

Introduction to Simulation - Lecture 13

Convergence of Multistep Methods

Jacob White

Thanks to Deepak Ramaswamy, Michal Rewienski, and
Karen Veroy

Outline

Small Timestep issues for Multistep Methods

Local truncation error

Selecting coefficients.

Nonconverging methods.

Stability + Consistency implies convergence

Next Time Investigate Large Timestep Issues

Absolute Stability for two time-scale examples.

Oscillators.

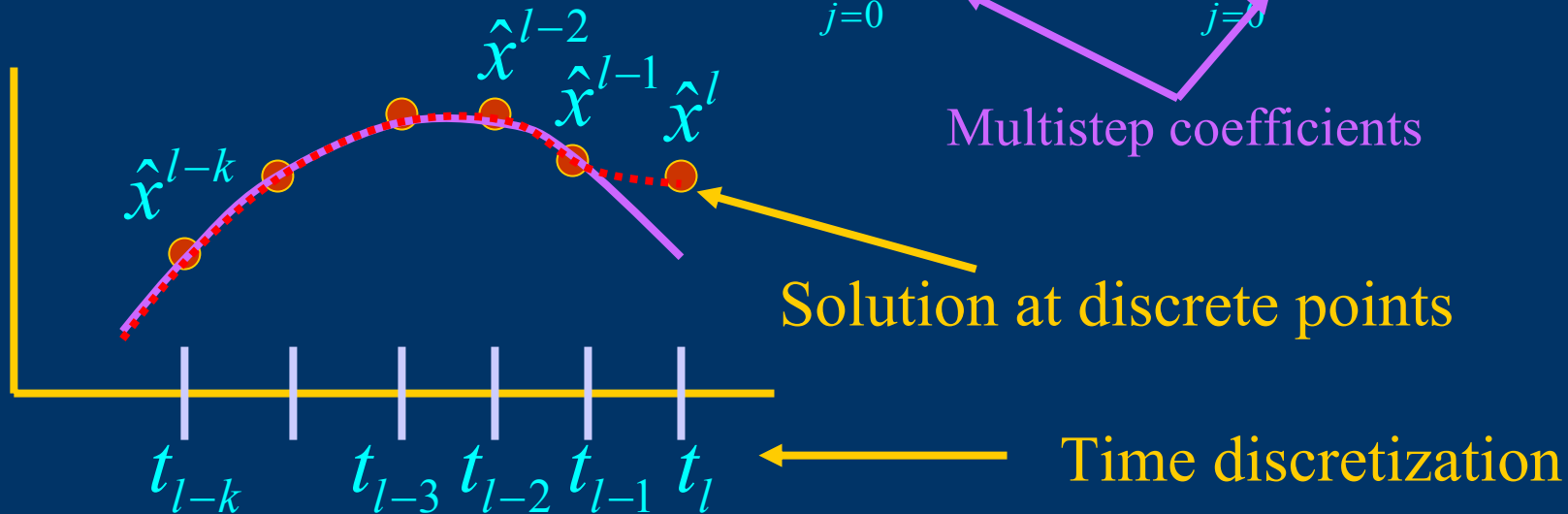
Multistep Methods

Basic Equations

General Notation

Nonlinear Differential Equation: $\frac{d}{dt}x(t) = f(x(t), u(t))$

k-Step Multistep Approach: $\sum_{j=0}^k \alpha_j \hat{x}^{l-j} = \Delta t \sum_{j=0}^k \beta_j f(\hat{x}^{l-j}, u(t_{l-j}))$



Multistep Methods

Basic Equations

Common Algorithms

Multistep Equation:
$$\sum_{j=0}^k \alpha_j \hat{x}^{l-j} = \Delta t \sum_{j=0}^k \beta_j f(\hat{x}^{l-j}, u(t_{l-j}))$$

Forward-Euler Approximation:
$$x(t_l) \approx x(t_{l-1}) + \Delta t f(x(t_{l-1}), u(t_{l-1}))$$

FE Discrete Equation:
$$\hat{x}^l - \hat{x}^{l-1} = \Delta t f(\hat{x}^{l-1}, u(t_{l-1}))$$

Multistep Coefficients: $k = 1, \alpha_0 = 1, \alpha_1 = -1, \beta_0 = 0, \beta_1 = 1$

BE Discrete Equation:
$$\hat{x}^l - \hat{x}^{l-1} = \Delta t f(\hat{x}^l, u(t_l))$$

Multistep Coefficients: $k = 1, \alpha_0 = 1, \alpha_1 = -1, \beta_0 = 1, \beta_1 = 0$

Trap Discrete Equation:
$$\hat{x}^l - \hat{x}^{l-1} = \frac{\Delta t}{2} \left(f(\hat{x}^l, u(t_l)) + f(\hat{x}^{l-1}, u(t_{l-1})) \right)$$

Multistep Coefficients: $k = 1, \alpha_0 = 1, \alpha_1 = -1, \beta_0 = \frac{1}{2}, \beta_1 = \frac{1}{2}$

Multistep Methods

Basic Equations

Definitions and Observations

Multistep Equation:
$$\sum_{j=0}^k \alpha_j \hat{x}^{l-j} = \Delta t \sum_{j=0}^k \beta_j f(\hat{x}^{l-j}, u(t_{l-j}))$$

- 1) If $\beta_0 \neq 0$ the multistep method is implicit
- 2) A k -step multistep method uses k previous x 's and f 's
- 3) A normalization is needed, $\alpha_0 = 1$ is common
- 4) A k -step method has $2k + 1$ free coefficients

How does one pick good coefficients?

Want the highest accuracy

Multistep Methods

Simplified Problem for Analysis

Scalar ODE: $\frac{d}{dt} v(t) = \lambda v(t), v(0) = v_0 \quad \lambda \in \mathbb{C}$

Why such a simple Test Problem?

- Nonlinear Analysis has many *unrevealing* subtleties
- Scalar is equivalent to vector for multistep methods.

$\frac{d}{dt} x(t) = Ax(t)$ multistep discretization $\longrightarrow \sum_{j=0}^k \alpha_j \hat{x}^{l-j} = \Delta t \sum_{j=0}^k \beta_j A \hat{x}^{l-j}$

Let $Ey(t) = x(t)$ $\longrightarrow \sum_{j=0}^k \alpha_j \hat{y}^{l-j} = \Delta t \sum_{j=0}^k \beta_j E^{-1} A E \hat{y}^{l-j}$

Decoupled Equations

$\longrightarrow \sum_{j=0}^k \alpha_j \hat{y}^{l-j} = \Delta t \sum_{j=0}^k \beta_j \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} \hat{y}^{l-j}$

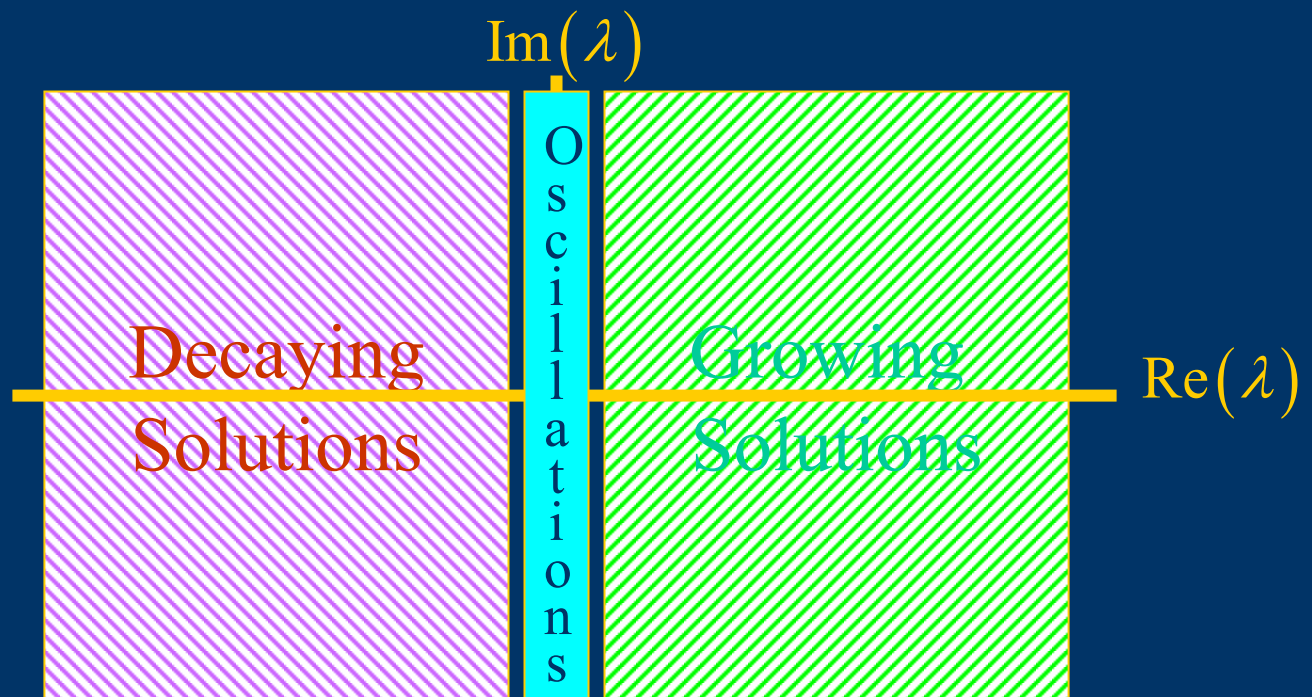
Multistep Methods

Simplified Problem for Analysis

Scalar ODE: $\frac{d}{dt}v(t) = \lambda v(t), v(0) = v_0 \quad \lambda \in \mathbb{C}$

Scalar Multistep formula: $\sum_{j=0}^k \alpha_j \hat{v}^{l-j} = \Delta t \sum_{j=0}^k \beta_j \lambda \hat{v}^{l-j}$

Must Consider ALL $\lambda \in \mathbb{C}$



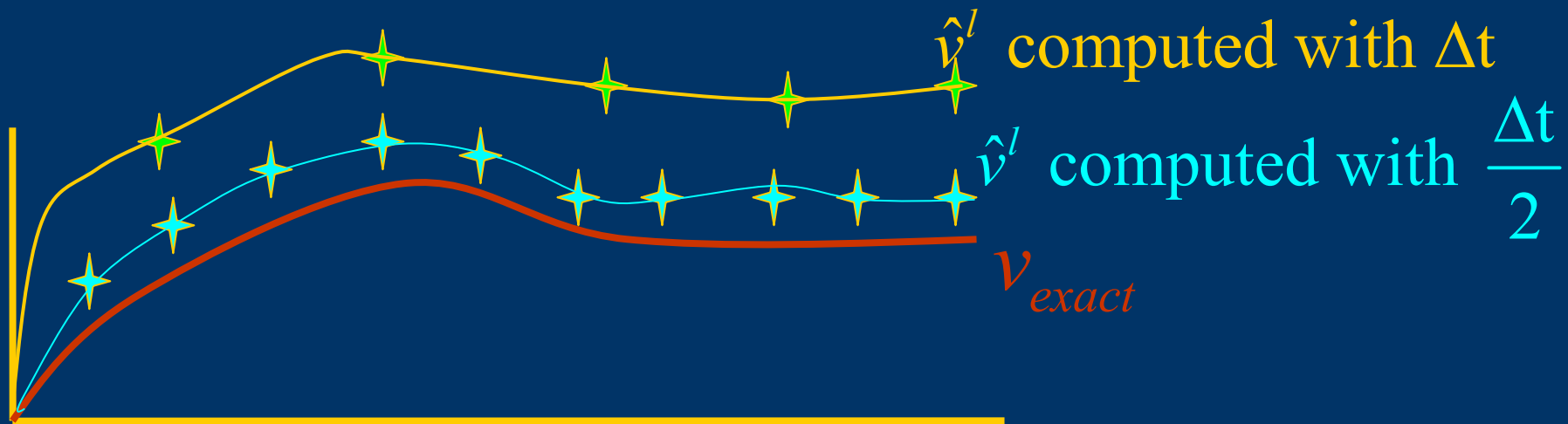
Multistep Methods

Convergence Analysis

Convergence Definition

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

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



Multistep Methods

Convergence Analysis

Order-p convergence

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

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

for all Δt less than a given Δt_0

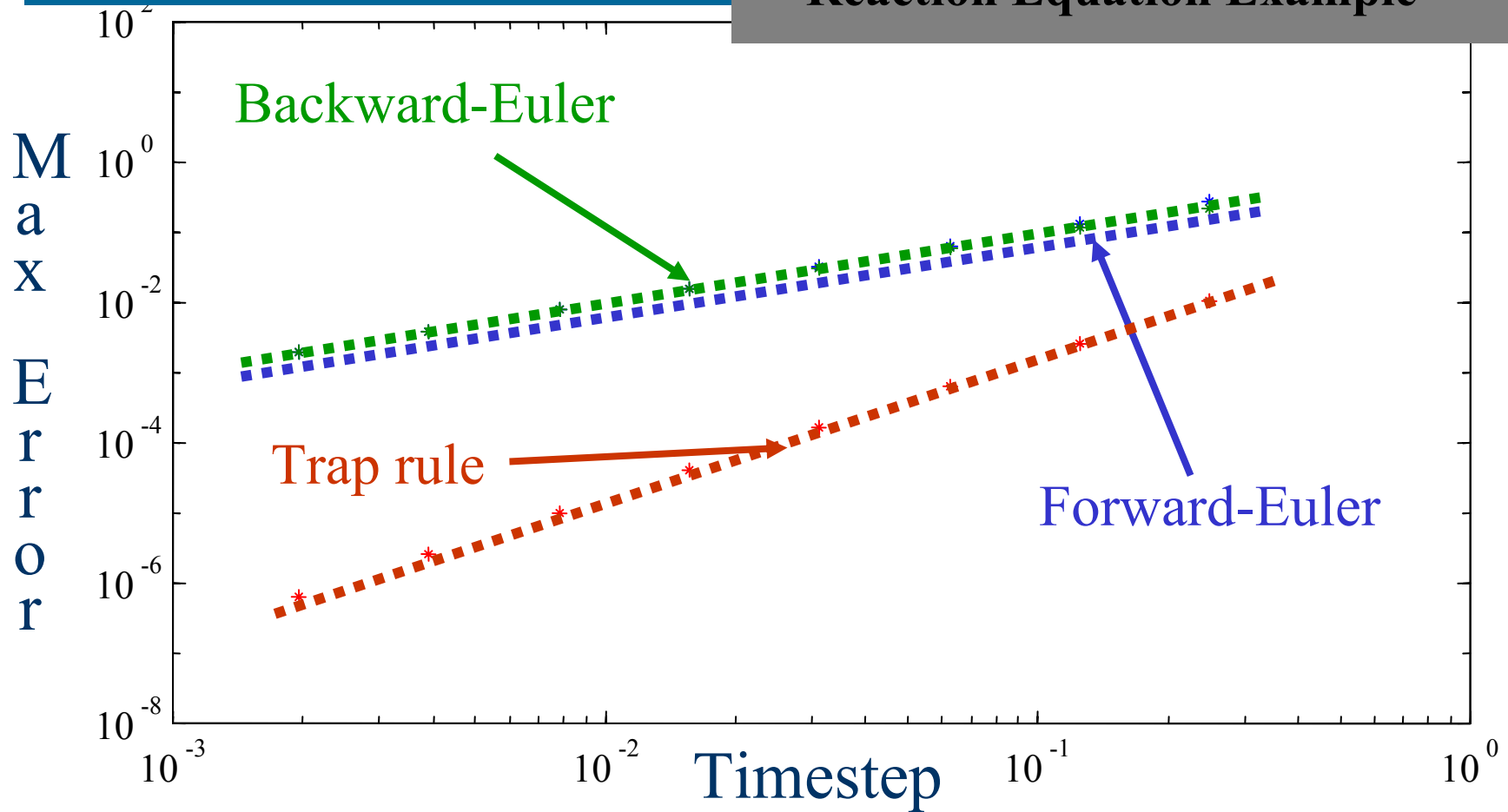
Forward- and Backward-Euler are order 1 convergent

Trapezoidal Rule is order 2 convergent

Multi-step Methods

Convergence Analysis

Reaction Equation Example



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

Multistep Methods

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 ($k=1$) methods are stable in this sense.
Multi-step ($k > 1$) methods require careful analysis.

Multistep Methods

Convergence Analysis

Global Error Equation

Multistep formula:

$$\sum_{j=0}^k \alpha_j \hat{v}^{l-j} - \Delta t \sum_{j=0}^k \beta_j \lambda \hat{v}^{l-j} = 0$$

Exact solution Almost satisfies Multistep Formula:

$$\sum_{j=0}^k \alpha_j v(t_{l-j}) - \Delta t \sum_{j=0}^k \beta_j \frac{d}{dt} v(t_{l-j}) = e^l$$

Local Truncation Error (LTE)

Global Error: $E^l \equiv v(t_l) - \hat{v}^l$

Difference equation relates LTE to Global error

$$(\alpha_0 - \lambda \Delta t \beta_0) E^l + (\alpha_1 - \lambda \Delta t \beta_1) E^{l-1} + \dots + (\alpha_k - \lambda \Delta t \beta_k) E^{l-k} = e^l$$

Forward-Euler

Convergence Analysis

Consistency for Forward Euler

Forward-Euler definition

$$\hat{v}^{l+1} - \hat{v}^l - \Delta t \lambda \hat{v}^l = 0$$

$$\tau \in [l\Delta t, (l+1)\Delta t]$$

Substituting the exact $v(t)$ and expanding

$$v((l+1)\Delta t) - v(l\Delta t) - \Delta t \frac{dv(l\Delta t)}{dt} = \underbrace{\frac{(\Delta t)^2}{2} \frac{d^2v(\tau)}{dt^2}}_{e^l}$$

$\frac{d}{dt}v = \lambda v$

where e^l is the LTE and is bounded by

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

Forward-Euler

Global Error Equation

Forward-Euler definition

$$\hat{v}^{l+1} = \hat{v}^l + \Delta t \lambda \hat{v}^l$$

Using the LTE definition

$$v((l+1)\Delta t) = v(l\Delta t) + \Delta t \lambda v(l\Delta t) + e^l$$

Subtracting yields global error equation

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

Using magnitudes and the bound on e^l

$$|E^{l+1}| \leq |I + \Delta t \lambda| |E^l| + |e^l| \leq (1 + \Delta t |\lambda|) |E^l| + C(\Delta t)^2$$

Forward-Euler

Convergence Analysis

A helpful bound on difference equations

A lemma bounding difference equation solutions

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

Then $|u^l| \leq \frac{e^{\varepsilon l}}{\varepsilon} |b|$

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

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

One-step Methods

Convergence Analysis

A helpful bound on difference equations cont.

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

$$|u^l| \leq \frac{1 - (1 + \varepsilon)^l}{1 - (1 + \varepsilon)} |b| = \frac{(1 + \varepsilon)^l - 1}{\varepsilon} |b| \leq \frac{e^{\varepsilon l}}{\varepsilon} |b|$$

One-step Methods

Convergence Analysis

Back to Forward Euler
Convergence analysis.

Applying the lemma and cancelling terms

$$|E^{l+1}| \leq \left(1 + \underbrace{\Delta t |\lambda|}_{\varepsilon} \right) |E^l| + \underbrace{C (\Delta t)^2}_b \leq \frac{e^{l\Delta t |\lambda|}}{\cancel{\Delta t |\lambda|}} C (\Delta t)^2$$

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

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

Forward-Euler

Convergence Analysis

Observations about the forward-Euler analysis.

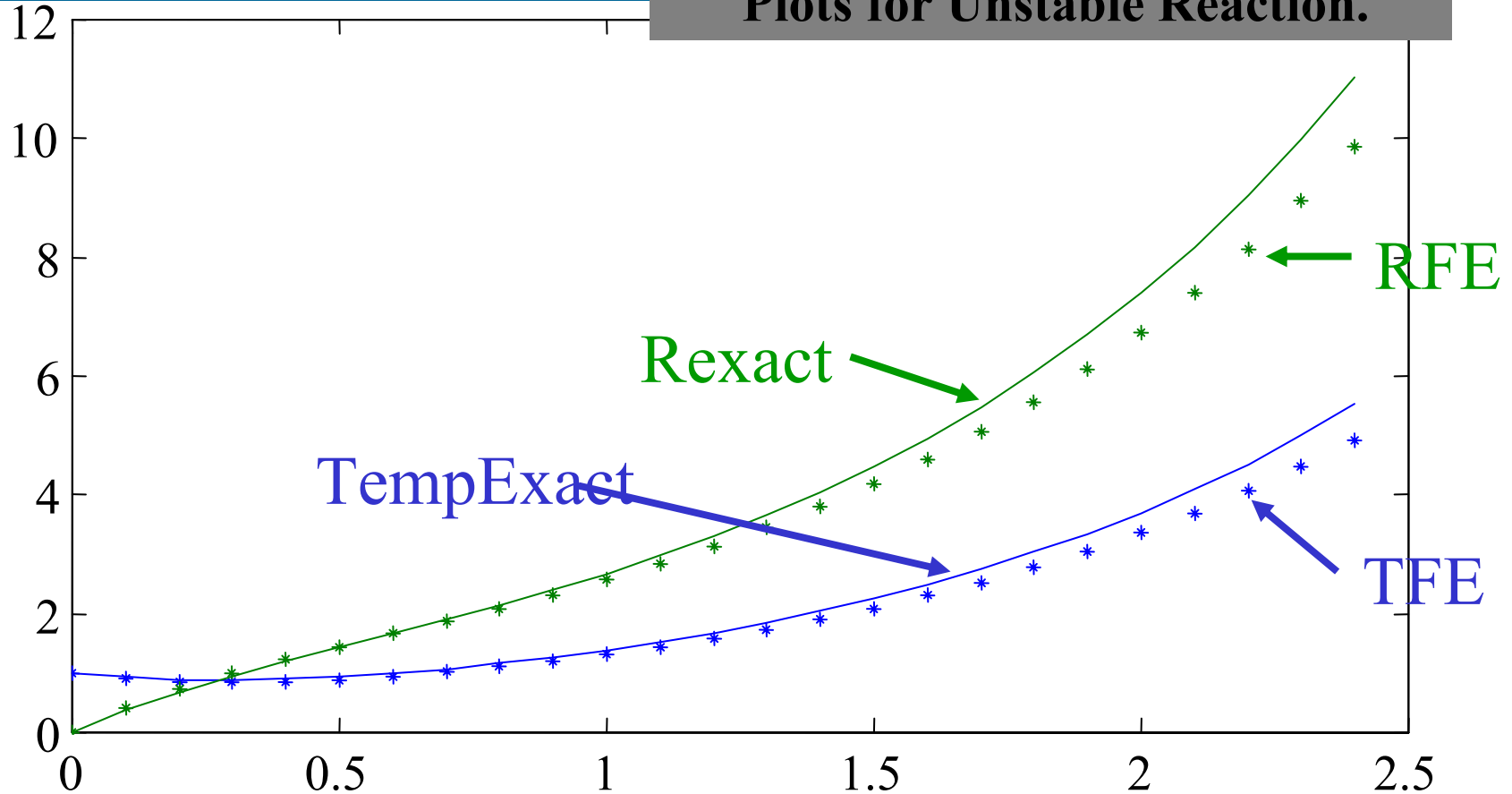
$$\max_{l \in [0, L]} |E^l| \leq e^{|\lambda|T} \frac{C}{|\lambda|} \Delta t$$

- forward-Euler is order 1 convergent
- Bound grows exponentially with time interval.
- C related to exact solution's second derivative.
- The bound grows exponentially with time.

Forward-Euler

Convergence Analysis

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

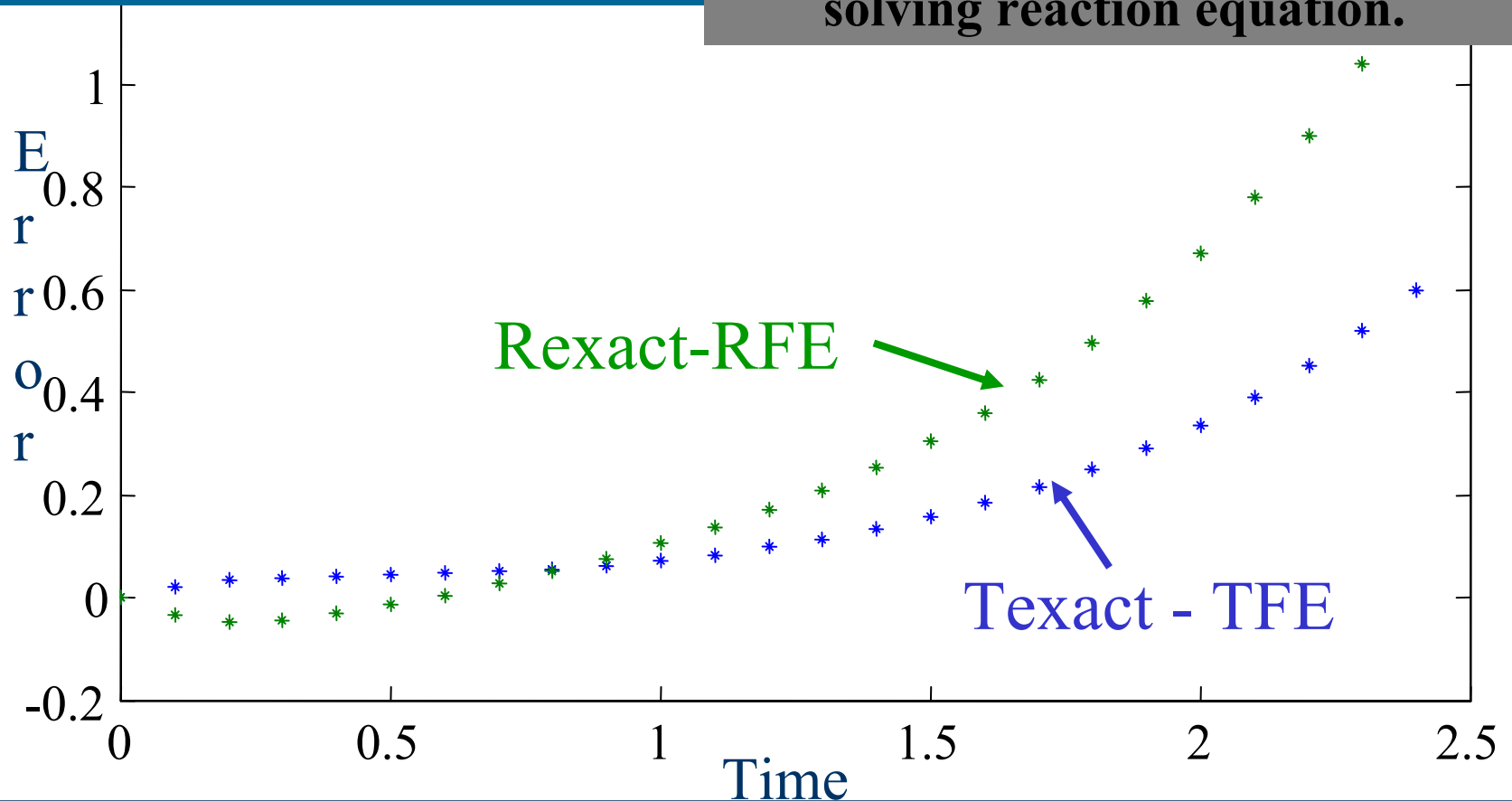


Forward-Euler Errors appear to grow with time

Forward-Euler

Convergence Analysis

forward-Euler errors for solving reaction equation.

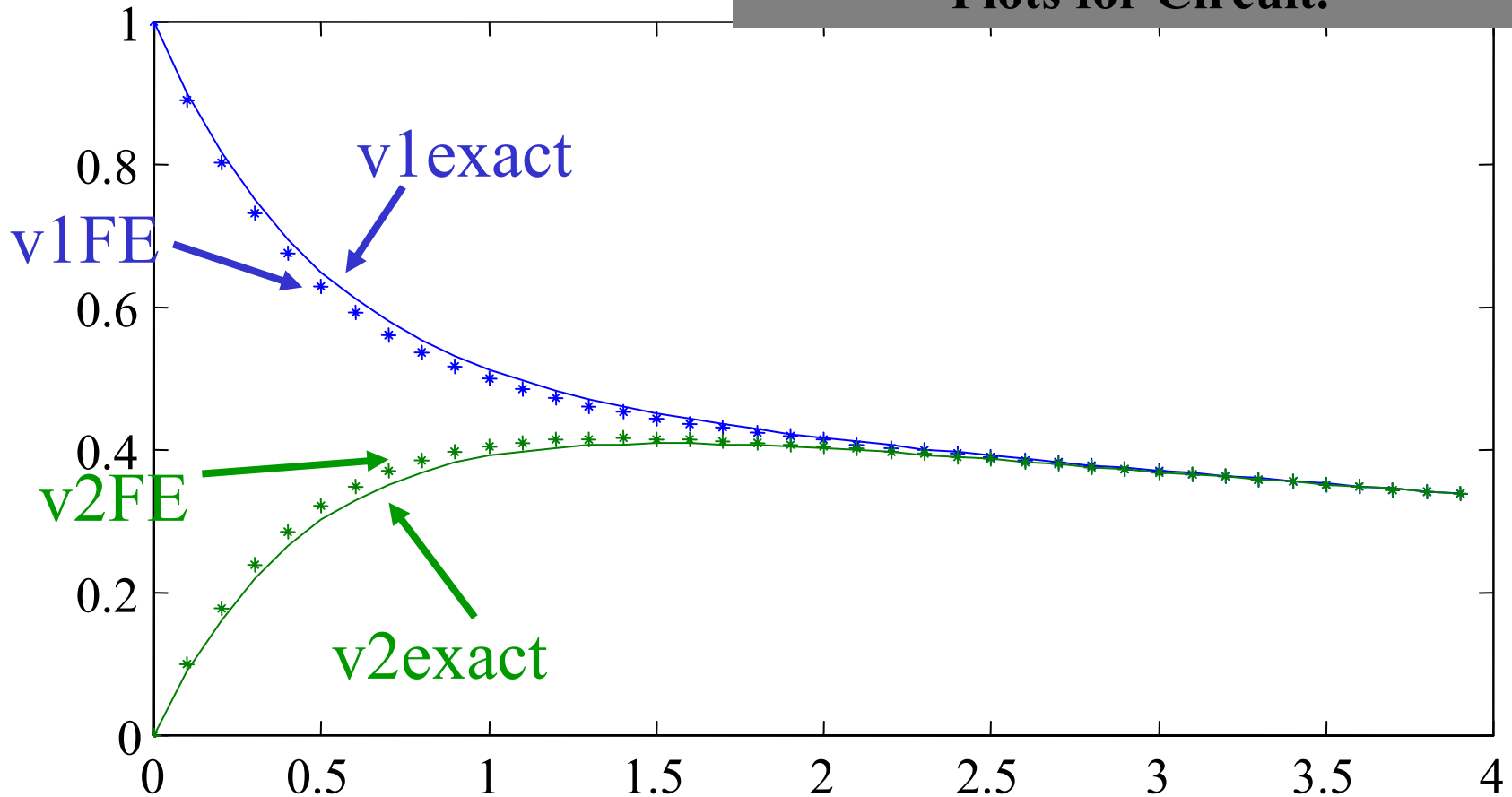


Note error grows exponentially with time, as bound predicts

Forward-Euler

Convergence Analysis

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

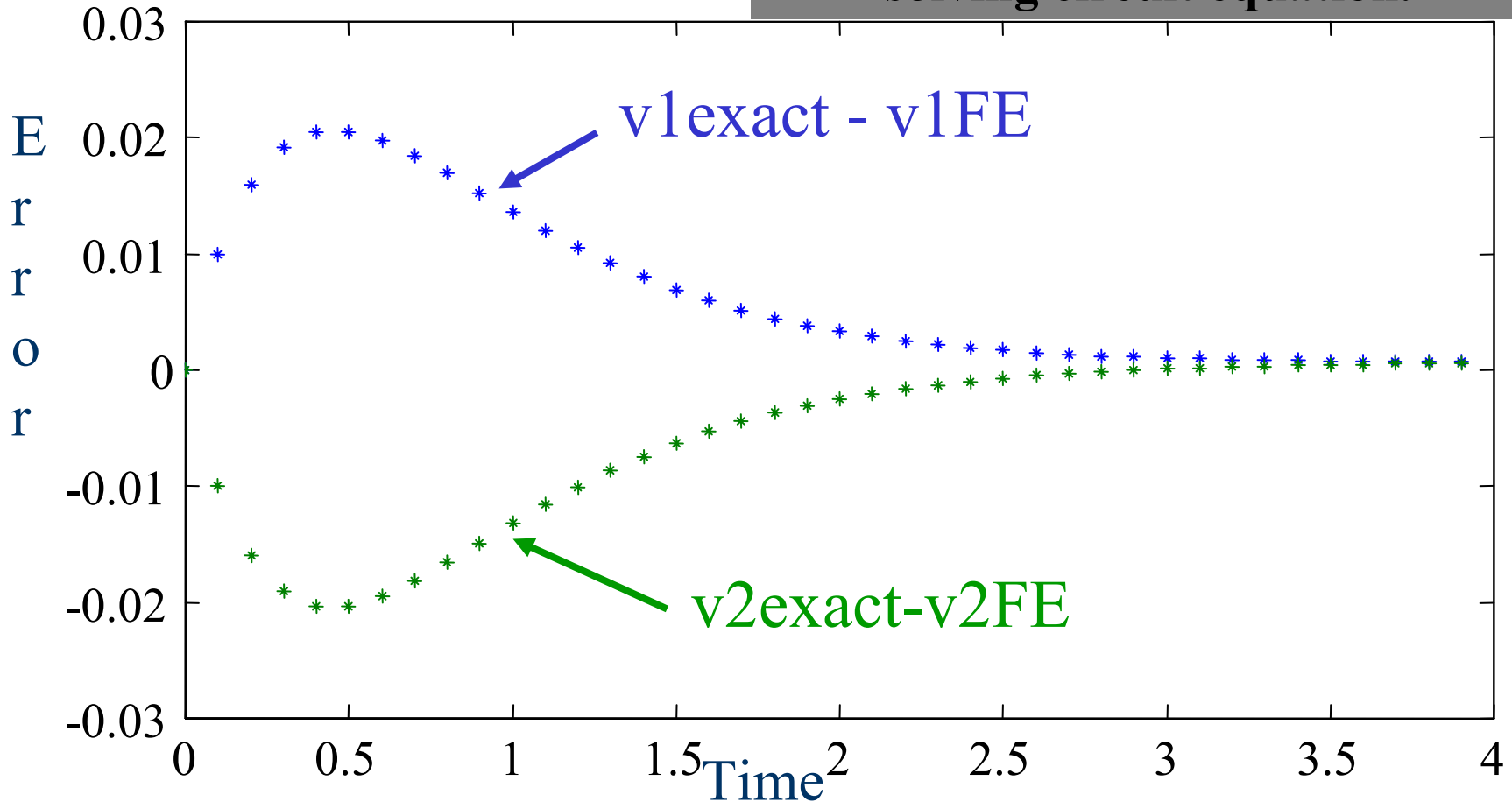


Forward-Euler Errors don't always grow with time

Forward-Euler

Convergence Analysis

forward-Euler errors for solving circuit equation.



Error does not always grow exponentially with time!

Bound is conservative

Multistep Methods

Making LTE Small

Exactness Constraints

Local Truncation Error:
$$\sum_{j=0}^k \alpha_j v(t_{l-j}) - \Delta t \sum_{j=0}^k \beta_j \frac{d}{dt} v(t_{l-j}) = e^l$$

Can't be from $\frac{d}{dt} v(t) = \lambda v(t)$

LTE

If $v(t) = t^p \Rightarrow \frac{d}{dt} v(t) = pt^{p-1}$

$$\sum_{j=0}^k \alpha_j \underbrace{\left((k-j) \Delta t \right)^p}_{v(t_{k-j})} - \Delta t \sum_{j=0}^k \beta_j \underbrace{p \left((k-j) \Delta t \right)^{p-1}}_{\frac{d}{dt} v(t_{k-j})} = e^k$$

Multistep Methods

Making LTE Small

Exactness Constraints Cont.

$$\sum_{j=0}^k \alpha_j ((k-j)\Delta t)^p - \Delta t \sum_{j=0}^k \beta_j p ((k-j)\Delta t)^{p-1} =$$
$$(\Delta t)^p \left(\sum_{j=0}^k \alpha_j (l-j)^p - \sum_{j=0}^k \beta_j p (l-j)^{p-1} \right) = e^k$$

If $\left(\sum_{j=0}^k \alpha_j ((k-j))^p - \sum_{j=0}^k \beta_j p (k-j)^{p-1} \right) = 0$ then $e^k = 0$ for $v(t) = t^p$

As any smooth $v(t)$ has a locally accurate Taylor series in t :

if $\left(\sum_{j=0}^k \alpha_j (k-j)^p - \sum_{j=0}^k \beta_j p (k-j)^{p-1} \right) = 0$ for all $p \leq p_0$

Then $\left(\sum_{j=0}^k \alpha_j v(t_{l-j}) - \sum_{j=0}^k \beta_j \frac{d}{dt} v(t_{l-j}) \right) = e^l = C(\Delta t)^{p_0+1}$

Multistep Methods

Making LTE Small

Exactness Constraint $k=2$

Example

Exactness Constraints:
$$\left(\sum_{j=0}^k \alpha_j (k-j)^p - \sum_{j=0}^k \beta_j p (k-j)^{p-1} \right) = 0$$

For $k=2$, yields a 5×6 system of equations for Coefficients

$$\begin{array}{l} p=0 \\ p=1 \\ p=2 \\ p=3 \\ p=4 \end{array} \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & -1 & -1 & -1 \\ 4 & 1 & 0 & -4 & -2 & 0 \\ 8 & 1 & 0 & -12 & -3 & 0 \\ 16 & 1 & 0 & -32 & -4 & 0 \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Note

$$\sum \alpha_i = 0$$

Always

Multistep Methods

Making LTE Small

Exactness Constraint $k=2$

Example Continued

Exactness
Constraints for $k=2$

$$\begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & -1 & -1 & -1 \\ 4 & 1 & 0 & -4 & -2 & 0 \\ 8 & 1 & 0 & -12 & -3 & 0 \\ 16 & 1 & 0 & -32 & -4 & 0 \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Forward-Euler $\alpha_0 = 1, \alpha_1 = -1, \alpha_2 = 0, \beta_0 = 0, \beta_1 = 1, \beta_2 = 0,$

FE satisfies $p = 0$ and $p = 1$ but not $p = 2 \Rightarrow LTE = C(\Delta t)^2$

Backward-Euler $\alpha_0 = 1, \alpha_1 = -1, \alpha_2 = 0, \beta_0 = 1, \beta_1 = 0, \beta_2 = 0,$

BE satisfies $p = 0$ and $p = 1$ but not $p = 2 \Rightarrow LTE = C(\Delta t)^2$

Trap Rule $\alpha_0 = 1, \alpha_1 = -1, \alpha_2 = 0, \beta_0 = 0.5, \beta_1 = 0.5, \beta_2 = 0,$

Trap satisfies $p = 0, 1, \text{ or } 2$ but not $p = 3 \Rightarrow LTE = C(\Delta t)^3$

Multistep Methods

Making LTE Small

Exactness Constraint $k=2$
example, generating methods

First introduce a normalization, for example $\alpha_0 = 1$

$$\begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & -1 & -1 & -1 \\ 1 & 0 & -4 & -2 & 0 \\ 1 & 0 & -12 & -3 & 0 \\ 1 & 0 & -32 & -4 & 0 \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} -1 \\ -2 \\ -4 \\ -8 \\ -16 \end{bmatrix}$$

Solve for the 2-step method with lowest LTE

$$\alpha_0 = 1, \alpha_1 = 0, \alpha_2 = -1, \beta_0 = 1/3, \beta_1 = 4/3, \beta_2 = 1/3$$

Satisfies all five exactness constraints $LTE = C(\Delta t)^5$

Solve for the 2-step explicit method with lowest LTE

$$\alpha_0 = 1, \alpha_1 = 4, \alpha_2 = -5, \beta_0 = 0, \beta_1 = 4, \beta_2 = 2$$

Can only satisfy four exactness constraints $LTE = C(\Delta t)^4$

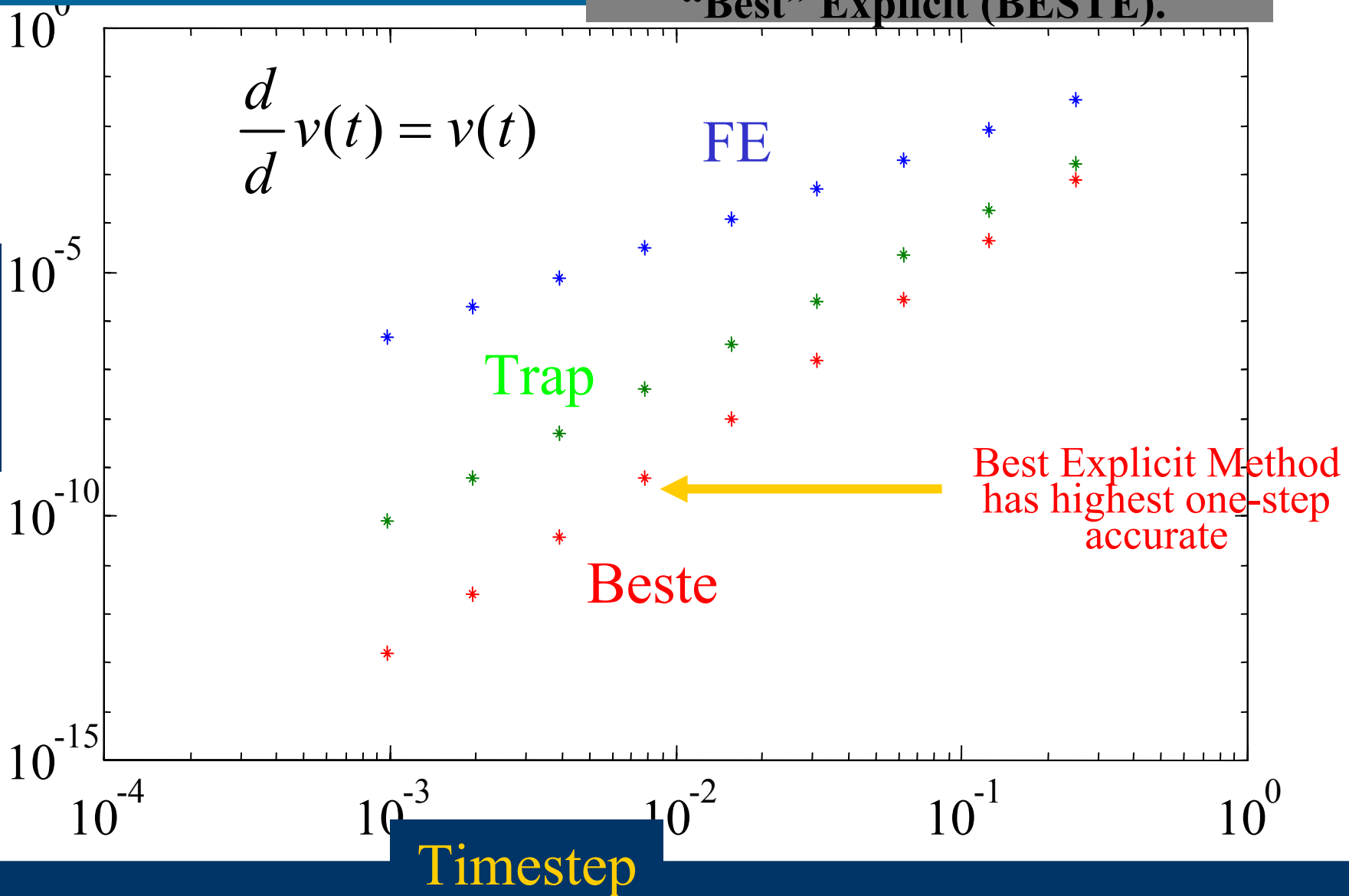
Multistep Methods

Making LTE Small

LTE Plots for the FE, Trap, and “Best” Explicit (BESTE).

L
T
E

$$\frac{d}{dt} v(t) = v(t)$$

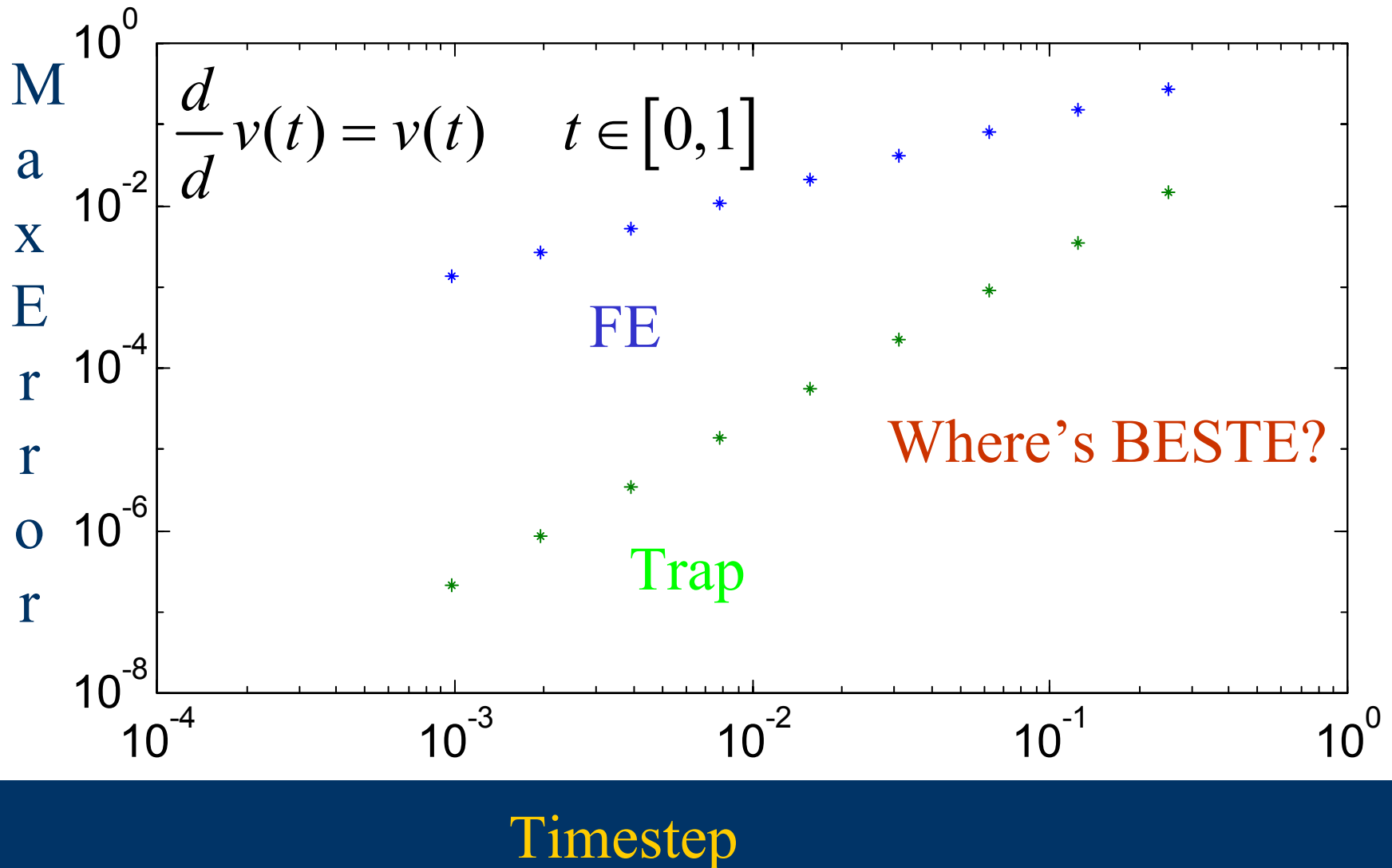


Timestep

Multistep Methods

Making LTE Small

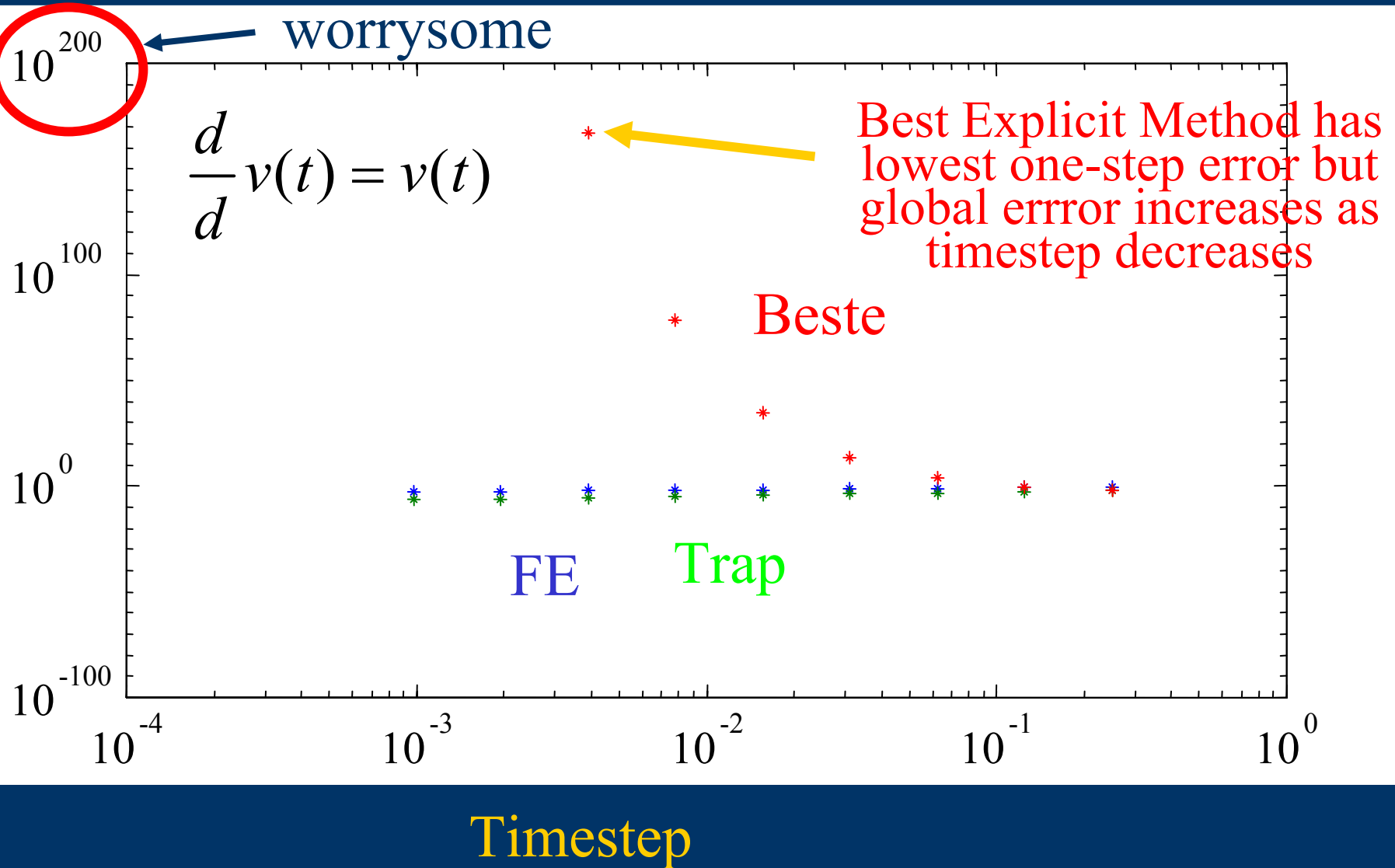
Global Error for the FE, Trap, and “Best” Explicit (BESTE).



Multistep Methods

Making LTE Small

Global Error for the FE, Trap, and “Best” Explicit (BESTE).



Multistep Methods

Stability of the method

Difference Equation

Why did the “best” 2-step explicit method fail to Converge?

Multistep Method Difference Equation

$$(\alpha_0 - \lambda \Delta t \beta_0) E^l + (\alpha_1 - \lambda \Delta t \beta_1) E^{l-1} + \dots + (\alpha_k - \lambda \Delta t \beta_k) E^{l-k} = e^l$$

$$v(l \Delta t) - \hat{v}^l$$

Global Error

LTE

We made the LTE so small, how come the Global error is so large?

An Aside on Solving Difference Equations

Consider a general k th order difference equation

$$a_0 x^l + a_1 x^{l-1} + \cdots + a_k x^{l-k} = u^l$$

Which must have k initial conditions

$$x^0 = x_0, \quad x^{-1} = x_1, \quad \cdots, \quad x^{-k} = x_k$$

As is clear when the equation is in update form

$$x^1 = -\frac{1}{a_0} \left(a_1 x^0 + \cdots + a_k x^{-k+1} - u^1 \right)$$

Most important difference equation result

$$x \text{ can be related to } u \text{ by } x^l = \sum_{j=0}^l h^{l-j} u^j$$

An Aside on Difference Equations Cont.

If $a_0 z^k + a_1 z^{k-1} + \cdots + a_k = 0$ has distinct roots

$$\zeta_1, \zeta_2, \dots, \zeta_k$$

Then $x^l = \sum_{j=0}^l h^{l-j} u^j$ where $h^l = \sum_{j=1}^k \gamma_j (\zeta_j)^l$

To understand how h is derived, first a simple case

Suppose $x^l = \zeta x^{l-1} + u^l$ and $x^0 = 0$

$$x^1 = \zeta x^0 + u^1 = u^1, \quad x^2 = \zeta x^1 + u^2 = \zeta u^1 + u^2$$

$$x^l = \sum_{j=0}^l \zeta^{l-j} u^j$$


An Aside on Difference Equations Cont.

Three important observations

If $|\zeta_i| < 1$ for all i , then $|x^l| \leq C \max_j |u^j|$
where C does not depend on l

If $|\zeta_i| > 1$ for any i , then there exists
a bounded u^j such that $|x^l| \rightarrow \infty$

If $|\zeta_i| \leq 1$ for all i , and if $|\zeta_i| = 1$, ζ_i is distinct
then $|x^l| \leq Cl \max_j |u^j|$



Multistep Methods

Stability of the method

Difference Equation

Multistep Method Difference Equation

$$(\alpha_0 - \lambda \Delta t \beta_0) E^l + (\alpha_1 - \lambda \Delta t \beta_1) E^{l-1} + \dots + (\alpha_k - \lambda \Delta t \beta_k) E^{l-k} = e^l$$

Definition: A multistep method is stable if and only if

$$\text{As } \Delta t \rightarrow 0 \quad \max_{l \in \left[0, \frac{T}{\Delta t}\right]} \|E^l\| \leq C \frac{T}{\Delta t} \max_{l \in \left[0, \frac{T}{\Delta t}\right]} \|e^l\| \quad \text{for any } e^l$$

Theorem: A multistep method is stable if and only if

The roots of $\alpha_0 z^k + \alpha_1 z^{k-1} + \dots + \alpha_k = 0$ are either

Less than one in magnitude or equal to one and distinct

Multistep Methods

Stability of the method

Stability Theorem “Proof”

Given the Multistep Method Difference Equation

$$(\alpha_0 - \lambda \Delta t \beta_0) E^l + (\alpha_1 - \lambda \Delta t \beta_1) E^{l-1} + \cdots + (\alpha_k - \lambda \Delta t \beta_k) E^{l-k} = e^l$$

If the roots of $\sum_{j=0}^k \alpha_j z^{k-j} = 0$ are either

- less than one in magnitude
- equal to one in magnitude but distinct

Then from the aside on difference equations

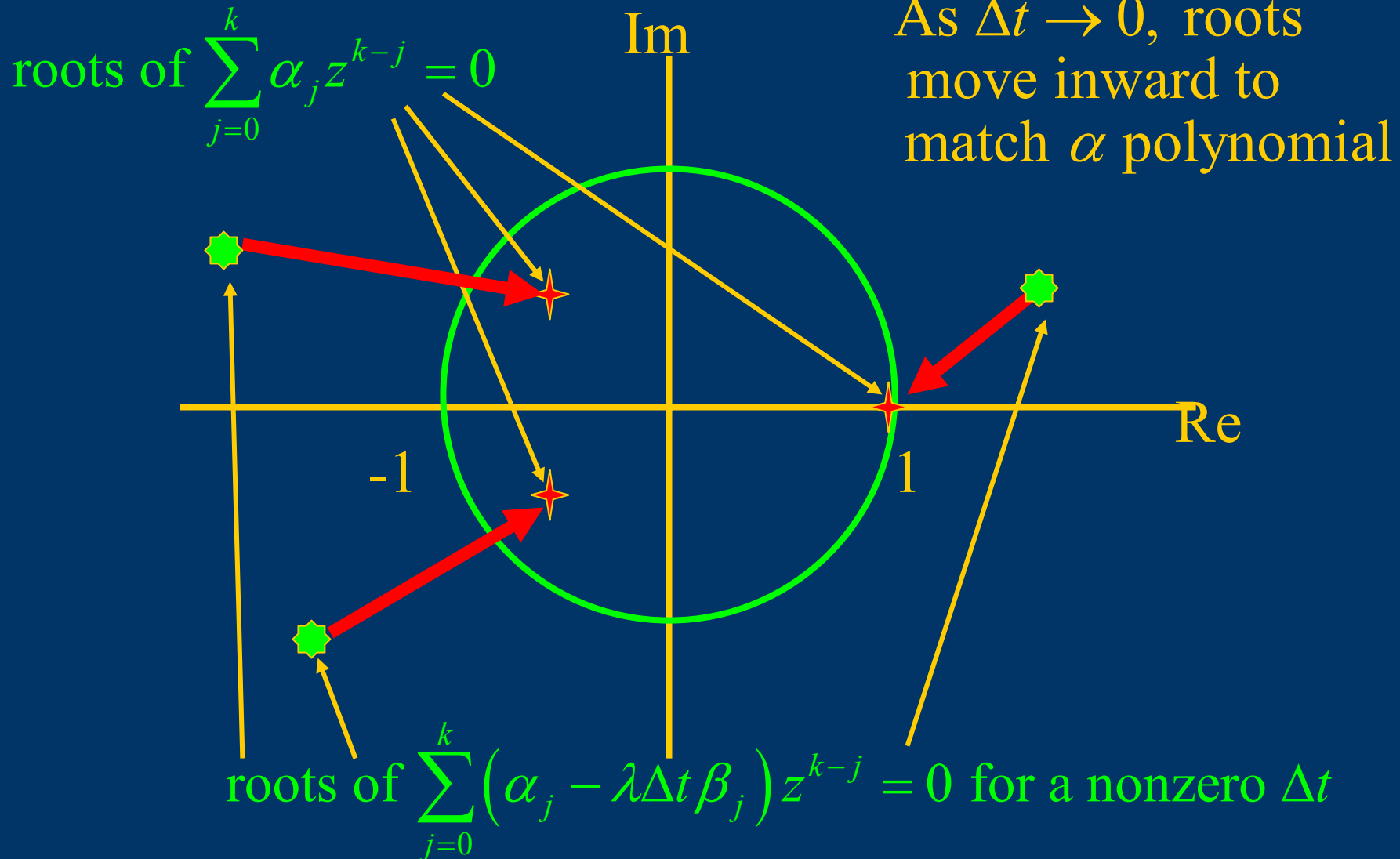
$$\|E^l\| \leq Cl \max_l \|e^l\|$$

From which stability easily follows.

Multistep Methods

Stability of the method

Stability Theorem “Proof”



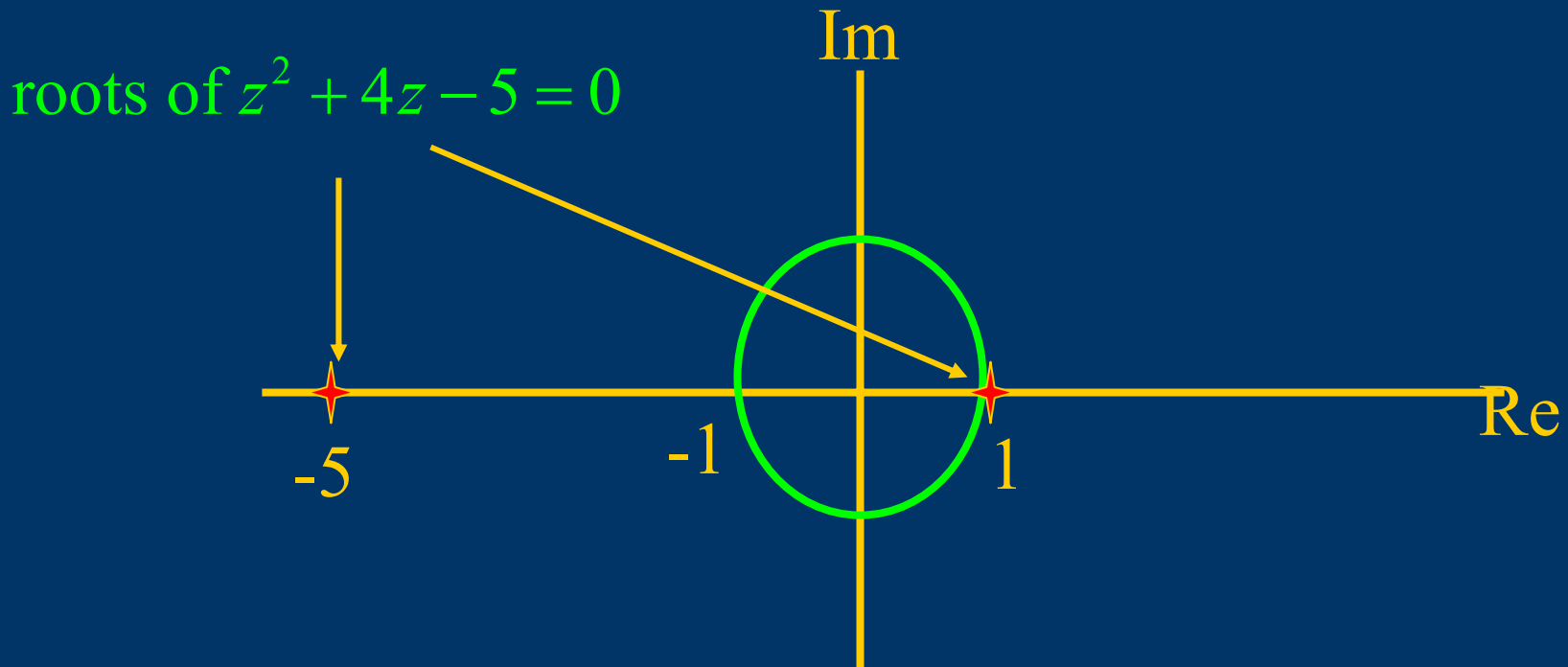
Multistep Methods

Stability of the method

The BESTE Method

Best explicit 2-step method

$$\alpha_0 = 1, \alpha_1 = 4, \alpha_2 = -5, \beta_0 = 0, \beta_1 = 4, \beta_2 = 2$$



Method is Wildly unstable!

Multistep Methods

Stability of the method

Dahlquist's First Stability Barrier

For a stable, explicit k -step multistep method, the maximum number of exactness constraints that can be satisfied is less than or equal to k (note there are $2k$ coefficients). For implicit methods, the number of constraints that can be satisfied is either $k+2$ if k is even or $k+1$ if k is odd.

Multistep Methods

Convergence Analysis

Conditions for convergence,
stability and consistency

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

Exactness Constraints up to p_0 (p_0 must be > 0)

$$\Rightarrow \max_{l \in \left[0, \frac{T}{\Delta t}\right]} \|e^l\| \leq C_1 (\Delta t)^{p_0+1} \text{ for } \Delta t < \Delta t_0$$

2) Global Condition: One step errors grow slowly (stability)

roots of $\sum_{j=0}^k \alpha_j z^{k-j} = 0$ inside or simple on unit circle

$$\Rightarrow \max_{l \in \left[0, \frac{T}{\Delta t}\right]} \|E^l\| \leq C_2 \frac{T}{\Delta t} \max_{l \in \left[0, \frac{T}{\Delta t}\right]} \|e^l\|$$

Convergence Result: $\max_{l \in \left[0, \frac{T}{\Delta t}\right]} \|E^l\| \leq CT (\Delta t)^{p_0}$

Summary

Small Timestep issues for Multistep Methods

Local truncation error and Exactness.

Difference equation stability.

Stability + Consistency implies convergence.

Next time

Absolute Stability for two time-scale examples.

Oscillators.

Maybe Runge-Kutta schemes