Simulation of Classical Dynamic Systems

N-dimension problems

Simulation of Classical Dynamic Systems

- Projectile Motion
- Planetary Motion
  - Single planet in a solar system
  - A binary system
- Molecular Dynamics

2nd Order ODE

- Problem: $\frac{d^2}{dt^2}\, x(t) = \frac{F(x,x',t)}{m}$

$$x(0) = x_0\,, \qquad x'(0) = v_0$$

- Change of variables

$$set: \quad \frac{d}{dt}x(t) = v(t)\,;$$

$$\frac{d^2}{dt^2}x(t) = \frac{d}{dt}v(t) = \frac{F(x,v,t)}{m}$$

$$x(0) = x_0, \qquad v(0) = v_0$$

System of 2nd Order ODE

- Problem: $\frac{d^2}{dt^2}\, x_i(t) = \frac{F_i(x_i, v_i, t)}{m_i}$

$$x_i(0) = x_{i0}\,, \qquad x_i'(0) = v_{i0}$$

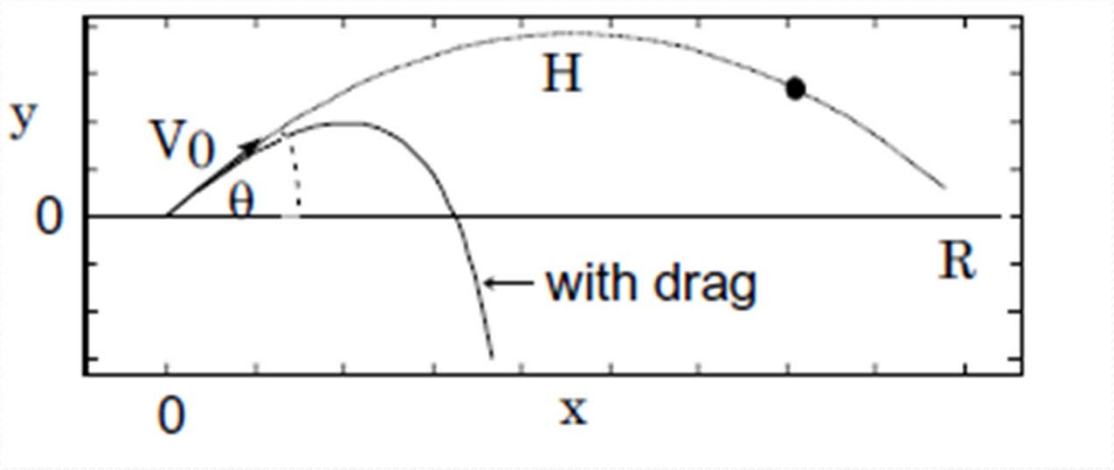
- Change of variables

$$set: \quad \frac{d}{dt} x_i(t) = v_i(t)\,;$$

$$\frac{d^2}{dt^2} x_i(t) = \frac{d}{dt} v_i(t) = \frac{F_i(x_i, v_i, t)}{m_i}$$

$$x_i(0) = x_0, \qquad v_i(0) = v_0$$

Projectile motion



$$\mathbf{F_{ext}} = m\frac{d^2}{dt^2}\boldsymbol{r}(t)$$

$$\frac{d^2}{dt^2}\,\mathbf{r}(t) = \frac{\mathbf{F_{ext}}(t)}{m}$$

$$\mathbf{F_{ext}} = \mathbf{W_m} + \mathbf{F_{drag}}$$
$$= -mg\hat{y} - b|v(t)|^n\,\hat{v}$$

Projectile motion

$$\frac{d^2}{dt^2}\,\mathbf{r}(t) = -g\,\hat{y} - \frac{b}{m}\,|\mathbf{v}(t)|^n\,\frac{\mathbf{v}(t)}{|\mathbf{v}(t)|}$$

$$\frac{d^2}{dt^2}x(t) = -\frac{b}{m}\left(\sqrt{v_x(t)^2 + v_y(t)^2}\right)^{n-1} v_x(t)$$

$$\frac{d^2}{dt^2}y(t) = -g - \frac{b}{m}\left(\sqrt{v_x(t)^2 + v_y(t)^2}\right)^{n-1} v_y(t)$$

Simultaneous 1st order ODE

$$\frac{d}{dt}x(t) = v_x(t)$$

$$\frac{d}{dt}v_x(t) = a_x(t) = -\frac{b}{m}\left(\sqrt{v_x(t)^2 + v_y(t)^2}\right)^{n-1} v_x(t)$$

$$\frac{d}{dt}y(t) = v_y(t)$$

$$\frac{d}{dt}v_y(t) = a_y(t) = -g - \frac{b}{m}\left(\sqrt{v_x(t)^2 + v_y(t)^2}\right)^{n-1} v_y(t)$$

Euler's Method

$$x(t + \Delta t) \approx x(t) + \Delta t * v_x(t)$$

$$v_x(t + \Delta t) \approx v_x(t) - \Delta t * \ b \left(\sqrt{v_x(t)^2 + v_y(t)^2}\right)^{n-1} \ v_x(t)$$

$$y(t + \Delta t) \approx y(t) + \Delta t * \ v_y(t)$$

$$v_y(t + \Delta t) \approx v_y(t) + \Delta t \ * (-g - b \left(\sqrt{v_x(t)^2 + v_y(t)^2}\right)^{n-1} \ v_y(t))$$

2nd Order Taylor method

- $x(t+\Delta t) \approx x(t) + \Delta t\, x'(t) + \frac{\Delta t^2}{2}\, x''(t)$

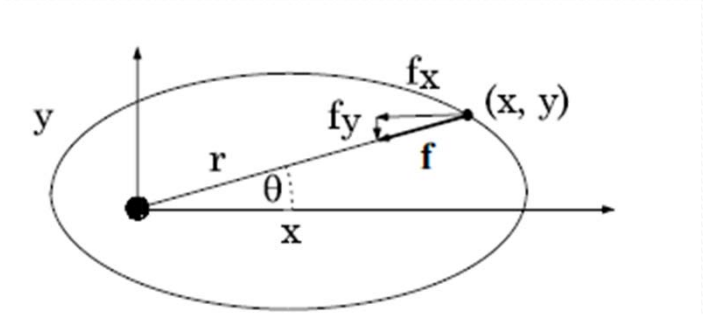
$$= x(t) + \Delta t\, v_x(t) + \frac{\Delta t^2}{2}\, a_x(t)$$

- $v_x(t+\Delta t) \approx v_x(t) + \Delta v_x'(t) + \frac{\Delta t^2}{2} v_x''(t)$

$$= v_x(t) + \Delta t\, a_x(t) + \frac{\Delta t^2}{2} a_x'(t)$$

- $y(t+\Delta t) \approx y(t) + \Delta t\, v_y(t) + \frac{\Delta t^2}{2}\, a_y(t)$
- $v_y(t+\Delta t) \approx v_y(t) + \Delta t\, a_y(t) + \frac{\Delta t^2}{2} a_y'(t)$

Planetary Motion



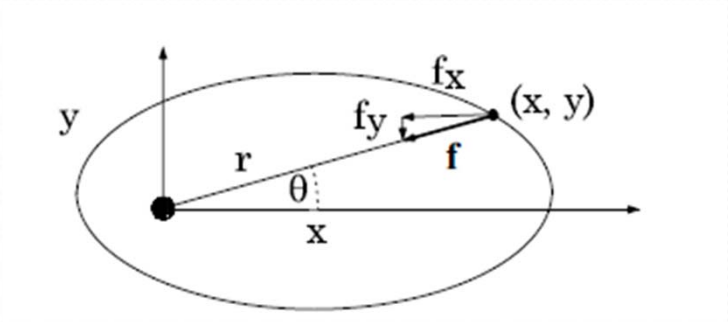
$$\frac{d^2}{dt^2}\,\mathbf{r_s}(t) = \frac{\mathbf{F_{es}}(t)}{M_s}$$

$$\frac{d^2}{dt^2}\,\mathbf{r_e}(t) = \frac{\mathbf{F_{se}}(t)}{m_e}$$

$$|\mathbf{F_{se}}| = |\mathbf{F_{es}}| = \frac{GM_S m_e}{|\mathbf{r_e}(t) - \mathbf{r_s}(t)|^2}$$

Planetary Motion

If $M_s \gg m_e$, then $\mathbf{r_s(t)}$~constant



$$\frac{d^2}{dt^2}\,\mathbf{r_e}(t) = \frac{\mathbf{F_{se}}(t)}{m_e},$$

$$\mathbf{r_e}(t) = x(t)\hat{\imath} + y(t)\hat{\jmath}$$

$$\frac{d^2}{dt^2}x(t) = -\frac{GM}{|\mathbf{r_e}(t)|^2}\frac{x(t)}{|\mathbf{r_e}(t)|}$$

$$\frac{d^2}{dt^2}y(t) = -\frac{GM}{|\mathbf{r_e}(t)|^2}\frac{y(t)}{|\mathbf{r_e}(t)|}$$

Planetary Motion

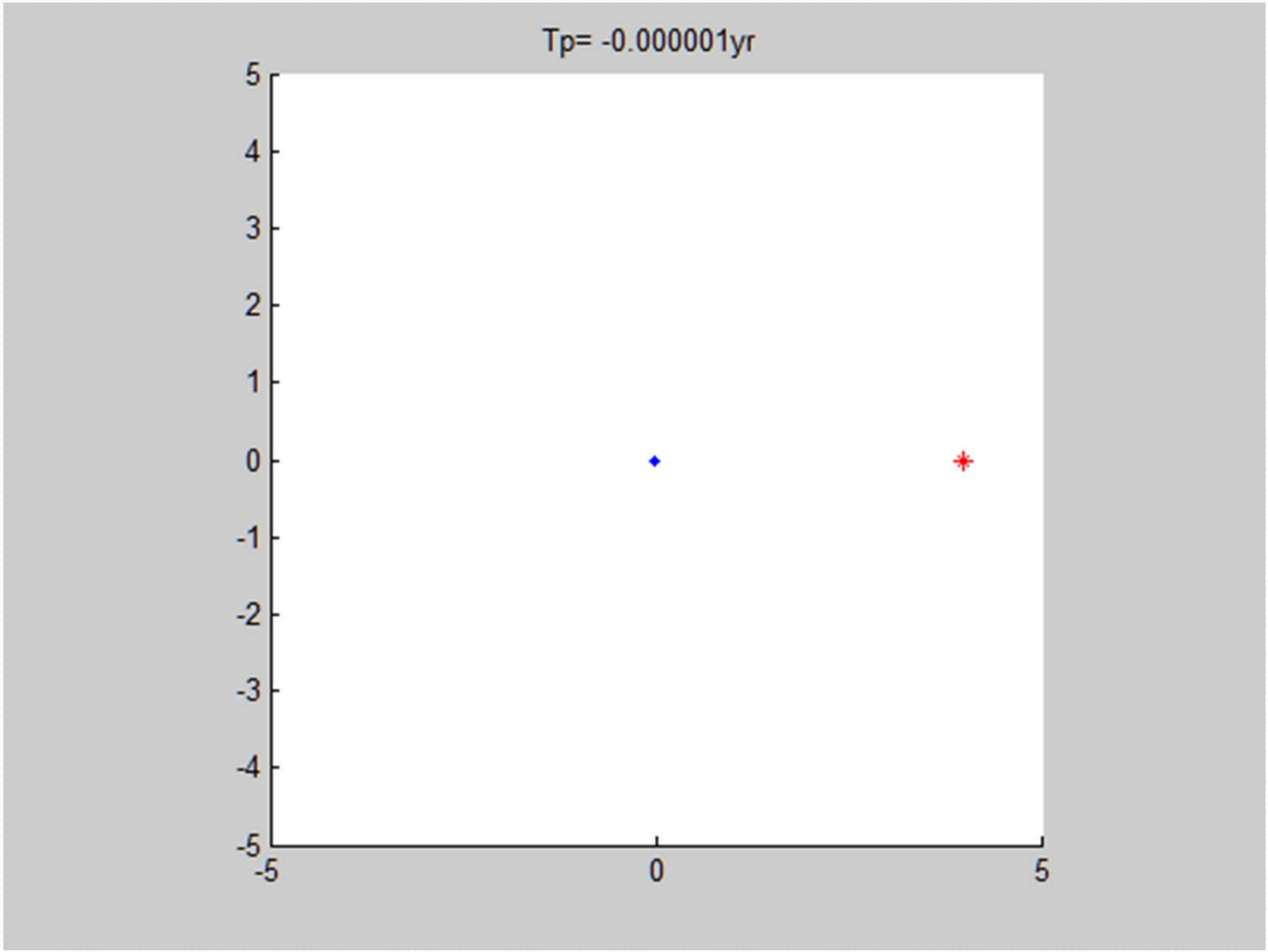
If $M_s \gg m_e$, then $\mathbf{r_s(t)}$~constant

$$\frac{d}{dt}x(t) = v_x(t)$$

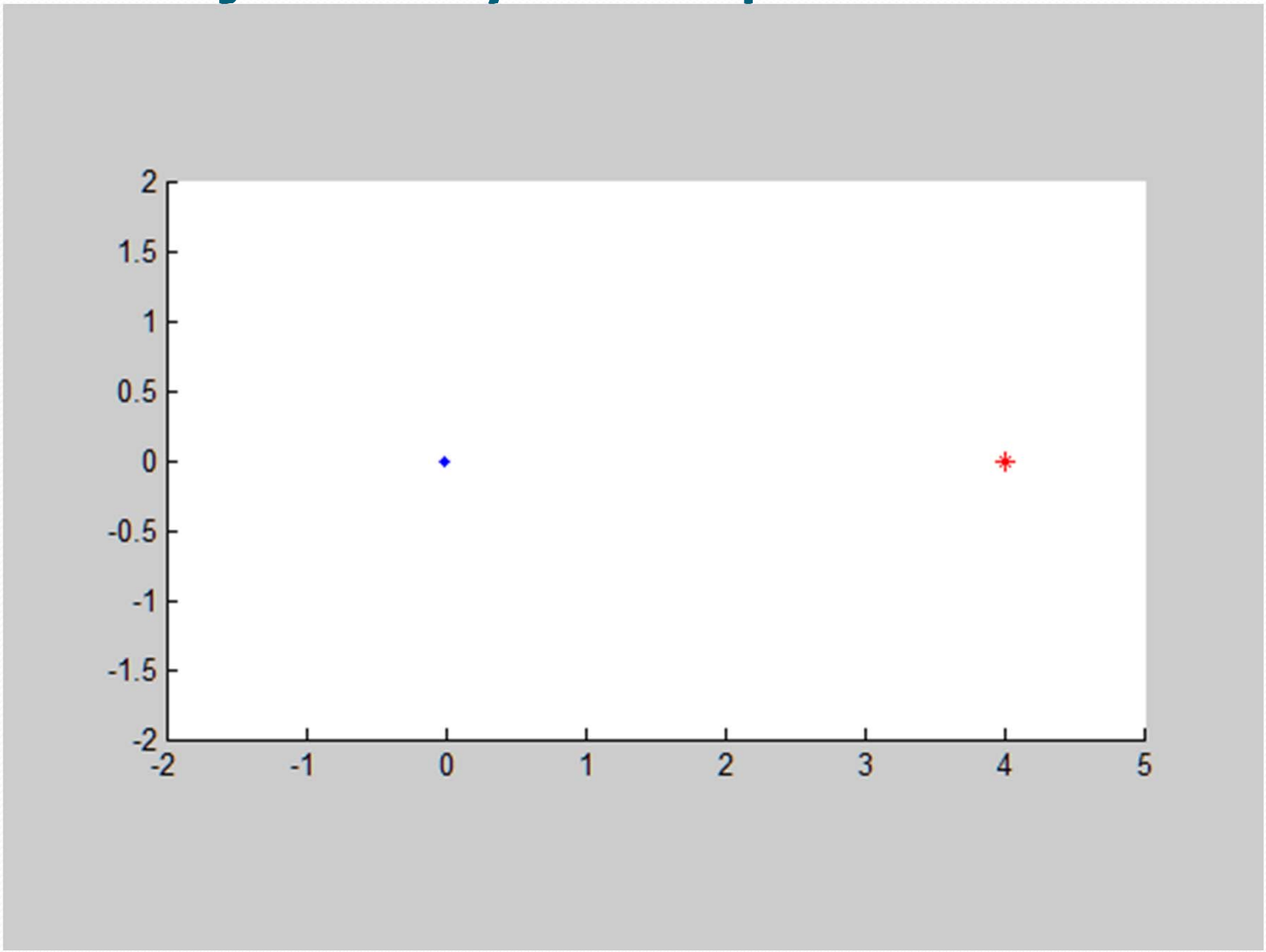
$$\frac{d}{dt}v_x(t) = -\frac{GM}{(x(t)^2 + y(t)^2)^{\frac{3}{2}}}x(t)$$

$$\frac{d}{dt}y(t) = v_y(t)$$

$$\frac{d}{dt}v_y(t) = -\frac{GM}{(x(t)^2 + y(t)^2)^{\frac{3}{2}}}y(t)$$


Tp= -0.000001yr
5
4
3
2
1
0
-1
-2
-3
-4
-5
-5
0
5

The trajectory of a planet



Planetary Motion

If $\boldsymbol{M_s}$ $\boldsymbol{and}$ $\boldsymbol{m_e}$ are compatible ($\vec{r} \equiv \vec{r}_e - \vec{r}_s$)

Equation of Motion for m_e

$$\frac{d^2}{dt^2} x_e(t) = -GM_s \frac{x_e(t) - x_s(t)}{|r(t)|^{\frac{3}{2}}}$$

$$\frac{d^2}{dt^2} y_e(t) = -GM_s \frac{y_e(t) - y_s(t)}{|r(t)|^{\frac{3}{2}}}$$

Equation of Motion for M_s

$$\frac{d^2}{dt^2} x_s(t) = -Gm_e \frac{x_s(t) - x_e(t)}{|r(t)|^{\frac{3}{2}}}$$

$$\frac{d^2}{dt^2} y_s(t) = -Gm_e \frac{y_s(t) - y_e(t)}{|r(t)|^{\frac{3}{2}}}$$

Planetary Motion: a binary star system

Equation of Motion for m_1

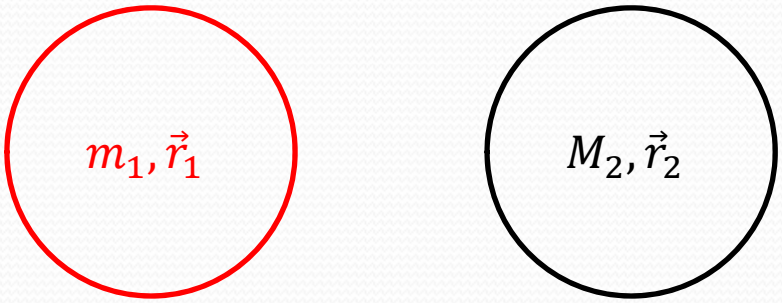
$$\frac{d^2}{dt^2}x_1(t) = -GM_2\frac{x_1(t)-x_2(t)}{|r(t)|^{\frac{3}{2}}}$$

$$\frac{d^2}{dt^2}y_1(t) = -GM_2\frac{y_1(t)-y_2(t)}{|r(t)|^{\frac{3}{2}}}$$

Equation of Motion for M_2

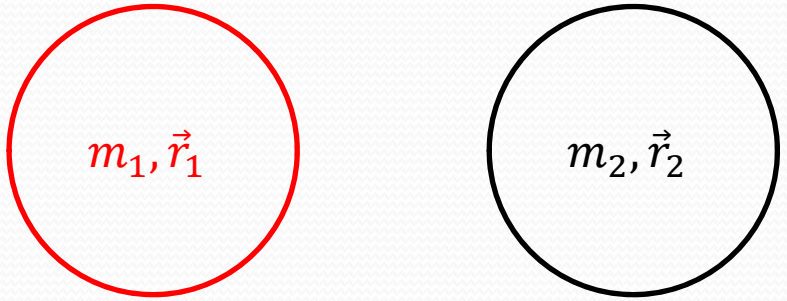
$$\frac{d^2}{dt^2}x_2(t) = -Gm_1\frac{x_2(t)-x_1(t)}{|r(t)|^{\frac{3}{2}}}$$

$$\frac{d^2}{dt^2}y_2(t) = -Gm_1\frac{y_2(t)-y_1(t)}{|r(t)|^{\frac{3}{2}}}$$



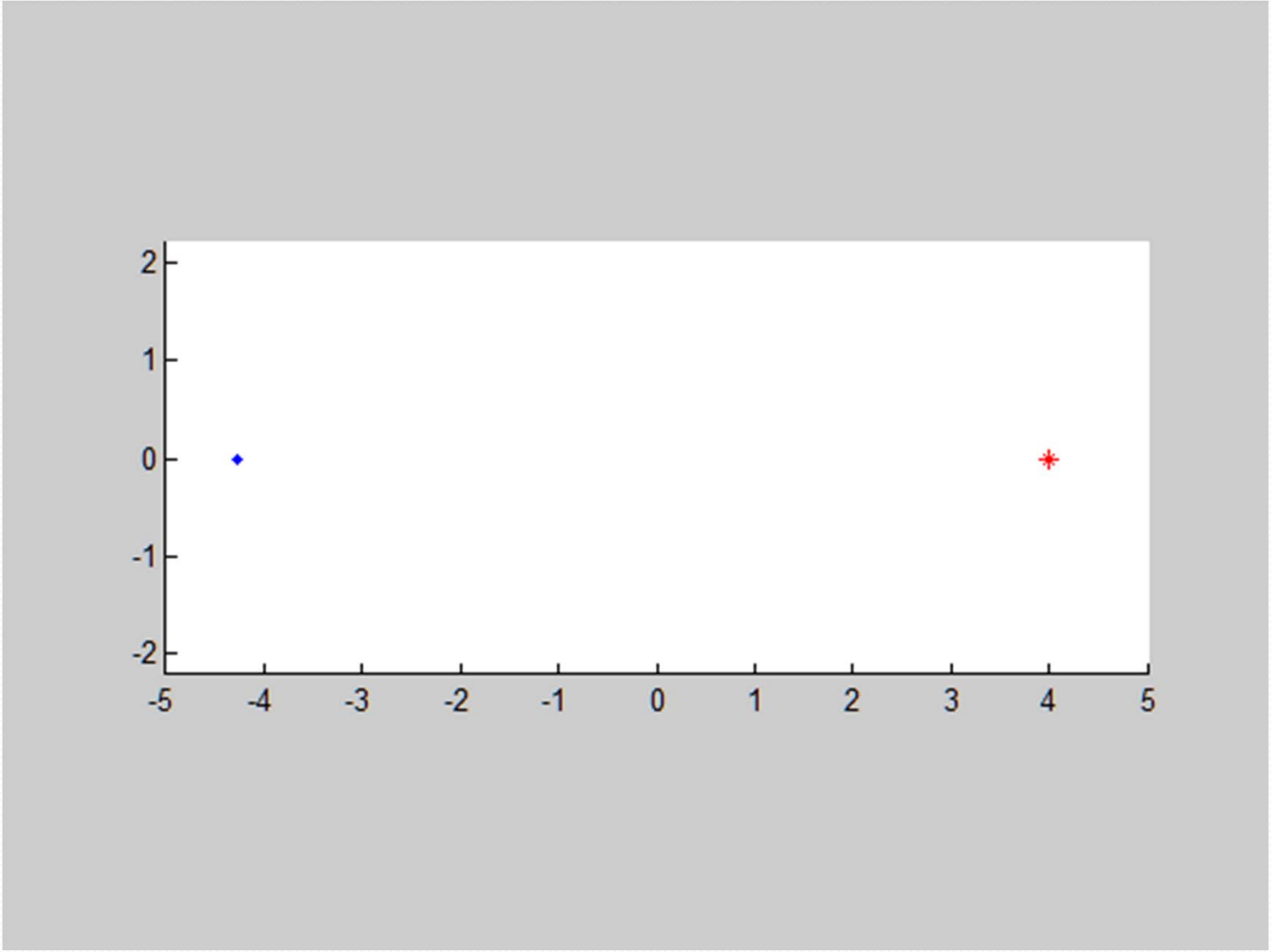
Dynamics of a binary star system

- $\frac{d^2}{dt^2} m_1 x_1(t) = -\frac{d^2}{dt^2} m_2 x_2(t)$
- $\frac{d^2}{dt^2} m_1 y_1(t) = -\frac{d^2}{dt^2} m_2 y_2(t)$

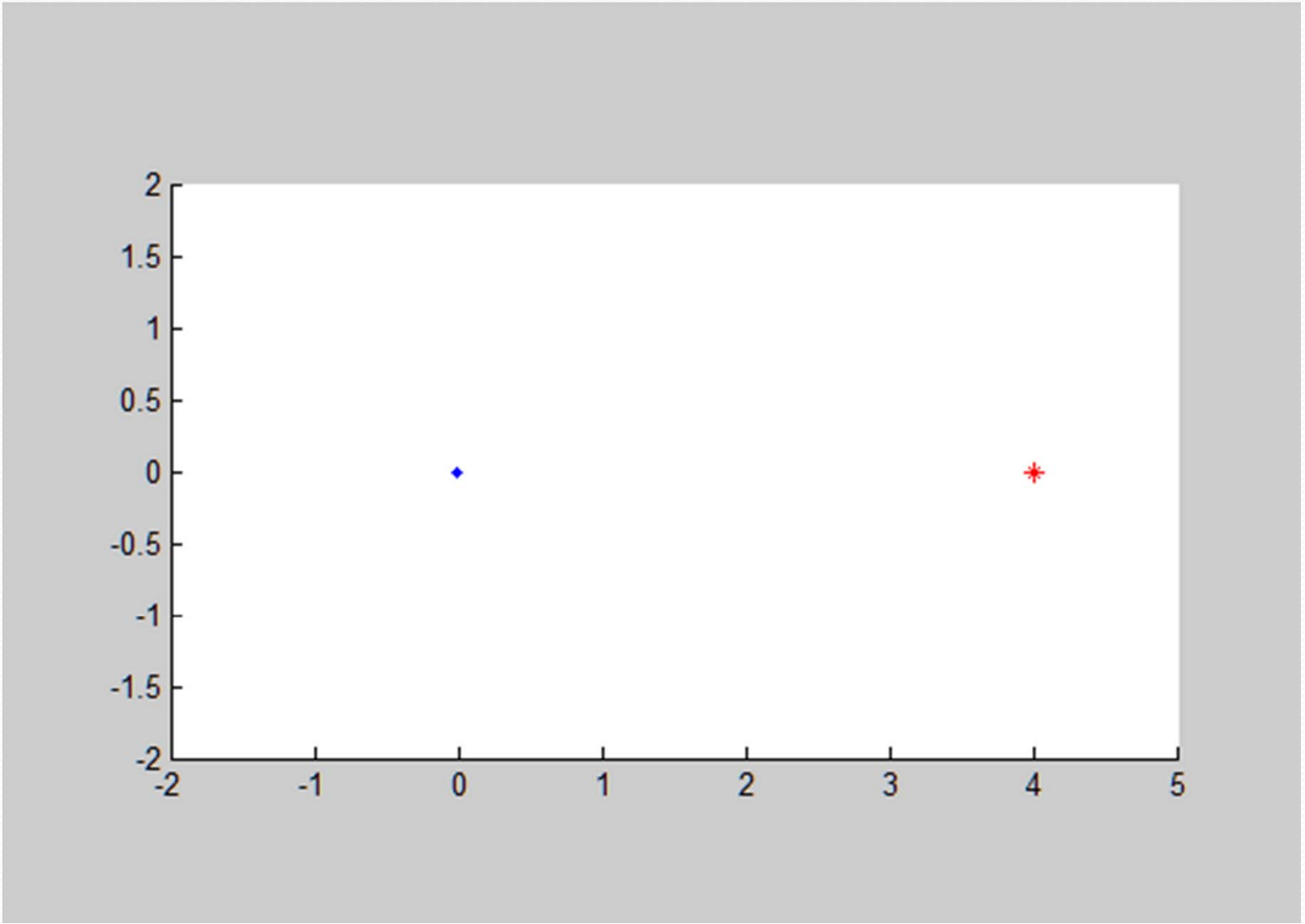


- Since m1 and m2 are constant with $\frac{d}{dt} x = v_x \; and \frac{d}{dt} y = v_y$
- Linear momentum of the system is conservative

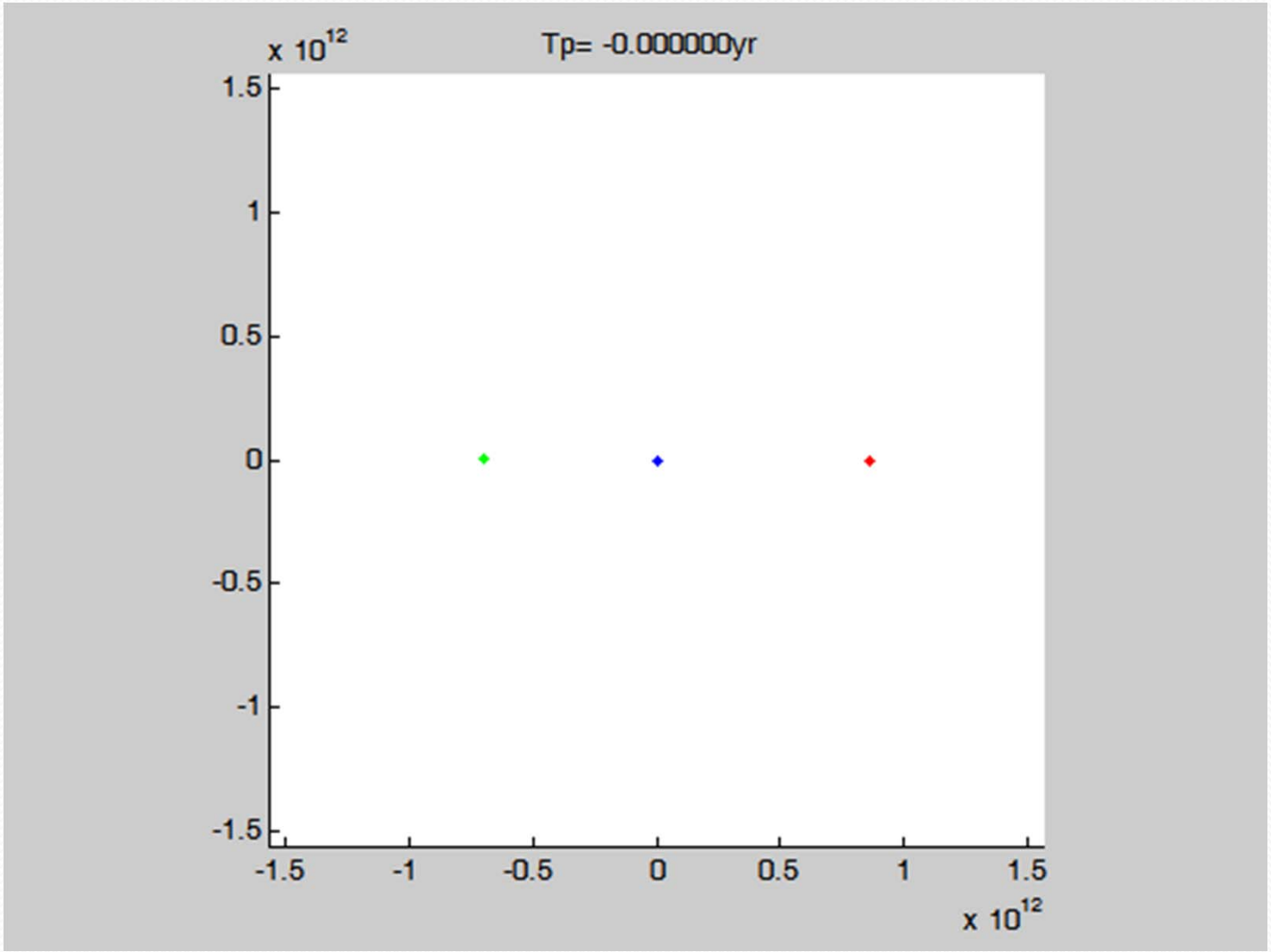
A binary star system



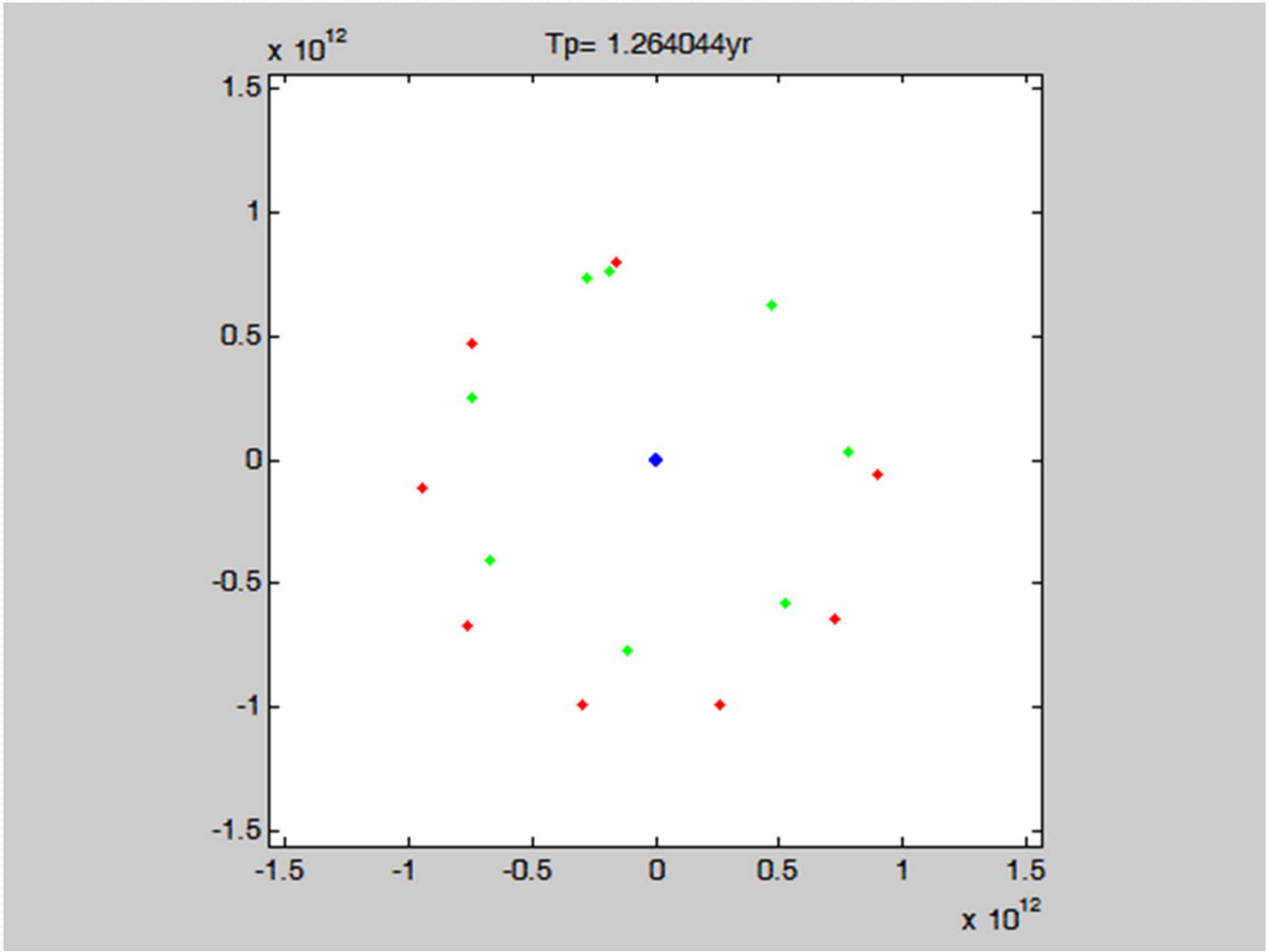
If $M_s \gg m_e$,



Three Body Interaction



Clearing the neighborhood



Conservation of linear momentum of a simulated system

- If the interaction between the objects in a system follows Newton's Third Law

$\Rightarrow$

- The momentum of the system is conservative
- The forces are regarded as internal forces of a system

Equation of Motion of the "Blues" N = 3

X-direction

$$\frac{d}{dt}x_i(t) = v_x^{(i)}(t)$$

$$\frac{d}{dt}v_x^{(i)}(t) = a_x^{(i)}(t) = \frac{F_x^{(i)}(t)}{m_i}$$

$$F_x^{(i)}(t) = \sum_{j=1}^{N} F_x^{(j,i)}(t)$$

$$F_x^{(j,i)}(t) = -F_x^{(i,j)}(t)$$

Y-direction

$$\frac{d}{dt}y_i(t) = v_y^{(i)}(t)$$

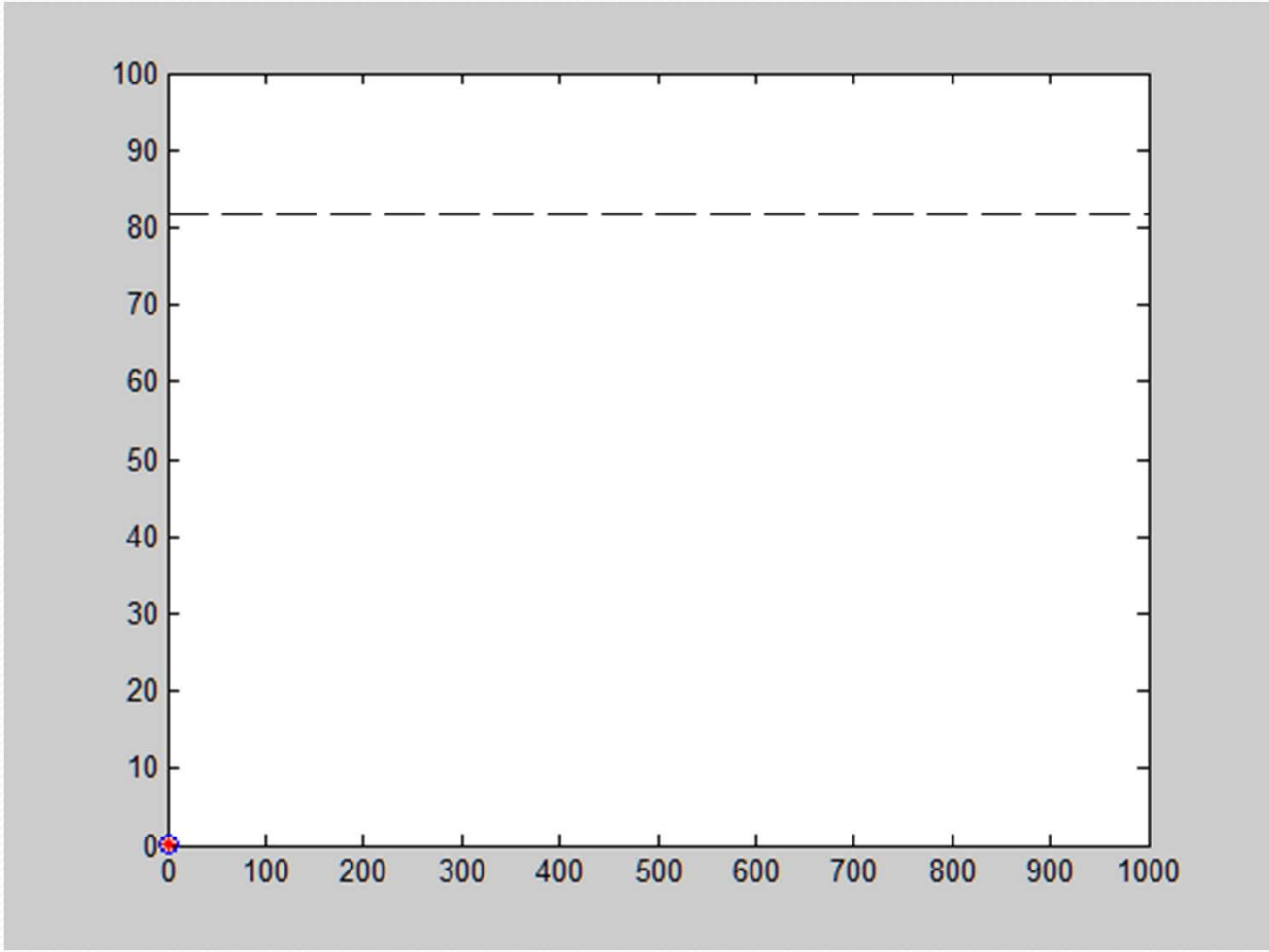
$$\frac{d}{dt}v_y^{(i)}(t) = a_y^{(i)}(t) = -g + \frac{F_y^{(i)}(t)}{m_i}$$

$$F_y^{(i)}(t) = \sum_{j=1}^{N} F_y^{(j,i)}(t)$$

$$F_y^{(j,i)}(t) = -F_y^{(i,j)}(t)$$

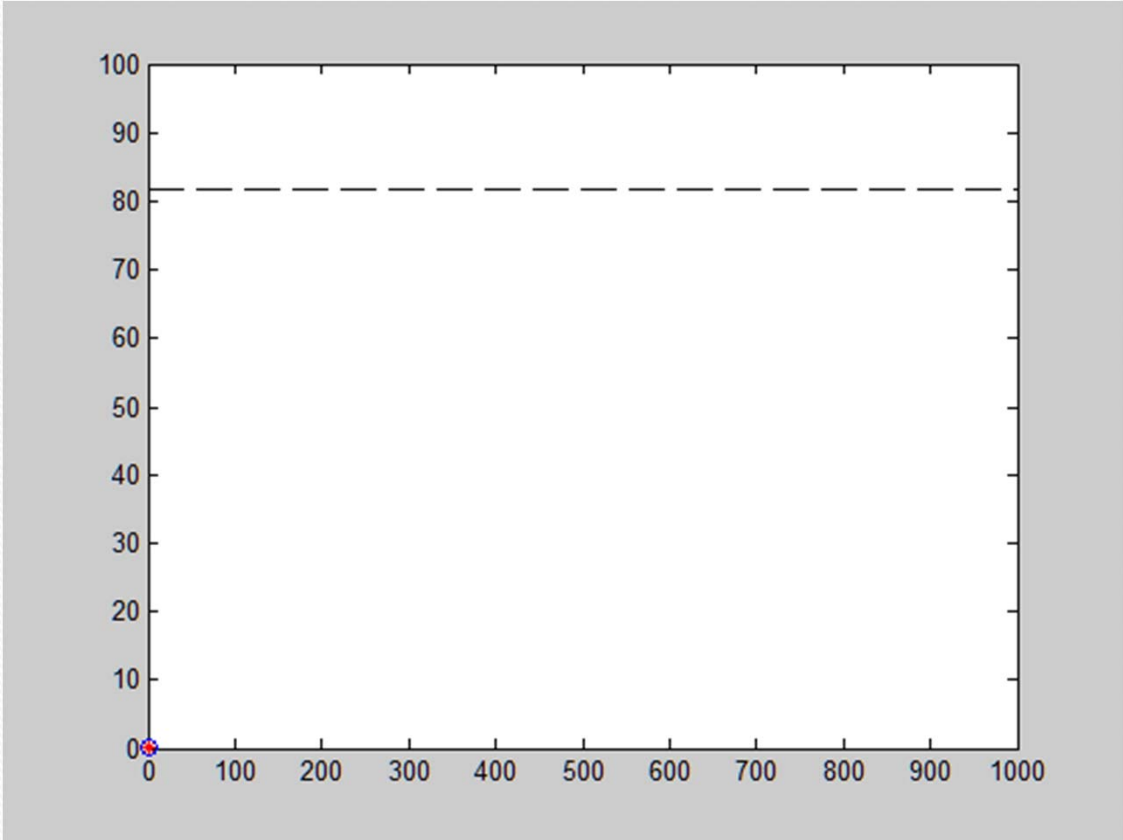
Equation of Motion of the “Blues” N = 3

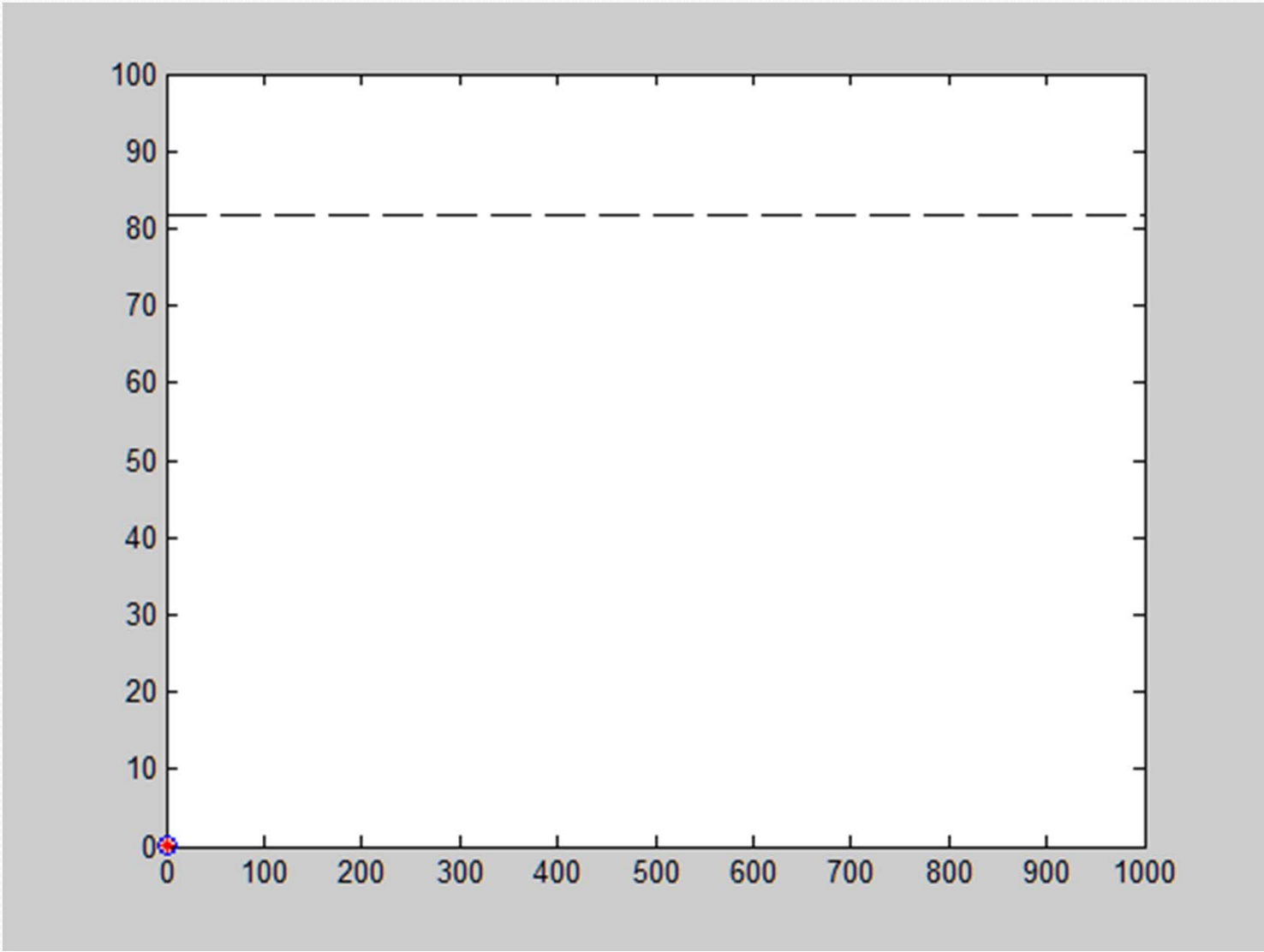
- If F (t) =o all the time



Equation of Motion of the "Blues" N = 3

- At the time when blues are separated
- $F_{12} = +5N\,\hat{x}, F_{21} = -5N\hat{x},$
- $F_{23} = +5N\,\hat{x}, F_{32} = -5N\hat{x},$




100
90
80
70
60
50
40
30
20
10
0
0
100
200
300
400
500
600
700
800
900
1000

Multi-variable ODE

- Rewrite the higher ODEs to simultaneous 1st order ODEs

- Solve the equation with existing methods:
  Euler's Method, Higher order Taylor Method, Runge-Kutta, ...

A General Equation of Motion
N objects with no external forces

X-direction

$$\frac{d}{dt}x_i(t) = v_x^{(i)}(t)$$

$$\frac{d}{dt}v_x^{(i)}(t) = a_x^{(i)}(t) = \frac{F_x^{(i)}(t)}{m_i}$$

$$F_x^{(i)}(t) = \sum_{j=1}^{N} F_x^{(j,i)}(t)$$

$$F_x^{(j,i)}(t) = -F_x^{(i,j)}(t)$$

Y-direction

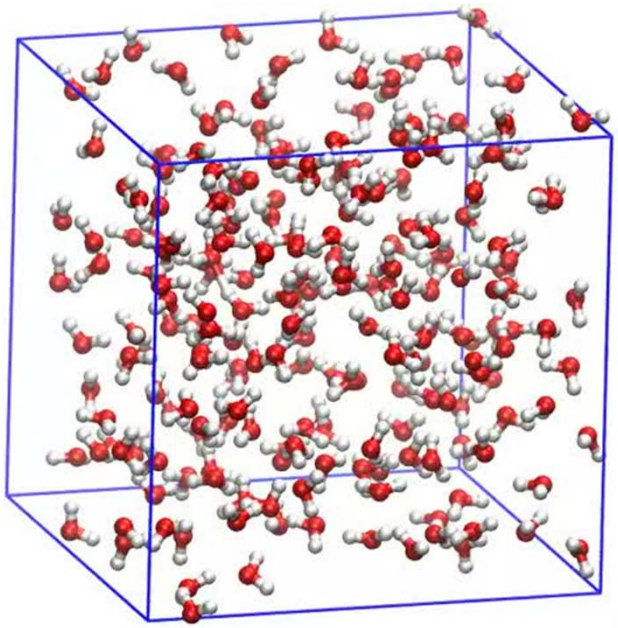
$$\frac{d}{dt}y_i(t) = v_y^{(i)}(t)$$

$$\frac{d}{dt}v_y^{(i)}(t) = a_y^{(i)}(t) = \frac{F_y^{(i)}(t)}{m_i}$$

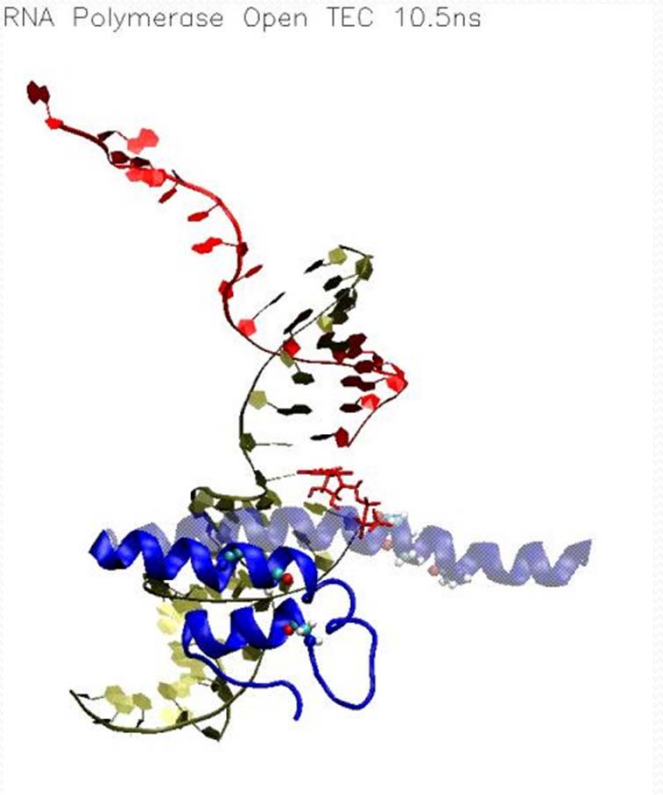
$$F_y^{(i)}(t) = \sum_{j=1}^{N} F_y^{(j,i)}(t)$$

$$F_y^{(j,i)}(t) = -F_y^{(i,j)}(t)$$

Simulation with Molecular Dynamics



http://commons.wikimedia.org/wiki/File:Isothermal-Isobaric_Molecular_Dynamics_Simulation_of_Water.webm



http://upload.wikimedia.org/wikipedia/commons/thumb/8/85/Molecular-dynamics-and-mutational-analysis-of-the-catalytic-and-translocation-cycle-of-RNA-2046-1682-5-11-S3.ogv/378px--Molecular-dynamics-and-mutational-analysis-of-the-catalytic-and-translocation-cycle-of-RNA-2046-1682-5-11-S3.ogv.jpg

Simulation with Molecular Dynamics

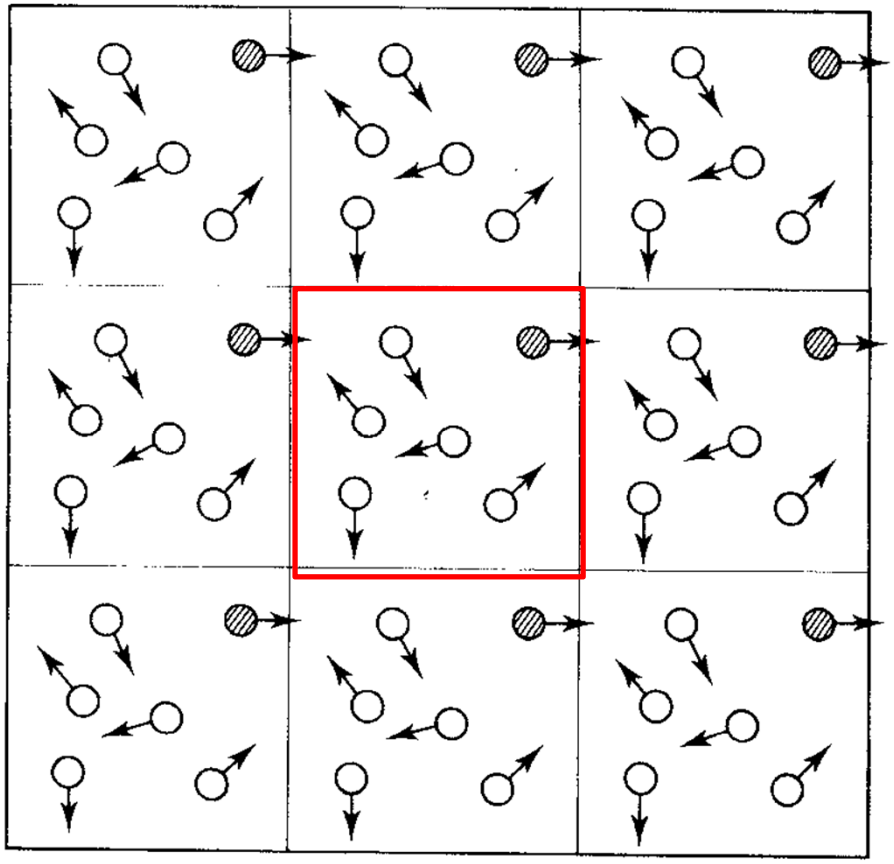
- Boundary Condition: Collision on the boundaries
- Collision between particles
- Solving a system of differential equation for multiple particles

Boundary Condition: Collision on the boundaries

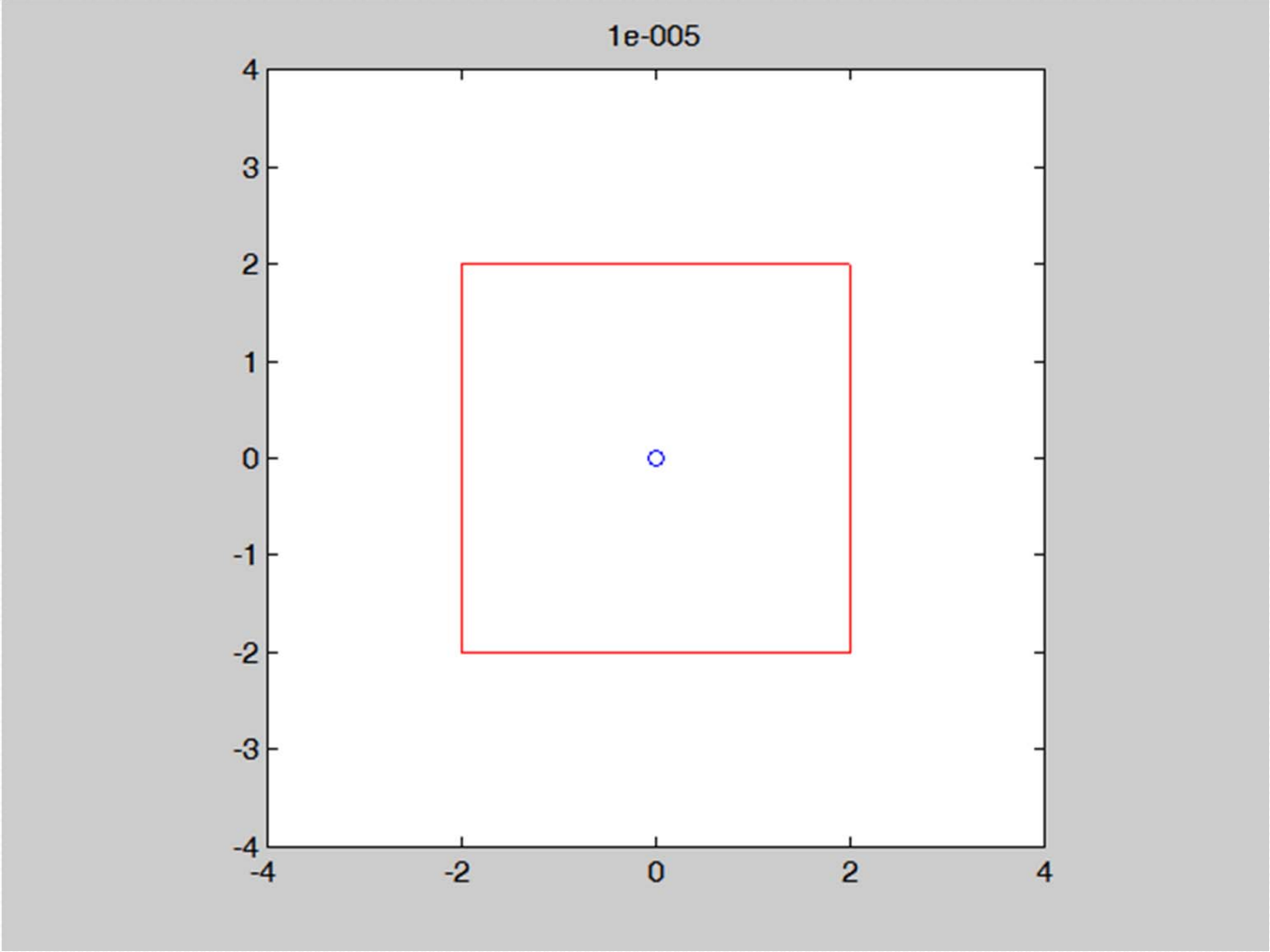
- A Thermal Dynamic System
  - Contains at least 6×10^{23} particles

- At equilibrium state
  - Dynamic properties of a smaller region resembles the properties of the entire system.

At equilibrium state



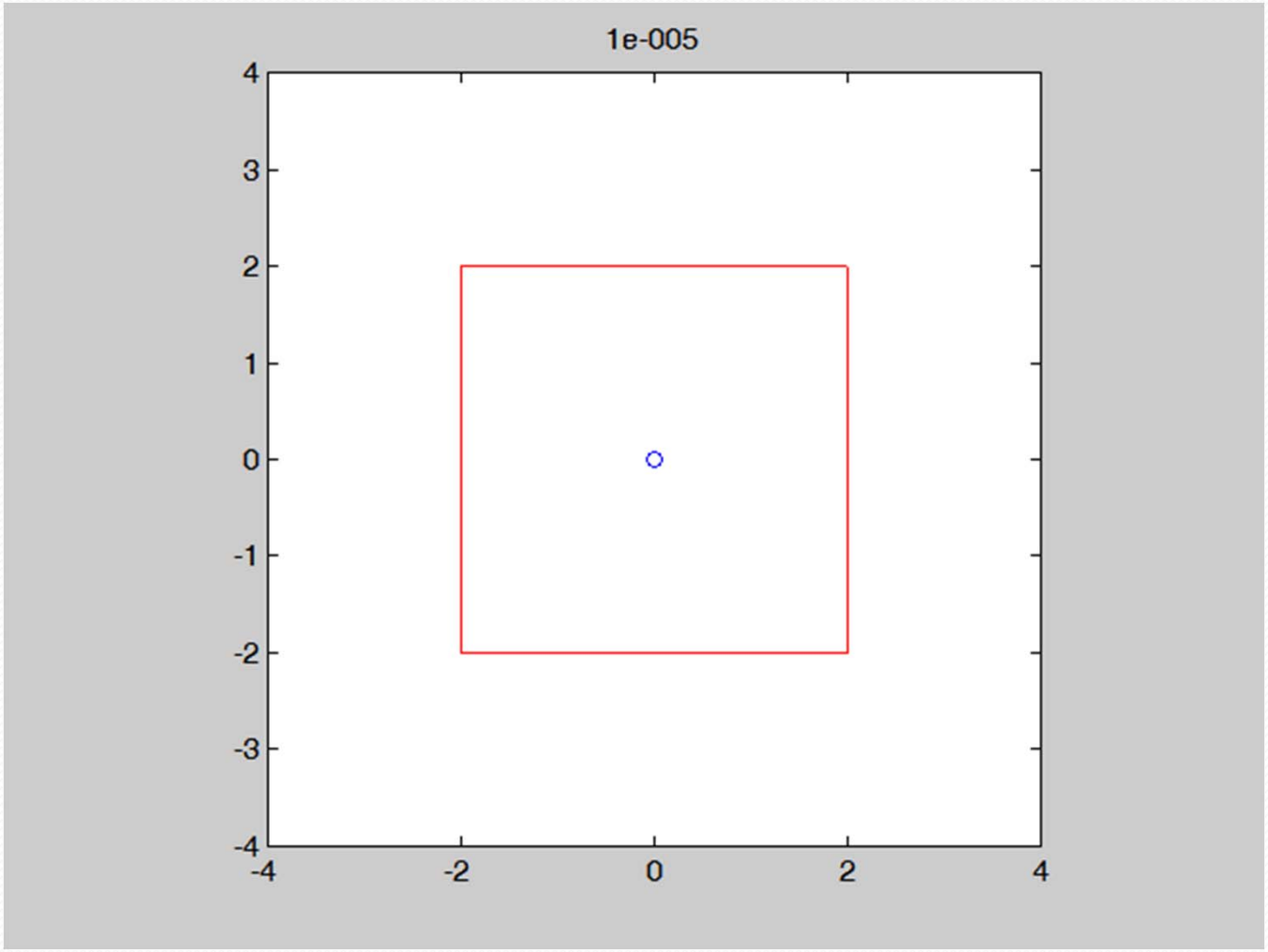
Without Boundary Condition



Boundary Condition:

- Reflective Boundary Condition
  - Each boundary works like a mirror and each one contains mirror objects of the particles in the system.
  - When a particle hits the boundary, it is replaced by the mirror object with respect to the hit boundary
- Periodic Boundary Condition

Reflective Boundary Condition



Reflective Boundary Condition

- If the particle does not exceed to the location twice as large as the original bounary

$$\vec{r}_i(t) = \frac{\vec{r}_i(t)}{|\vec{r}_i(t)|} * 2 * L_i - \vec{r}_i(t)$$

  - where i are 1,2,3 representing x, y, and z components respectively

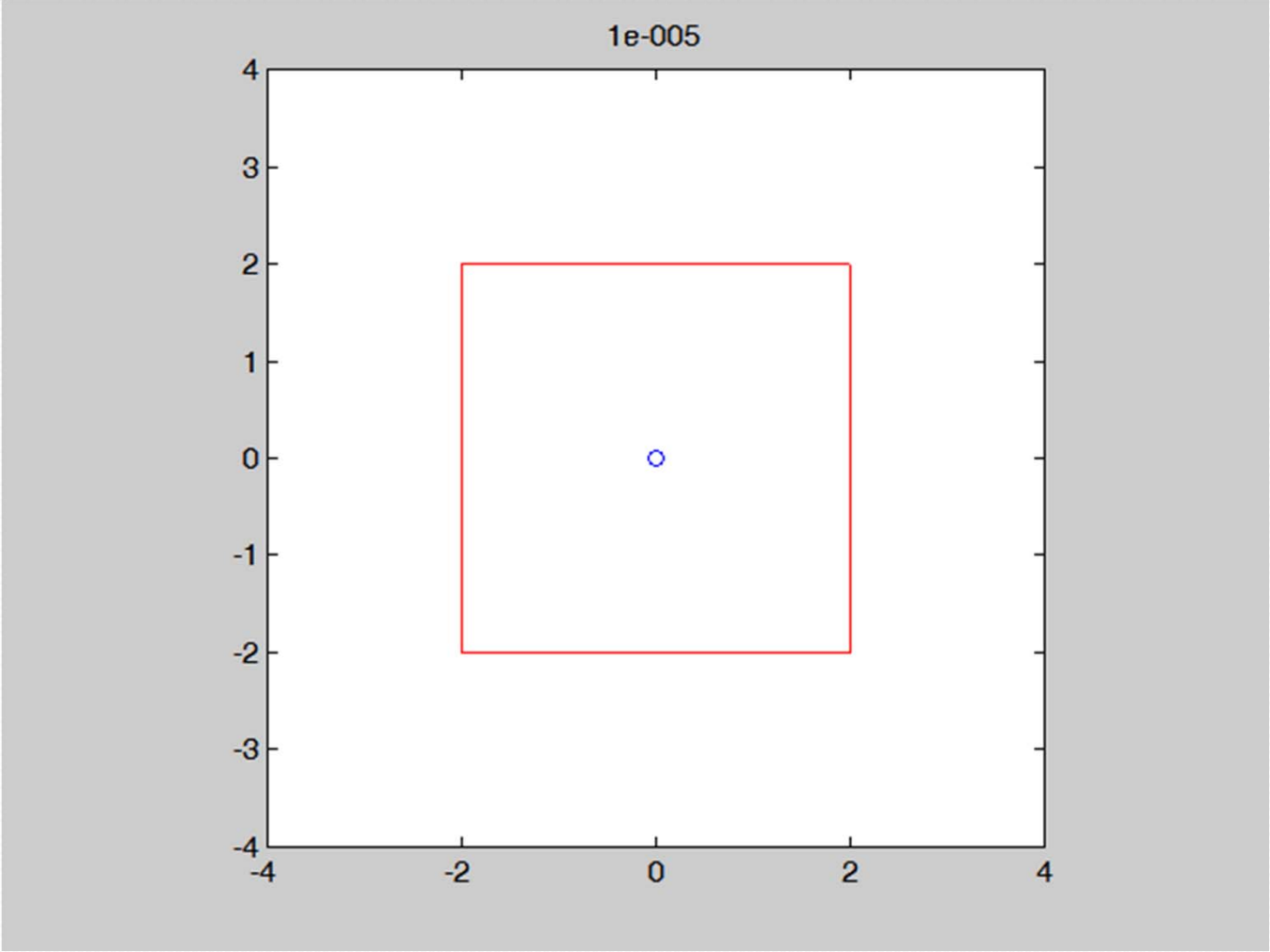
- $\vec{v}_i(t) = -\vec{v}_i(t)$

Boundary Condition:

- Reflective Boundary Condition

- Periodic Boundary Condition
  - Each boundary is identical to that of the other side across the system
  - When a particle hits the boundary, it returns to the system from the other corresponding boundary

Periodic Boundary Condition



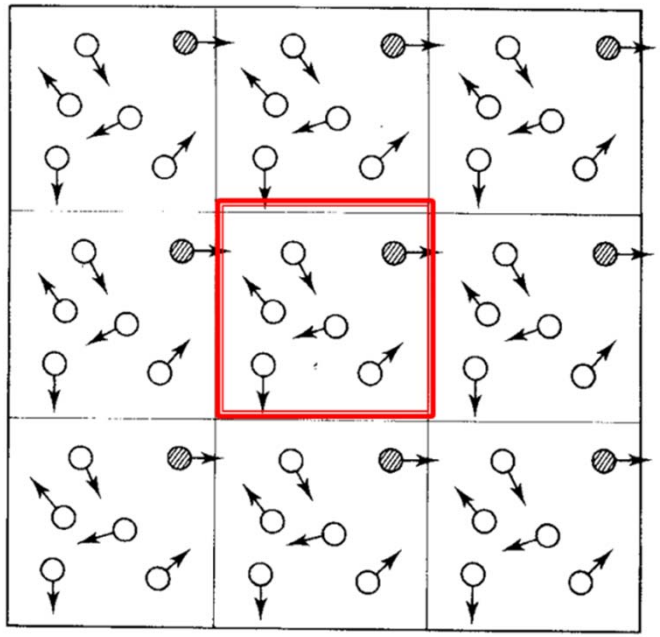
Periodic Boundary Condition

- If the particle does not exceed to the location twice as large as the original bounary

$$\vec{r}_i(t) = \vec{r}_i(t) - 2L_i$$

  - where i are 1,2,3 representing x, y, and z components respectively

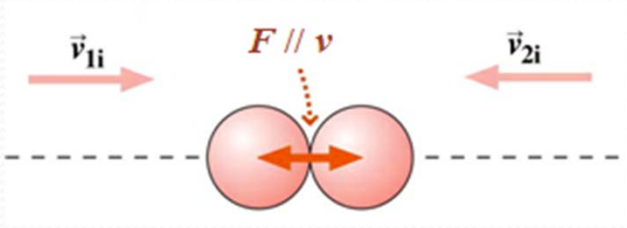
- $\vec{v}_i(t) = \vec{v}_i(t)$



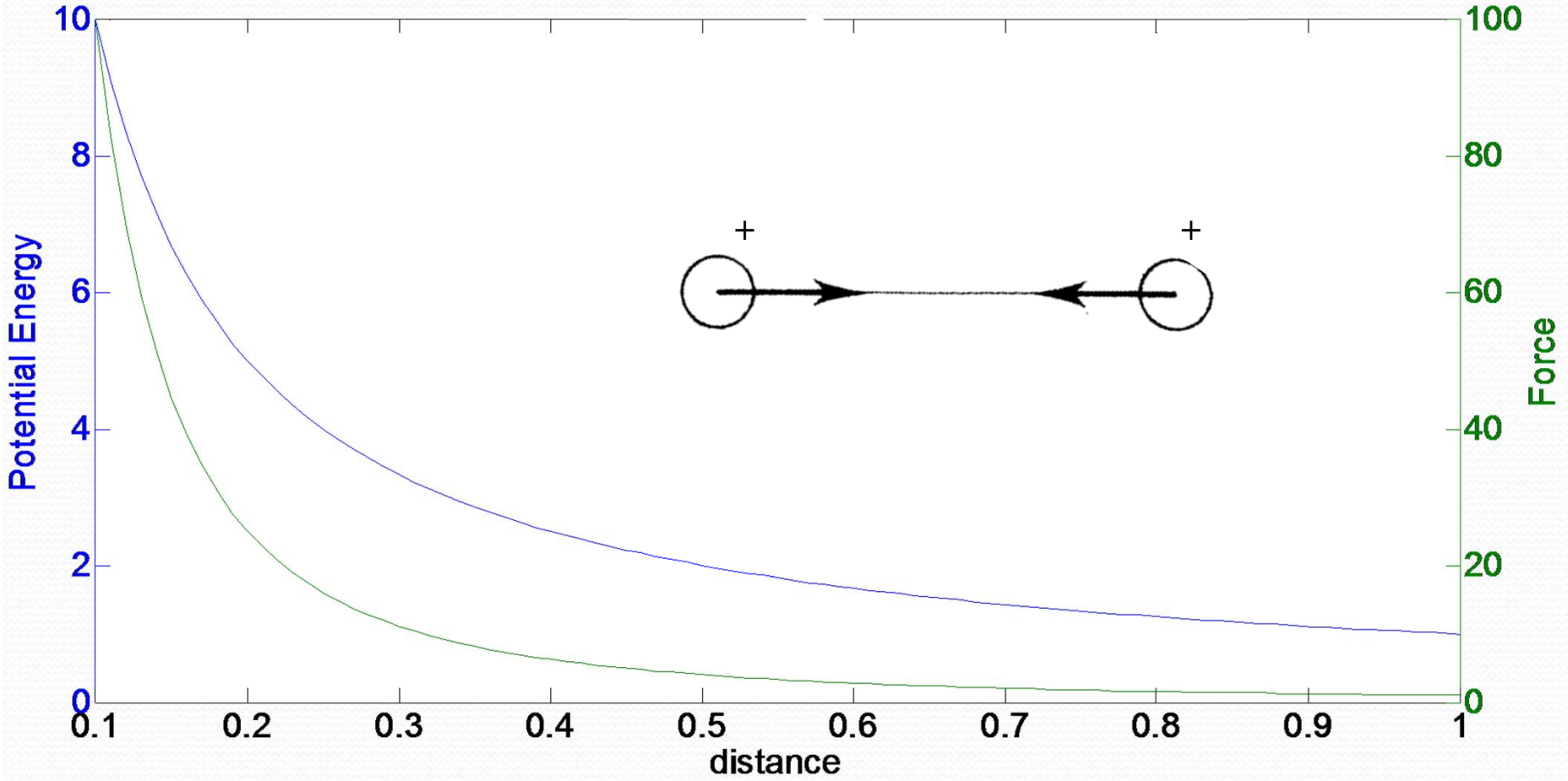
Simulation with Molecular Dynamics

- Boundary Condition: Collision on the boundaries
- Collision between particles
- Solving a system of differential equation for multiple particles

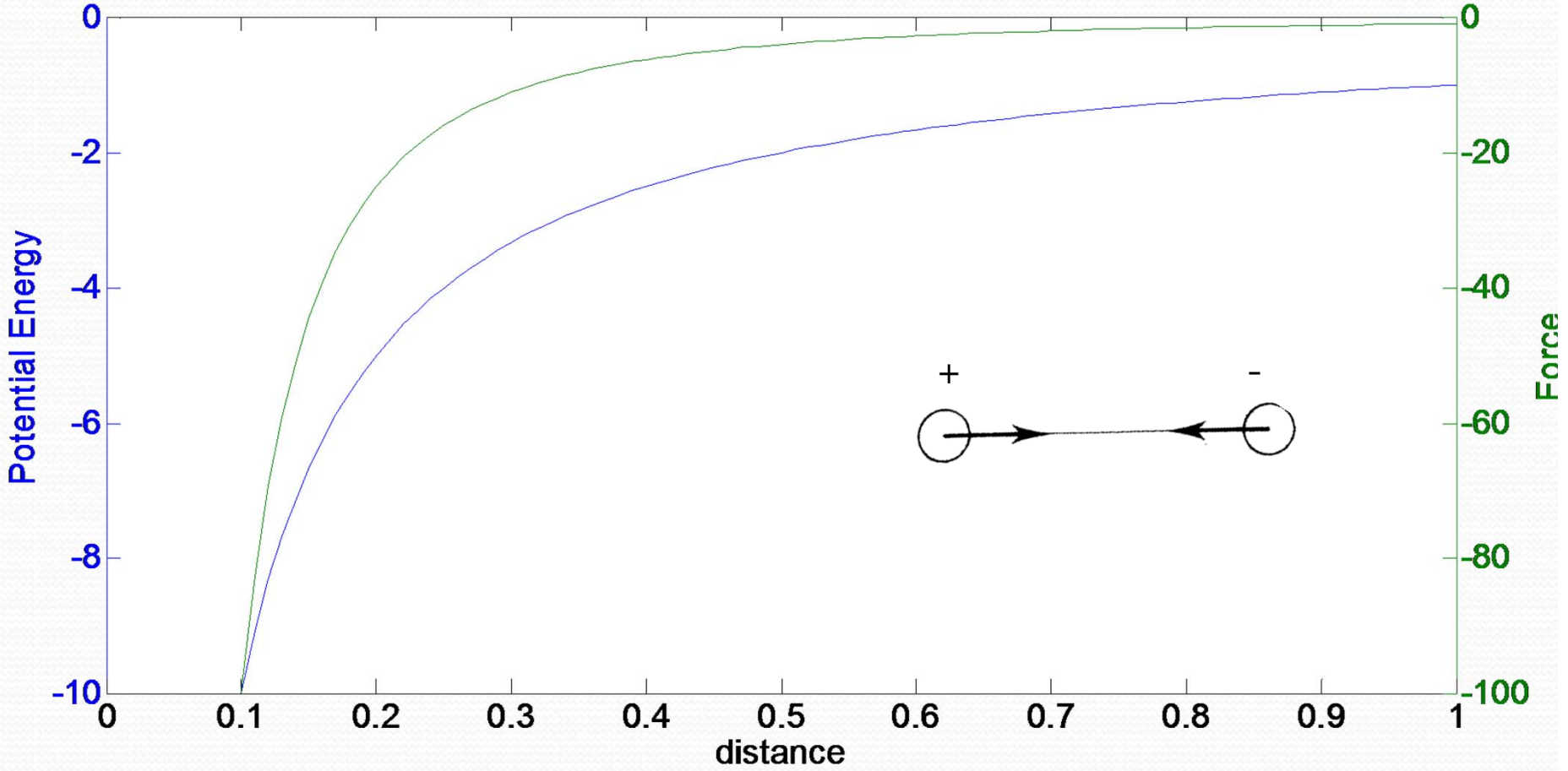
Collision



Potential Energy bewteen two charged particles

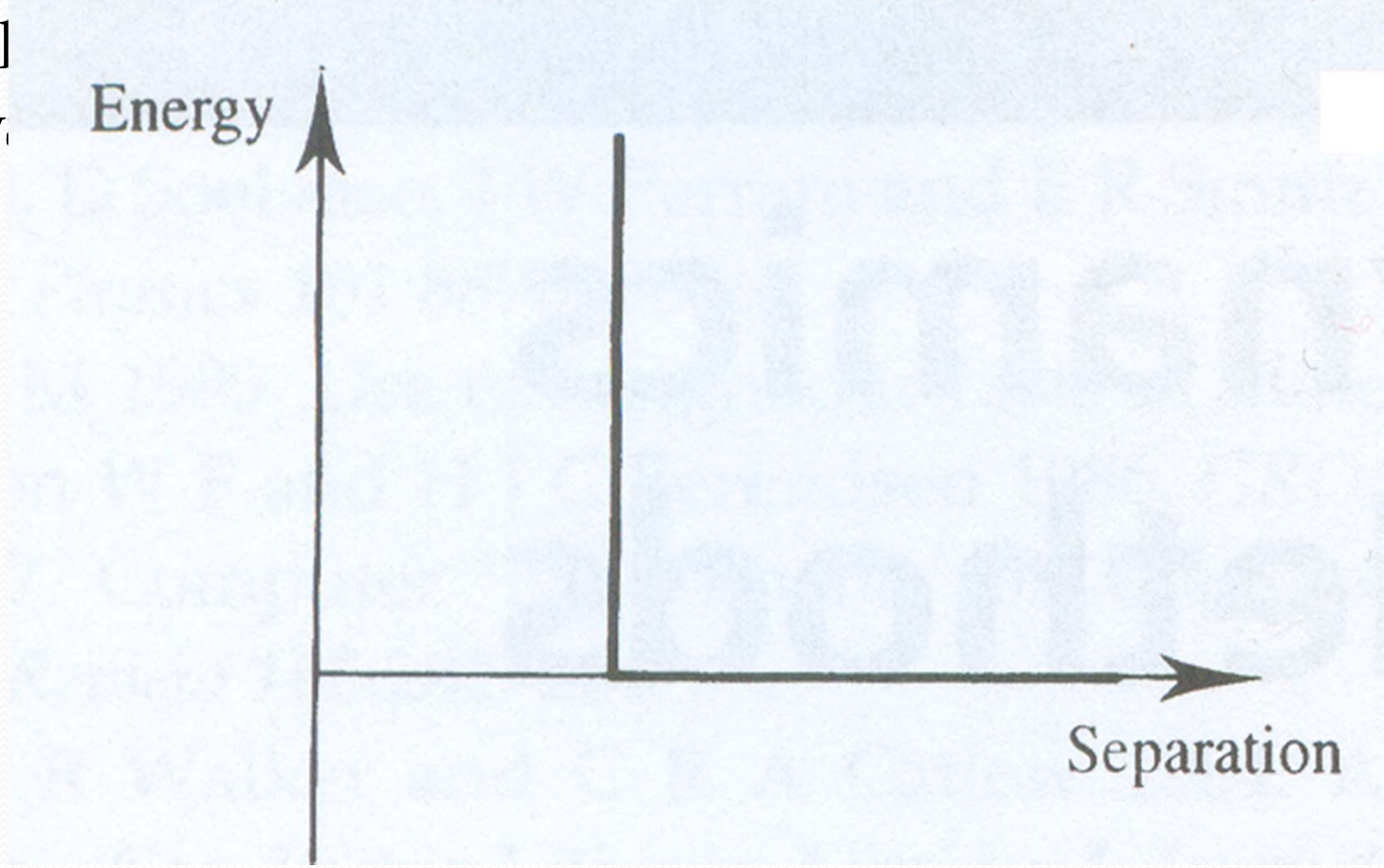


Potential Energy bewteen two charged particles



Collision Model for Molecular Dynamics

- Tl
  w
  -
  -



The steps involved in the hard-sphere calculation are as follows:

1. Identify the next pair of spheres to collide and calculate when the collision will occur.
2. Calculate the positions of all the spheres at the collision time.
3. Determine the new velocities of the two colliding spheres after the collision.
4. Repeat from 1 until finished.

The new velocities of the colliding spheres are calculated by applying the principle of conservation of linear momentum.

Conservation Laws

$$\frac{1}{2}m_1v_1^2+\frac{1}{2}m_2v_2^2=\frac{1}{2}m_1v_1'^2+\frac{1}{2}m_2v_2'^2$$

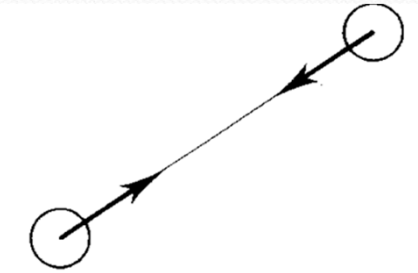
$$m_1v_1+m_2v_2=m_1v_1'+m_2v_2'$$

Velocities after collision

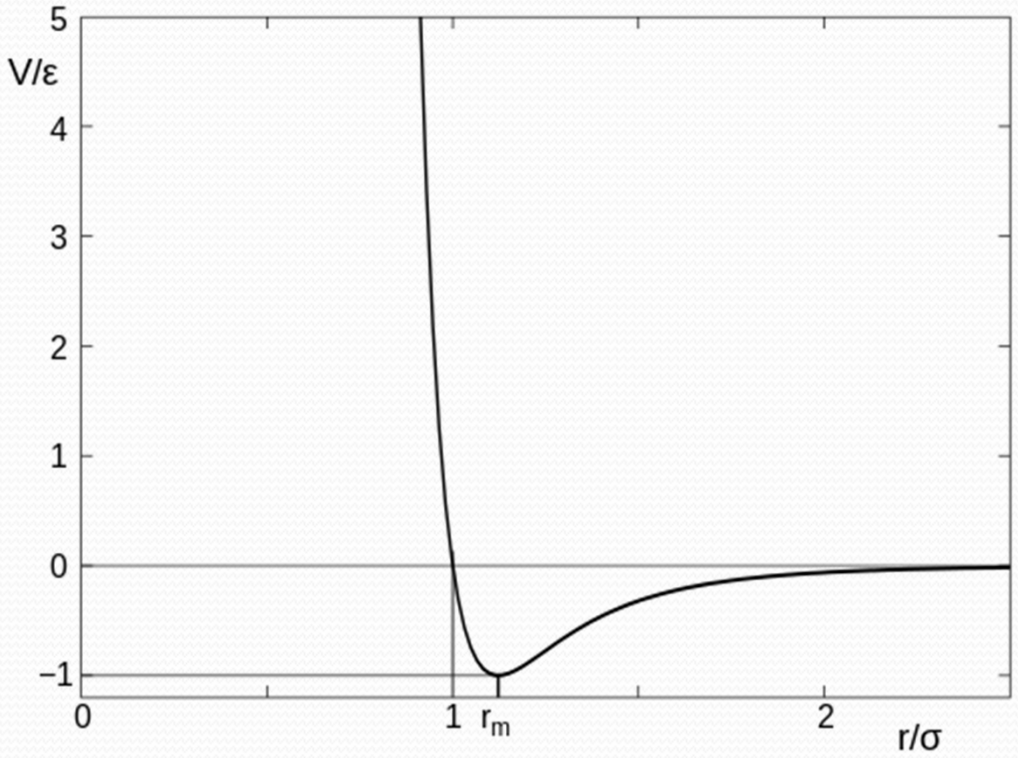
$$v_1'=\frac{(m_1-m_2)v_1+2m_2v_2}{m_1+m_2}$$

$$v_2'=\frac{(m_2-m_1)v_2+2m_1v_1}{m_1+m_2}$$

Lennard Jones Potential



$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] = \varepsilon\left[\left(\frac{r_m}{r}\right)^{12} - 2\left(\frac{r_m}{r}\right)^{6}\right],$$



$$\begin{aligned} F(r) &= -V'(r) \\ &= -\epsilon\left[-\frac{12}{r_m}\left(\frac{r_m}{r}\right)^{13} + \frac{12}{r_m}\left(\frac{r_m}{r}\right)^{7}\right] \\ &= \frac{12\epsilon}{r_m}\left[\left(\frac{r_m}{r}\right)^{13} - \left(\frac{r_m}{r}\right)^{7}\right] \end{aligned}$$

$$F_x = F(r) * \frac{x}{\sqrt{x^2 + y^2 + z^2}}$$

$$F_y = F(r) * \frac{y}{\sqrt{x^2 + y^2 + z^2}}$$

$$F_z = F(r) * \frac{z}{\sqrt{x^2 + y^2 + z^2}}$$

Forces between two molecules from Lennard Jones Potential

- $U_{ij} = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$
- $F_{from\ i\ to\ j} = F_{ij} = -\frac{\partial}{\partial r} U\,\hat{r} =$

$$4\epsilon\left(\frac{12}{\sigma}\left(\frac{\sigma}{r_{ij}}\right)^{13} - \frac{6}{\sigma}\left(\frac{\sigma}{r_{ij}}\right)^{7}\right)\widehat{r_{ij}}$$

- $r_{ij} \equiv \vec{r_j}(t) - \vec{r_i}(t)$

Parameters for water

- If taking two water molecules as two spheres

$$\sigma = 0.32 \times 10^{-9}\,\mathrm{m}$$
$$\epsilon = 1.08 \times 10^{-21}\,\mathrm{J}$$

- As for the other terms such as hydrogen bond, there will be a very long story. So the discussion of other forces are left for the advanced topics.

Simulation with Molecular Dynamics

- Boundary Condition: Collision on the boundaries
- Collision between particles
- Solving a system of differential equation for multiple particles

System of 2nd Order ODE

- Problem: $\frac{d^2}{dt^2}\, x_i(t) = \frac{\sum_j F_{ij}\left(x_j, x_j', t\right)}{m_i}$

$$x_i(0) = x_{i0}\,, \qquad x_i'(0) = v_{i0}$$

- Change of variables

$$set: \quad \frac{d}{dt} x_i(t) = v_i(t)\,;$$

$$\frac{d^2}{dt^2} x_i(t) = \frac{d}{dt} v_i(t) = \frac{\sum_j F_{ij}\left(x_j, x_j', t\right)}{m_i}$$

$$x_i(0) = x_0, \qquad v_i(0) = v_0$$

Verlet Algorithm

- Using simpler method to achieve higher order Taylor's method

- $\vec{r}(t+\Delta t) = \vec{\mathrm{r}}(t) + \Delta t \frac{d}{dt}\vec{\mathrm{r}}(t) + \frac{\Delta t^2}{2!}\frac{d^2}{dt^2}\vec{r}(t) + \frac{\Delta t^3}{3!}\frac{d^3}{dt^3}\vec{r}(t) + \cdots$
- $\vec{r}(t-\Delta t) = \vec{\mathrm{r}}(t) - \Delta t \frac{d}{dt}\vec{\mathrm{r}}(t) + \frac{\Delta t^2}{2!}\frac{d^2}{dt^2}\vec{r}(t) - \frac{\Delta t^3}{3!}\frac{d^3}{dt^3}\vec{r}(t) + \ldots$

- Verlet Algorithm
-

$$\vec{r}(t+\Delta t) \approx 2 * \vec{r}(t) - \vec{r}(t-\Delta t) + \Delta t^2 * \frac{F(\vec{r},\vec{v},t)}{m};$$

Verlet Algorithm

- $\vec{r}(t+\Delta t) = \vec{\mathrm{r}}(t) + \Delta t \frac{d}{dt}\vec{\mathrm{r}}(t) + \frac{\Delta t^2}{2!}\frac{d^2}{dt^2}\vec{r}(t) + \frac{\Delta t^3}{3!}\frac{d^3}{dt^3}\vec{r}(t) + \cdots$
- $\vec{r}(t-\Delta t) = \vec{\mathrm{r}}(t) - \Delta t \frac{d}{dt}\vec{\mathrm{r}}(t) + \frac{\Delta t^2}{2!}\frac{d^2}{dt^2}\vec{r}(t) - \frac{\Delta t^3}{3!}\frac{d^3}{dt^3}\vec{r}(t) + \ldots$

- Verlet Algorithm
-

$$\vec{r}(t+\Delta t) = 2 * \vec{r}(t) - \vec{r}(t-\Delta t) + \Delta t^2 * \frac{F(\vec{r},\vec{v},t)}{m};$$

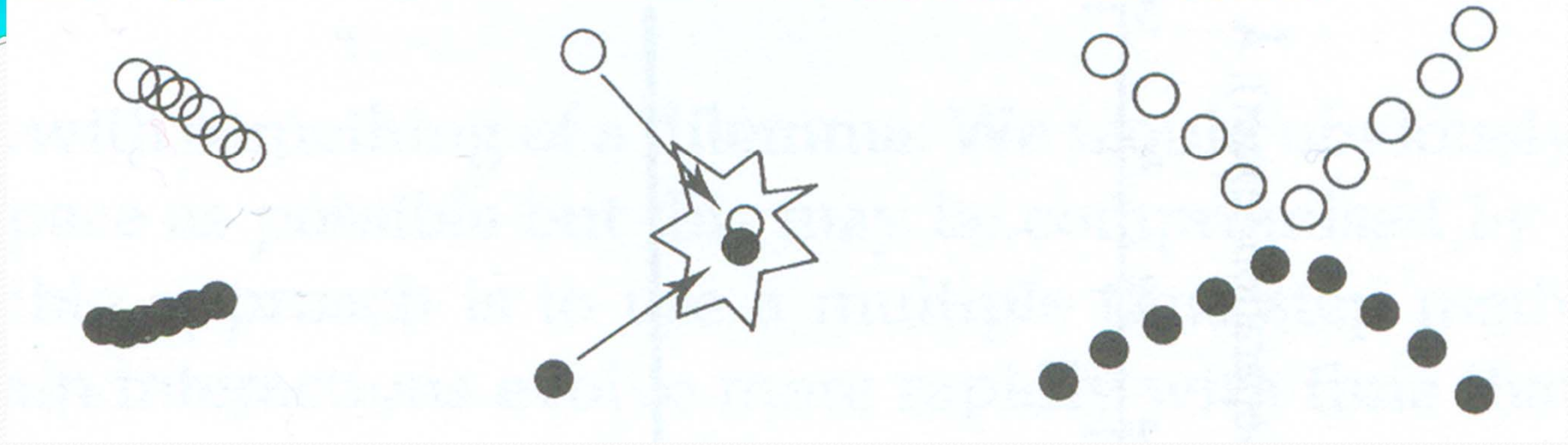
$$\vec{v}(t) = \frac{\vec{r}(t+\Delta t) - \vec{r}(t-\Delta t)}{2\Delta t}$$

Choosing the Time Step

- There are no hard and fast rules for calculating the most appropriate time step to use in a molecular dynamics simulation;

too small : it takes much longer time to reach the equilibrium state.

too large and instabilities may arise in the integration algorithm due to high energy overlaps between atoms. Such instabilities would certainly lead to a violation of energy and linear momentum conservation and could result in a program failure due to numerical overflow.



small time step

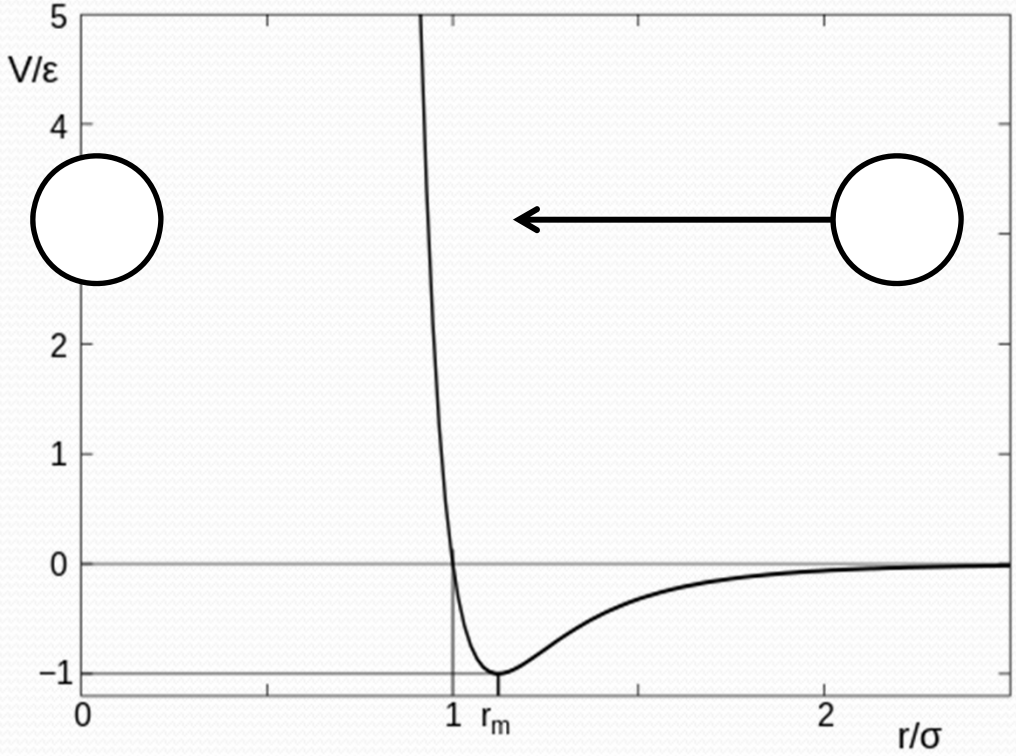
large time step

appropriate time step

With a very small time step (left) phase space is covered very slowly; a large time step (middle) gives instabilities. With an appropriate time step (right) phase space is covered efficiently and collisions occur smoothly.

Guide Line for choosing time steps

- At least 10~1000 steps between L-J potential dip



$$V_{rms} = \sqrt{\frac{3kT}{M}} \sim 10^3 m/s$$

$$\sigma \sim 10^{-10}\ m$$

$$\Delta t \sim 0.1 * \frac{\sigma}{V_{rms}} \sim 10^{-14}\ sec$$

The different types of motion present in various systems together with suggested time steps.

System	Types of motion present	Suggested time step (*s*)
Atoms	Translation	10^{-14} (10fs)
Rigid molecules	Translation, rotation	5×10^{-15}
Flexible molecules, rigid bonds	Translation, rotation, torsion	2×10^{-15}
Flexible molecules, flexible bonds	Translation, rotation, torsion, vibration	10^{-15} or 5×10^{-16}

Setting up the system for simulation

1. Set a total number of molecules : N
2. Set the boundary of the system : Lx, Ly, Lz
3. Give each molecular a specific location but randomly distributed within the boundaries.
   - Don't overlap any two of them overlap
4. Give each molecular a velocity
   - Constant speed but toward different direction for each molecule
   - $\frac{1}{2}m|\bar{v}|^2 = \frac{3}{2}kT$
5. Now you have $\vec{r}_i(0)\ and\ \vec{v}_i(0)\ and\ F_{ij}(0)$
   - Use Euler Method or higher order Tylor's Method to find $\vec{r}_i(\Delta t)$
   - Then proceed to Verlet's Algorithm using $\vec{r}_i(0)\ and\ \vec{r}_i(\Delta t)$ for following location estimation

Setting up the system for simulation

5. Now you have $\vec{r}_i(0)$ *and* $\vec{v}_i(0)$ *and* $F_{ij}(0)$

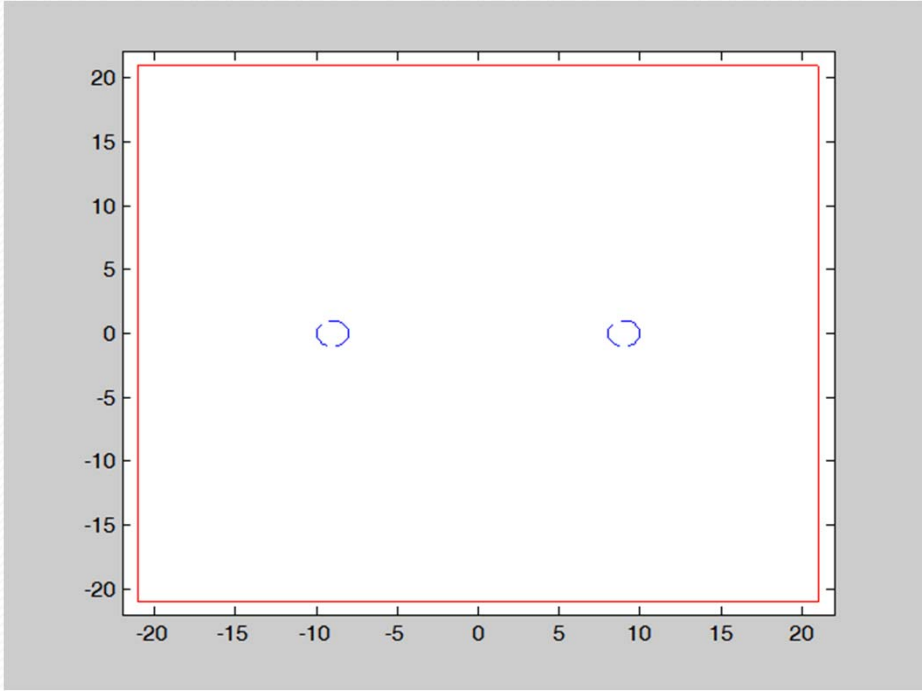
6. Use Euler Method or higher order Tylor's Method to find $\vec{r}_i(\Delta t)$

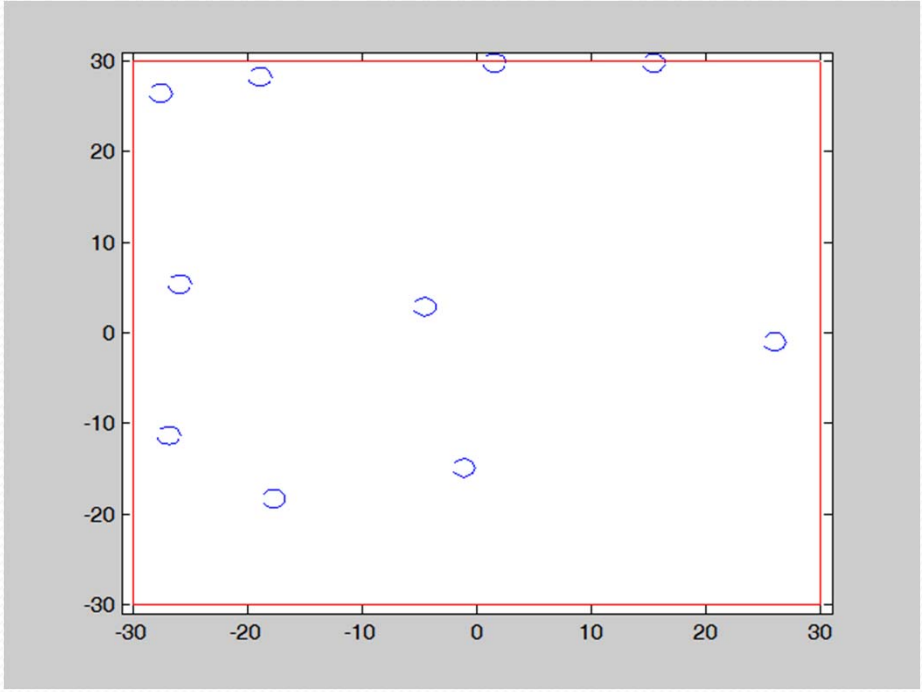
7. Then proceed to Verlet's Algorithm using $\vec{r}_i(0)$ *and* $\vec{r}_i(\Delta t)$ for following location estimation

8. Calculate Thermal Dynamic Properties
   - Total Energy → Temperature
   - Average Pressure
     (from the impact when a particle hits a wall)
   - Velocity Distribution

Practice

- Write a program to create two particle collision then proceed to multiple particles





Summary

Simulation of a classical dynamic system

- $\frac{d^2}{dt^2}\,\vec{r}_i(t) = \left(F_{ext}^{(i)}(t) + F_{int}^{(i)}(t)\right)/m_i$

- For the internal forces within a system, Newton's Third Law must apply.

- $Drag\ Force: F_{drag} \propto -|v|^n \hat{v}$
- Gravitational Force, Electrostatic Force, ….
- Lennard-Jones Forces

$$F(r) = -\left(\frac{d}{dx}\hat{\imath} + \frac{d}{dy}\hat{\jmath} + \frac{d}{dz}\hat{k}\right)\left(4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)\right)$$