Module 3C - Generic Time Stepping

Omar Betancourt, Payton Goodrich, Emre Mengi

July 24, 2021

Contents

Objectives:
Review temporal discretization tools needed for simulation of the upcoming systems that are built on differential equations.
Prerequisite Knowledge: N/A
Prerequisite Modules: 1A - Calculus, 1D - Differential Equations, 2C - Particle Dynamics
Difficulty: Easy

Summary: In this module, you will learn how to implement three different time-stepping schemes that are commonly used in modeling and simulation of systems, particularly ones defined by differential equations. This module teaches the concept of time-stepping using particle dynamics simulation as a use-case example.

1 Theory

1.1 Isolating a single particle:

In order to motivate the time-stepping process, we first start with the dynamics of a single point mass under the force $\boldsymbol{\Psi}$. The equation of motion is given by (Newton's Law)

$$m\dot{\boldsymbol{v}} = \boldsymbol{\Psi}, \tag{1.1}$$

where $\boldsymbol{\Psi}$ is the force provided from interactions with other particles in the external environment. Expanding the velocity in a Taylor series about $t + \phi\Delta t$ we obtain $(0 \le \phi \le 1)$

$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}(t+\phi\Delta t) + \frac{d\boldsymbol{v}}{dt}|_{t+\phi\Delta t}(1-\phi)\Delta t + \frac{1}{2}\frac{d^2\boldsymbol{v}}{dt^2}|_{t+\phi\Delta t}(1-\phi)^2(\Delta t)^2 + \mathcal{O}(\Delta t)^3 \tag{1.2}$$

and

$$\boldsymbol{v}(t) = \boldsymbol{v}(t+\phi\Delta t) - \frac{d\boldsymbol{v}}{dt}|_{t+\phi\Delta t}\phi\Delta t + \frac{1}{2}\frac{d^2\boldsymbol{v}}{dt^2}|_{t+\phi\Delta t}\phi^2(\Delta t)^2 + \mathcal{O}(\Delta t)^3. \tag{1.3}$$

Subtracting the two expressions yields

$$\frac{d\boldsymbol{v}}{dt}|_{t+\phi\Delta t} = \frac{\boldsymbol{v}(t+\Delta t) - \boldsymbol{v}(t)}{\Delta t} + \hat{\mathcal{O}}(\Delta t), \tag{1.4}$$

where $\hat{\mathcal{O}}(\Delta t) = \mathcal{O}(\Delta t)^2$ when $\phi = \frac{1}{2}$. Inserting this into the equation of motion yields

$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}(t) + \frac{\Delta t}{m}\boldsymbol{\Psi}(t+\phi\Delta t) + \hat{\mathcal{O}}(\Delta t)^2. \tag{1.5}$$

Note that adding a weighted sum of Equations 1.2 and 1.3 yields

$$\boldsymbol{v}(t+\phi\Delta t) = \phi\boldsymbol{v}(t+\Delta t) + (1-\phi)\boldsymbol{v}(t) + \mathcal{O}(\Delta t)^2, \tag{1.6}$$

which will be useful shortly. Now expanding the position of the center of mass in a Taylor series about $t + \phi\Delta t$ we obtain

$$\boldsymbol{r}(t+\Delta t) = \boldsymbol{r}(t+\phi\Delta t) + \frac{d\boldsymbol{r}}{dt}|_{t+\phi\Delta t}(1-\phi)\Delta t + \frac{1}{2}\frac{d^2\boldsymbol{r}}{dt^2}|_{t+\phi\Delta t}(1-\phi)^2(\Delta t)^2 + \mathcal{O}(\Delta t)^3 \tag{1.7}$$

and

$$\boldsymbol{r}(t) = \boldsymbol{r}(t+\phi\Delta t) - \frac{d\boldsymbol{r}}{dt}|_{t+\phi\Delta t}\phi\Delta t + \frac{1}{2}\frac{d^2\boldsymbol{r}}{dt^2}|_{t+\phi\Delta t}\phi^2(\Delta t)^2 + \mathcal{O}(\Delta t)^3. \tag{1.8}$$

Subtracting the two expressions yields

$$\frac{\boldsymbol{r}(t+\Delta t) - \boldsymbol{r}(t)}{\Delta t} = \boldsymbol{v}(t+\phi\Delta t) + \hat{\mathcal{O}}(\Delta t). \tag{1.9}$$

Inserting Equation 1.6 yields

$$\boldsymbol{r}(t+\Delta t) = \boldsymbol{r}(t) + (\phi \boldsymbol{v}(t+\Delta t) + (1-\phi)\boldsymbol{v}(t))\,\Delta t + \hat{\mathcal{O}}(\Delta t)^2 \tag{1.10}$$

and thus using Equation 1.5 yields

$$\boldsymbol{r}(t+\Delta t) = \boldsymbol{r}(t) + \boldsymbol{v}(t)\Delta t + \frac{\phi(\Delta t)^2}{m}\boldsymbol{\Psi}(t+\phi\Delta t) + \hat{\mathcal{O}}(\Delta t)^2. \tag{1.11}$$

The term $\boldsymbol{\Psi}(t+\phi\Delta t)$ can be approximated by

$$\boldsymbol{\Psi}(t+\phi\Delta t) \approx \phi\boldsymbol{\Psi}(\boldsymbol{r}(t+\Delta t)) + (1-\phi)\boldsymbol{\Psi}(\boldsymbol{r}(t)), \tag{1.12}$$

yielding

$$\boldsymbol{r}(t+\Delta t) = \boldsymbol{r}(t) + \boldsymbol{v}(t)\Delta t + \frac{\phi(\Delta t)^2}{m}\left(\phi\boldsymbol{\Psi}(\boldsymbol{r}(t+\Delta t)) + (1-\phi)\boldsymbol{\Psi}(\boldsymbol{r}(t))\right) + \hat{\mathcal{O}}(\Delta t)^2. \tag{1.13}$$

We note that

- When $\phi = 1$, then this is the (implicit) Backward Euler scheme, which is very stable (very dissipative) and $\mathcal{O}(\Delta t)^2$ locally in time,
- When $\phi = 0$, then this is the (explicit) Forward Euler scheme, which is conditionally stable and $\mathcal{O}(\Delta t)^2$ locally in time,
- When $\phi = 0.5$, then this is the (implicit) "Midpoint" scheme, which is stable and $\hat{\mathcal{O}}(\Delta t)^2 = \mathcal{O}(\Delta t)^3$ locally in time.

Typically, if the systems are relatively simple, and if small times steps can be used, Explicit methods are preferred. We will use such methods in this monograph. However, in passing we remark that efficient methods for complex multiparticle systems have been developed by use of adaptive iterative schemes in Zohdi [1]-[3]. Implicit time-stepping methods, with time step size adaptivity, built on approaches found in Zohdi [2]. They are beyond the scope of this monograph, but are discussed in the context of PDE's associated with the Navier-Stokes equations.

2 Example

EXAMPLE PROBLEM 1: Consider the dynamics of a single point mass under a force $\boldsymbol{\Psi}$

$$m\dot{\boldsymbol{v}} = \boldsymbol{\Psi}$$

Derive Eq. 2.1 for the time update equation for the position of the point mass obtained by numerical integration for a generic time stepping scaling factor $\phi \in [0,1]$.

$$\boldsymbol{u}(t+\Delta t) = \boldsymbol{u}(t) + \boldsymbol{v}(t)\Delta t + \frac{\phi(\Delta t)^2}{m}\left(\phi\boldsymbol{\Psi}(\boldsymbol{u}(t+\Delta t)) + (1-\phi)\boldsymbol{\Psi}(\boldsymbol{u}(t))\right) + \hat{\mathcal{O}}(\Delta t)^2. \tag{2.1}$$

EXAMPLE PROBLEM 2:
Denote the differences in the scheme and solution for $\phi = (0, 0.5, 1)$. Which scheme is the most stable? Least stable?

EXAMPLE PROBLEM 3: Consider the following differential equation

$$\rho c \frac{\partial \theta}{\partial t} = \nabla \cdot (k \nabla \theta) \tag{2.2}$$

where ρ, c, k are constants. Rewrite this equation for a generic time stepping scaling factor $\phi \in [0,1]$.

EXAMPLE PROBLEM 1 SOLUTION:
Given that the equation of motion is:

$$m\dot{\boldsymbol{v}} = \boldsymbol{\Psi}$$

where $\boldsymbol{\Psi}$ denotes the forces applied on the point mass. To obtain the time update equation, velocity terms $\dot{\boldsymbol{v}}(t+\Delta t)$ and $\dot{\boldsymbol{v}}(t)$ can be expanded at using Taylor series about $t+\phi\Delta t$, where $0 \le \phi \le 1$.

$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}(t+\phi\Delta t) + \dot{\boldsymbol{v}}(t+\phi\Delta t)(1-\phi)\Delta t + \frac{1}{2}\ddot{\boldsymbol{v}}(t+\phi\Delta t)(1-\phi)^2(\Delta t)^2 + O(\Delta t)^3$$

$$\boldsymbol{v}(t) = \boldsymbol{v}(t+\phi\Delta t) - \dot{\boldsymbol{v}}(t+\phi\Delta t)\phi\Delta t + \frac{1}{2}\ddot{\boldsymbol{v}}(t+\phi\Delta t)\phi^2(\Delta t)^2 + O(\Delta t)^3$$

If we subtract the second equation from the first:

$$\dot{\boldsymbol{v}}(t+\phi\Delta t) = \frac{\boldsymbol{v}(t+\Delta t) - \boldsymbol{v}(t)}{\Delta t} + \hat{O}(\Delta t)$$

in which $\hat{O}(\Delta t)$ depends on the value of ϕ. When $\phi = 0.5$, $\hat{O}(\Delta t)$=$O(\Delta t)^2$ and otherwise $\hat{O}(\Delta t)$=$O(\Delta t)$. The expression can also be written in form:

$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}(t) + \Delta t\dot{\boldsymbol{v}}(t+\phi\Delta t) + \hat{O}(\Delta t)^2$$

Replacing the derivative of velocity using the equation of motion given:

$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}(t) + \frac{\Delta t}{m}\boldsymbol{\Psi}(t+\phi\Delta t) + \hat{O}(\Delta t)^2$$

If the weighted sum for the Taylor expansions is taken instead:

$$\boldsymbol{v}(t+\phi\Delta t) = \phi\boldsymbol{v}(t+\Delta t) + (1-\phi)\boldsymbol{v}(t) + O(\Delta t)^2$$

Now, the position of the point mass can be expanded the same way as it was done for velocity above:

$$\boldsymbol{u}(t+\Delta t) = \boldsymbol{u}(t+\phi\Delta t) + \dot{\boldsymbol{u}}(t+\phi\Delta t)(1-\phi)\Delta t + \frac{1}{2}\ddot{\boldsymbol{u}}(t+\phi\Delta t)(1-\phi)^2(\Delta t)^2 + O(\Delta t)^3$$

$$\boldsymbol{u}(t) = \boldsymbol{u}(t+\phi\Delta t) - \dot{\boldsymbol{u}}(t+\phi\Delta t)\phi\Delta t + \frac{1}{2}\ddot{\boldsymbol{u}}(t+\phi\Delta t)\phi^2(\Delta t)^2 + O(\Delta t)^3$$

Subtracting:

$$\dot{\boldsymbol{u}}(t+\phi\Delta t) = \frac{\boldsymbol{u}(t+\Delta t) - \boldsymbol{u}(t)}{\Delta t} + \hat{O}(\Delta t)$$

$\dot{\boldsymbol{u}}$ is equal to $\boldsymbol{v}$:

$$\boldsymbol{v}(t+\phi\Delta t) = \frac{\boldsymbol{u}(t+\Delta t) - \boldsymbol{u}(t)}{\Delta t} + \hat{O}(\Delta t)$$

$$\boldsymbol{u}(t+\Delta t) = \boldsymbol{u}(t) + \Delta t\boldsymbol{v}(t+\phi\Delta t) + \hat{O}(\Delta t)^2$$

Using the previously derived weighted sum equation:

$$\boldsymbol{u}(t+\Delta t) = \boldsymbol{u}(t) + \Delta t(\phi\boldsymbol{v}(t+\Delta t) + (1-\phi)\boldsymbol{v}(t) + O(\Delta t)^2) + \hat{O}(\Delta t)^2$$

Replacing $\boldsymbol{v}(t+\Delta t)$ with the equation that contains mass and forcing function:

$$\boldsymbol{u}(t+\Delta t) = \boldsymbol{u}(t) + \Delta t(\phi(\boldsymbol{v}(t) + \frac{\Delta t}{m}\boldsymbol{\Psi}(t+\phi\Delta t) + \hat{O}(\Delta t)^2) + (1-\phi)\boldsymbol{v}(t) + O(\Delta t)^2) + \hat{O}(\Delta t)^2$$

$$\boldsymbol{u}(t+\Delta t) = \boldsymbol{u}(t) + \boldsymbol{v}(t)\Delta t + \frac{\phi(\Delta t)^2}{m}\boldsymbol{\Psi}(t+\phi\Delta t) + \hat{O}(\Delta t)^2$$

Getting rid of higher order terms and making the approximation that $\boldsymbol{\Psi}(t+\phi\Delta t) \approx \phi\boldsymbol{\Psi}(t+\Delta t)+(1-\phi)\boldsymbol{\Psi}(t)$:

For displacement:

$$\boldsymbol{u}(t+\Delta t) = \boldsymbol{u}(t) + \boldsymbol{v}(t)\Delta t + \frac{\phi(\Delta t)^2}{m}(\phi\boldsymbol{\Psi}(t+\Delta t) + (1-\phi)\boldsymbol{\Psi}(t))$$

For velocity:

$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}(t) + \frac{\Delta t}{m}(\phi\boldsymbol{\Psi}(t+\Delta t) + (1-\phi)\boldsymbol{\Psi}(t))$$

EXAMPLE PROBLEM 2 SOLUTION:

The differences in the scheme and solution for different values of ϕ is:

$\phi = 1$: Backward Euler (Implicit) Scheme

- Very stable.
- Very dissipative.
- Truncation error in order $\hat{\mathcal{O}}(\Delta t)^2 = \mathcal{O}(\Delta t)^2$.
- Harder to implement due to implicit nature, but can use larger time steps.

$\phi = 0$: Forward Euler (Explicit) Scheme

- Conditionally stable (depending on time step size).
- Truncation error in order $\hat{\mathcal{O}}(\Delta t)^2 = \mathcal{O}(\Delta t)^2$.
- Needs smaller time steps for accuracy, but can be iterated directly due to explicit nature.
- Mass matrix can be approximated.

$\phi = 0.5$: Midpoint (Implicit) Scheme

- Stable.
- Truncation error in order $\hat{\mathcal{O}}(\Delta t)^2 = \mathcal{O}(\Delta t)^3$.
- Harder to implement due to implicit nature, but can use larger time steps.

Among these schemes, Forward Euler is the least stable and Backward Euler is the most stable.

EXAMPLE PROBLEM 3 SOLUTION:

The given heat equation is:

$$\rho c\dot{\theta} = \nabla \cdot (k\nabla\theta)$$

The right side of the equation can be written as a function $\boldsymbol{\Psi}(\boldsymbol{x}, t)$:

$$\rho c\dot{\theta} = \boldsymbol{\Psi}(\boldsymbol{x}, t)$$

Density can be assumed to be uniform and constant $\rho = \rho_0$. We can use the velocity of the point mass equation from Q1 as it is the DE is the same order:

$$\rho_0 c\theta(t+\Delta t) = \rho_0 c\theta(t) + \Delta t(\phi\boldsymbol{\Psi}(t+\Delta t) + (1-\phi)\boldsymbol{\Psi}(t))$$

3 Assignment

Given the following differential equation:

$$\rho C\dot{\theta} = -Bcos(2t)\boldsymbol{x} + \rho aI$$

where ρ, C, B, a and I are constants, provide the following:

(a) Set up the solution for θ using a Foward Euler, Backward Euler, and Midpoint Schemes

(b) Given the initial condition $\theta(t=0) = \theta_0$ and a time step size of Δt, write an expression for θ at $t = \Delta t, t = 2\Delta t$, and $t = 3\Delta t$ *only* for the Forward Euler scheme. You may write the temperature at each time step in terms of the temperature at previous time steps.

4 Solution

A: Rewriting our equation so that only $\dot{\theta}$ is by itself on the left hand hand side

$$\dot{\theta} = -B\frac{cos(2t)}{\rho C}\boldsymbol{x} + \frac{aI}{C}$$

The right side of the equation can be written as a function $\boldsymbol{\Psi}(\boldsymbol{x}, t)$:

$$\dot{\theta} = \boldsymbol{\Psi}(\boldsymbol{x}, t)$$

We can use the velocity of the point mass equation from Q1 as it is the DE is the same order:

$$\theta(t+\Delta t) = \theta(t) + \Delta t(\phi\boldsymbol{\Psi}(t+\Delta t) + (1-\phi)\boldsymbol{\Psi}(t))$$

Back substitute the value $\boldsymbol{\Psi}(\boldsymbol{x}, t)$

$$\theta(t+\Delta t) = \theta(t) + \Delta t(\phi(-B\frac{cos(2(t+\Delta t))}{\rho C}\boldsymbol{x} + \frac{aI}{C}) + (1-\phi)(-B\frac{cos(2t)}{\rho C}\boldsymbol{x} + \frac{aI}{C}))$$

For forward Euler scheme, $\phi = 0$

$$\theta(t+\Delta t) = \theta(t) + \Delta t(-B\frac{cos(2t)}{\rho C}\boldsymbol{x} + \frac{aI}{C})$$

For backward Euler scheme, $\phi = 1$

$$\theta(t+\Delta t) = \theta(t) + \Delta t(-B\frac{cos(2(t+\Delta t))}{\rho C}\boldsymbol{x} + \frac{aI}{C})$$

For Midpoint scheme, $\phi = 0.5$

$$\theta(t+\Delta t) = \theta(t) + \Delta t(0.5(-B\frac{cos(2(t+\Delta t))}{\rho C}\boldsymbol{x} + \frac{aI}{C}) + (0.5)(-B\frac{cos(2t)}{\rho C}\boldsymbol{x} + \frac{aI}{C}))$$

B: Using Forward Euler:

$$\theta(t+\Delta t) = \theta(t) + \Delta t(-B\frac{cos(2t)}{\rho C}\boldsymbol{x} + \frac{aI}{C})$$

At $t = \Delta t$:

$$\theta(\Delta t) = \theta_0 + \Delta t\left(-B\frac{1}{\rho C}\boldsymbol{x} + \frac{aI}{C}\right)$$

At $t = 2\Delta t$:

$$\theta(2\Delta t) = \theta(\Delta t) + \Delta t\left(-B\frac{cos(2\Delta t)}{\rho C}\boldsymbol{x} + \frac{aI}{C}\right)$$

$$\Rightarrow \theta(2\Delta t) = \theta_0 + \Delta t\left(-B\frac{1+cos(2\Delta t)}{\rho C}\boldsymbol{x} + \frac{2aI}{C}\right)$$

At $t = 3\Delta t$:

$$\theta(3\Delta t) = \theta(2\Delta t) + \Delta t\left(-B\frac{cos(4\Delta t)}{\rho C}\boldsymbol{x} + \frac{aI}{C}\right)$$

$$\Rightarrow \theta(3\Delta t) = \theta_0 + \Delta t\left(-B\frac{1+cos(2\Delta t)}{\rho C}\boldsymbol{x} + \frac{2aI}{C}\right) + \Delta t\left(-B\frac{cos(4\Delta t)}{\rho C}\boldsymbol{x} + \frac{aI}{C}\right)$$

$$\Rightarrow \theta(3\Delta t) = \theta_0 + \Delta t\left(-B\frac{1+cos(2\Delta t)+cos(4\Delta t)}{\rho C}\boldsymbol{x} + \frac{3aI}{C}\right)$$

5 References

1. Zohdi, T. I. (2002). An adaptive-recursive staggering strategy for simulating multifield coupled processes in microheterogeneous solids. *The International Journal of Numerical Methods in Engineering.* **53**, 1511-1532.

2. Zohdi, T. I. (2003). Computational design of swarms. *The International Journal of Numerical Methods in Engineering.* **57**, 2205-2219.

3. Zohdi, T. I. (2010). Simulation of coupled microscale multiphysical-fields in particulate-doped dielectrics with staggered adaptive FDTD. *Computer Methods in Applied Mechanics and Engineering.* Volume 199, 79-101.

4. Zohdi, T. I. (Book, 2018) A finite element primer for beginners-extended version including sample tests and projects. Second Edition.

5. Zohdi, T. I. (Book, 2018) Modeling and simulation of functionalized materials for additive manufacturing and 3D printing: continuous and discrete media.