Lecture 3

Convergence of Multi-Step Methods

In Lecture 2, we began the discussion of convergence. In this lecture, we will complete that discussion for the class of numerical methods known as multi-step methods (a class that includes the forward Euler and midpoint methods we have previously discussed).

3.1 Multi-step Methods

The class of finite difference methods known as multi-step methods is one of the most widely-used approaches for solving ordinary differential equations, and forms the basis for solving partial differential equations as well.

Definition 3.1 (Multi-step Methods) *The generic form of an s-step multi-step method is,*

$$v^{n+1} + \sum_{i=1}^{s} \alpha_i v^{n+1-i} = \Delta t \sum_{i=0}^{s} \beta_i f^{n+1-i}.$$

A multi-step method with $\beta_0 = 0$ is known as an ***explicit*** *method since in this case the new value v^{n+1} can be determined as an explicit function of known values (i.e. from v^i and f_i with $i \leq n$). A multi-step method with $\beta_0 \neq 0$ is known as an* ***implicit*** *method since in this case the new value v^{n+1} is an implicit function of itself through the forcing function, $f^{n+1} = f(v^{n+1}, t^{n+1})$.*

Example 3.1 *Using the notation given in Definition 3.1, the forward Euler method is:*

$$\alpha_1 = -1 \quad \textit{all other} \quad \alpha_i = 0$$

$$\beta_1 = 1 \quad \textit{all other} \quad \beta_i = 0$$

Example 3.2 *Using the notation given in Definition 3.1, the midpoint method is:*

$$\alpha_2 = -1 \quad \textit{all other} \quad \alpha_i = 0$$

$$\beta_1 = 2 \quad \textit{all other} \quad \beta_i = 0$$

Example 3.3 *In this example, we will derive the most accurate multi-step method of the following form:*

$$v^{n+1} + \alpha_1 v^n + \alpha_2 v^{n-1} = \Delta t\left[\beta_1 f^n + \beta_2 f^{n-1}\right]$$

The local truncation error for this method is,

$$\tau = -\alpha_1 u^n - \alpha_2 u^{n-1} + \Delta t\left[\beta_1 f^n + \beta_2 f^{n-1}\right] - u^{n+1}$$

Substitution of $f^n = u_t^n$ *and* $f^{n-1} = u_t^{n-1}$ *gives,*

$$\tau = -\alpha_1 u^n - \alpha_2 u^{n-1} + \Delta t\left[\beta_1 u_t^n + \beta_2 u_t^{n-1}\right] - u^{n+1}$$

Then, Taylor series about $t = t^n$ *are substituted for* u^{n-1}, u_t^{n-1}, *and* u^{n+1} *to give,*

$$\begin{aligned}\tau &= -\alpha_1 u^n - \alpha_2\left[u^n - \Delta t u_t^n + \frac{1}{2}\Delta t^2 u_{tt}^n - \frac{1}{6}\Delta t^3 u_{ttt}^n + \frac{1}{24}\Delta t^4 u_{tttt}^n + O(\Delta t^5)\right] \\ &\quad + \Delta t\beta_1 u_t^n + \Delta t\beta_2\left[u_t^n - \Delta t u_{tt}^n + \frac{1}{2}\Delta t^2 u_{ttt}^n - \frac{1}{6}\Delta t^3 u_{tttt}^n + O(\Delta t^4)\right] \\ &\quad - \left[u^n + \Delta t u_t^n + \frac{1}{2}\Delta t^2 u_{tt}^n + \frac{1}{6}\Delta t^3 u_{ttt}^n + \frac{1}{24}\Delta t^4 u_{tttt}^n + O(\Delta t^5)\right]\end{aligned}$$

Next, collect the terms in powers of Δt, *which gives the following coefficients:*

$$\begin{array}{rcccccccccc} u^n: & - & \alpha_1 & - & \alpha_2 & & & & & - & 1 \\ \Delta t u_t^n: & & & & \alpha_2 & + & \beta_1 & + & \beta_2 & - & 1 \\ \Delta t^2 u_{tt}^n: & & & - & \frac{\alpha_2}{2} & & & - & \beta_2 & - & \frac{1}{2} \\ \Delta t^3 u_{ttt}^n: & & & & \frac{\alpha_2}{6} & & & + & \frac{\beta_2}{2} & - & \frac{1}{6} \\ \Delta t^4 u_{tttt}^n: & & & - & \frac{\alpha_2}{24} & & & - & \frac{\beta_2}{6} & - & \frac{1}{24} \end{array}$$

To find the most accurate multi-step method of the given form, we solve for the values of α_1, α_2, β_1, *and* β_2 *that result in the coefficients of the first four terms being identically zero. The resulting values are:*

$$\alpha_1 = 4 \qquad \alpha_2 = -5 \qquad \beta_1 = 4 \qquad \beta_2 = 2$$

Note, with these values, the leading error term is $-\frac{1}{6}\Delta t^4 u_{tttt}^n$. *Thus, the scheme is third order accurate* ($p = 3$).

3.2 Dahlquist Equivalence Theorem

In order for a multi-step method to be convergent (as described in Definition 2.1), two conditions must be met:

Consistency: In the limit of $\Delta t \to 0$, the method must be a consistent discretization of the ordinary differential equation.

Stability: In the limit of $\Delta t \to 0$, the method must not have solutions that can grow unbounded as $n = T/\Delta t \to \infty$.

The Dahlquist Equivalence Theorem in fact guarantees that a consistent and stable multi-step method is convergent, and vice-versa:

Theorem 3.1 (Dahlquist Equivalence Theorem) *A multi-step method is convergent if and only if it is consistent and stable.*

3.3 Consistency

As given in Definition 3.1, a s-step multi-step method can be written as,

$$v^{n+1} + \sum_{i=1}^{s} \alpha_i v^{n+1-i} - \Delta t \sum_{i=0}^{s} \beta_i f^{n+1-i} = 0,$$

where the forcing terms have been moved to the left-hand side. Substituting the exact solution, $u(t)$, into the left-hand side will produce a remainder which is in fact the opposite of the truncation error (see Equation 2.2),

$$u^{n+1} + \sum_{i=1}^{s} \alpha_i u^{n+1-i} - \Delta t \sum_{i=0}^{s} \beta_i f^{n+1-i} = u^{n+1} - N(u^{n+1}, u^n, \ldots, \Delta t) = -\tau \tag{3.1}$$

If we only require that $\tau \to 0$ (i.e. $\tau = O(\Delta t)$) as $\Delta t \to 0$, the method will not generally be consistent with the ODE. To see why, note that in the limit of $\Delta t \to 0$, the forcing terms will vanish since they are scaled by Δt. Thus, $\tau \to 0$ would place a constraint only on the α's. Let's look at that constraint on the α's to build some insight. Substituting Taylor series about $t = t^n$ for the values of u gives,

$$u^{n+1} + \sum_{i=1}^{s} \alpha_i u^{n+1-i} = \left(1 + \sum_{i=1}^{s} \alpha_i\right) u^n + O(\Delta t).$$

Thus, for $\tau \to 0$ as $\Delta t \to 0$ requires,

$$1 + \sum_{i=1}^{s} \alpha_i = 0. \tag{3.2}$$

This constraint can be interpreted as requiring a constant solution, i.e. $u(t) =$ constant, to be a valid solution of the multi-step method. Clearly, this is not enough to guarantee consistency with the ODE since the ODE requires $u_t = f(u,t)$.

To achieve a consistent discretization, we force $\tau/\Delta t \to 0$ (i.e. $\tau = O(\Delta t^2)$). This stronger constraint can be shown to enforce that the ODE is satisfied in the limit of $\Delta t \to 0$:

$$\begin{aligned}
\frac{\tau}{\Delta t} &= \frac{N(u^{n+1}, u^n, \ldots, \Delta t) - u^{n+1}}{\Delta t} \\
&= \frac{N(u^{n+1}, u^n, \ldots, \Delta t) - (u^n + \Delta t u_t^n + O(\Delta t^2))}{\Delta t} \\
&= \frac{N(u^{n+1}, u^n, \ldots, \Delta t) - u^n}{\Delta t} - u_t^n + O(\Delta t) \\
&= \frac{N(u^{n+1}, u^n, \ldots, \Delta t) - u^n}{\Delta t} - f(u^n, t^n) + O(\Delta t)
\end{aligned}$$

Thus, in the limit of $\tau/\Delta t \to 0$ as $\Delta t \to 0$, then the slope of the numerical method (i.e. the first term) must be equal to the forcing at t^n. In other words, the multi-step discretization would satisfy the governing equation in the limit. An equivalent way to write this consistency constraint is,

$$\lim_{\Delta t \to 0} \frac{1}{\Delta t}\left[u^{n+1} + \sum_{i=1}^{s} \alpha_i u^{n+1-i}\right] - \sum_{i=0}^{s} \beta_i f^{n+1-i} = u_t(t^n) - f(u(t^n), t^n) = 0. \tag{3.3}$$

In terms of the local accuracy, consistency requires that the multi-step method be at least first-order ($p = 1$) since $\tau = O(\Delta t^{p+1})$ and consistency requires that $\tau/\Delta t = O(\Delta t^p)$ must go to zero (i.e. $p \geq 1$).

3.4 Stability

The remaining issue to determine is whether the solutions to the multi-step method can grow unbounded as $\Delta t \to 0$ for finite time T. Consider again the s-step multi-step method:

$$v^{n+1} + \sum_{i=1}^{s} \alpha_i v^{n+1-i} = \Delta t \sum_{i=0}^{s} \beta_i f^{n+1-i}.$$

In the limit of $\Delta t \to 0$, the multi-step approximation will satisfy the following recurrence relationship,

$$v^{n+1} + \sum_{i=1}^{s} \alpha_i v^{n+1-i} = 0. \tag{3.4}$$

This recurrence relationship can be viewed a providing the characteristic or unforced behavior of the multi-step method. In terms of stability, the question is whether or not the solutions to Equation 3.4 can grow unbounded.

Definition 3.2 (Stability) *A multi-step method is stable (also known as zero stable) if all solutions to*

$$v^{n+1} + \sum_{i=1}^{s} \alpha_i v^{n+1-i} = 0,$$

are bounded as $n \to \infty$.

To determine if a method if stable, we assume that the solution to the recurrence has the following form,

$$v^n = v^0 z^n,$$

where the superscript in the z^n term is in fact a power. Note: z can be a complex number. If the recurrence relationship has solutions with $|z| > 1$, then the multi-step method would be unstable.

Example 3.4 *In Example 3.3, the most accurate two-step, explicit method was found to be,*

$$v^{n+1} + 4v^n - 5v^{n-1} = \Delta t\left(4f^n + 2f^{n-1}\right).$$

We will determne if this algorithm is stable. The recurrence relationship is,

$$v^{n+1} + 4v^n - 5v^{n-1} = 0.$$

Then, substitution of $v^n = v^0 z^n$ *gives,*

$$z^{n+1} + 4z^n - 5z^{n-1} = 0.$$

Factoring this relationship gives,

$$z^{n-1}\left(z^2 + 4z - 5\right) = z^{n-1}(z-1)(z+5) = 0.$$

Thus, the recurrence relationship has roots at $z = 1$, $z = -5$, *and* $z = 0$ *(*$n-1$ *of these roots). The root at* $z = -5$ *will grow unbounded as* n *increases so this method is not stable. By the Dahlquist Equivalence Theorem, this means the method is not convergent (even though it has local accuracy* $p = 3$ *and is therefore consistent).*

To demonstrate the lack of convergence for this method (due to its lack of stability), we again consider the solution of $u_t = -u^2$ *with* $u(0) = 1$. *These results are shown in Figure 3.1 These results clearly show the instability. Note that the solution oscillates as is expected since the large parasitic root is negative (*$z = -5$*). Furthermore, decreasing* Δt *from* 0.1 *to* 0.05 *only causes the instability to manifest itself in shorter time (though the same number of steps). Clearly, though the method is consistent, it will not converge because of this instability.*

In-class Discussion 3.1 (Stability of the midpoint method)

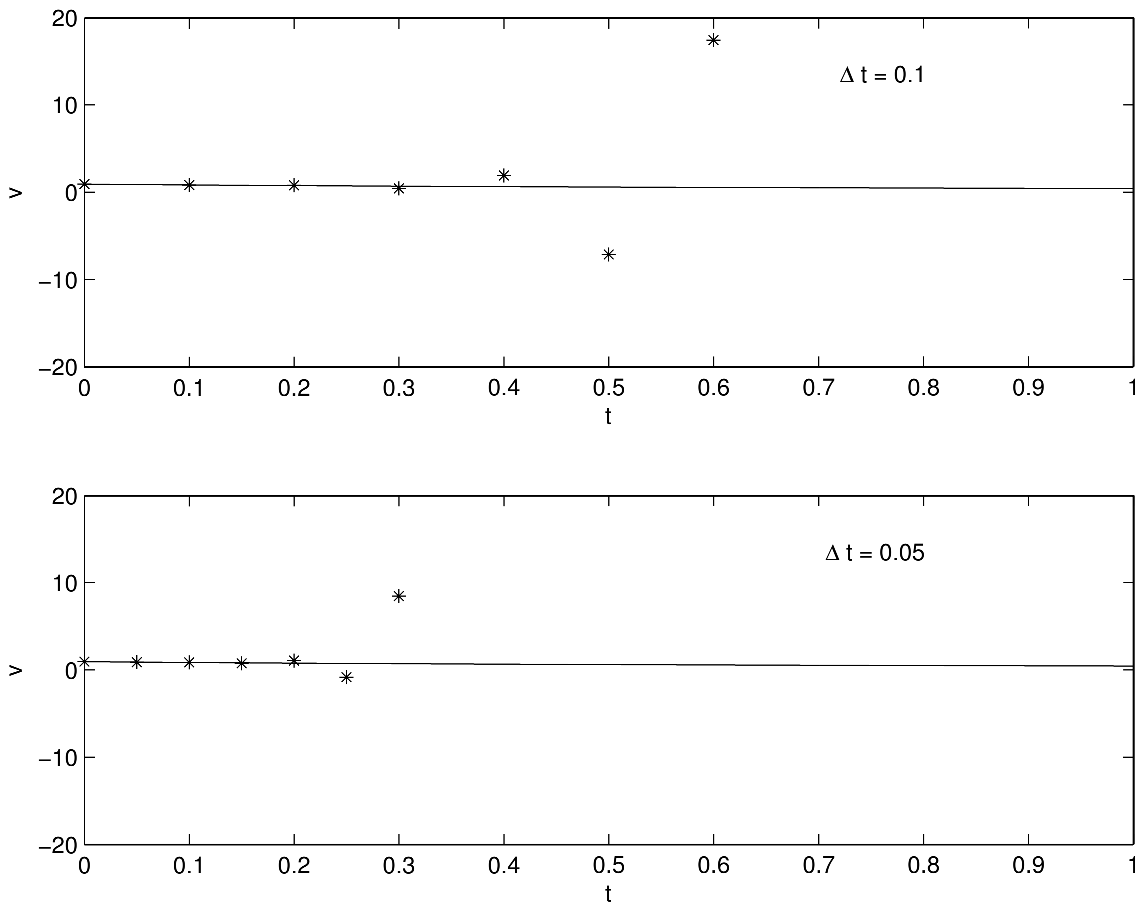

Figure 3.1: Most-accurate explicit, two-step multi-step method applied to $\dot{u} = -u^2$ with $u(0) = 1$ with $\Delta t = 0.1$ (upper plot) and 0.05 (lower plot).