<u>Leap Frog Method and its Application-I</u>

Course: MPHYCC-05 Modeling and Simulation, MPHYCC-09 Lab-II
<u>(M.Sc. Sem-II)</u>

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Unit-3 of CC-05

<u>Leap Frog Method</u>

Leap Frog method is generally useful in solving the equation of motion (i.e., the Newton' s second law) of a dynamical system in classical mechanics, which is of the form:

$$\frac{d^2 y}{dt^2} = a(y) \qquad \text{----------} \ (1)$$

The above equation of motion can also be written in the form:

$$a = \frac{dv}{dt}; v = \frac{dy}{dt} \qquad \text{---------} \ (2)$$

Now our aim is to calculate position y(t) and velocity v(t) by solving two coupled first order ordinary differential equations (1). For this, first of all, we descretize the time domain i.e.,

The figure shows the descretization of the time domain, staring with t_0, into evenly spaced time points t_i *where* $t_i=t_0+i\Delta t$ *(i=1,2,3...n and size of each time step* $\Delta t=t_1-t_0=t_2-t_1$ *and so on).* The values of y and v at the first point t_0 is known to us by the initial conditions. Moreover, the values of y and v at time t_i (i^{th} time point) are denoted by y_i and v_i where y_i = y(t_i)=y($t_0+i\Delta t$) *and* v_i = v(t_i)=v($t_0+i\Delta t$).

To achieve the second order accuracy, in the Leap-Frog method, the position y is evaluated at the end-points of the time points (at t_0, t_1, t_2 ...) and velocity v is evaluated at the *mid-points* of the time points (at $t_{1/2}$, $t_{3/2}$, $t_{5/2}$ ...), i.e., y and v are staggered in such a way that they "leapfrog" over each other as shown in the figure.

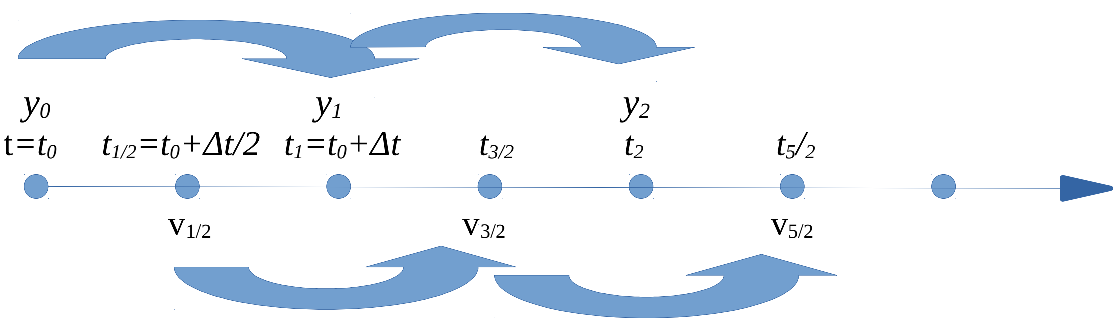


Figure: The leapfrog scheme.

With this definition, the Leapfrog scheme can be obtained that advances y_i to y_{i+1} and $v_{i+1/2}$ to $v_{i+3/2}$:

$$y_{i+1} = y_i + \Delta t \ v_{i+1/2} \quad \text{------------} \ (3)$$

$$v_{i+1/2} = v_{i-1/2} + \Delta t \ a_i \quad \text{------------}(4)$$

The graphical representation of the scheme is shown in the above figure. In general, the initial conditions are specified for $t=t_0$ time, i.e., $y(t=t_0)=y_0$ and $v(t=t_0)=v_0$ are specified; and they are rarely specified at the midpoints of time interval (the staggered times). However, to initiate the Leapfrog scheme, we require the specification of $v(t=t_0- \Delta t/2)=v_{-1/2}$ in equation (4). Therefore, for the initiation we use the Euler's scheme to evaluate $v_{-1/2}$ from the given v_0. From the Euler's scheme,

$$v_{-1/2} = v_0 - (\Delta t/2) \ a_0 \quad \text{-----------} \ (5)$$

Using the Taylor's series expansion of equations (3) and (4), we can easily show that the Leapfrog scheme is second order accurate, i.e., the truncation error associated with the scheme $e \sim O(\Delta t^{\,3})$. Hence, in terms of accuracy, the Leapfrog scheme is better than the Euler's scheme but inferior than the Runge-Kutta 4th order scheme. Here it is important to mention the two primary strengths of Leapfrog Scheme when applied to mechanics problems. The first is the time-reversibility of the Leapfrog method i.e., we can calculate the solution in forward *n* time steps, and then reverse the direction of integration and can otbain the solution in backwards *n* time steps to arrive at the same starting time. The second strength is that the scheme conserves the energy of dynamical systems (a slight change is possible). Particularly, this strength becomes crucial when computing orbital dynamics. In comparison, many other integration schemes such as the Runge-Kutta 4th order, do not conserve energy.

As an application of the Leapfrog method, in the following, we solve the equation of motion of a charged particle in a uniform electric field and magnetic field using this method.

Application of Leapfrog Method
Motion of a Charged Particle in a Uniform Electric field

Equation of motion of a charged particle q in an static 1D Electric field $\mathbf{E}=E_0\,\hat{e}_y$:

$$m\frac{d^2 y}{dt^2}=q\,E_0$$

or $$\frac{d\,v}{dt}=\frac{q\,E_0}{m} \quad ; \quad v=\frac{d\,y}{dt} \qquad \text{---------} \ (6)$$

We need to solve the above equation of motion with the specified initial conditions $v(t=0)=v_0$ and $y(t=0)=y_0$. We can analytically solve the equation and determine that the charged particle moves in the parallel direction to **E** if the q> 0 and anti-parallel to **E** if q<0. If we solve for velocity, we get

$$v(t)=\frac{q\,E_0}{m}t+v_0 \qquad \text{-----------} \ (7)$$

and, if we solve for position we get

$$y(t)=\frac{q\,E_0}{m}\frac{t^2}{2}+v_0 t+y_0 \quad \text{---------} \ (8)$$

Clearly, velocity increases linearly with time i.e., acceleration of the particle remains constant.

Now, we want to solve equation (6) using the Leapfrog method. Applying Leapfrog scheme given by equations (3) & (4) for equation (6), we have

$$y_{i+1} = y_i + \Delta t\ v_{i+1/2} \qquad \text{------------} \ (9)$$

$$v_{i+1/2} = v_{i-1/2} + \Delta t\ (qE_0/m) \quad \text{------------}(10)$$

In addition, using equation (5), we do one time adjustment for obtaining velocity at $t=0-\Delta t/2$

$$v_{-1/2} = v_0 - (\Delta t/2)\ (qE_0/m) \quad \text{------------}(11)$$

Algorithm to Solve Eq^n of Motion of Charged Particle in Uniform Electric Field using Leapfrog Method

1. Define the values of constant: q, E_0, m

2. Define initial time and time step: t_0, Δt

3. Define total number of steps: n [then final time $t_f = t_0 + (n+1)\,\Delta t$]

4. Specify initial conditions for $t=t_0$: y, v

5. Calculate velocity $v_{-1/2}$: $v = v - (\Delta t/2)\ (qE_0/m)$

6. Start iteration ($i=0$, n)

{ $v = v + \Delta t\ (qE_0/m)$

$y = y + \Delta t\ v$

write v, y }

7. end

C-Program to Solve Eq^n of Motion of Charged Particle in Uniform Electric Field using Leapfrog Method

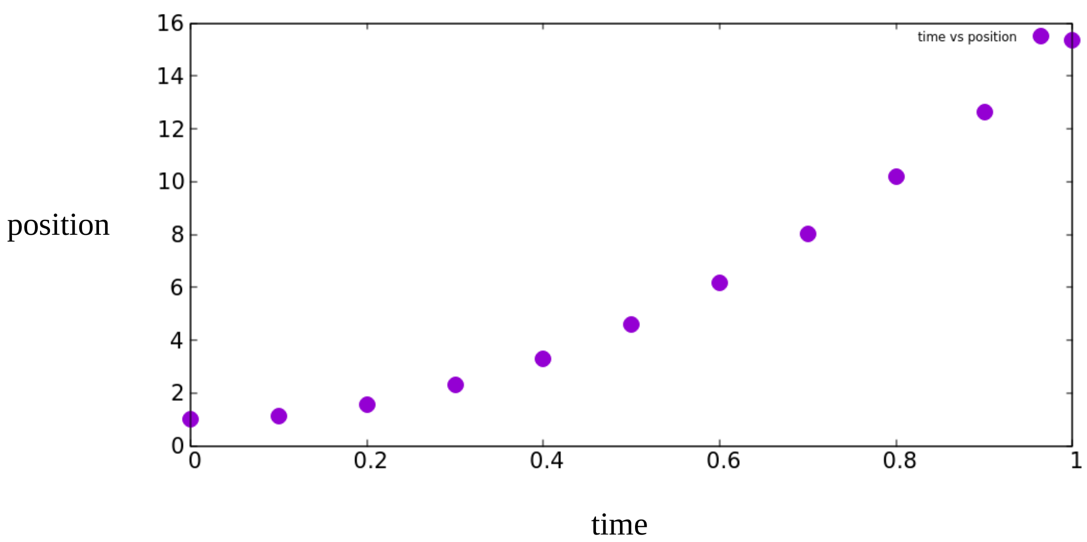
```
#include <stdio.h>
#include <math.h>
int main(void)
  { FILE *fp;
   fp=fopen("leafE0.dat","w");
   const double q = 4.8E-10;
   const double m = 1.67E-27;
   const double E0 = 1.0E-16;
   int i;
   int n = 9;
   double t=0.0;
   double dt = 0.1;
   double pos = 1.0;
   double vel = 0.0;
   fp=fopen("leafE0.dat","w");
   fprintf(fp,"%f %f %f\n", t, pos, vel); // write initial data
   vel = vel - 0.5*(q/m)*E0*dt;  // this is a one-step adjustment
```

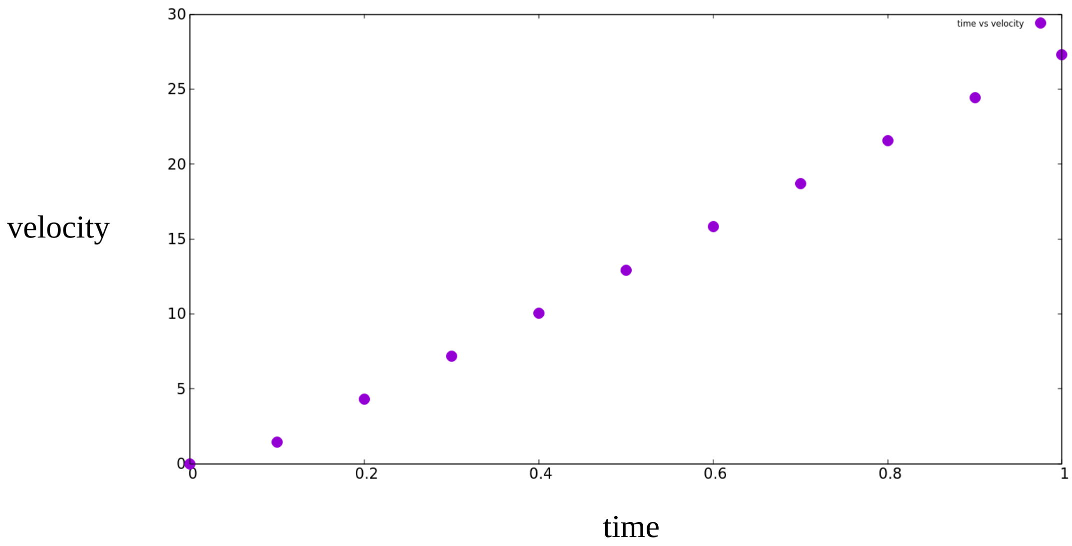
```
   for(i = 0; i <= n; i++)
    {vel =vel+ E0 *(q/m)* dt;
     pos = pos+ vel*dt;
     t=t+dt;
     printf("%f %f %f\n", t, pos, vel);
     fprintf(fp,"%f %f %f\n", t, pos, vel);}

 return 0;}
```

Output of the program:

```
0.100000   1.143713   1.437126
0.200000   1.574850   4.311377
0.300000   2.293413   7.185629
0.400000   3.299401   10.059880
0.500000   4.592814   12.934132
0.600000   6.173653   15.808383
0.700000   8.041916   18.682635
0.800000   10.197605  21.556886
0.900000   12.640719  24.431138
1.000000   15.371257  27.305389
```

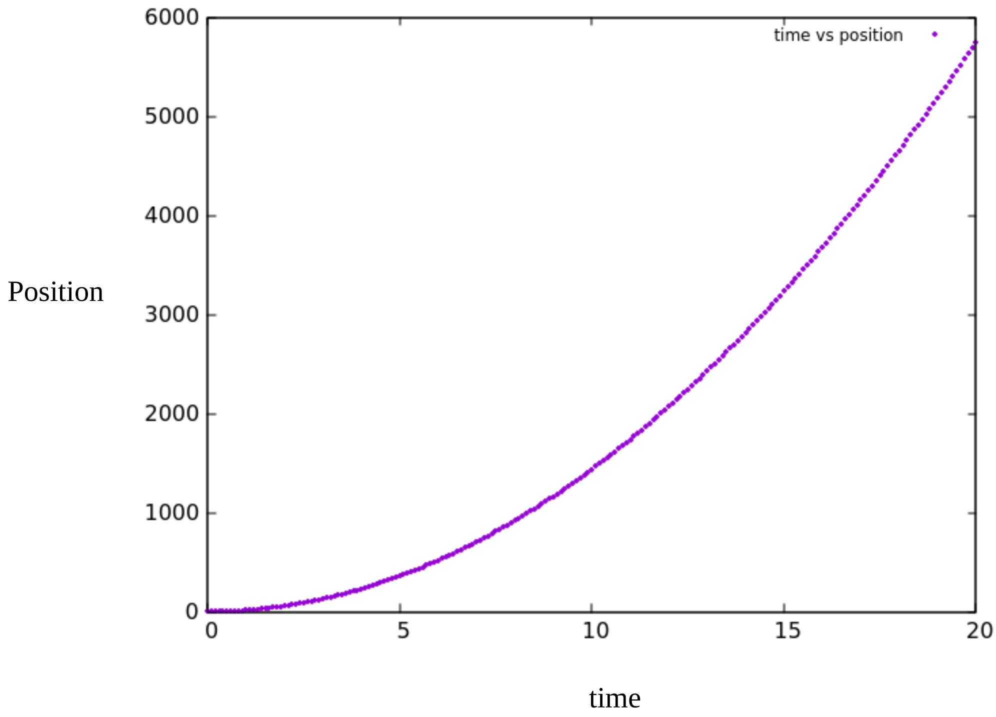
Important Note: In the above program, initial time is set to be zero, i.e., t_0 =0 and time step dt=0.1 and total number of steps n=9. Initial conditions are v_0 =0 and y_0 =1. Therefore, total time=0+(9+1)(0.1)=1. In the output, we have printed t, position and velocity. Moreover, when we run the program, an output file is also generated "leafE0.dat" in which same output data is written. We can use this file to generate plot between velocity vs. Time or position vs. Time or velocity vs position to verify our numerical results with analytical ones. For the above output, we get following plots:

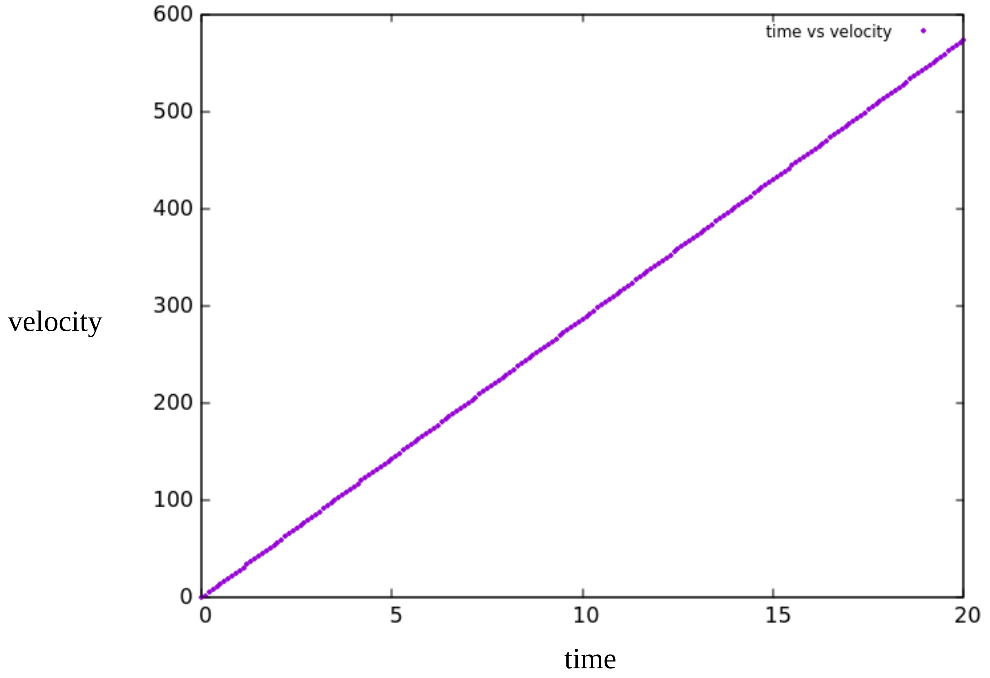




From the above plots, it appears that plot between velocity and time is linear and, plot between position and time is parabolic. This indicates that our numerical solution shows a reasonable match with analytical solutions given by equations (7) & (8).

To further show the accuracy, we set n=199 in the above program and keep all the other parameters same. Now, total time=0+(199+1)(0.1)=20.





The above plots shows a good match with analytical solutions given by equations (7) & (8) with obtained numerical solution.

Next, we aim to solve the equation of motion of a charged particle moving in a uniform magnetic field using the Leapfrog Method.