Numerical Lecture #3: Initializing Higher Order Schemes, Third-Order Adams-Bashforth

I. Initializing Higher Order Schemes

A. Single Particle Motion $\frac{dx}{dt} = v$

1. Euler: $x_{j+1} = x_j + v_j \Delta t$ ← Requires only information at step j to obtain step j+1

2. Leapfrog: $x_{j+1} = x_{j-1} + 2\Delta t\, v_j$
   a. Second-order scheme requires information at step j **and** step j-1 to obtain step j+1.

3. But, initial conditions provide only $\underset{\sim}{x}_0, \underset{\sim}{v}_0$.

$$\boxed{\text{How do we obtain } \underset{\sim}{x}_1, \underset{\sim}{v}_1 \text{ to compute } \underset{\sim}{x}_2, \underset{\sim}{v}_2 \text{ using leapfrog?}}$$

4. ANSWER: Use a lower order scheme to initialize.
   a. First step:
   $$\left.\begin{aligned} \underset{\sim}{x}_1 &= \underset{\sim}{x}_0 + \underset{\sim}{v}_0 \Delta t \\ \underset{\sim}{v}_1 &= \underset{\sim}{v}_0 + \left.\frac{dv}{dt}\right|_{t_0} \Delta t \end{aligned}\right\} \text{Now we have } \underset{\sim}{x}_0, \underset{\sim}{v}_0 \text{ and } \underset{\sim}{x}_1, \underset{\sim}{v}_1$$
   b. Second step:
   $$\underset{\sim}{x}_2 = \underset{\sim}{x}_0 + \underset{\sim}{v}_1 \Delta t$$
   $$\underset{\sim}{v}_2 = \underset{\sim}{v}_0 + 2\left.\frac{dv}{dt}\right|_{t_1} \Delta t$$

II. Adams-Bashforth

A. Concept:

1. Use past value to obtain a better numerical approximation of $\frac{dx}{dt}$ (derivative).

II. (Continued)

B. Adams-Bashforth Methods $\frac{dx}{dt} = v$

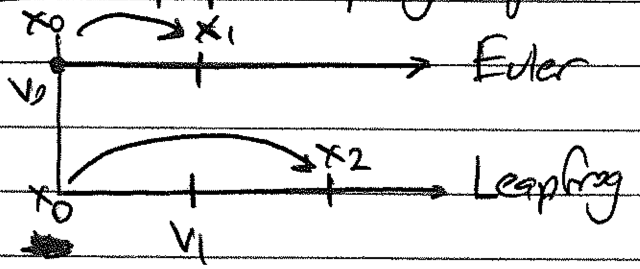
1. Second-order: $x_{j+1} = x_j + \frac{\Delta t}{2}\left[3v_j - v_{j-1}\right]$

2. Third-order: $$\boxed{x_{j+1} = x_j + \frac{\Delta t}{12}\left[23v_j - 16v_{j-1} + 5v_{j-2}\right]}$$

3. 3rd-order Adams-Bashforth (AB3) is very simple to implement, and is generally a great choice for 3rd-order integration in time.

C. Initializing 3rd-order Adams Bashforth

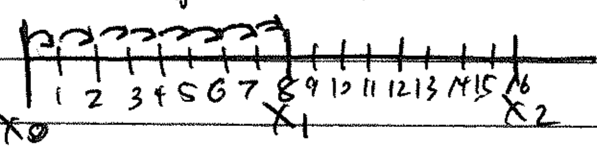
1. Euler step plus Leapfrog step:



Together, we obtain x_0, x_1, x_2 needed to start AB3

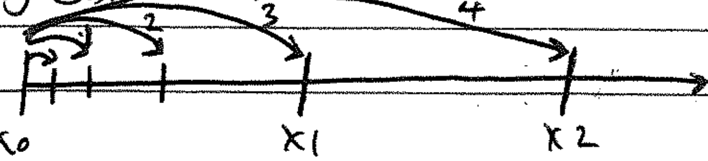
2. BUT: Euler is only first-order accurate, Leapfrog only 2nd-order.
$\Rightarrow$ Thus, error in first two steps is larger than AB3 steps.

3. Alternative: Use multiple Euler steps $\quad \Delta t_{Euler} = \frac{\Delta t_{AB3}}{8}$



$\Rightarrow$ 16 Euler steps to get x_0, x_1, x_2

4. Better: Leapfrog Geometric after 1 small Euler step.



1 Euler plus 4 Leapfrog Steps.