Lecture 1

Numerical Integration of Ordinary Differential Equations: An Introduction

Ordinary differential equations (ODE's) occur throughout science and engineering.

Example 1.1 *A model for the velocity u of a spherical object falling freely through the atmosphere can be derived by applying Newton's Law. Specifically,*

$$m_p \dot{u} = m_p g - D(u) \tag{1.1}$$

where m_p is the mass of the particle, g is the gravity, and D is the aerodynamic drag acting on the particle. For low speeds, this drag can be modeled as,

$$D = \frac{1}{2}\rho_g \pi a^2 u^2 C_D(Re) \tag{1.2}$$

$$Re = \frac{2\rho_g u a}{\mu_g} \tag{1.3}$$

$$C_D = \frac{24}{Re} + \frac{6}{1+\sqrt{Re}} + 0.4 \tag{1.4}$$

where ρ_g and μ_g are the density and dynamic viscosity of the atmosphere, a is the sphere radius, Re is the Reynolds number for the sphere, and C_D is the drag coefficient. To complete the problem specification, an initial condition is required on the velocity. For example, at time $t = 0$, let $u(0) = u_0$. By solving Equation 1.1 with this initial condition, the velocity at any time $u(t)$ can be found.

A general ODE is typically written in the form,

$$\dot{u} = f(u, t), \tag{1.5}$$

where $f(u, t)$ is the forcing function that results in the evolution of u in time. When $f(u, t)$ depends on u in a nonlinear manner, then the ODE is called a nonlinear ODE.

Example 1.2 *For Example 1.1, the forcing function is,*

$$f(u,t) = g - \frac{1}{m_p} D(u)$$

From the definition of $D(u)$, $f(u,t)$ is nonlinear in u. Note also that in this example, f does not depend on t directly rather $f(u,t) = f(u)$.

Although the use of numerical integration is most important for nonlinear ODE's (since analytic solutions rarely exist), the study of numerical methods applied to linear ODE's is often quite helpful in understanding the behavior for nonlinear problems. The general form For a single, linear ODE, is

$$\dot{u} = \lambda(t)u + g(t), \tag{1.6}$$

where $\lambda(t)$ is independent of u. When $\lambda(t)$ is a constant, the ODE is referred to as a linear ODE with constant coefficients.

In many situations, the linear ODE is derived by linearizing a nonlinear ODE about a constant state. Specifically, define the dependent state $u(t)$ as a sum of u_0 and a perturbation, $\tilde{u}(t)$,

$$u(t) = u_0 + \tilde{u}(t). \tag{1.7}$$

A linearized equation for the evolution of $\tilde{u}$ can be derived by substitution of this into Equation 1.5:

$$\begin{aligned}
\dot{u} &= f(u,t), \\
\dot{\tilde{u}} &= f(u_0 + \tilde{u}, t) \\
\dot{\tilde{u}} &= f(u_0, 0) + \left.\frac{\partial f}{\partial u}\right|_{u_0,0} \tilde{u} + \left.\frac{\partial f}{\partial t}\right|_{u_0,0} t + O(t^2, \tilde{u}t, \tilde{u}^2).
\end{aligned}$$

Thus, when t and $\tilde{u}$ are small, the perturbation satisfies the linear equation,

$$\dot{\tilde{u}} \approx f(u_0, 0) + \left.\frac{\partial f}{\partial u}\right|_{u_0,0} \tilde{u} + \left.\frac{\partial f}{\partial t}\right|_{u_0,0} t \tag{1.8}$$

Comparing Equation 1.6 to 1.8, we see that in this example,

$$\begin{aligned}
\lambda(t) &= \left.\frac{\partial f}{\partial u}\right|_{u_0,0}, \\
g(t) &= f(u_0, 0) + \left.\frac{\partial f}{\partial t}\right|_{u_0,0} t
\end{aligned}$$

Note, this is a constant coefficient linear ODE.

Example 1.3 *For the falling sphere problem in Examples 1.1 and 1.2, a linear ODE can be derived by linearizing about the initial velocity u_0. As shown above, this requires the calculation of $\partial f/\partial u$ and $\partial f/\partial t$. For the sphere,*

$$\frac{\partial f}{\partial u} = \frac{\partial}{\partial u}\left[g - \frac{1}{m_p} D(u)\right] = -\frac{1}{m_p}\frac{\partial D}{\partial u}$$

The value of $\partial D/\partial u$ is

$$\begin{aligned}\frac{\partial D}{\partial u} &= \frac{\partial}{\partial u}\left[\frac{1}{2}\rho_g \pi a^2 u^2 C_D(Re)\right], \\ &= \rho_g \pi a^2 u C_D(Re) + \frac{1}{2}\rho_g \pi a^2 u^2 \frac{\partial C_D}{\partial Re}\frac{\partial Re}{\partial u},\end{aligned}$$

and $\partial C_D/\partial Re$ and $\partial Re/\partial u$ can be found from their definitions given in Example 1.1. Also, since f does not directly depend on t for this problem, $\partial f/\partial t = 0$.

1.1 The Forward Euler Method

We now consider our first numerical method for ODE integration, the forward Euler method. The general problem we wish to solve is to approximate the solution $u(t)$ for Equation 1.5 with an appropriate initial condition, $u(0) = u_0$. Usually, we are interesting in approximating this solution over some range of t, say from $t = 0$ to $t = T$. Or, we may not know a precise final time but wish to integrate forward in time until an event occurs (e.g. the problem reaches a steady state). In either case, the basic philosophy of numerical integration is to start from a known initial state, $u(0)$, and somehow approximate the solution a small time forward, $u(\Delta t)$ where Δt is a small time increment. Then, we repeat this process and move forward to the next time to find, $u(2\Delta t)$, and so on. Initially, we will consider the situation in which Δt is fixed for the entire integration from $t = 0$ to T. However, the best methods for solving ODE's tend to be adaptive methods in which Δt is adjusted depending on the current approximation.

Before moving on to the specific form of the forward Euler method, let's put some notations in place. Superscripts will be used to indicate a particular iteration. Thus, assuming constant Δt,

$$t^n = n\Delta t.$$

The approximation from the numerical integration will be defined as v. Thus, using the superscript notation,

$$v^n = \text{the approximation of } u(t^n).$$

Now, let's derive the forward Euler method. There are several ways to motivate the forward Euler method. We will start with an approach based on Taylor series. Specifically, the Taylor expansion of $u(t^{n+1})$ about t^n is,

$$u(t^{n+1}) = u(t^n) + \Delta t \dot{u}(t^n) + \frac{1}{2}\Delta t^2 \ddot{u}(t^n) + O(\Delta t^3).$$

Using only the first two terms in this expansion,

$$u(t^{n+1}) \approx u(t^n) + \Delta t \dot{u}(t^n).$$

Finally, the term $\dot{u}(t^n)$ is in fact just $f(u(t^n), t^n)$ since the governing equation is Equation 1.5. Thus,

$$u(t^{n+1}) \approx u(t^n) + \Delta t f(u(t^n), t^n). \tag{1.9}$$

In-class Discussion 1.1 (Graphical interpretation of Equation 1.9)

Since we do not know $u(t^n)$, we will instead use the approximation from the previous timestep, v^n. Thus, the forward Euler algorithm is,

$$v^{n+1} = v^n + \Delta t f(v^n, t^n) \qquad \text{for} \qquad n \geq 0, \tag{1.10}$$

and $v^0 = u(0)$.

Example 1.4 *Now, let's apply the forward Euler method to solving the falling sphere problem. Suppose the sphere is actually a small particle of ice falling in the atmosphere at an altitude of approximately 3000 meters. Specifically, let's assume the radius of the particle is* $a = 0.01m$. *Then, since the density of ice is approximately* $\rho_p = 917\,kg/m^3$, *the mass of the particle can be calculated from,*

$$m_p = \rho_p\, Volume_p = \rho_p \frac{4}{3}\pi a^3 = 0.0038\,kg$$

At that altitude, the properties of the atmosphere are:

$$\begin{aligned} \rho_g &= 0.9\,kg/m^3 \\ \mu_g &= 1.69E\text{-}5\,kg/(m\,sec) \\ g &= 9.8m/sec^2 \end{aligned}$$

We expect the particle to accelerate until it reaches its terminal velocity which will occur when the drag force is equal to the gravitational force. But, a priori, we do not know how long that will take (see In-class Discussion 1.2 for someways to make this estimate). For now, let's set $T = 25\,sec$ *and use a timestep of* $\Delta t = 0.25\,sec$. *The results are shown in Figure 1.1.*

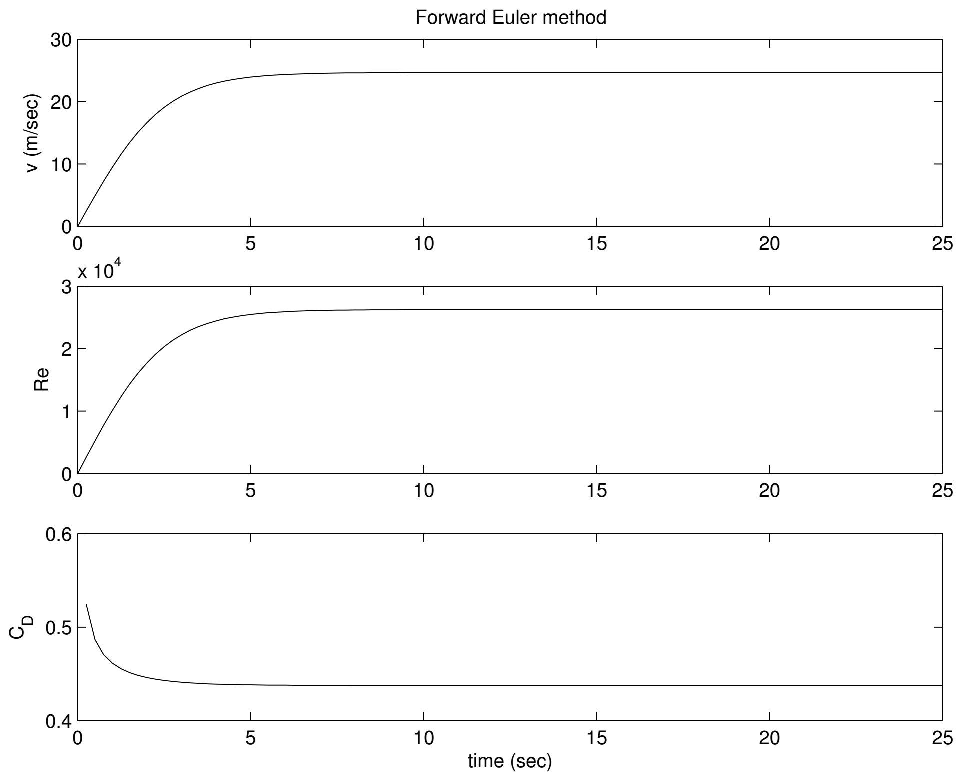

Figure 1.1: Behavior of velocity, Reynolds number, and drag coefficient as a function of time for an ice particle falling through the atmosphere. Simulation performed using the forward Euler method with $\Delta t = 0.25\, sec$.

In-class Discussion 1.2 (Estimating time to reach terminal velocity)

1.2 The Midpoint Method

Now, let's look at a second integration method known as the midpoint method. For this method, we will use a slightly different point of view to derive it. Specifically, let's start from the definition of a derivative,

$$\dot{u}(t) = \lim_{\Delta t \to 0} \frac{u(t + \Delta t) - u(t - \Delta t)}{2\Delta t}$$

Now, instead of taking the limit, assume a finite Δt. Then, we end up with an approximation to du/dt:

$$\dot{u}(t) \approx \frac{u(t + \Delta t) - u(t - \Delta t)}{2\Delta t} \qquad \text{for small } \Delta t$$

Then, we can re-arrange this to the following estimate for $u(t + \Delta t)$,

$$u(t + \Delta t) \approx u(t - \Delta t) + 2\Delta t \dot{u}(t) \tag{1.11}$$

In-class Discussion 1.3 (Graphical interpretation of Equation 1.11)

Then, following the same process as in the forward Euler method, we arrive at the midpoint method,

$$v^{n+1} = v^{n-1} + 2\Delta t f(v^n, t^n) \qquad \text{for} \qquad n \geq 1. \tag{1.12}$$

However, because of the use of v^{n-1}, the midpont method can only be applied for $n \geq 1$. Thus, for the first timestep a different numerical method must be applied (e.g. the forward Euler method).

Example 1.5 *We will now solve the same problem as in Example 1.4 using the midpoint method. Using the same values of Δt and T as before, the results are shown in Figure 1.2. Clearly, something has gone wrong here as the results show non-physical oscillations. Perhaps the oscillations will disappear if we take a smaller timestep. To test out this hypothesis, let's re-run the midpoint method with $\Delta t = 0.025\,sec$ which is one-tenth the previous timestep. Those results are shown in Figure 1.3. Unfortunately, while the results are better, the oscillations are clearly still present. For this problem, clearly the forward Euler method is a better choice than the midpoint method. We will see why this has happened in a few lectures.*

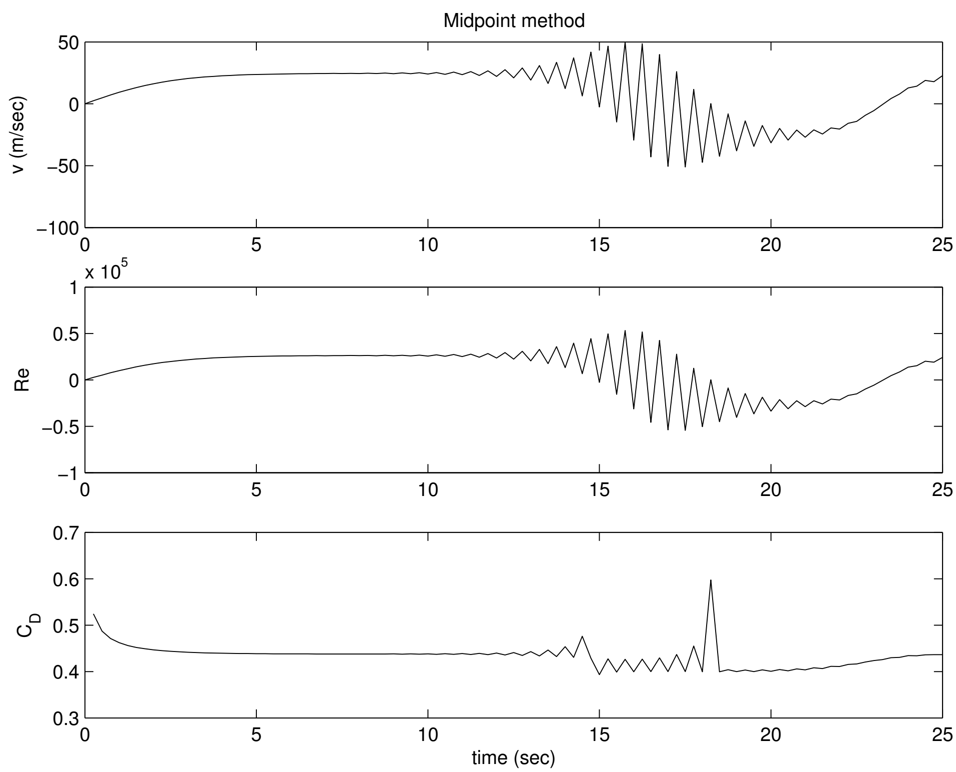

Figure 1.2: Behavior of velocity, Reynolds number, and drag coefficient as a function of time for an ice particle falling through the atmosphere. Simulation performed using the midpoint method with $\Delta t = 0.25\,sec$.

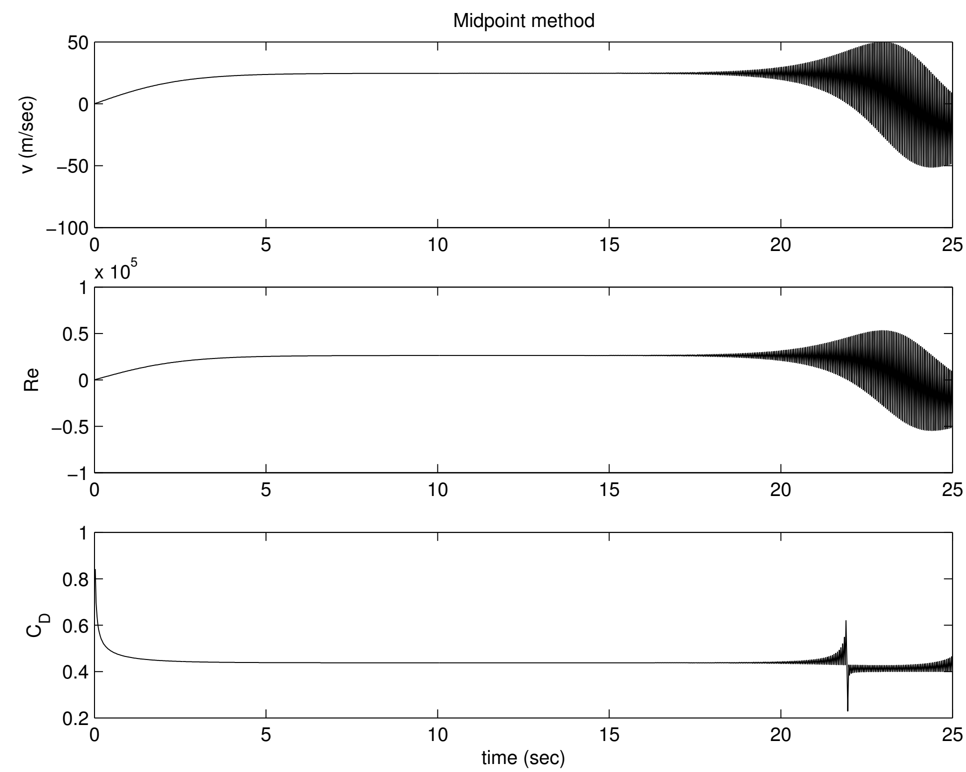

Figure 1.3: Behavior of velocity, Reynolds number, and drag coefficient as a function of time for an ice particle falling through the atmosphere. Simulation performed using the midpoint method with $\Delta t = 0.025\, sec.$