Introduction to Simulation - Lecture 14

Multistep Methods II

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Thanks to Deepak Ramaswamy, Michal Rewienski, and
Karen Veroy

Outline

- Small Timestep issues for Multistep Methods
  - Reminder about LTE minimization
  - A nonconverging example
  - Stability + Consistency implies convergence
- Investigate Large Timestep Issues
  - Absolute Stability for two time-scale examples.
  - Oscillators.

Multistep Methods

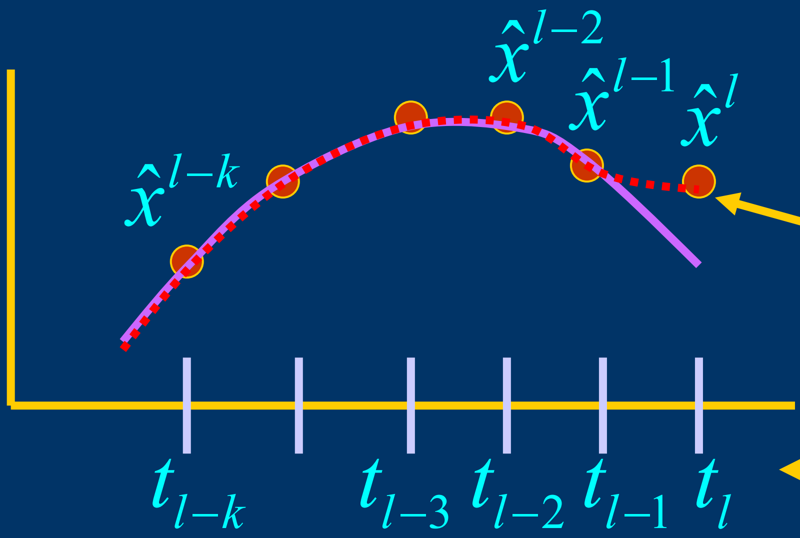
Basic Equations

General Notation

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

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

Multistep coefficients



Solution at discrete points

Time discretization

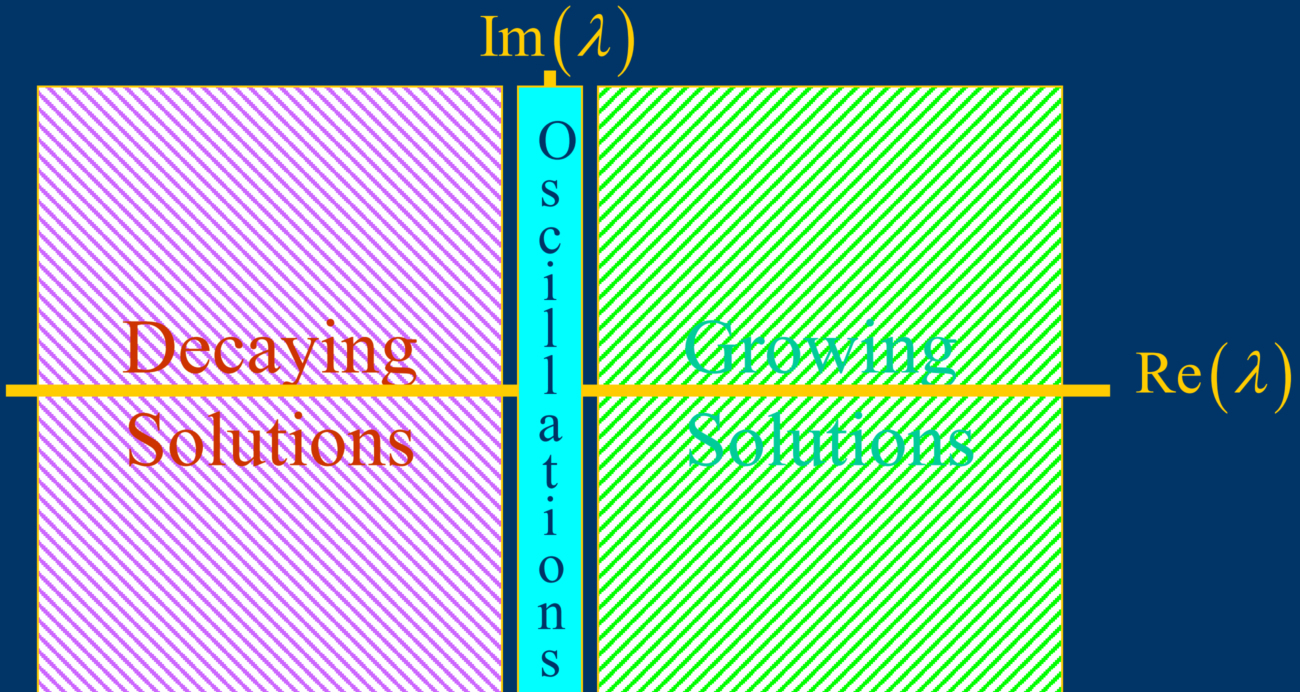
Multistep Methods

Simplified Problem for Analysis

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

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 $\lambda \in \mathbb{C}$



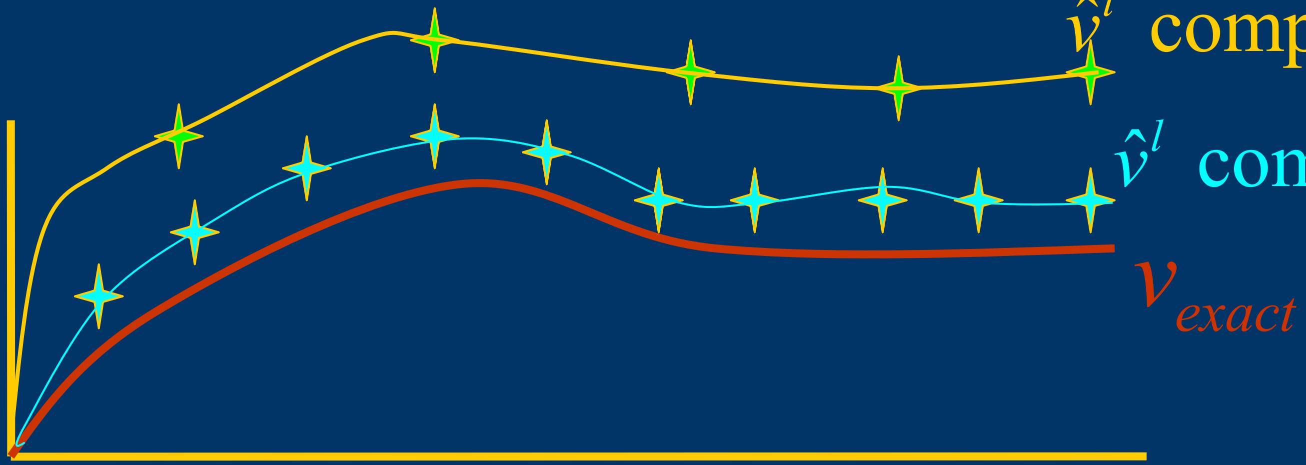
Multistep Methods

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

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)

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:

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

Local Truncation Error (LTE)

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

Difference equation relates LTE to Global error

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

Multistep Methods

Making LTE Small

Exactness Constraints

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

LTE

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

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

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

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 5x6 system of equations for Coefficients

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

Note

$\sum \alpha_i = 0$

Always

Multistep Methods

Making LTE Small

Exactness Constraint k=2 example, 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 $LTE = C(\Delta t)^5$

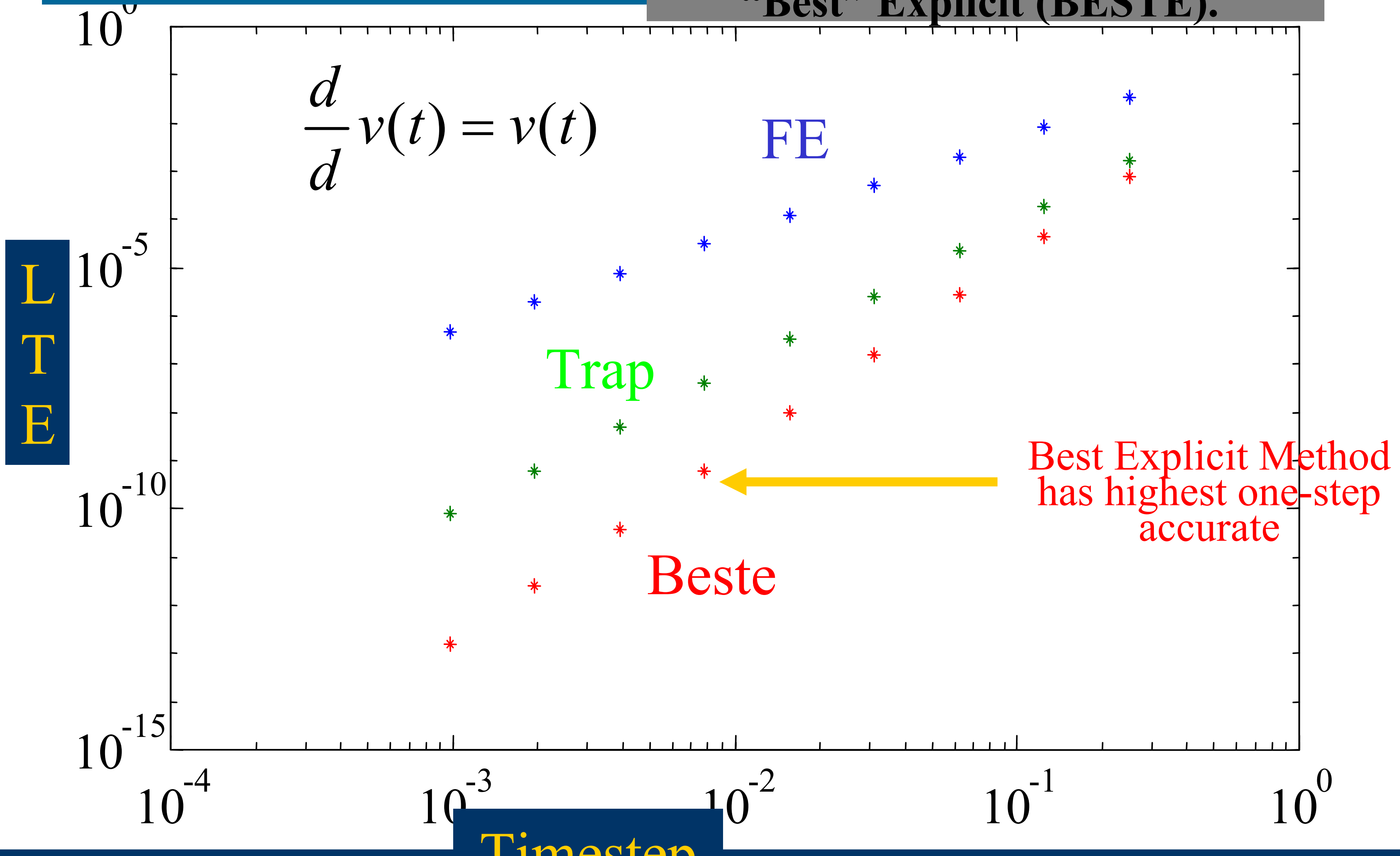
Solve for the 2-step explicit method with lowest LTE

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

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

Making LTE Small

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

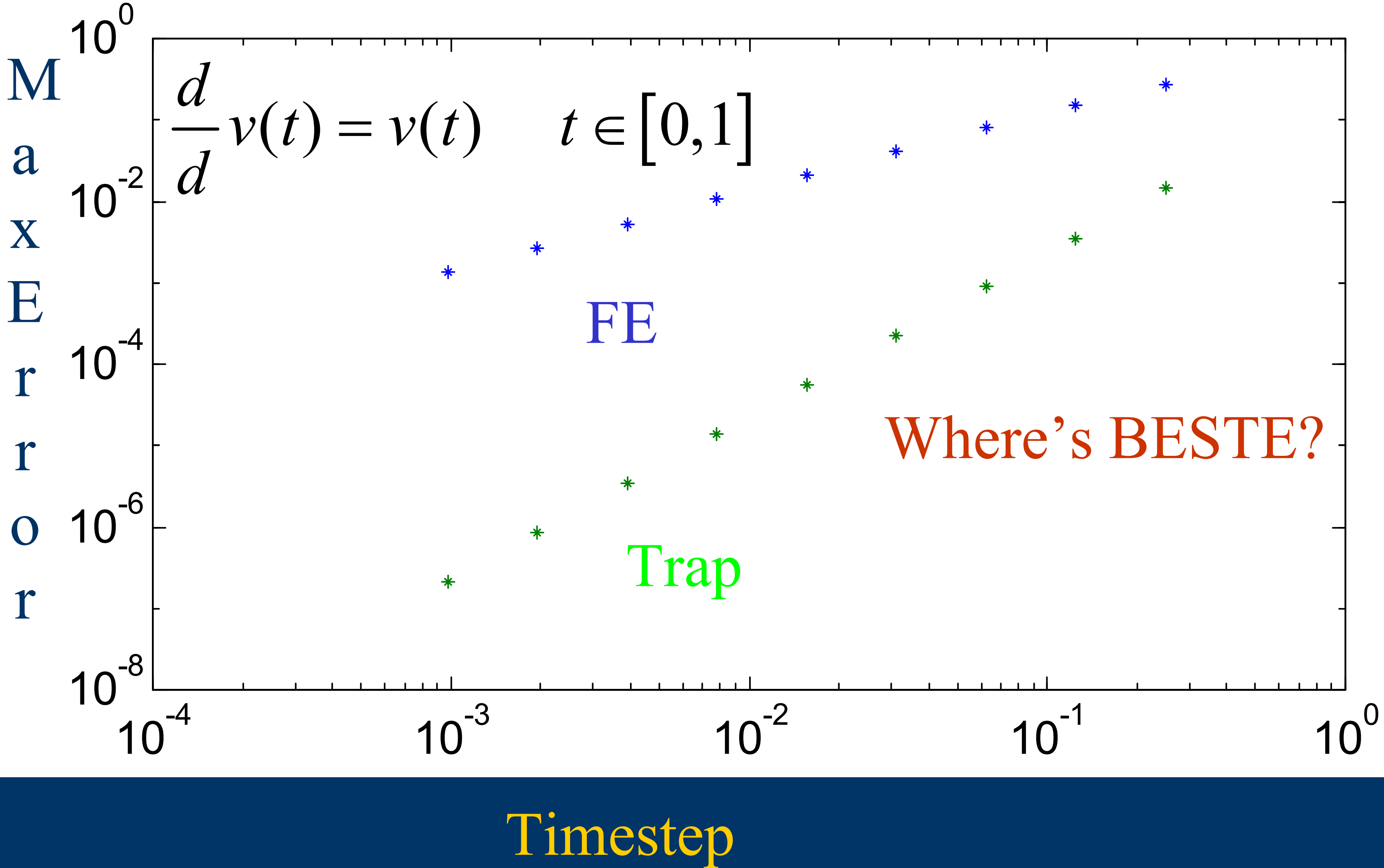


Best Explicit Method has highest one-step accurate

Multistep Methods

Making LTE Small

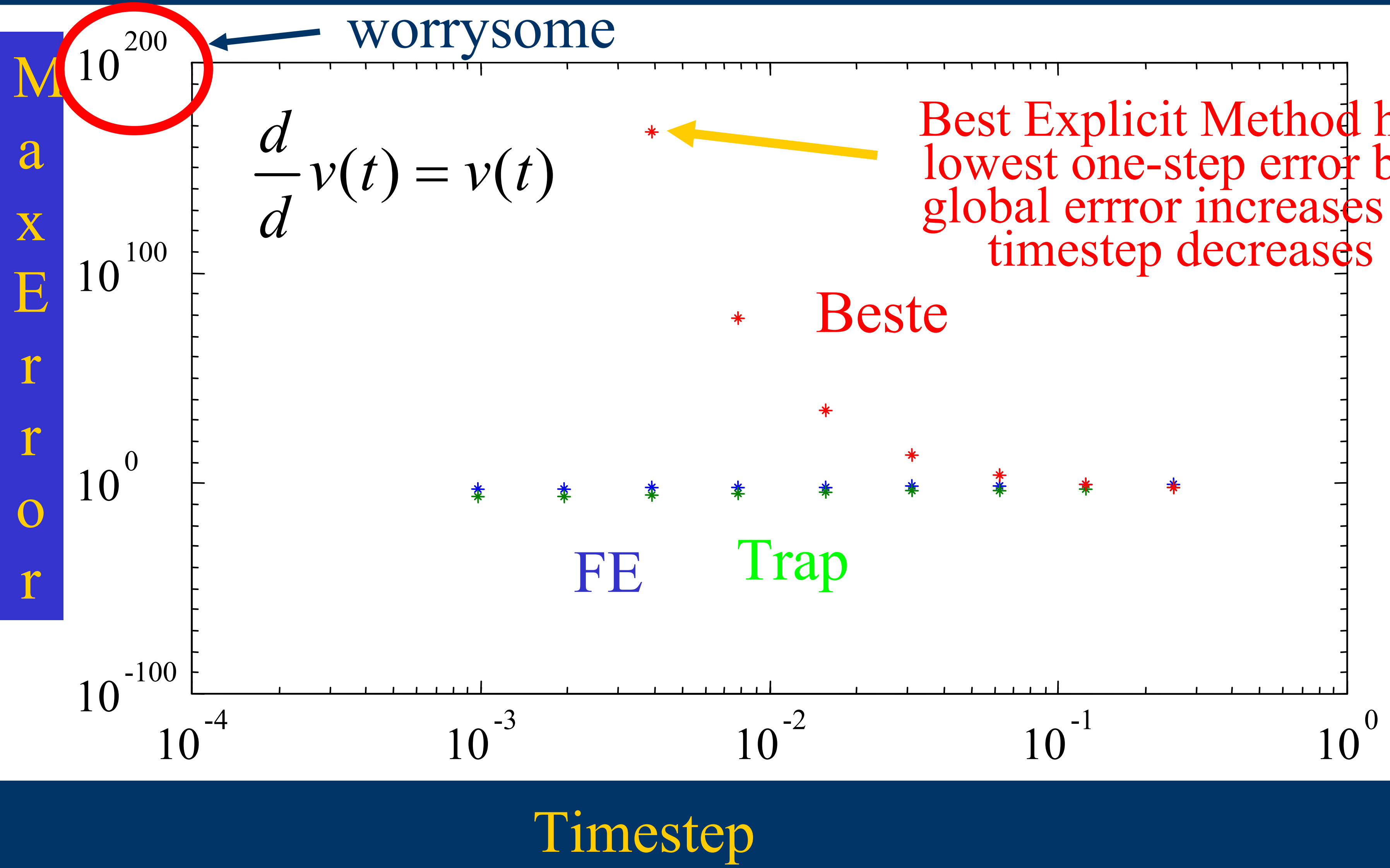
Global Error for the FE, Trap, and “Best” Explicit (BESTE).



Multistep Methods

Making LTE Small

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



worrysome

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

Best Explicit Method has lowest one-step error but global errror increases as timestep decreases

Multistep Methods

Stability of the method

Difference Equation

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

Multistep Method Difference Equation

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

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

Global Error

LTE

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

Multistep Methods

Stability of the method

Stability Definition

Multistep Method Difference Equation

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

Definition: A multistep method is stable if as $\Delta t \rightarrow 0$

$$\max_{l\in\left[0,\frac{T}{\Delta t}\right]} \left|E^l\right| \le \underbrace{C\left(T\right)}_{\substack{\text{interval}\\\text{dependent}}} \frac{T}{\Delta t} \max_{l\in\left[0,\frac{T}{\Delta t}\right]} \left|e^l\right|$$

Stability means: Global Error is bounded by a constant times the sum of the LTE’s

Aside on difference Equations

Convolution Sum

Root Relation

Given a kth order difference eqn with zero initial conditions

$$a_0 x^l + \cdots + a_k x^{l-k} = u^l, \quad x^{-1} = 0, \quad \cdots, x^{-k} = 0$$

x can be related to the input u by $\underbrace{x^l = \sum_{j=0}^{l} h^{l-j} u^j}_{\text{convolution sum}}$

Root multiplicity

$$h^l = \sum_{q=1}^{Q} \sum_{m=0}^{M_q - 1} \gamma_{q,m} (l)^m (\varsigma_q)^l$$

Roots of

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

Aside on difference Equations

Convolution Sum

Bounding Terms

$$x^l = \sum_{q=1}^{Q} \sum_{m=0}^{M_q - 1} \underbrace{\left(\sum_{j=0}^{l} \gamma_{q,m} (l-j)^m (\varsigma_q)^{l-j} u^j \right)}_{R_{q,m}}$$

If $\left|\varsigma_q\right| < 1$, then $\left|R_{q,m}\right| \le C \max_j \left|u^j\right|$

Independent of l

If $\left|\varsigma_{\text{q}}\right| < (1+\varepsilon)$, then $\left|R_{q,0}\right| \le C \frac{e^{\varepsilon l}}{\varepsilon} \max_j \left|u^j\right|$

Bounds **distinct** Roots

Multistep Methods

Stability of the method

Stability Theorem

Theorem: A multistep method is stable if and only if

Roots of $\alpha_0 z^k + \alpha_1 z^{k-1} + \cdots + \alpha_k = 0$ either:

1. Have magnitude less than one
2. Have magnitude equal to one and are distinct

Multistep Methods

Stability of the method

Stability Theorem "Proof"

Given the Multistep Method Difference Equation

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

If, as $\Delta t \rightarrow 0$, roots of $\left(\alpha_0 - \lambda\Delta t\,\beta_0\right)z^l + \cdots + \left(\alpha_k - \lambda\Delta t\,\beta_k\right) = 0$

- less than one in magnitude or
- are distinct and bounded by $1 + \kappa\Delta t,\ \kappa > 0$

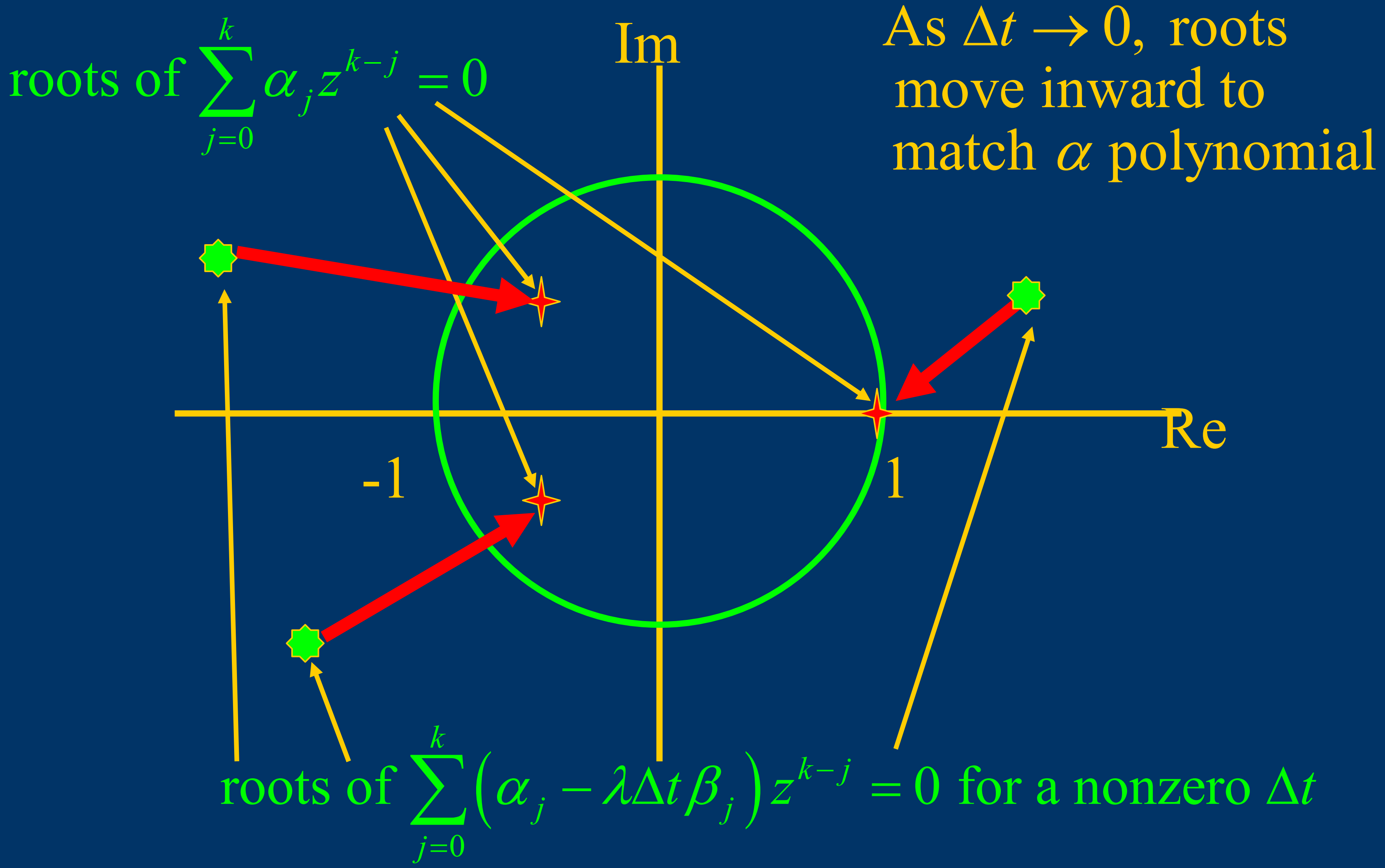
Then from the aside on difference equations

$$\max_{l \in \left[0, \frac{T}{\Delta t}\right]} \left|E^l\right| \le C\frac{e^{\kappa l \Delta t}}{\Delta t} \max_{l \in \left[0, \frac{T}{\Delta t}\right]} \left|e^l\right| \le \underbrace{\frac{Ce^{\kappa T}}{T}}_{C(T)} \frac{T}{\Delta t} \max_{l \in \left[0, \frac{T}{\Delta t}\right]} \left|e^l\right|$$

Multistep Methods

Stability of the method

Stability Theorem Picture



roots of $\sum_{j=0}^{k} \alpha_j z^{k-j} = 0$

As $\Delta t \rightarrow 0$, roots move inward to match α polynomial

roots of $\sum_{j=0}^{k} \left(\alpha_j - \lambda \Delta t \beta_j\right) z^{k-j} = 0$ for a nonzero Δt

Multistep Methods

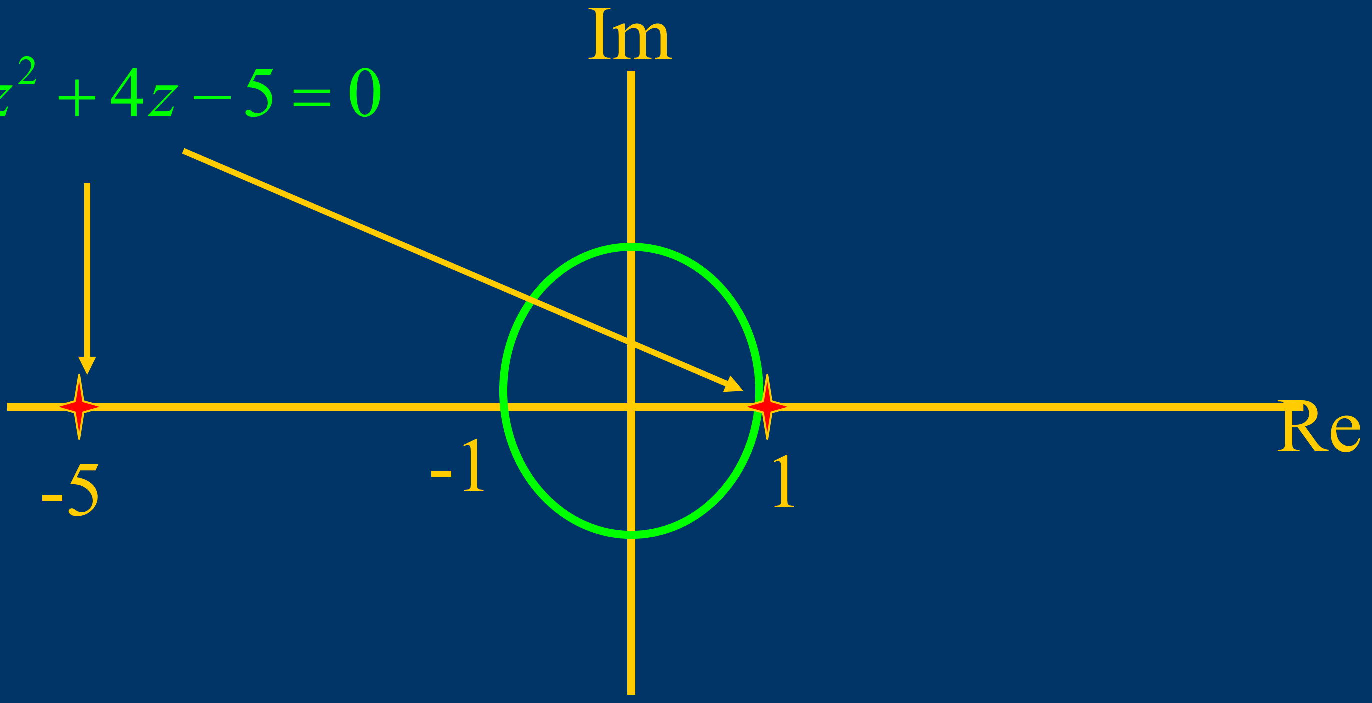
Stability of the method

The BESTE Method

Best explicit 2-step method

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

roots of $z^2 + 4z - 5 = 0$



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-1 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)

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

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

$$\text{roots of } \sum_{j=0}^{k} \alpha_j z^{k-j} = 0$$

Inside the unit circle or on the unit circle and distinct

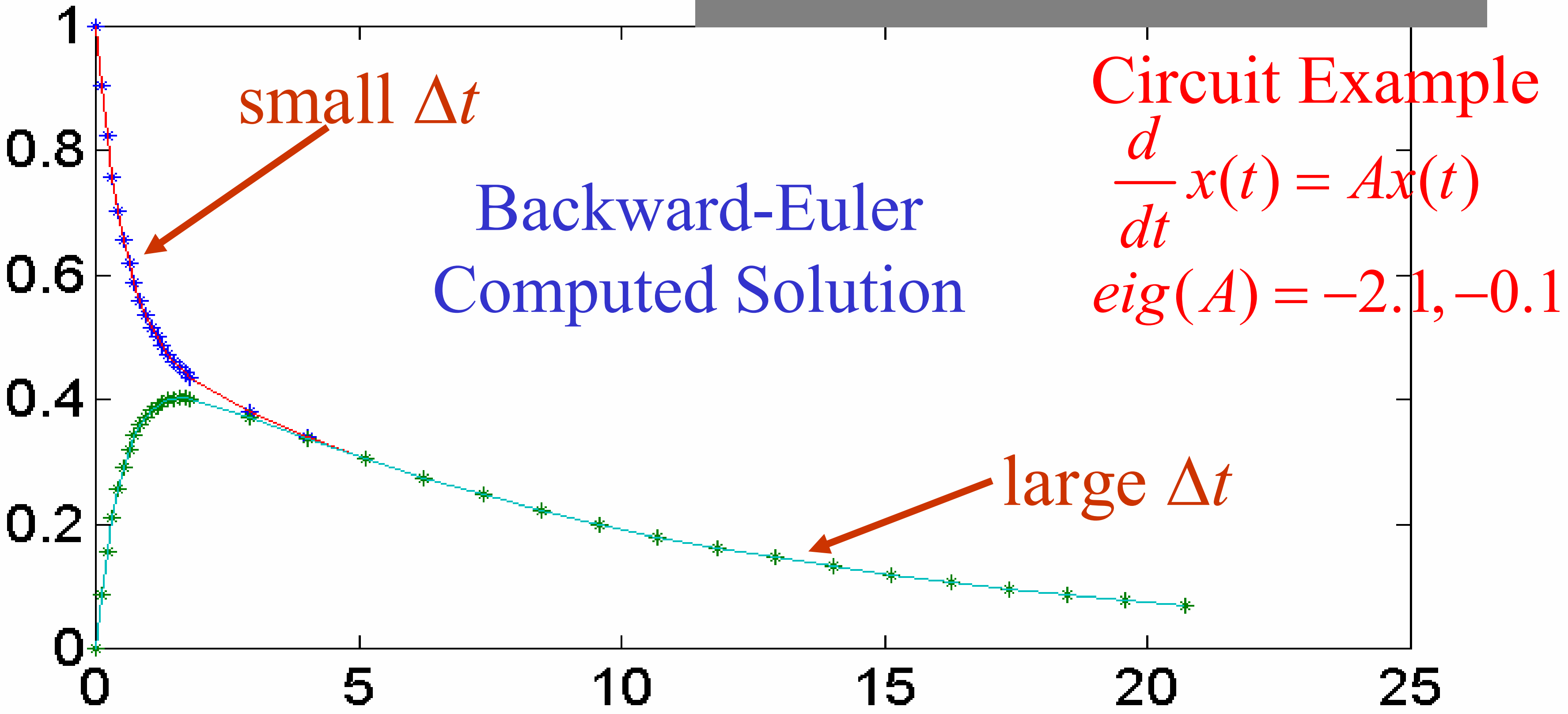
$$\Rightarrow \max_{l \in \left[0, \frac{T}{\Delta t}\right]} \left\| E^l \right\| \leq C_2 \frac{T}{\Delta t} \max_{l \in \left[0, \frac{T}{\Delta t}\right]} \left\| e^l \right\|$$

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

Multistep Methods

Large timestep stability

Two time-constant circuit



Circuit Example

$$\frac{d}{dt}x(t) = Ax(t)$$

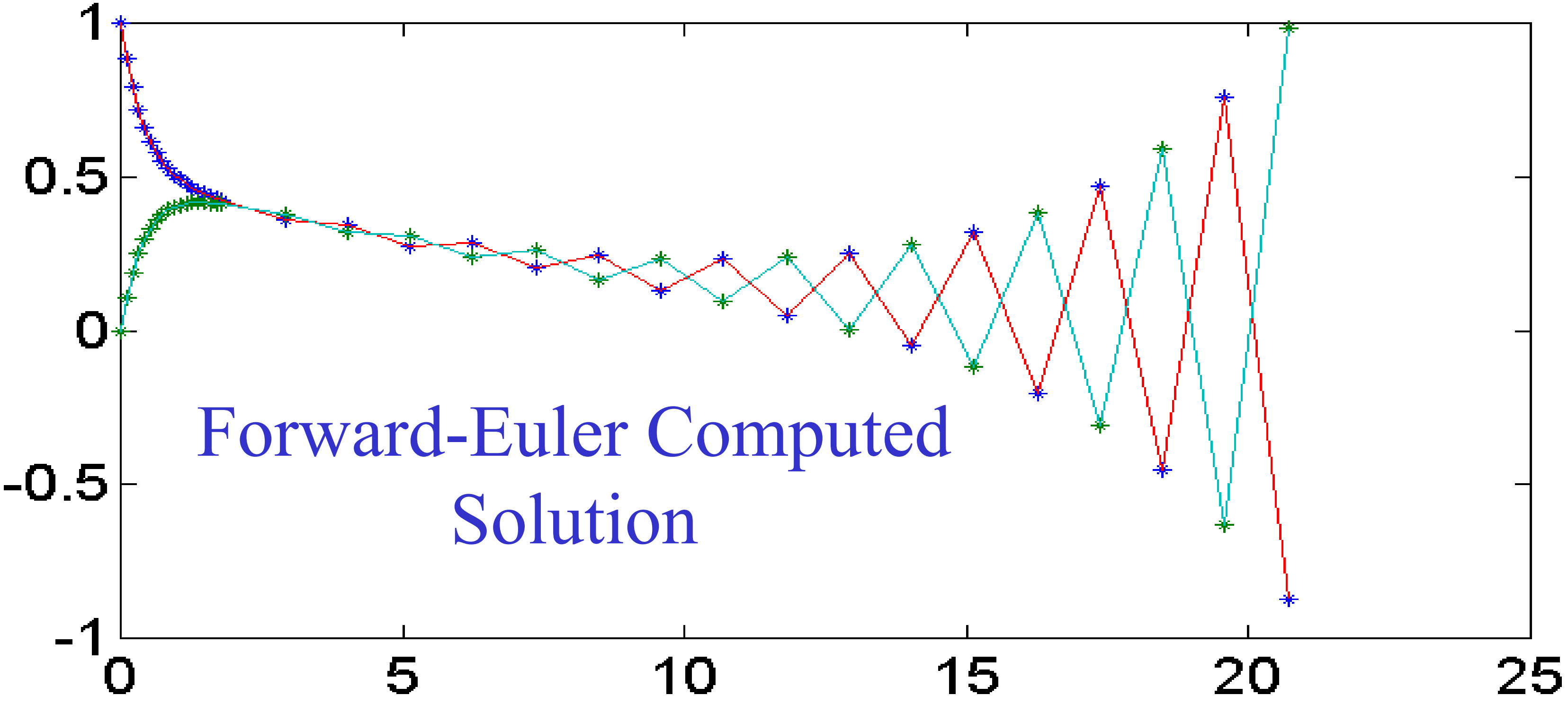
$$eig(A) = -2.1, -0.1$$

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

Multistep Methods

Large Timestep Stability

FE on two time-constant circuit?



Forward-Euler Computed Solution

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

Multistep Methods

Large Timestep Stability

FE, BE and Trap on the scalar ode problem

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

Forward-Euler: $$\hat{v}^{l+1}=\hat{v}^{l}+\Delta t\lambda\hat{v}^{l}=\left(1+\Delta t\lambda\right)\hat{v}^{l}$$

If $\left|1+\Delta t\lambda\right|>1$ the solution grows even if $\lambda<0$

Backward-Euler: $$\hat{v}^{l+1}=\hat{v}^{l}+\Delta t\lambda\hat{v}^{l+1}\Rightarrow\hat{v}^{l+1}=\frac{1}{\left(1-\Delta t\lambda\right)}\hat{v}^{l}$$

If $\left|\frac{1}{1-\Delta t\lambda}\right|<1$ the solution decays even if $\lambda>0$

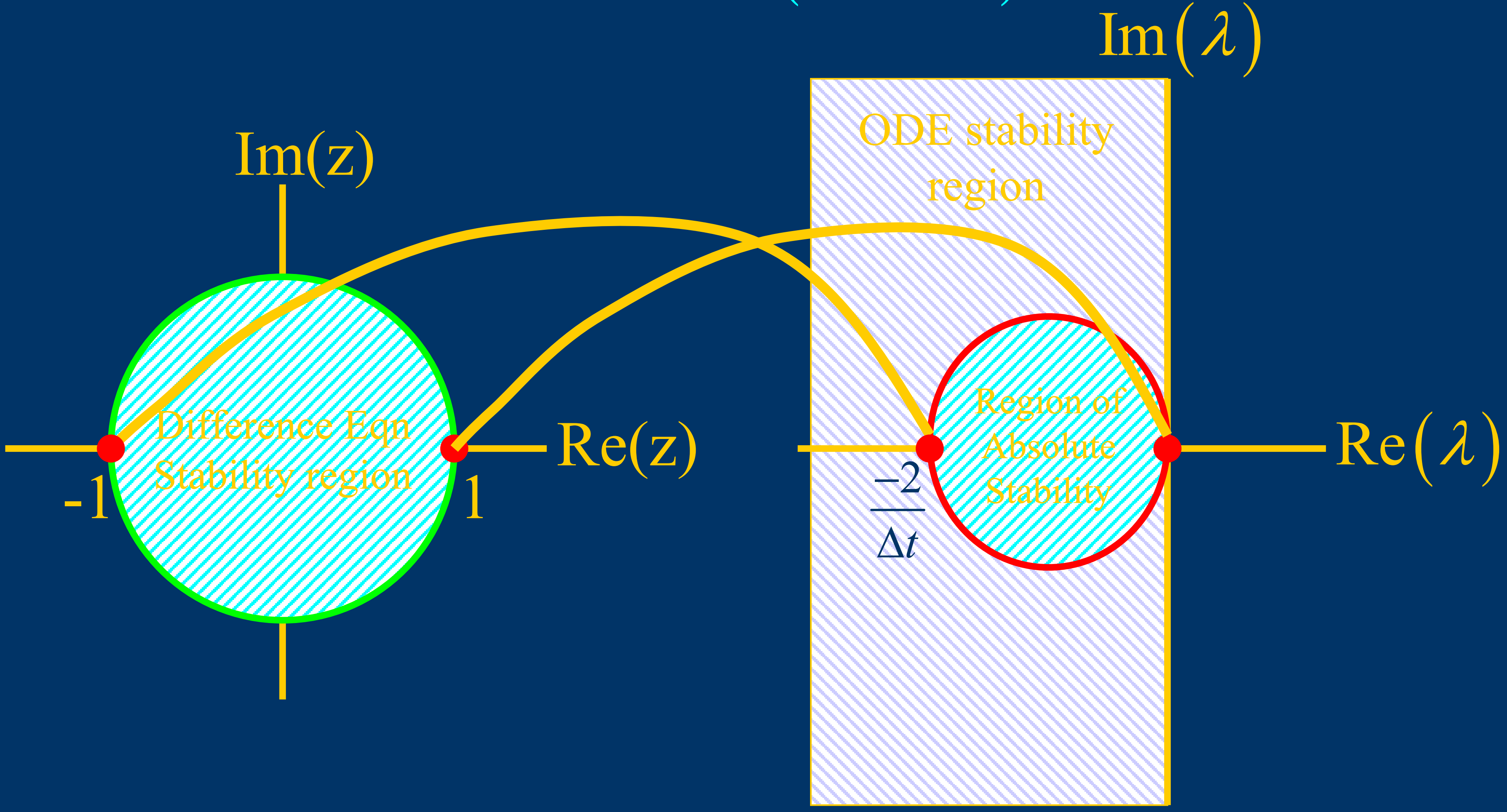
Trap Rule: $$\hat{v}^{l+1}=\hat{v}^{l}+0.5\Delta t\lambda\left(\hat{v}^{l+1}+\hat{v}\right)^{l}\Rightarrow\hat{v}^{l+1}=\frac{\left(1+0.5\Delta t\lambda\right)}{\left(1-0.5\Delta t\lambda\right)}\hat{v}^{l}$$

Multistep Methods

Large Timestep Stability

FE large timestep region of absolute stability

Forward Euler $z = \left(1 + \Delta t \lambda\right)$

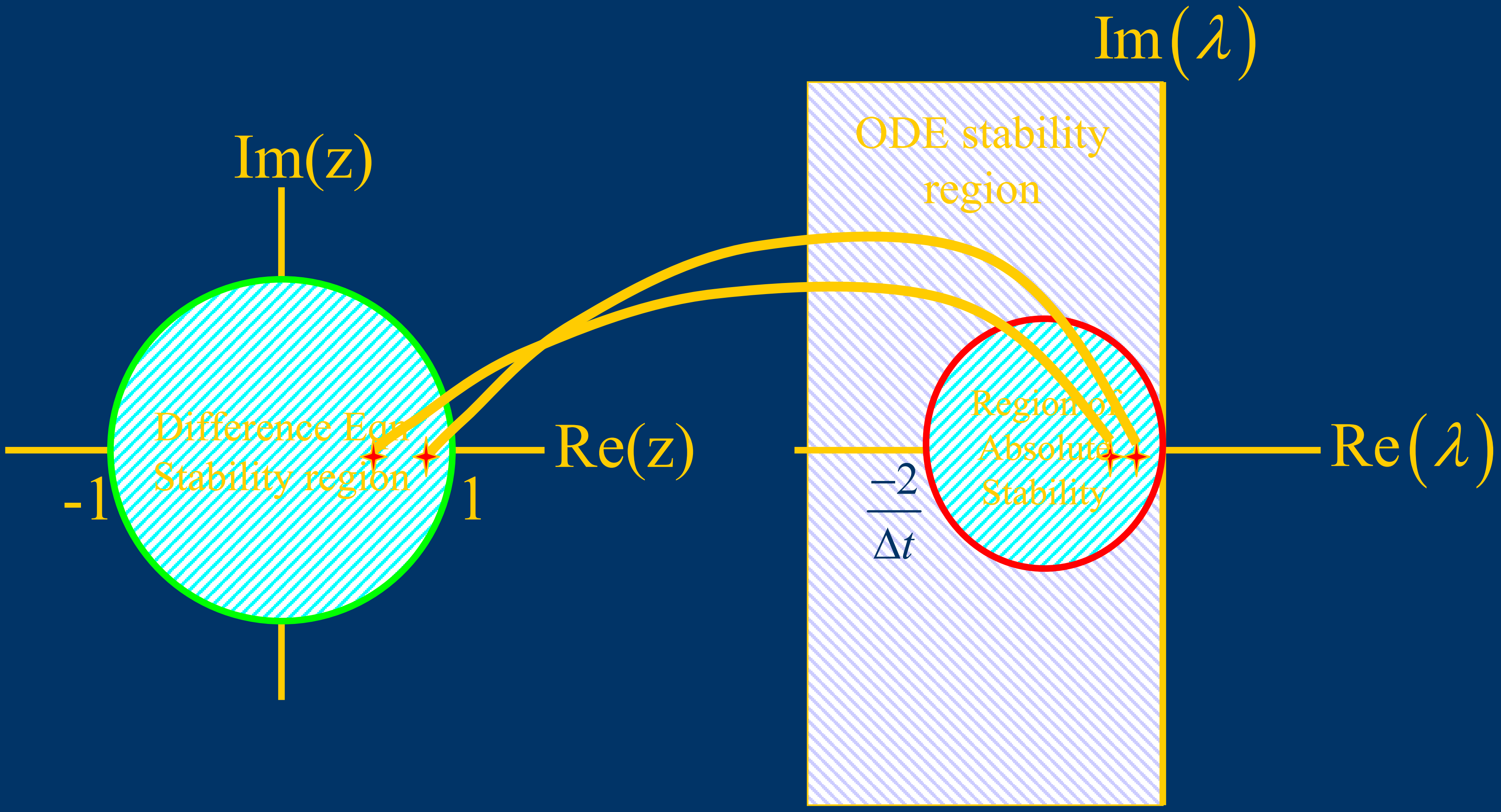


Multistep Methods

Large Timestep Stability

FE large timestep stability, circuit example

Circuit example with $\Delta t = 0.1, \ \lambda = -2.1, -0.1$

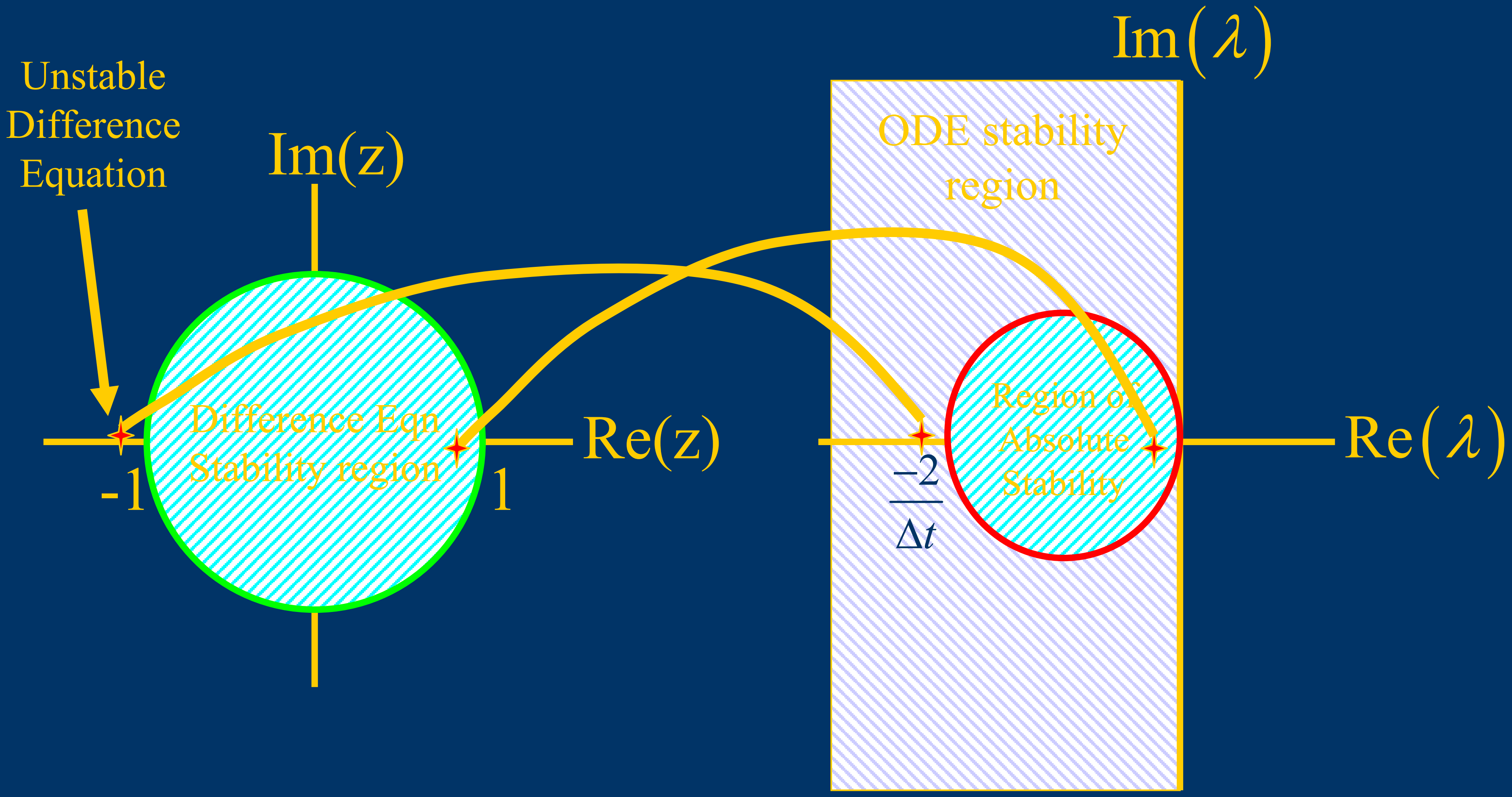


Multistep Methods

Large Timestep Stability

FE large timestep stability, circuit example

Circuit example with $\Delta t=1.0,\ \lambda = -2.1, -0.1$

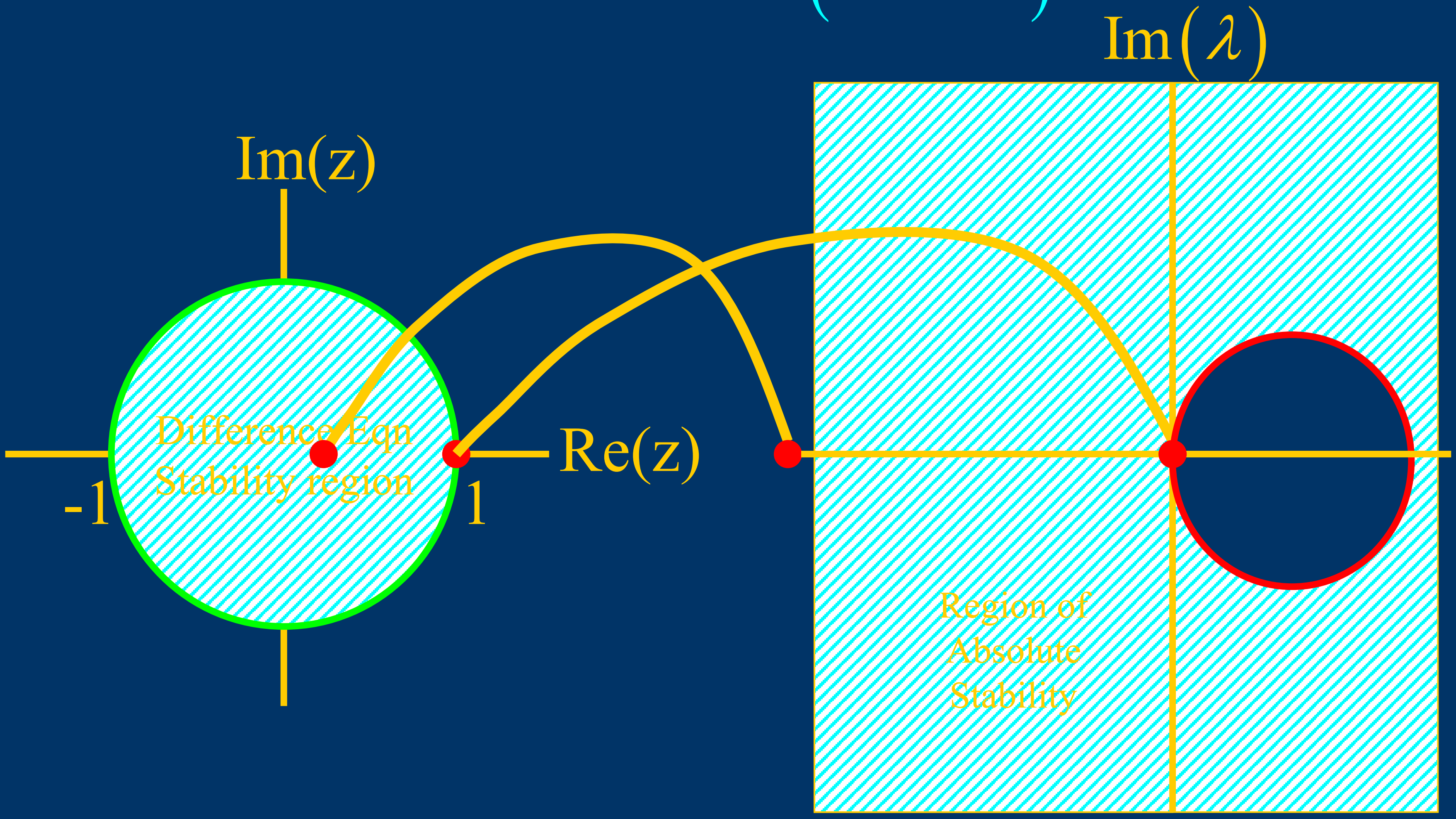


Multistep Methods

Large Timestep Stability

BE large timestep region of absolute stability

Backward Euler $z = \left(1 - \Delta t \lambda\right)^{-1}$

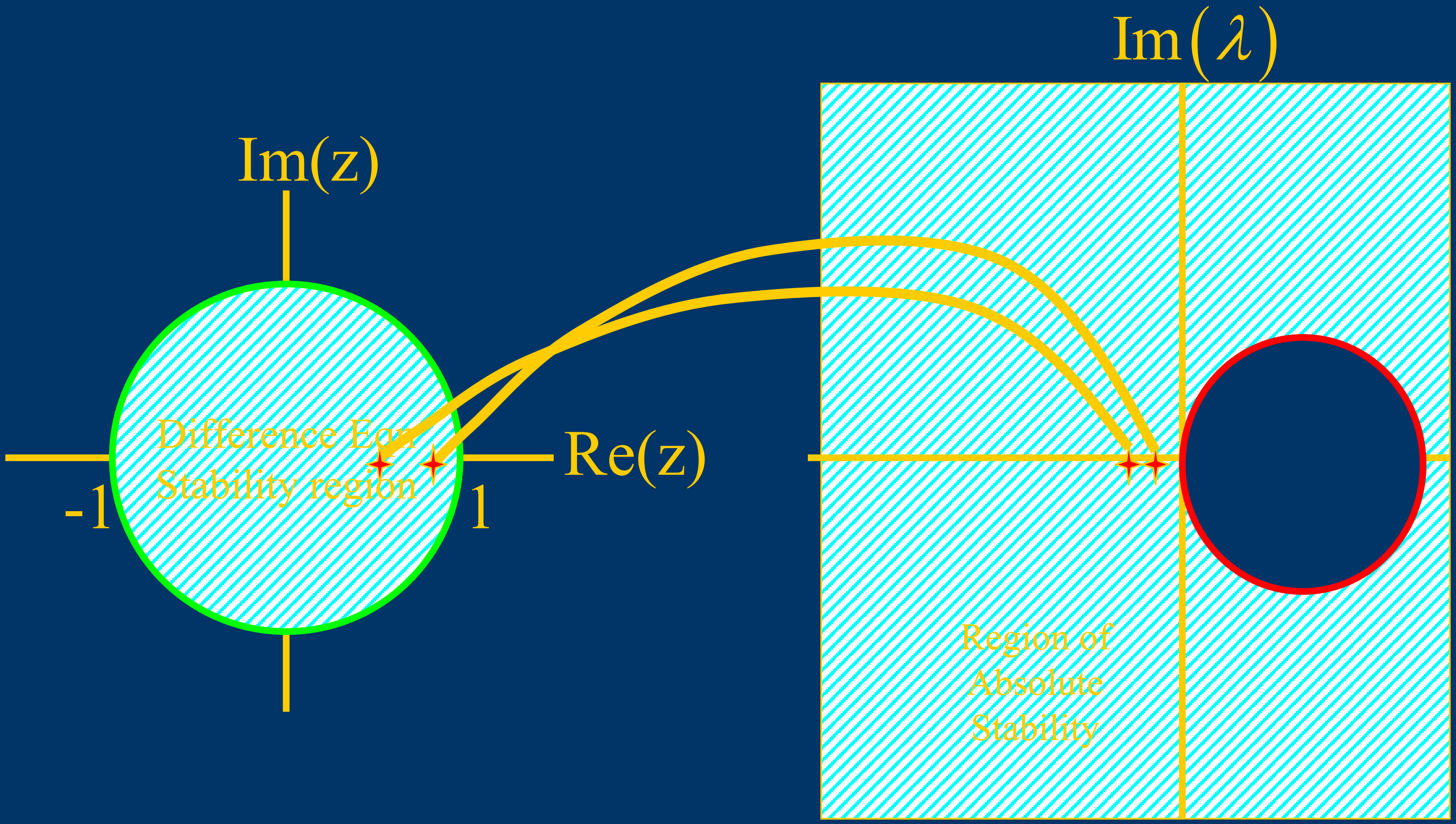


Multistep Methods

Large Timestep Stability

BE large timestep stability, circuit example

Circuit example with $\Delta t = 0.1,\ \lambda = -2.1,\ -0.1$

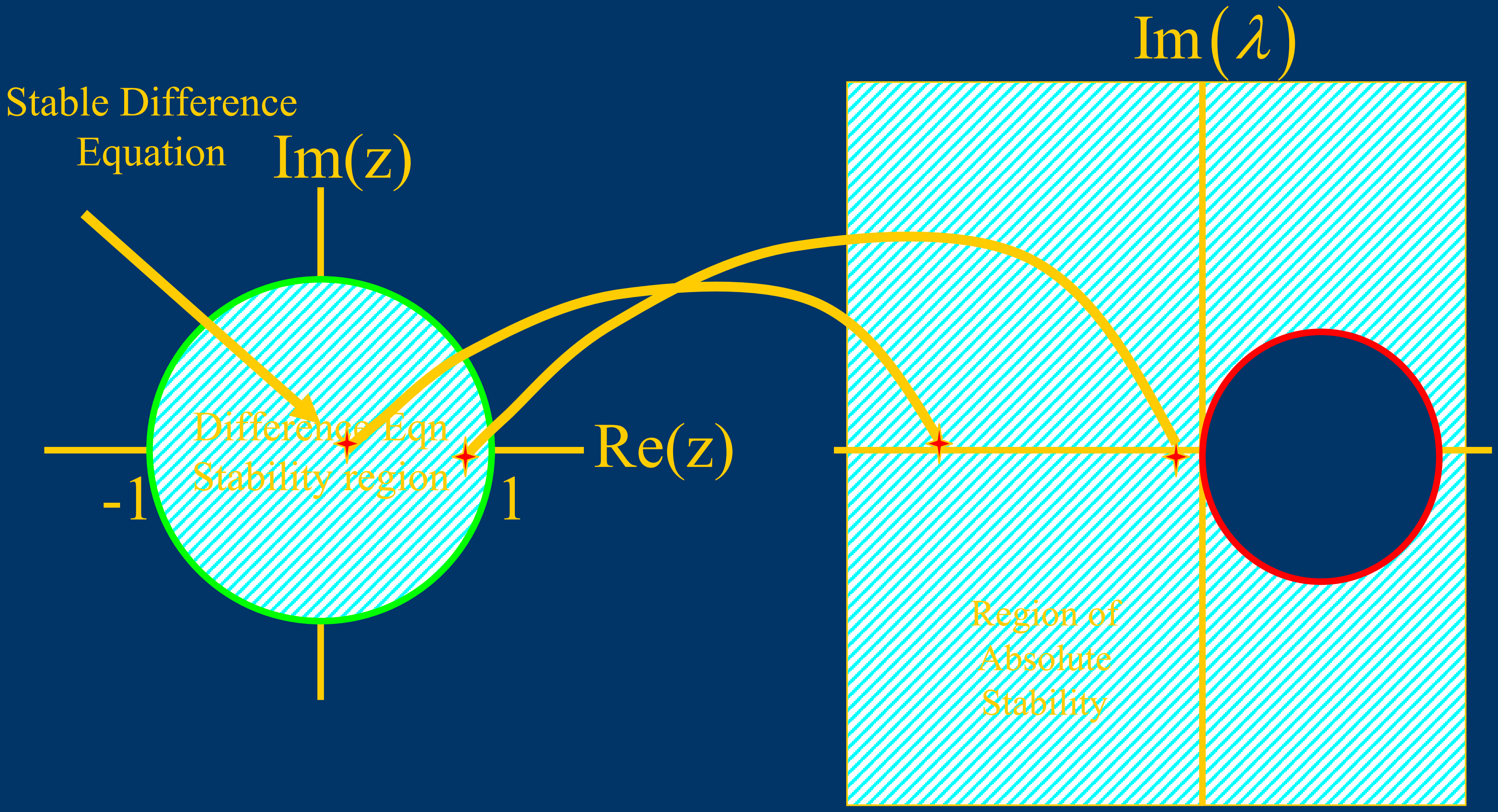


Multistep Methods

Large Timestep Stability

BE large timestep stability, circuit example

Circuit example with $\Delta t = 1.0,\ \lambda = -2.1, -0.1$



Multistep Methods

Large Timestep Stability

Stability Definitions

Region of Absolute Stability for a Multistep method:

Values of $\lambda\Delta t$ where roots of $\sum_{j=0}^{k}\left(\alpha_j - \lambda\Delta t\,\beta_j\right)z^{k-j} = 0$ are inside the unit circle.

A-stable:

A method is A-stable if its region of absolute stability includes the entire left-half of the complex plane

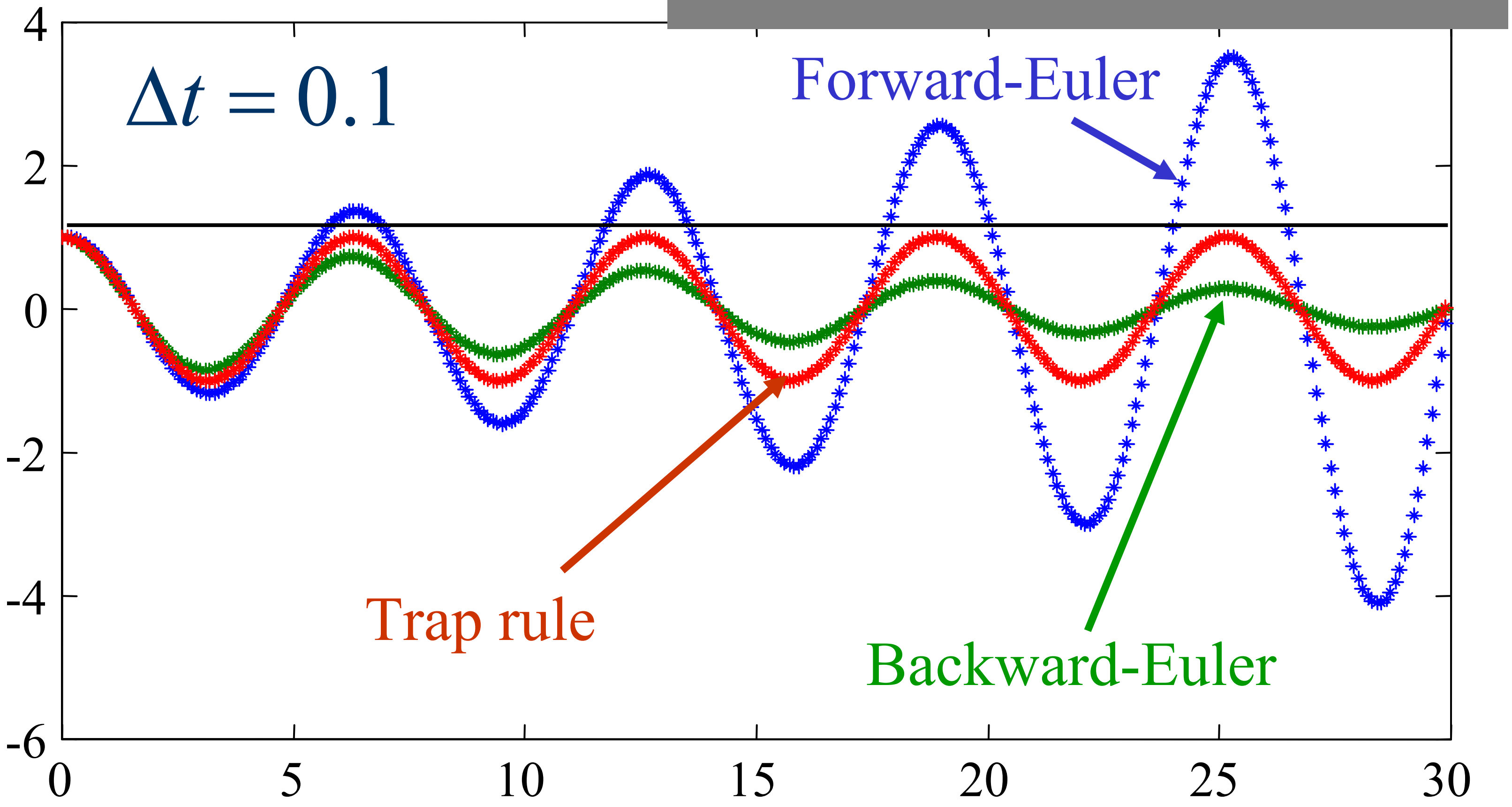
Dahlquist's second Stability barrier:

There are no A-stable multistep methods of convergence order greater than 2, and the trap rule is the most accurate.

Multistep methods

Numerical Experiments

Oscillating Strut and Mass



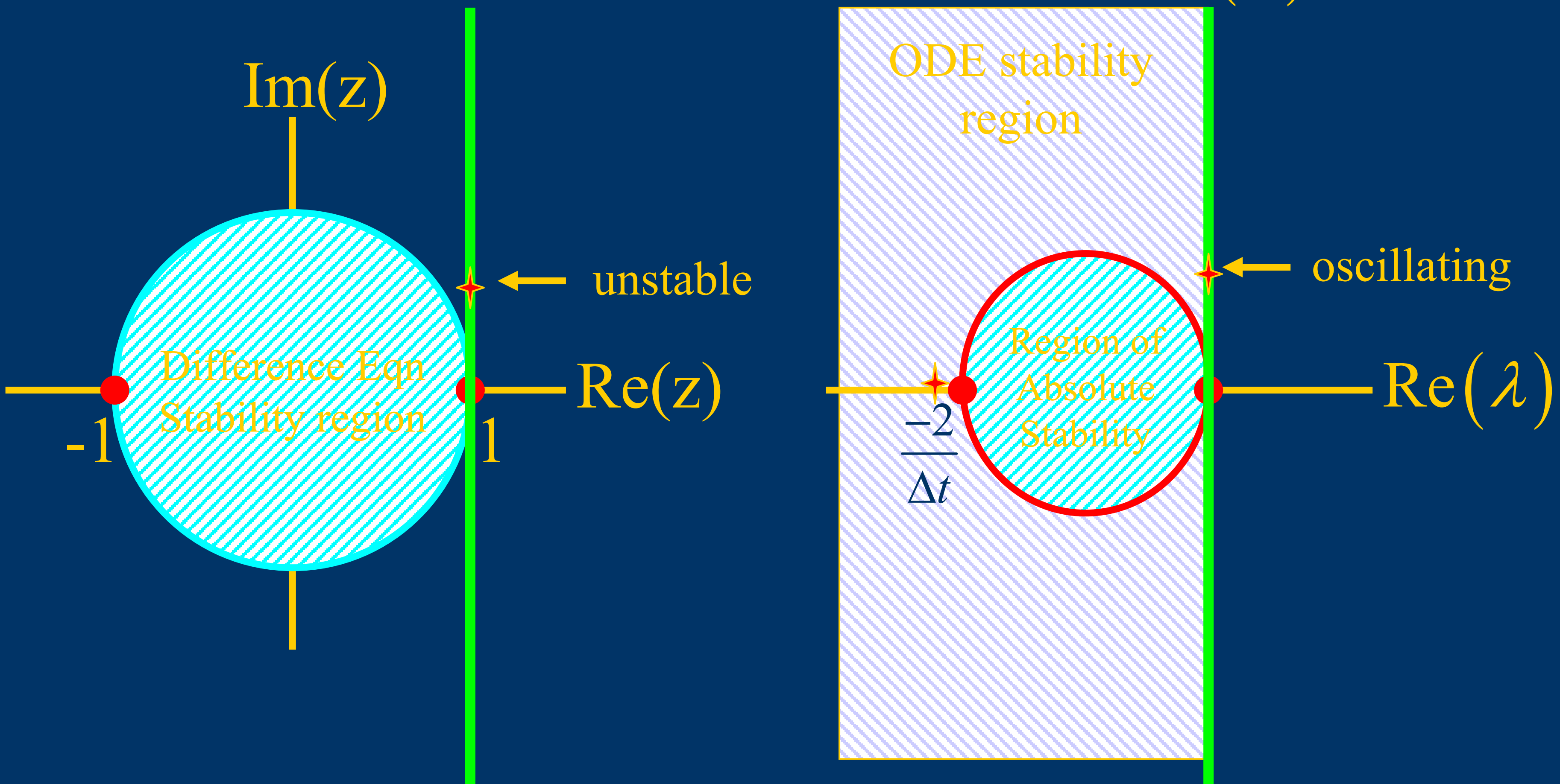
Why does FE result grow, BE result decay and the Trap rule preserve oscillations

Multistep Methods

Large Timestep Stability

FE large timestep oscillator example

Forward Euler $z = \left(1 + \Delta t \lambda\right)$

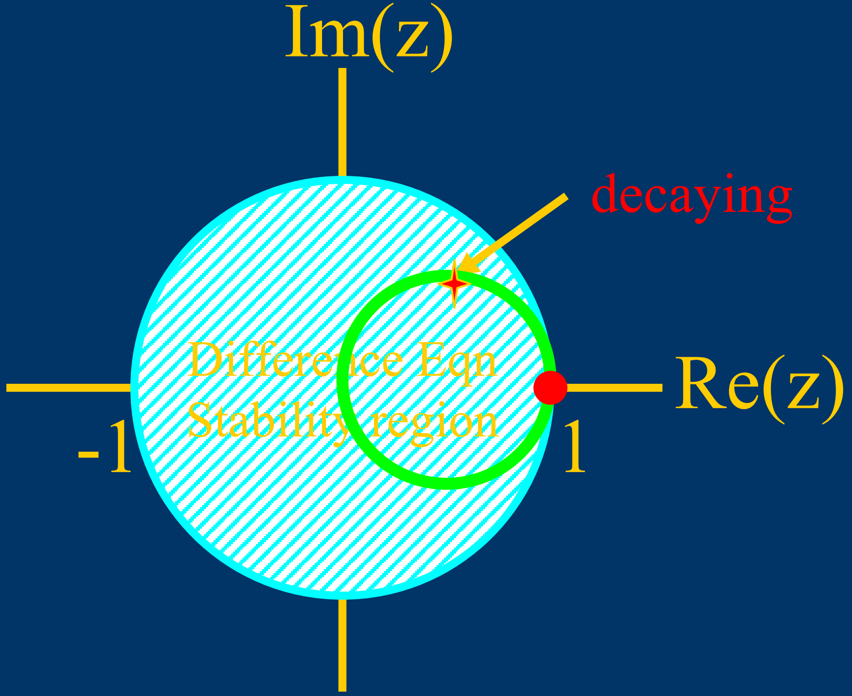


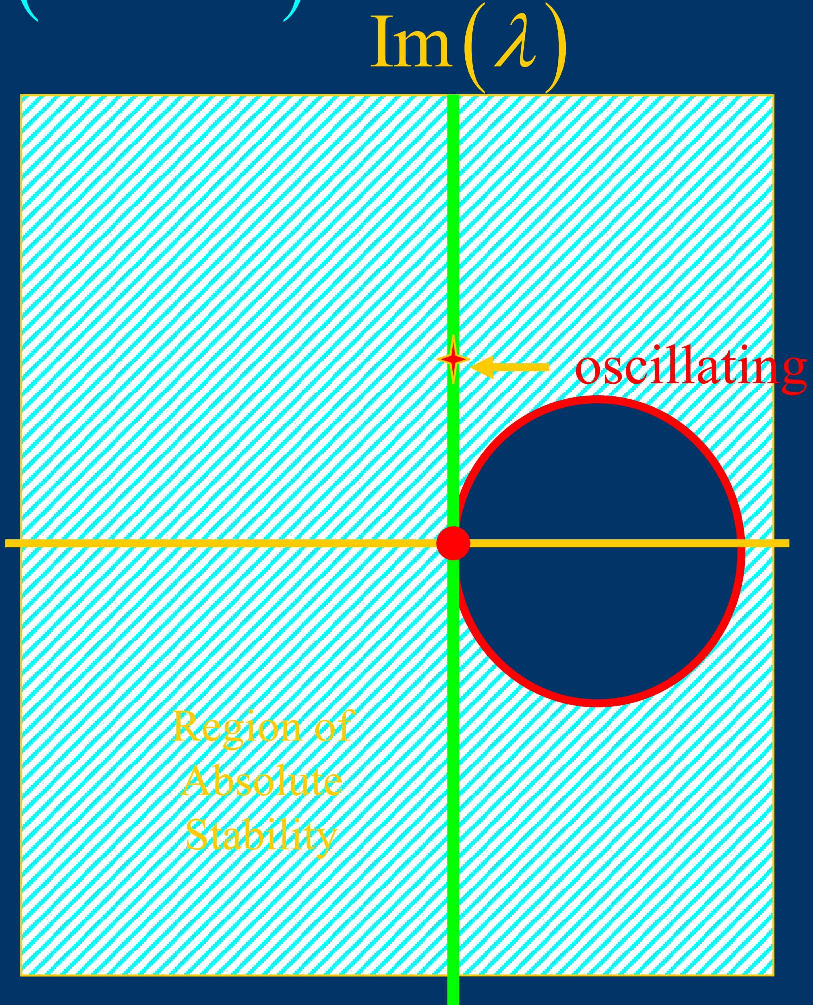
Multistep Methods

Large Timestep Stability

BE large timestep oscillator example

Backward Euler $z = \left(1 - \Delta t \lambda\right)^{-1}$



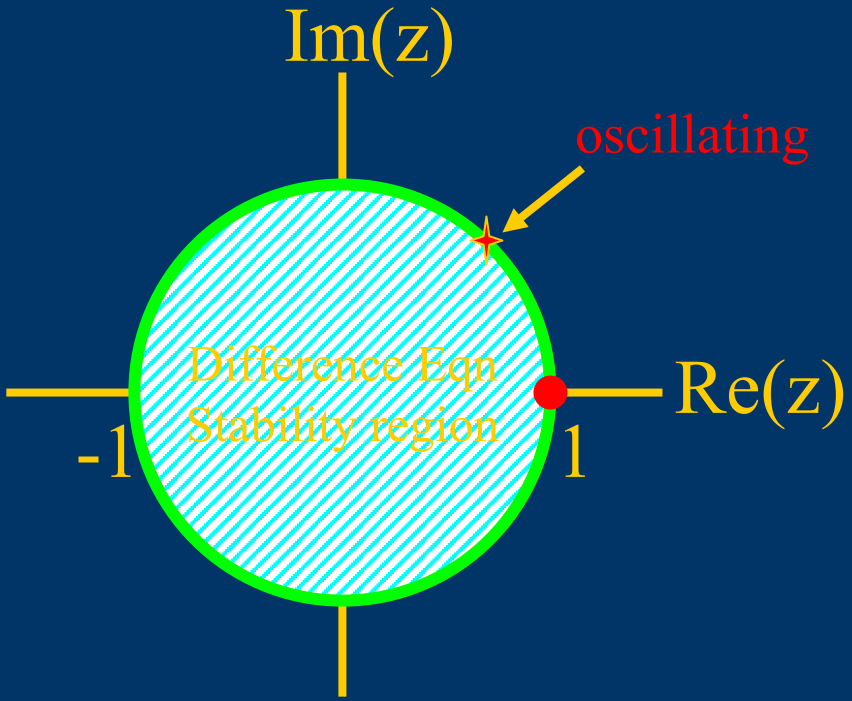


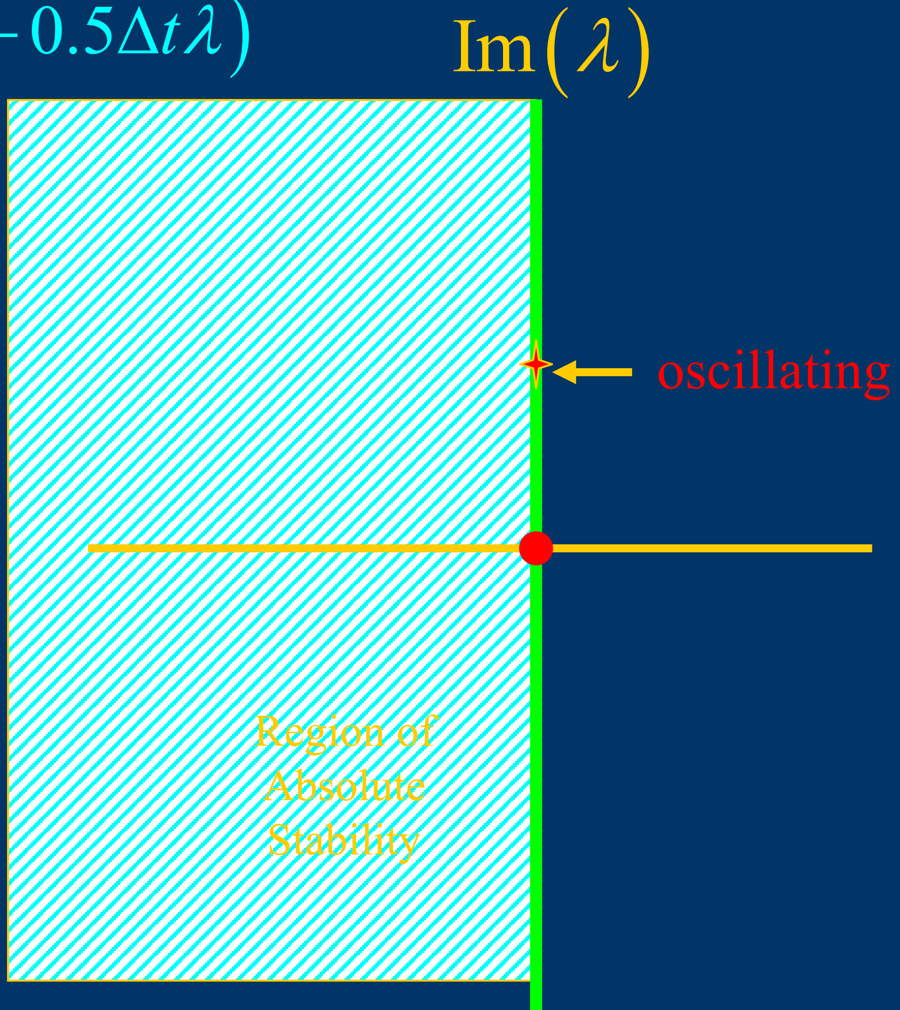
Multistep Methods

Large Timestep Stability

Trap large timestep oscillator example

Trap Rule $$z = \frac{\left(1 + 0.5\Delta t \lambda\right)}{\left(1 - 0.5\Delta t \lambda\right)}$$





Multistep Methods

Large Timestep Issues

Two Time-Constant Stable problem (Circuit)

FE: stability, not accuracy, limited timestep size.

BE was A-stable, any timestep could be used.

Trap Rule most accurate A-stable m-step method

Oscillator Problem

Forward-Euler generated an unstable difference equation regardless of timestep size.

Backward-Euler generated a stable (decaying) difference equation regardless of timestep size.

Trapezoidal rule mapped the imaginary axis

Summary

Small Timestep issues for Multistep Methods

- Local truncation error and Exactness.
- Difference equation stability.
- Stability + Consistency implies convergence.

Investigate Large Timestep Issues

- Absolute Stability for two time-scale examples.
- Oscillators.

Didn’t talk about

- Runge-Kutta schemes, higher order A-stable methods.