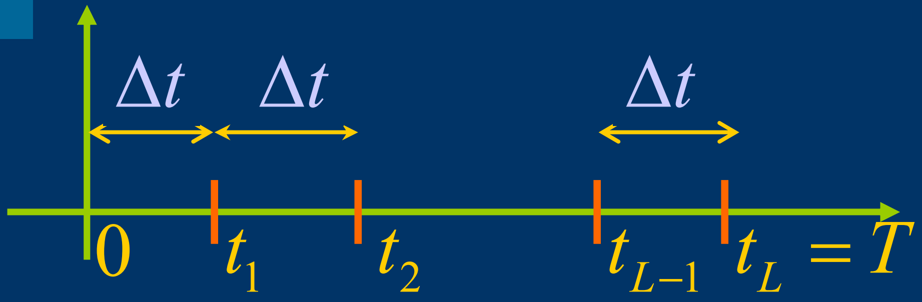
Note the system has a positive eigenvalue

- Solutions grow exponentially with time.

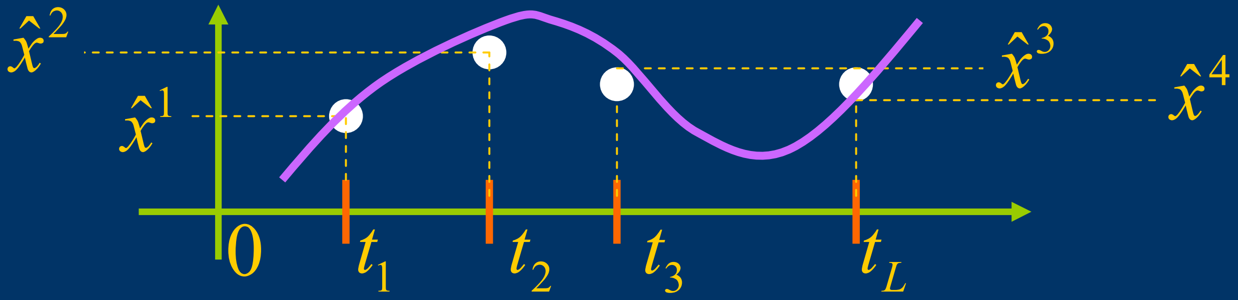
Finite Difference Methods

Basic Concepts

First - Discretize Time



Second - Represent *x(t)* using values at t_i



$$\hat{x}^l \simeq x(t_l)$$

Approx. sol'n

Exact sol'n

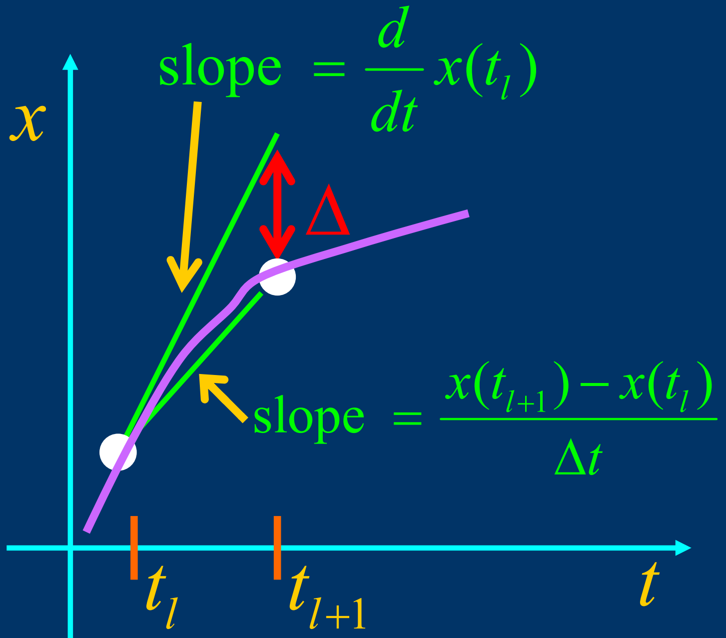
Third - Approximate $\frac{d}{dt}x(t_l)$ using the discrete $\hat{x}^l$'s

Example: $\frac{d}{dt}x(t_l) \simeq \frac{\hat{x}^l - \hat{x}^{l-1}}{\Delta t_l}$ *or* $\frac{\hat{x}^{l+1} - \hat{x}^l}{\Delta t_{l+1}}$

Finite Difference Methods

Basic Concepts

Forward Euler Approximation



$$\frac{d}{dt}x(t_l) = A\,x(t_l) \cong \frac{x(t_{l+1}) - x(t_l)}{\Delta t}$$

or

$$x(t_{l+1}) \cong x(t_l) + \Delta t\,A\,x(t_l)$$

$$\Delta = x(t_{l+1}) - \left(x(t_l) + \Delta t\,A\,x(t_l)\right)$$

Finite Difference Methods

Basic Concepts

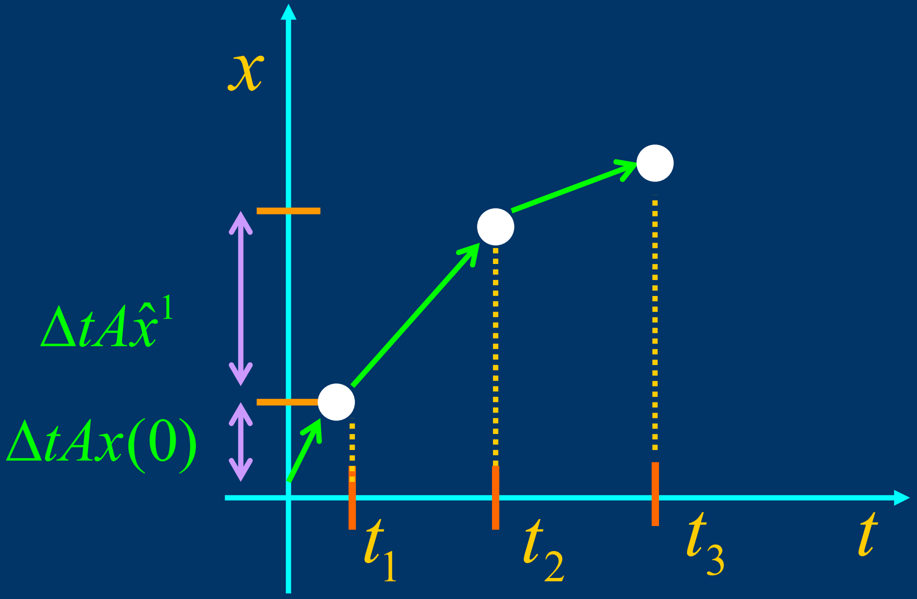
Forward Euler Algorithm

$$x(t_1) \simeq \hat{x}^1 = x(0) + \Delta t A x\left(0\right)$$

$$x(t_2) \simeq \hat{x}^2 = \hat{x}^1 + \Delta t A \hat{x}^1$$

$$\vdots$$

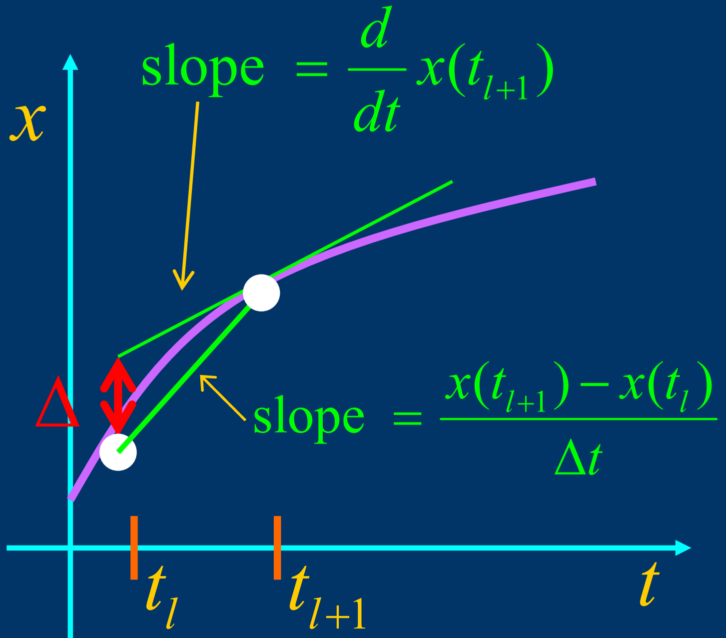
$$x(t_L) \simeq \hat{x}^L = \hat{x}^{L-1} + \Delta t A \hat{x}^{L-1}$$



Finite Difference Methods

Basic Concepts

Backward Euler Approximation



$$\frac{d}{dt}x(t_{l+1}) = A\,x(t_{l+1}) \cong \frac{x(t_{l+1}) - x(t_l)}{\Delta t}$$

or

$$x(t_{l+1}) \cong x(t_l) + \Delta t\, A\, x(t_{l+1})$$

$$\Delta = x(t_{l+1}) - \left(x(t_l) + \Delta t\, A\, x(t_{l+1})\right)$$

Finite Difference Methods

Basic Concepts

Backward Euler Algorithm

Solve with Gaussian Elimination

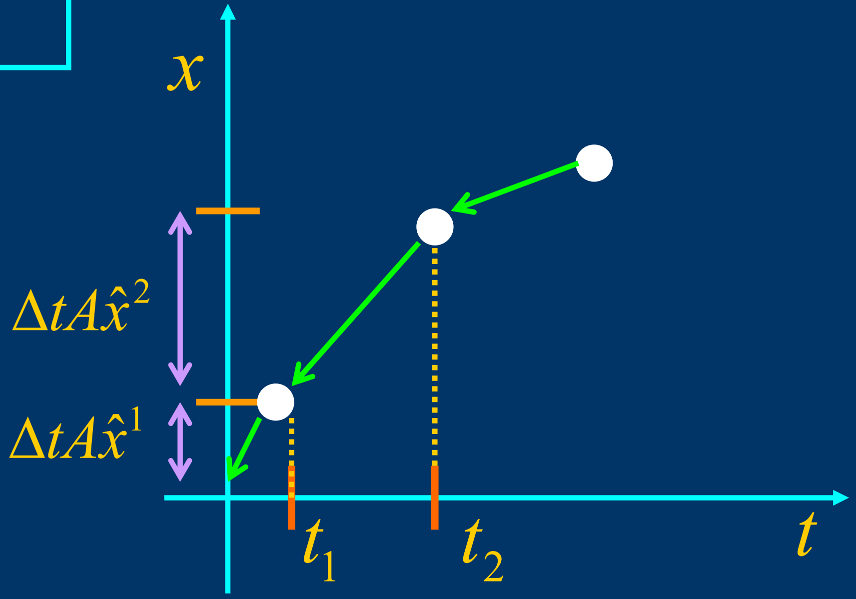
$$x(t_1) \simeq \hat{x}^1 = x(0) + \Delta t A \hat{x}^1$$

$$\Rightarrow [I - \Delta t A]\,\hat{x}^1 = x(0)$$

$$x(t_2) \simeq \hat{x}^2 = [I - \Delta t A]^{-1}\,\hat{x}^1$$

$$\vdots$$

$$x(t_L) \simeq \hat{x}^L = [I - \Delta t A]^{-1}\,\hat{x}^{L-1}$$



Finite Difference Methods

Basic Concepts

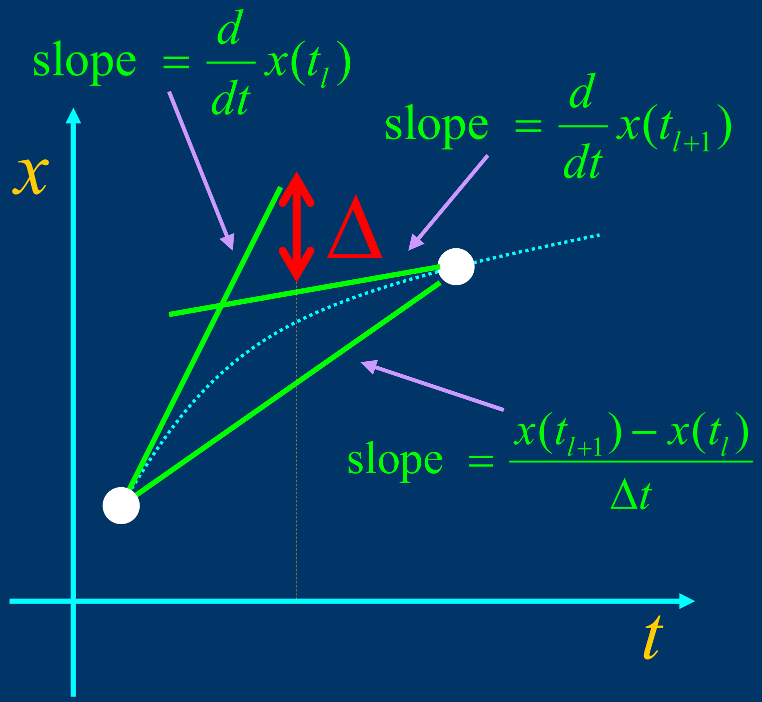
Trapezoidal Rule

$$\frac{1}{2}\left(\frac{d}{dt}x(t_{l+1})+\frac{d}{dt}x(t_l)\right)$$

$$=\frac{1}{2}\left(Ax(t_{l+1})+Ax(t_l)\right)$$

$$\simeq\frac{x(t_{l+1})-x(t_l)}{\Delta t}$$

$$x(t_{l+1})\simeq x(t_l)+\frac{1}{2}\Delta t A(x(t_{l+1})+x(t_l))$$



$$\Delta=\left(x(t_{l+1})-\frac{1}{2}\Delta t Ax(t_l)\right)-\left(x(t_l)+\frac{1}{2}\Delta t Ax(t_{l+1})\right)$$

Finite Difference Methods

Basic Concepts

Trapezoidal Rule Algorithm

Solve with Gaussian Elimination

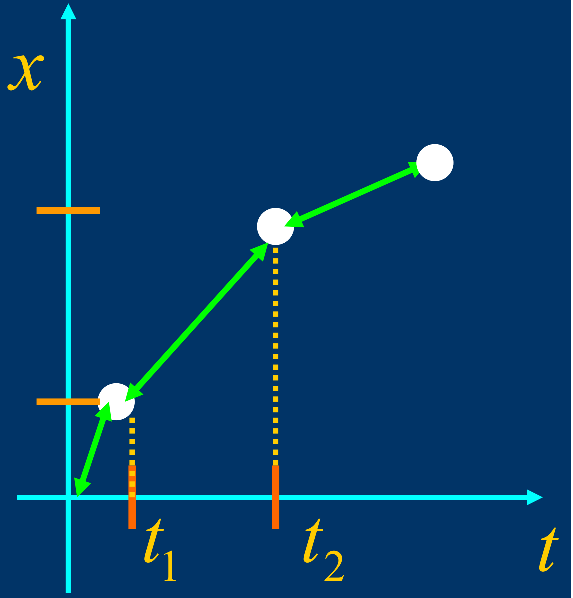
$$x(t_1) \simeq \hat{x}^1 = x(0) + \frac{\Delta t}{2}\left(Ax(0) + A\hat{x}^1\right)$$

$$\Rightarrow \left[I - \frac{\Delta t}{2}A\right]\hat{x}^1 = \left[I + \frac{\Delta t}{2}A\right]x(0)$$

$$x(t_2) \simeq \hat{x}^2 = \left[I - \frac{\Delta t}{2}A\right]^{-1}\left[I + \frac{\Delta t}{2}A\right]\hat{x}^1$$

$$\vdots$$

$$x(t_L) \simeq \hat{x}^L = \left[I - \frac{\Delta t}{2}A\right]^{-1}\left[I + \frac{\Delta t}{2}A\right]\hat{x}^{L-1}$$



Finite Difference Methods

Basic Concepts

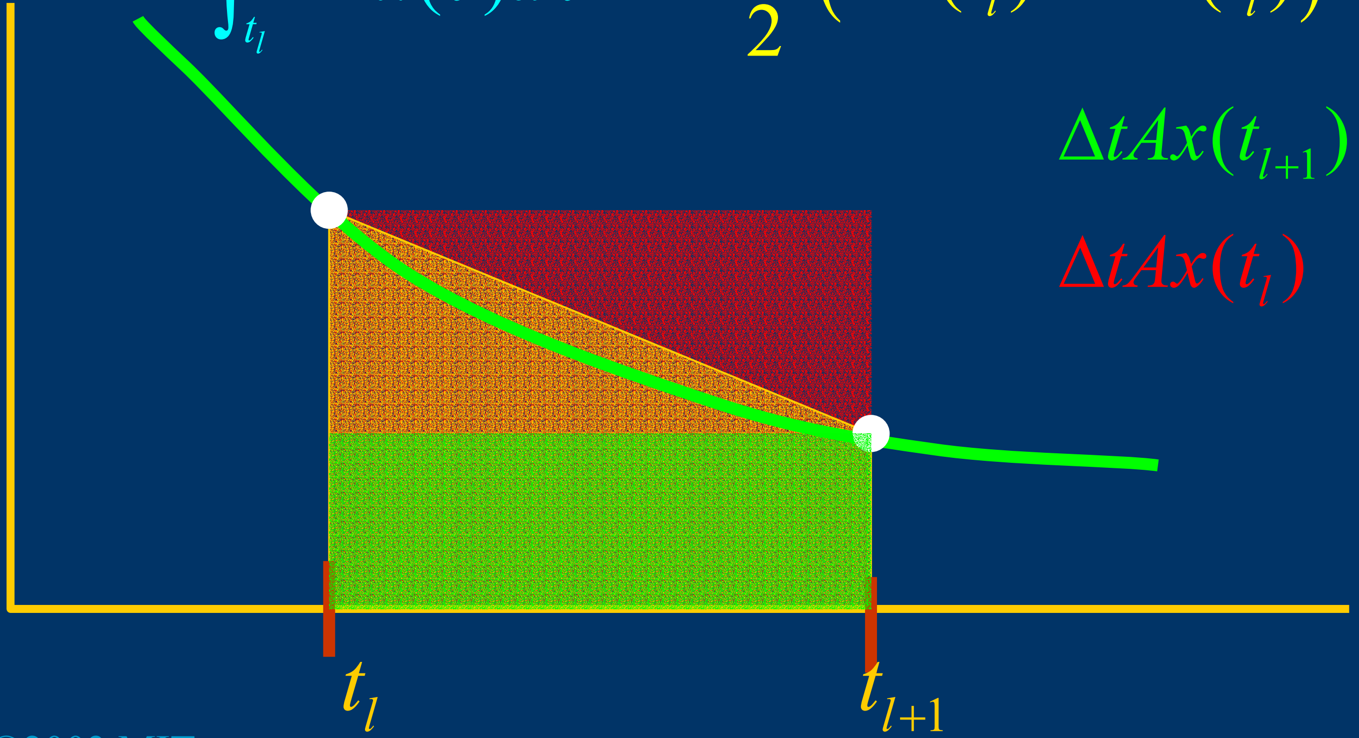
Numerical Integration View

$$\frac{d}{dt}x(t) = Ax(t) \Rightarrow x(t_{l+1}) = x(t_l) + \int_{t_l}^{t_{l+1}} Ax(\tau)d\tau$$

$$\int_{t_l}^{t_{l+1}} Ax(\tau)d\tau \approx \quad \frac{\Delta t}{2}\left(Ax(t_l) + Ax(t_l)\right) \quad \text{Trap}$$

$$\Delta t A x(t_{l+1}) \quad \text{BE}$$

$$\Delta t A x(t_l) \quad \text{FE}$$



Finite Difference Methods

Basic Concepts

Summary

Trap Rule, Forward-Euler, Backward-Euler

- Are all one-step methods
- $\hat{x}^{l}$ is computed using only $\hat{x}^{l-1}$, not $\hat{x}^{l-2}, \hat{x}^{l-3}$, etc.

Forward-Euler is simplest

- No equation solution → explicit method.
- Boxcar approximation to integral

Backward-Euler is more expensive

- Equation solution each step → implicit method

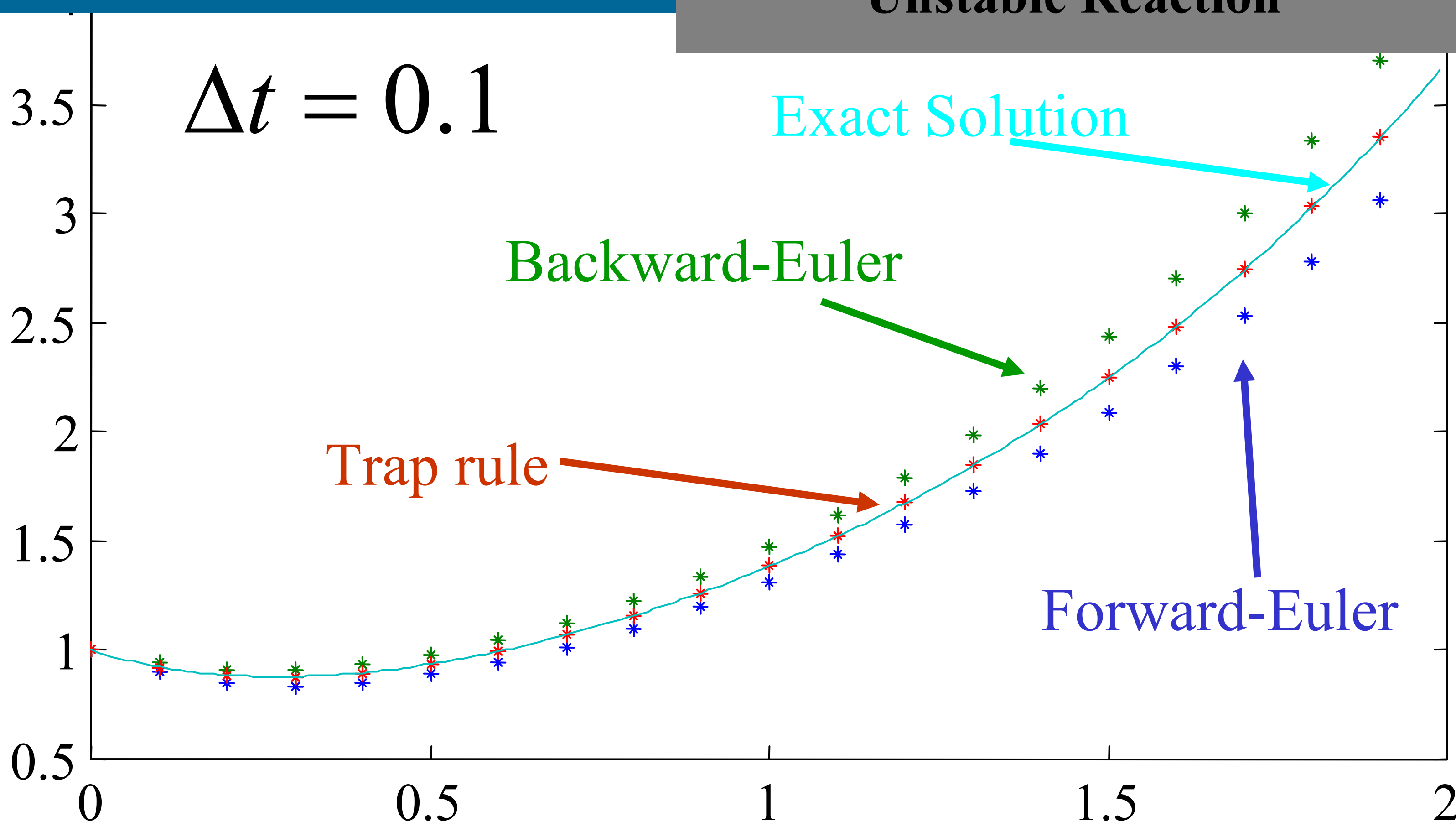
Trapezoidal Rule might be more accurate

- Equation solution each step → implicit method
- Trapezoidal approximation to integral

Finite Difference Methods

Numerical Experiments

Unstable Reaction

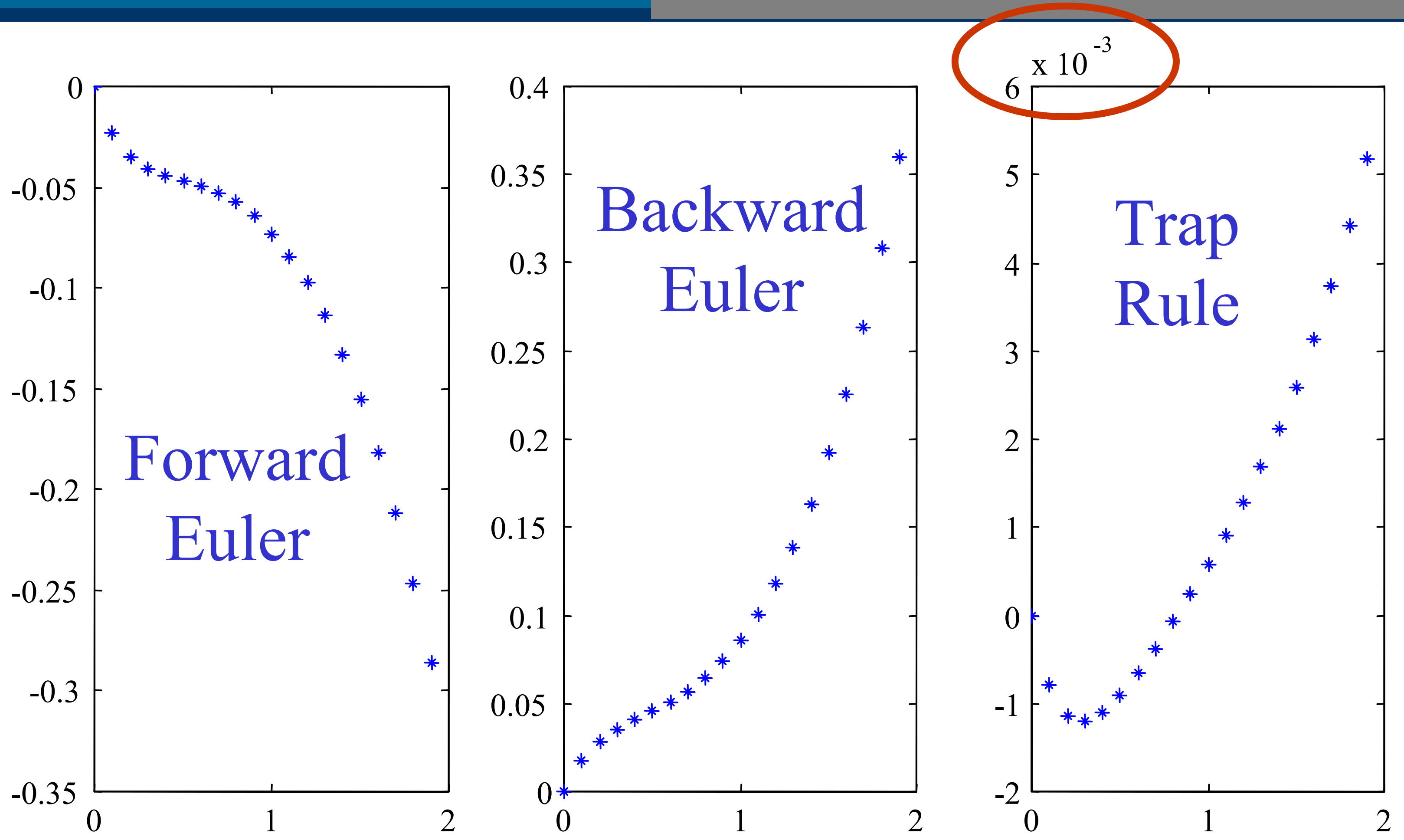


FE and BE results have larger errors than Trap Rule, and the errors grow with time.

Finite Difference Methods

Numerical Experiments

Unstable Reaction-Error Plots

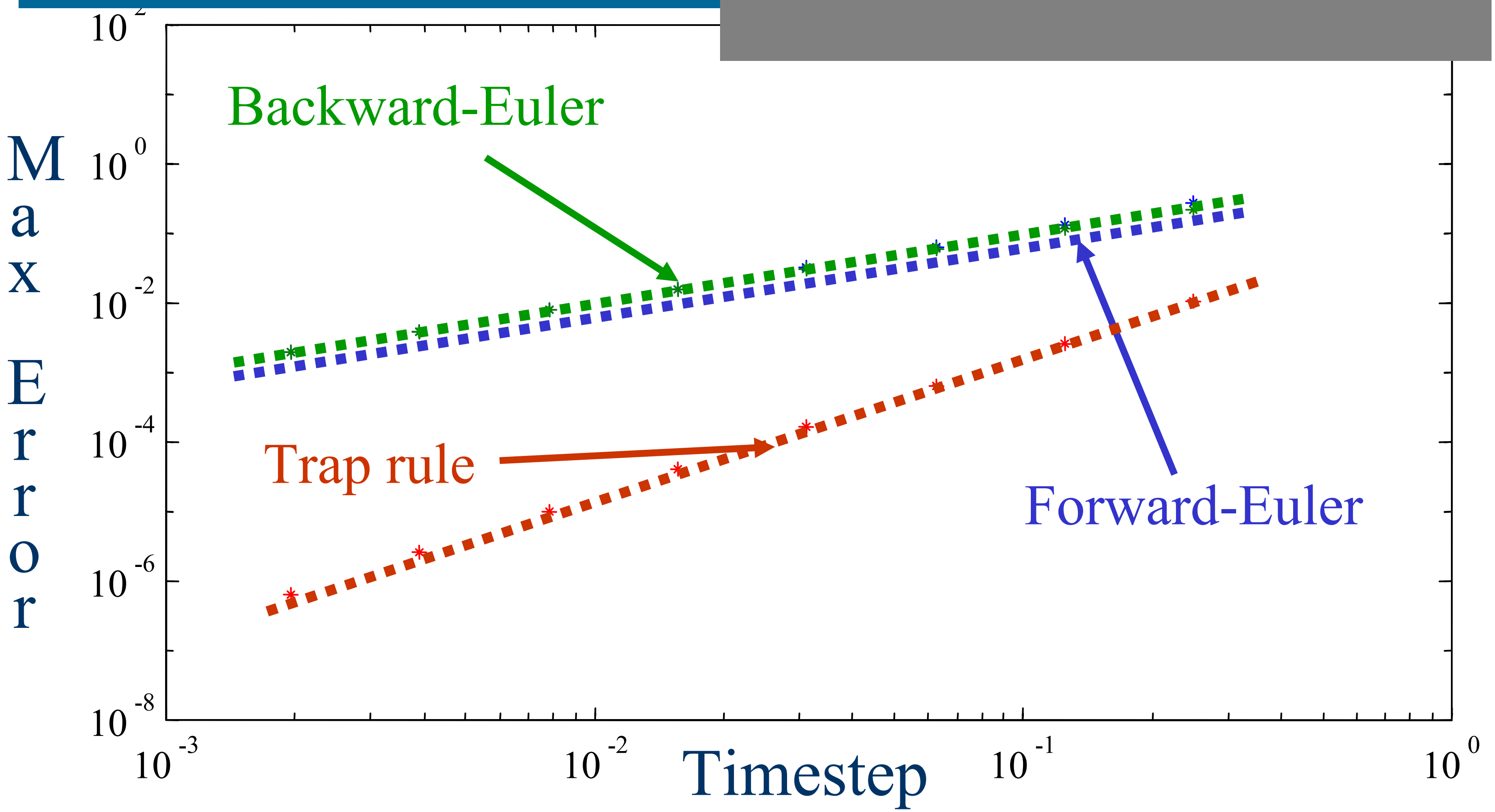


All methods have errors which grow exponentially

Finite Difference Methods

Numerical Experiments

Unstable Reaction-Convergence

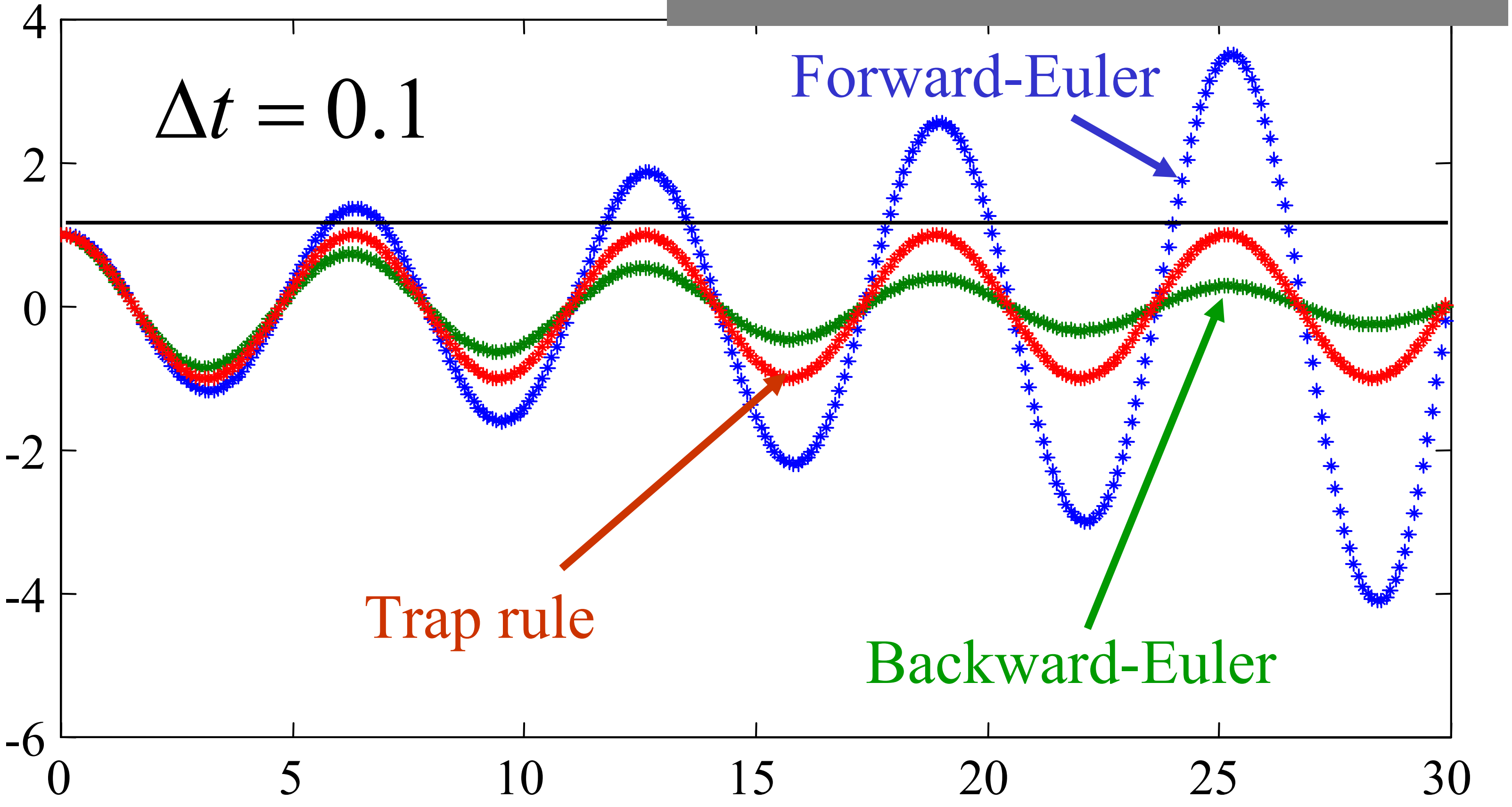


For FE and BE, $Error \propto \Delta t$ For Trap, $Error \propto \left(\Delta t\right)^2$

Finite Difference Methods

Numerical Experiments

Oscillating Strut and Mass

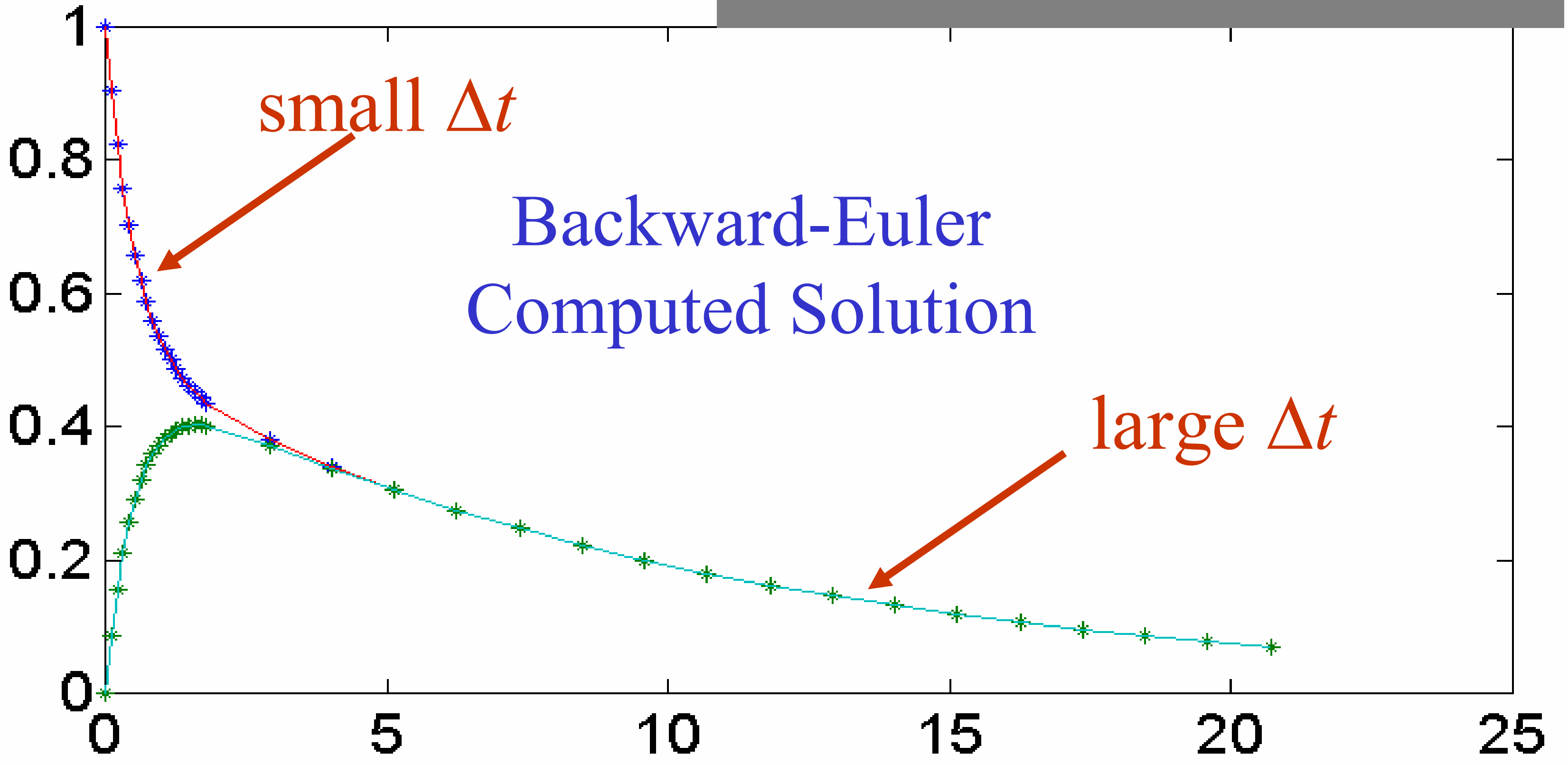


Why does FE result grow, BE result decay and the Trap rule preserve oscillations

Finite Difference Methods

Numerical Experiments

Two timescale RC Circuit

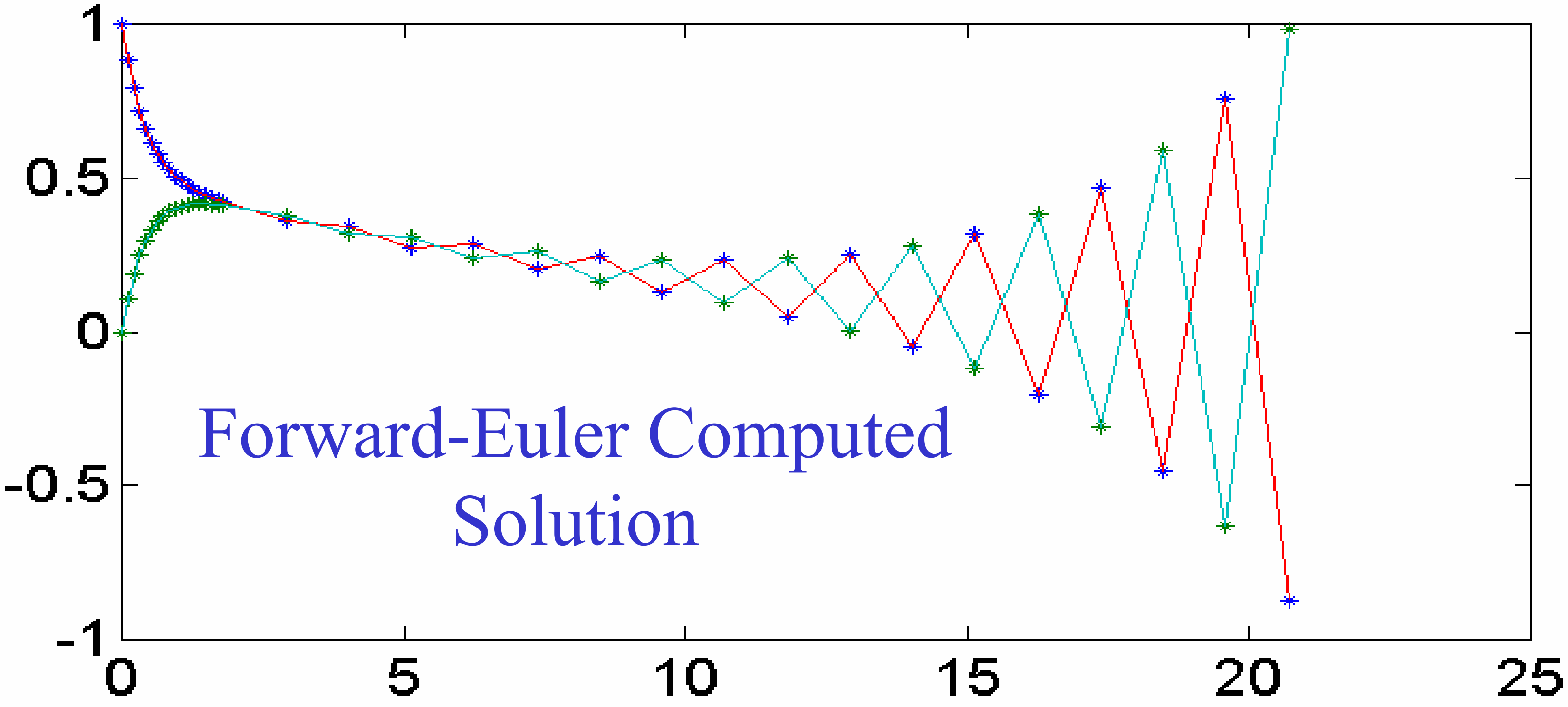


With Backward-Euler it is easy to use small timesteps for the fast dynamics and then switch to large timesteps for the slow decay

Finite Difference Methods

Numerical Experiments

Two timescale RC Circuit



Forward-Euler Computed Solution

The Forward-Euler is accurate for small timesteps, but goes unstable when the timestep is enlarged

Numerical Experiments

Summary

- Convergence
  - Did the computed solution approach the exact solution?
  - Why did the trap rule approach faster than BE or FE?
- Energy Preservation
  - Why did BE produce a decaying oscillation?
  - Why did FE produce a growing oscillation?
  - Why did trap rule maintain oscillation amplitude?
- Two timeconstant (stiff) problems
  - Why did FE go unstable when the timestep increased?

We will focus on convergence today

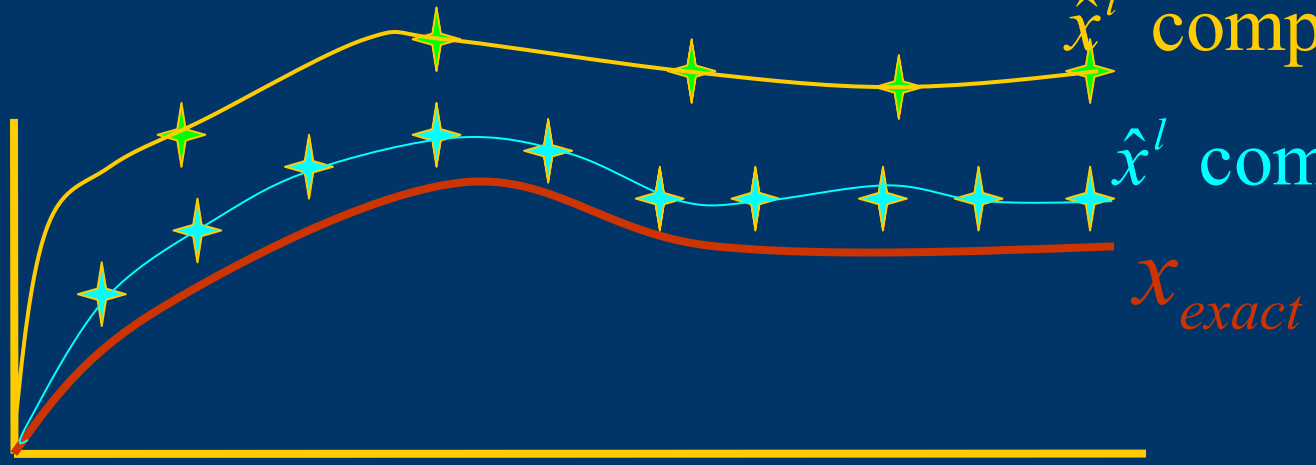
Finite Difference Methods

Convergence Analysis

Convergence Definition

Definition: A finite-difference method for solving initial value problems on [0,T] is said to be convergent if given any A and any initial condition

$$\max_{l \in \left[0, \frac{T}{\Delta t}\right]} \left\| \hat{x}^l - x(l\Delta t) \right\| \to 0 \text{ as } \Delta t \to 0$$



Finite Difference Methods

Convergence Analysis

Order-p convergence

Definition: A finite-difference method for solving initial value problems on [0,T] is said to be order p convergent if given any A and any initial condition

$$\max_{l \in \left[0, \frac{T}{\Delta t}\right]} \left\| \hat{x}^l - x\left(l\Delta t\right) \right\| \leq C\left(\Delta t\right)^p$$

for all Δt less than a given Δt_0

Forward- and Backward-Euler are order 1 convergent
Trapezoidal Rule is order 2 convergent

Convergence Analysis

Two Conditions for Convergence

1) Local Condition: One step errors are small (consistency)

Typically verified using Taylor Series

2) Global Condition: The single step errors do not grow too quickly (stability)

All one-step methods are stable in this sense.

Finite Difference Methods

Convergence Analysis

Consistency Definition

Definition: A one-step method for solving initial value problems on an interval [0,T] is said to be consistent if for any A and any initial condition

$$\frac{\left\| \hat{x}^{1} - x\left(\Delta t\right) \right\|}{\Delta t} \rightarrow 0 \text{ as } \Delta t \rightarrow 0$$

Finite Difference Methods

Convergence Analysis

Consistency for Forward Euler

Forward-Euler definition

$$\hat{x}^1 = x(0) + \Delta t A x(0)$$

$\tau \in [0, \Delta t]$

Expanding in t about zero yields

$$x(\Delta t) = x(0) + \Delta t \frac{dx(0)}{dt} + \frac{(\Delta t)^2}{2} \frac{d^2 x(\tau)}{dt^2}$$

Noting that $\frac{d}{dt} x(0) = Ax(0)$ and subtracting

$$\left\| \hat{x}^1 - x(\Delta t) \right\| \le \frac{(\Delta t)^2}{2} \left\| \frac{d^2 x(\tau)}{dt^2} \right\|$$

Proves the theorem if derivatives of x are bounded

Convergence Analysis for Forward Euler

Forward-Euler definition

$$\hat{x}^{l+1} = \hat{x}^{l} + \Delta t A \hat{x}^{l}$$

Expanding in t about $l\Delta t$ yields

$$x\left(\left(l+1\right)\Delta t\right) = x\left(l\Delta t\right) + \Delta t A x\left(l\Delta t\right) + e^{l}$$

where e^{l} is the "one-step" error bounded by

$$e^{l} \leq C\left(\Delta t\right)^{2}, \text{ where } C = 0.5 \max_{\tau \in [0,T]} \left\| \frac{d^{2}x\left(\tau\right)}{dt^{2}} \right\|$$

Finite Difference Methods

Convergence Analysis

Convergence Analysis for Forward Euler Continued

Subtracting the previous slide equations

$$\hat{x}^{l+1} - x\left(\left(l+1\right)\Delta t\right) = \left(I + \Delta t A\right)\left(\hat{x}^{l} - x\left(l\Delta t\right)\right) + e^{l}$$

Define the "Global" error $E^{l} \equiv x^{l} - \hat{x}\left(l\Delta t\right)$

$$E^{l+1} = \left(I + \Delta t A\right)E^{l} + e^{l}$$

Taking norms and using the bound on e^{l}

$$\left\|E^{l+1}\right\| \leq \left\|\left(I + \Delta t A\right)\right\|\left\|E^{l}\right\| + C\left(\Delta t\right)^{2}$$

$$\leq \left(1 + \Delta t\left\|A\right\|\right)\left\|E^{l}\right\| + C\left(\Delta t\right)^{2}$$

Finite Difference Methods

Convergence Analysis

A helpful bound on difference equations

A lemma bounding difference equation solutions

If $\left|u^{l+1}\right| \leq (1+\varepsilon)\left|u^{l}\right| + b, \quad u^{0} = 0, \quad \varepsilon > 0$

Then $\left|u^{l}\right| \leq \dfrac{e^{\varepsilon l}}{\varepsilon}|b|$

To prove, first write u^{l} as a power series and sum

$$\left|u^{l}\right| \leq \sum_{j=0}^{l-1}(1+\varepsilon)^{j}\,|b| = \frac{1-(1+\varepsilon)^{j}}{1-(1+\varepsilon)}|b|$$

Finite Difference Methods

Convergence Analysis

A helpful bound on difference equations cont.

To finish, note $(1+\varepsilon) \le e^{\varepsilon} \Rightarrow (1+\varepsilon)^l \le e^{\varepsilon l}$

$$\left|u^l\right| \le \frac{1-(1+\varepsilon)^j}{1-(1+\varepsilon)}|b| = \frac{(1+\varepsilon)^j - 1}{\varepsilon}|b| \le \frac{e^{\varepsilon l}}{\varepsilon}|b|$$

Mapping the global error equation to the lemma

$$\left\|E^{l+1}\right\| \le \left(1+\underbrace{\Delta t\left\|A\right\|}_{\varepsilon}\right)\left\|E^l\right\| + \underbrace{C\left(\Delta t\right)^2}_{b}$$

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Back to Forward Euler Convergence analysis.

Applying the lemma and cancelling terms

$$\left\|E^l\right\| \le \left(1+\underbrace{\Delta t\left\|A\right\|}_{\varepsilon}\right)\left\|E^{l-1}\right\| + \underbrace{C\left(\Delta t\right)^2}_{b} \le \frac{e^{l\Delta t\|A\|}}{\cancel{\Delta t}\left\|A\right\|}C\left(\Delta t\right)^{\cancel{2}}$$

Finally noting that $l\Delta t \le T$,

$$\max_{l\in[0,L]}\left\|E^l\right\| \le e^{\|A\|T}\frac{C}{\left\|A\right\|}\Delta t$$

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Convergence Analysis

Observations about the forward-Euler analysis.

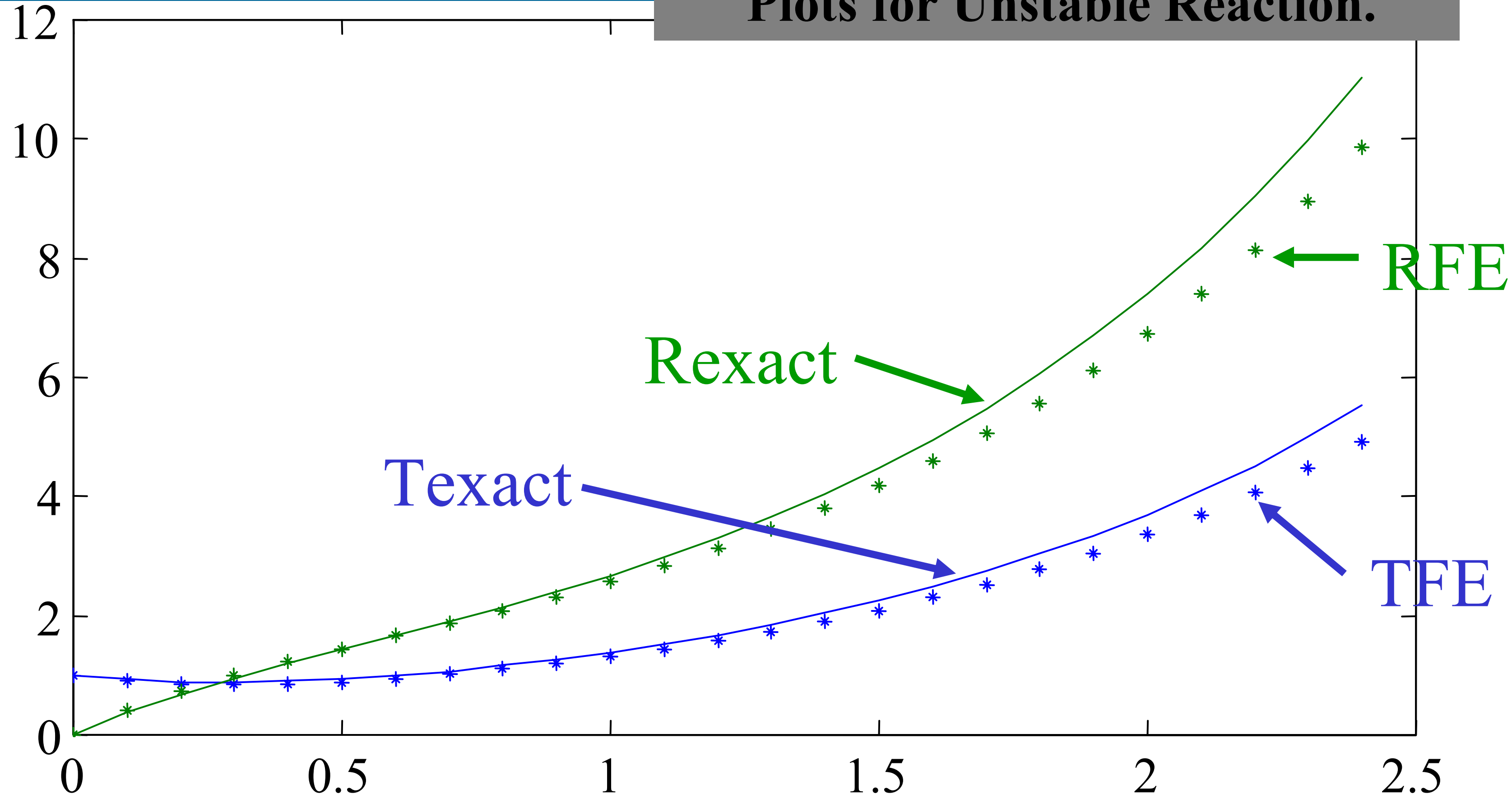
$$\max_{l \in [0,L]} \left\| E^l \right\| \leq e^{\|A\| T} \frac{C}{\|A\|} \Delta t$$

- forward-Euler is order 1 convergent
- The bound grows exponentially with time interval
- C is related to the solution second derivative
- The bound grows exponentially fast with norm(A).

Finite Difference Methods

Convergence Analysis

Exact and forward-Euler(FE) Plots for Unstable Reaction.

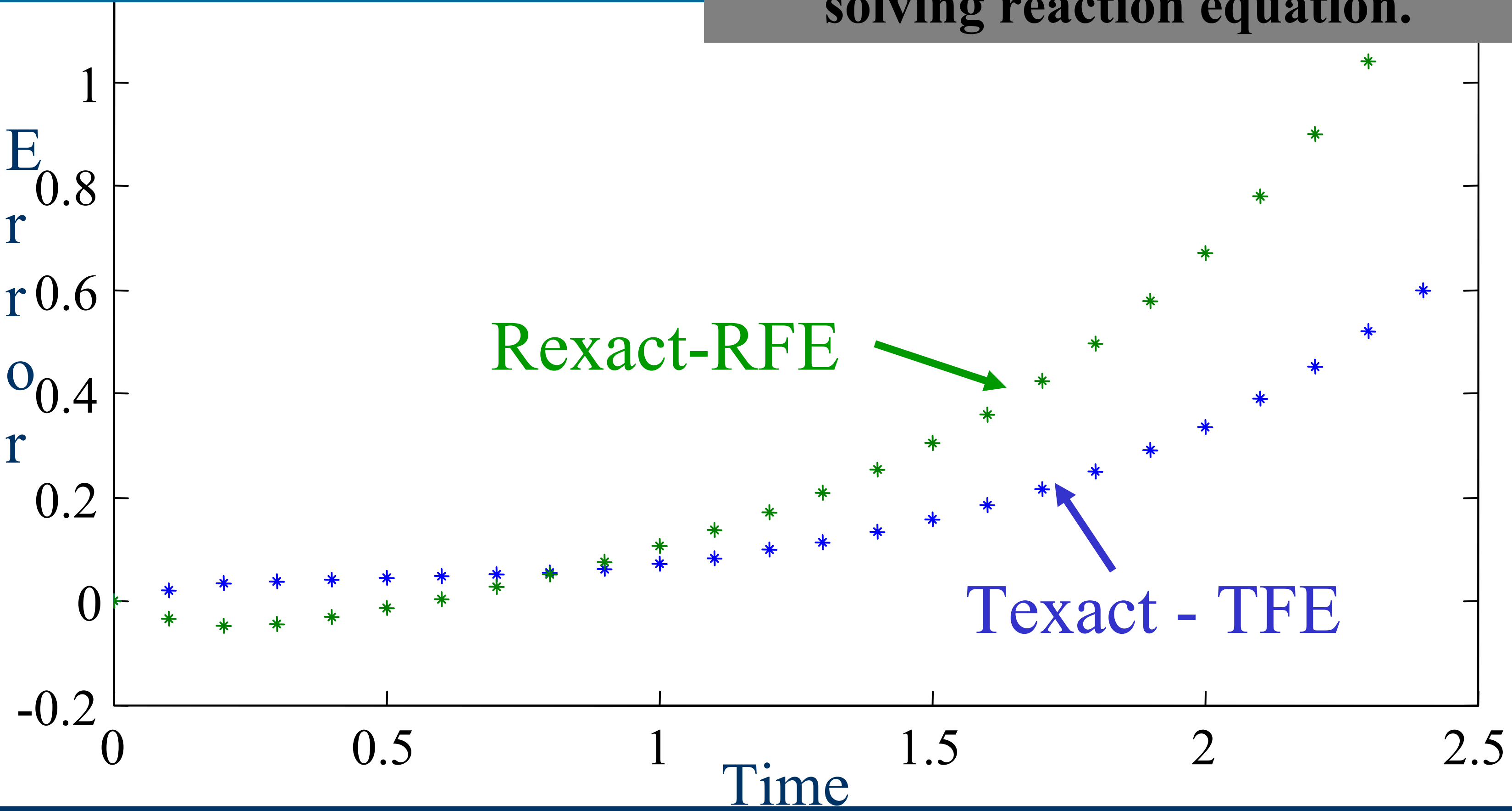


Forward-Euler Errors appear to grow with time

Finite Difference Methods

Convergence Analysis

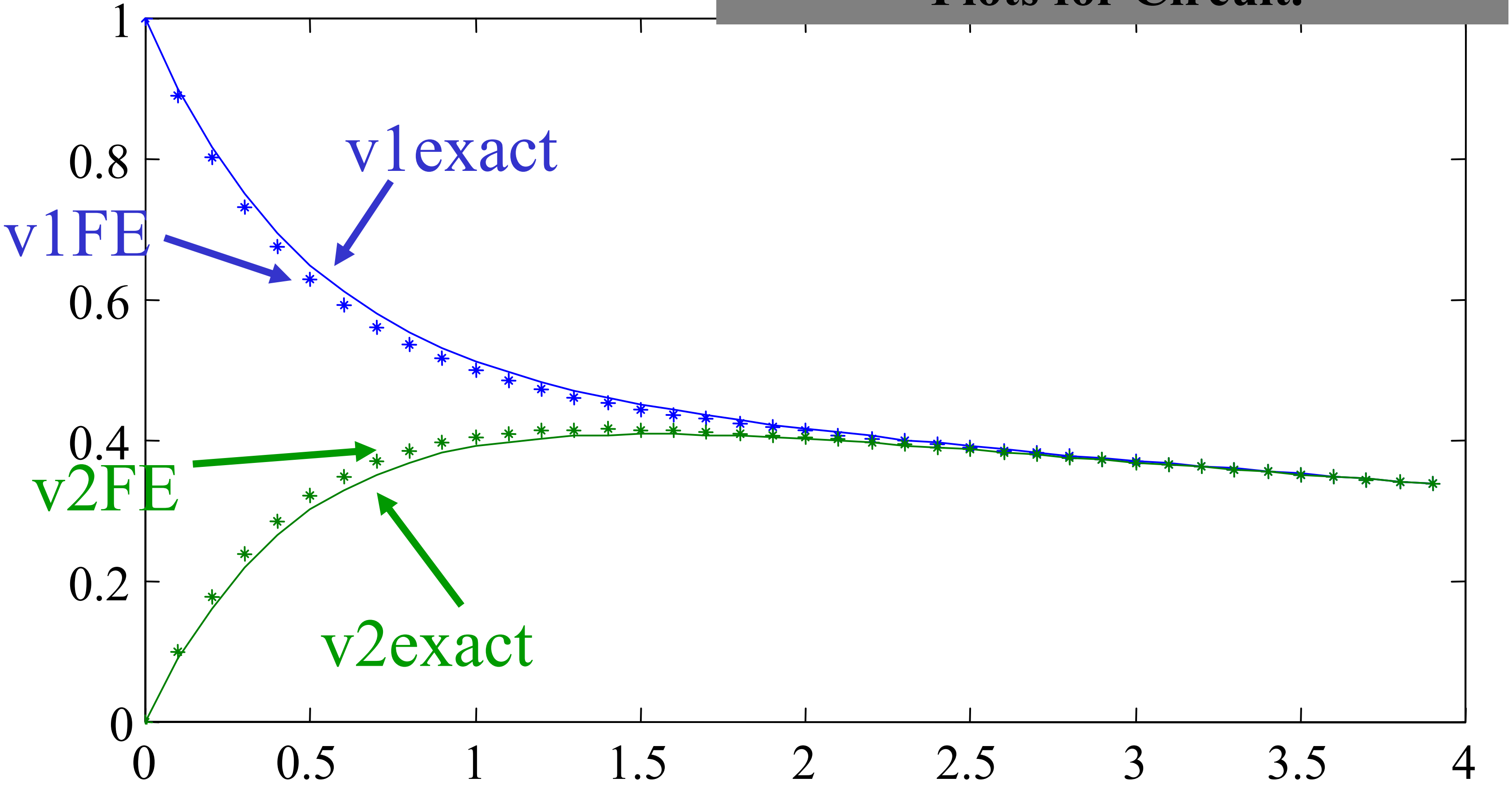
forward-Euler errors for solving reaction equation.



Note error grows exponentially with time, as bound predicts

Convergence Analysis

Exact and forward-Euler(FE) Plots for Circuit.

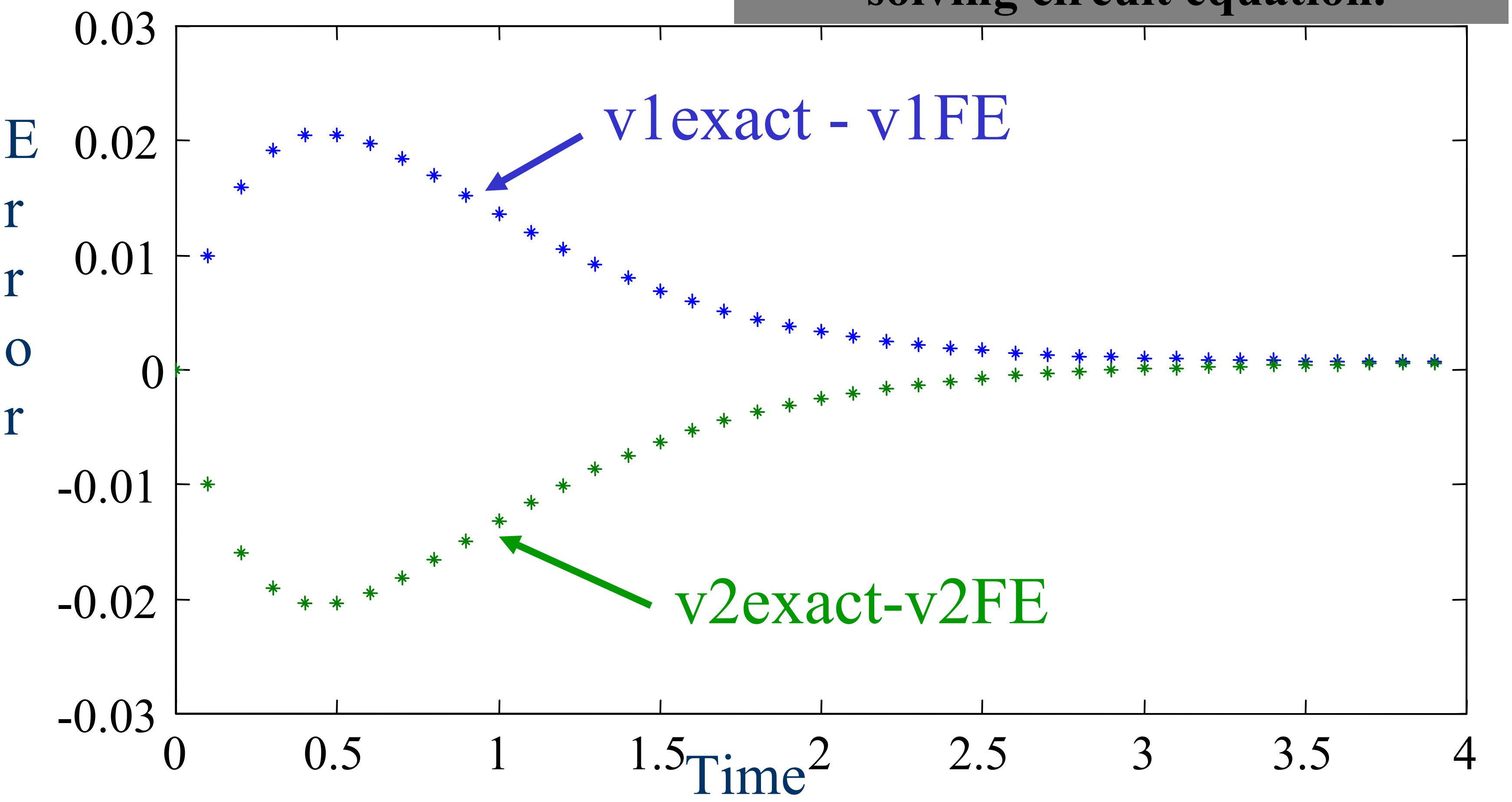


Forward-Euler Errors don’t always grow with time

Finite Difference Methods

Convergence Analysis

forward-Euler errors for solving circuit equation.



Error does not always grow exponentially with time!

Bound is conservative

Summary

- Initial Value problem examples
  - Signal propagation (two time scales).
  - Space frame dynamics (oscillator).
  - Chemical reaction dynamics (unstable system).
- Looked at the simple finite-difference methods
  - Forward-Euler, Backward-Euler, Trap Rule.
  - Look at the approximations and algorithms
  - Experiments generated many questions
- Analyzed Convergence for Forward-Euler

Many more questions to answer, some next time