Introduction to Simulation - Lecture 14

**Multistep Methods II**

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

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

- **Solution at discrete points**
- **Time discretization**
- **Multistep coefficients**
Multistep Methods

Simplified Problem for Analysis

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

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 \( \lambda \in \mathbb{C} \)

Decaying Solutions

Growing Solutions

Oscillations

Im(\( \lambda \))

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

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

$\hat{v}^l$ computed with $\frac{\Delta t}{2}$

$v_{\text{exact}}$
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:

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

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

Difference equation relates LTE to Global error

\( (\alpha_0 - \lambda \Delta t \beta_0) E^l + (\alpha_1 - \lambda \Delta t \beta_1) E^{l-1} + \cdots + (\alpha_k - \lambda \Delta t \beta_k) E^{l-k} = e^l \)
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 \[ \frac{d}{dt} v(t) = \lambda v(t) \]

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

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

\[ \frac{d}{dt} v(t_{k-j}) \]
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

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

Note

\[\sum \alpha_i = 0\]

Always

\[\sum \alpha_i = 0\]
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).

\[ \frac{d}{dt} v(t) = v(t) \]

Best Explicit Method has highest one-step accurate
Multistep Methods

Making LTE Small

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

\[
\frac{d}{dt} v(t) = v(t) \quad t \in [0, 1]
\]

Where’s BESTE?
Multistep Methods

Making LTE Small

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

Multistep Methods

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

Best Explicit Method has lowest one-step error but global error 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

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

Global Error

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

We made the LTE so small, how come the Global error is so large?
Multistep Method Difference Equation

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

**Definition:** A multistep method is stable if as \( \Delta t \to 0 \)

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

**Stability means:** Global Error is bounded by a constant times the sum of the LTE’s
Given a kth order difference eqn with zero initial conditions

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

\( x \) can be related to the input \( u \) by

\[ x^l = \sum_{j=0}^{l} h^{l-j} u^j \]

Root multiplicity

\[ h^l = \sum_{q=1}^{Q} \sum_{m=0}^{M_q-1} \gamma_{q,m}(l)^m \left( \zeta_q \right)^l \]

Roots of

\[ a_0 z^k + a_1 z^{k-1} + \cdots + a_k = 0 \]
Aside on difference Equations

Convolution Sum

Bounding Terms

\[ x^l = \sum_{q=1}^{Q} \sum_{m=0}^{M_q-1} \left( \sum_{j=0}^{l} \gamma_{q,m} (l-j)^m \left( \zeta_q \right)^{l-j} u^j \right) \]

If \(|\zeta_q| < 1\), then \(|R_{q,m}| \leq C \max_j |u^j|\)

If \(|\zeta_q| < (1+\varepsilon)\), then \(|R_{q,0}| \leq C \frac{e^{\varepsilon l}}{\varepsilon} \max_j |u^j|\)

Bounds distinct Roots
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

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

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

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

Then from the aside on difference equations

\[
\max_{l \in \left[0, \frac{T}{\Delta t}\right]} |E^l| \leq C e^{\kappa l \Delta t} \max_{l \in \left[0, \frac{T}{\Delta t}\right]} |e^l| \leq \frac{C e^{\kappa T}}{T} \frac{T}{\Delta t} \max_{l \in \left[0, \frac{T}{\Delta t}\right]} |e^l|
\]
Multistep Methods

Stability of the method

Stability Theorem Picture

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

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

roots of $\sum_{j=0}^{k} (\alpha_j - \lambda \Delta t \beta_j) z^{k-j} = 0$ for a nonzero $\Delta t$
Best explicit 2-step method

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

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

Method is Wildly unstable!
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.
1) Local Condition: One step errors are small (consistency)

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

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

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

roots of $\sum_{j=0}^{k} \alpha_j z^{k-j} = 0$ Inside 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: $\max_{l \in \left[0, \frac{T}{\Delta t}\right]} \left\| E^l \right\| \leq C T (\Delta t)^{p_0}$
With Backward-Euler it is easy to use small timesteps for the fast dynamics and then switch to large timesteps for the slow decay.
The Forward-Euler is accurate for small timesteps, but goes unstable when the timestep is enlarged.
Multistep Methods

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

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

If \( |1 + \Delta t \lambda| > 1 \) the solution grows even if \( \lambda < 0 \)

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

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

Trap Rule: \( \hat{v}^{t+1} = \hat{v}^t + 0.5 \Delta t \lambda (\hat{v}^{t+1} + \hat{v}) \Rightarrow \hat{v}^{t+1} = \frac{(1 + 0.5 \Delta t \lambda)}{(1 - 0.5 \Delta t \lambda)} \hat{v}^t \)
Multistep Methods

Large Timestep Stability

FE large timestep region of absolute stability

Forward Euler

\[ z = (1 + \Delta t \lambda) \]

Difference Eqn

Stability region

ODE stability region

Region of Absolute Stability

-1

Re(z)

Im(z)

1

Im(\lambda)

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

**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

\[ z = \left(1 - \Delta t \lambda \right)^{-1} \]

Region of Absolute Stability

\[ \text{Im}(\lambda) \]

\[ \text{Re}(z) \]

\[ \text{Im}(z) \]

Difference Eqn Stability region
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 $\Delta t = 1.0, \lambda = -2.1, -0.1$

Stable Difference Equation

$\text{Im}(z)$

$\text{Re}(z)$

Region of Absolute Stability

$\text{Im}(\lambda)$
Region of Absolute Stability for a Multistep method:
Values of $\lambda \Delta t$ where roots of $\sum_{j=0}^{k} (\alpha_j - \lambda \Delta t \beta_j) z^{k-j} = 0$
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

\[ \Delta t = 0.1 \]

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

\[ z = \left( 1 + \Delta t \lambda \right) \]

Difference Eqn Stability region

Im(z)

Re(z)

ODE stability region

Region of Absolute Stability

-1

1

Unstable

Oscillating

Im(\lambda)

Re(\lambda)

-2

\Delta t
Multistep Methods

Large Timestep Stability

BE large timestep oscillator example

Backward Euler

\[ z = (1 - \Delta t \lambda)^{-1} \]

Difference Eqn

Stability region

Decaying

Im(z)

Re(z)

Im(\lambda)

oscillating

Region of Absolute Stability
\[ z = \frac{1 + 0.5 \Delta t \lambda}{1 - 0.5 \Delta t \lambda} \]
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.