MD-Assignment 2

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1 Assignment

Implement the force-field equations derived in class to obtain a box of particles bouncing off walls and off each other. We can think of the normalized x-direction and y-direction as (ξ,ν). Determining newton second law motion equations can be seen in the following steps:

$$\vec{F} = -\nabla \cdot \phi\left(\xi, \nu\right) \tag{1}$$

$$-\nabla = \begin{bmatrix} -\frac{\partial}{\partial \xi} \\ -\frac{\partial}{\partial \nu} \end{bmatrix} \tag{2}$$

$$\phi\left(\xi, \nu\right) = \phi\left(\xi\right) + \phi\left(l - \xi\right) + \phi\left(\nu\right) + \phi\left(l - \nu\right) \tag{3}$$

1.1 Wall-Potentials:

$$\phi\left(\xi\right) = \left[\left(\frac{1}{\xi}\right)^{12} - 2\left(\frac{1}{\xi}\right)^{6}\right] \tag{4}$$

$$\phi\left(l - \xi\right) = \left[\left(\frac{1}{l - \xi}\right)^{12} - 2\left(\frac{1}{l - \xi}\right)^{6}\right] \tag{5}$$

$$\phi\left(\nu\right) = \left[\left(\frac{1}{\nu}\right)^{12} - 2\left(\frac{1}{\nu}\right)^{6}\right] \tag{6}$$

$$\phi\left(l - \nu\right) = \left[\left(\frac{1}{l - \nu}\right)^{12} - 2\left(\frac{1}{l - \nu}\right)^{6}\right] \tag{7}$$

1.2 Wall-Forces:

1.2.1 F_x :

Derivative of first potential term

$$-\frac{\partial}{\partial \xi} \cdot \phi\left(\xi\right) = -\frac{\partial}{\partial \xi} \cdot \left\{\left(\frac{1}{\xi}\right)^{12} - 2\left(\frac{1}{\xi}\right)^{6}\right\} \tag{8}$$

$$= -\left\{-12\left(\frac{1}{\xi}\right)^{13} \frac{\partial}{\partial \xi} \cdot \xi + 12\left(\frac{1}{\xi}\right)^{7} \frac{\partial}{\partial \xi} \cdot \xi\right\} \tag{9}$$

$$= 12\left\{\left(\frac{1}{\xi}\right)^{13} - \left(\frac{1}{\xi}\right)^{7}\right\} \tag{10}$$

$$\boxed{-\frac{\partial\left\{\phi\left(\xi\right)\right\}}{\partial\xi} = 12\left[\left(\frac{1}{\xi}\right)^{13} - \left(\frac{1}{\xi}\right)^{7}\right]}$$

Derivative of second potential term

$$-\frac{\partial}{\partial\xi}\cdot\phi\left(l-\xi\right) = -\frac{\partial}{\partial\xi}\cdot\left\{\left(\frac{1}{l-\xi}\right)^{12} - 2\left(\frac{1}{l-\xi}\right)^{6}\right\} \tag{11}$$

$$= -\left\{-12\left(\frac{1}{l-\xi}\right)^{13}\frac{\partial}{\partial\xi}\cdot\left(l-\xi\right) + 12\left(\frac{1}{l-\xi}\right)^{7}\frac{\partial}{\partial\xi}\cdot\left(l-\xi\right)\right\} \tag{12}$$

$$= -\left\{12\left(\frac{1}{l-\xi}\right)^{13} - 12\left(\frac{1}{l-\xi}\right)^{7}\right\} \tag{13}$$

$$= -12\left\{\left(\frac{1}{l-\xi}\right)^{13} - \left(\frac{1}{l-\xi}\right)^{7}\right\} \tag{14}$$

$$\boxed{-\frac{\partial\left\{\phi\left(l-\xi\right)\right\}}{\partial\xi} = -12\left[\left(\frac{1}{l-\xi}\right)^{13} - \left(\frac{1}{l-\xi}\right)^{7}\right]}$$

Derivative of third potential term

$$\boxed{-\frac{\partial\left\{\phi\left(\nu\right)\right\}}{\partial\xi} = 0}$$

Derivative of fourth potential term

$$\boxed{-\frac{\partial}{\partial\xi}\cdot\phi\left(l-\nu\right) = 0}$$

Therefore

$$\begin{aligned} F_x = \frac{\partial\left\{\phi\left(\xi,\nu\right)\right\}}{\partial\xi} &= \frac{\partial\left\{\phi\left(\xi\right)\right\}}{\partial\xi} + \frac{\partial\left\{\phi\left(l-\xi\right)\right\}}{\partial\xi} + \cancelto{0}{\frac{\partial\left\{\phi\left(\nu\right)\right\}}{\partial\xi}} + \cancelto{0}{\frac{\partial\left\{\phi\left(l-\nu\right)\right\}}{\partial\xi}} \\ &= \boxed{12\left[\left(\frac{1}{\xi}\right)^{13} - \left(\frac{1}{\xi}\right)^{7}\right] + -12\left[\left(\frac{1}{l-\xi}\right)^{13} - \left(\frac{1}{l-\xi}\right)^{7}\right] + 0 + 0} \end{aligned}$$

1.2.2 F_y :

$$\begin{aligned} F_y = \frac{\partial\left\{\phi\left(\xi,\nu\right)\right\}}{\partial\nu} &= \cancelto{0}{\frac{\partial\left\{\phi\left(\xi\right)\right\}}{\partial\nu}} + \cancelto{0}{\frac{\partial\left\{\phi\left(l-\xi\right)\right\}}{\partial\nu}} + \frac{\partial\left\{\phi\left(\nu\right)\right\}}{\partial\nu} + \frac{\partial\left\{\phi\left(l-\nu\right)\right\}}{\partial\nu} \\ &= \boxed{0 + 0 + 12\left[\left(\frac{1}{\nu}\right)^{13} - \left(\frac{1}{\nu}\right)^{7}\right] + -12\left[\left(\frac{1}{l-\nu}\right)^{13} - \left(\frac{1}{l-\nu}\right)^{7}\right]} \end{aligned}$$

1.3 Lennard-Jones Potential

$$|\vec{\eta}_i - \vec{\eta}_j| = \theta_{i,j}\left(\xi_i, \nu_i, \xi_j, \nu_j\right) = \sqrt{(\xi_i - \xi_j)^2 + (\nu_i - \nu_j)^2}$$

$$U_{LJ}\left(\theta_{i,j}\right) = \left\{\left(\frac{1}{|\vec{\eta}_i - \vec{\eta}_j|}\right)^{12} - 2\left(\frac{1}{|\vec{\eta}_i - \vec{\eta}_j|}\right)^{6}\right\}$$

$$= \boxed{\left\{\left(\frac{1}{\sqrt{(\xi_i - \xi_j)^2 + (\nu_i - \nu_j)^2}}\right)^{12} - 2\left(\frac{1}{\sqrt{(\xi_i - \xi_j)^2 + (\nu_i - \nu_j)^2}}\right)^{6}\right\}}$$

2 Tasks

- Things to do:
  1. Calculate and display a trace of the particles motion as it is making a reasonable number of collisions with each of the walls.
  2. Calculate the potential and kinetic energies as a function of time (KE(t), PE_Wall(t), PE_LJ(t))
  3. Calculate the total energies as a function of time (KE(t)+PE_Wall(t)+PE_LJ(t))
  4. Show (Total Energy vs. dt)

3 Motion

An example of a single particle in a box only interacting with the walls Figure 1 and Figure 2. Weird stuff

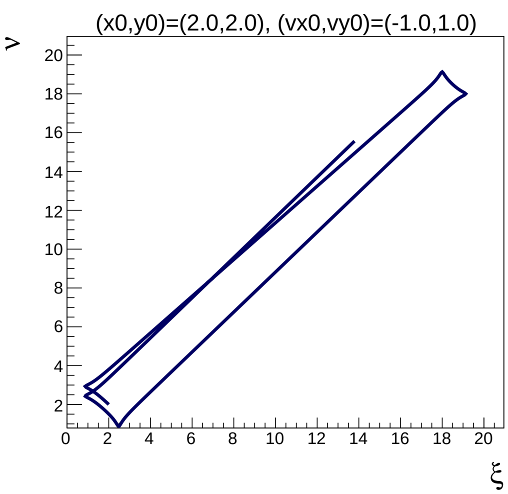

Figure 1: Motion particle trace

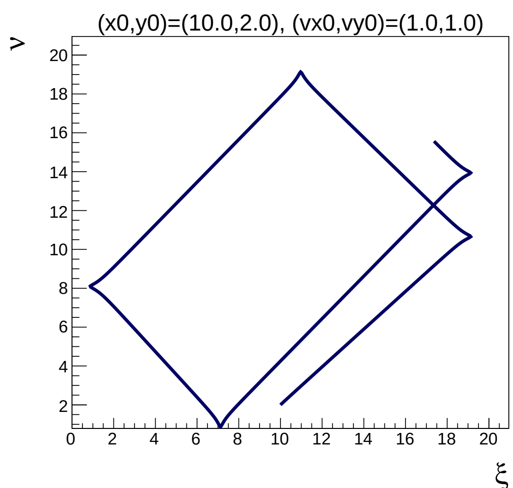

Figure 2: Different initial conditions

happens when I change the initial conditions to $(x_0, y_0) = (5, 5), (vx_0, vy_0) = (2, 3)$ as seen in Figure 3 and Figure 4. It is as though the particle goes through the bottom boundary, which should not happen. Several times before the bottom boundary has demonstrated a force, but at later times the boundary seems to disappear. A look at the force with respect to time and energy will be examined in the following sections.

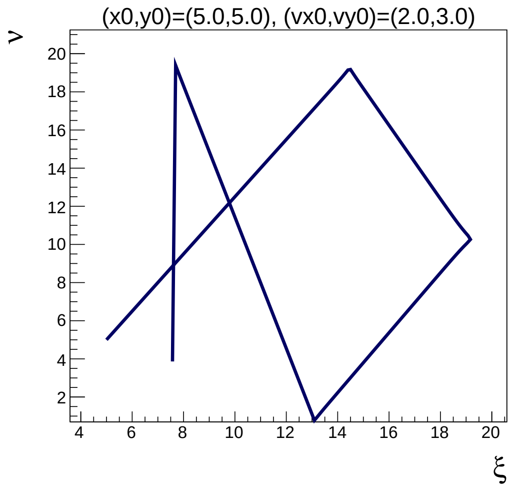

Figure 3: Motion particle trace

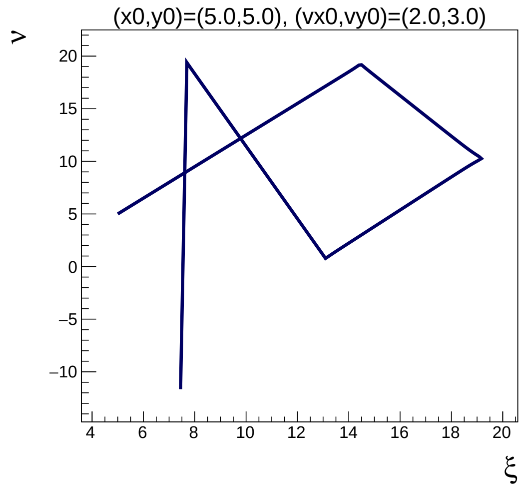

Figure 4: Different initial conditions

4 Force and Energy Analysis

A look at the x (ξ) and y (ν) wall-boundary forces with respect to time.

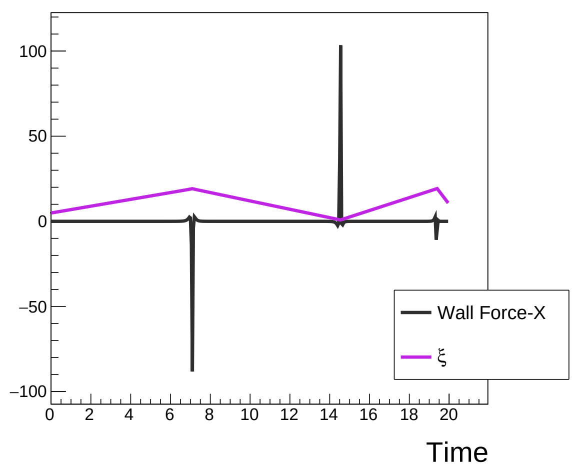

Figure 5: Motion particle trace

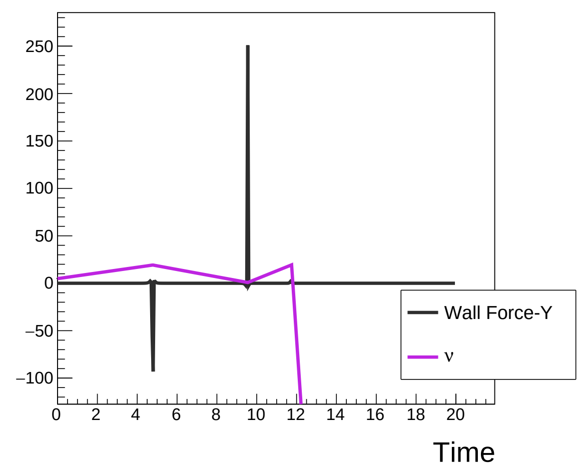

Figure 6: Different initial conditions

4.1 Energy

4.1.1 Kinetic Energy

Kinetic energy shoots off to inf near time of 12.

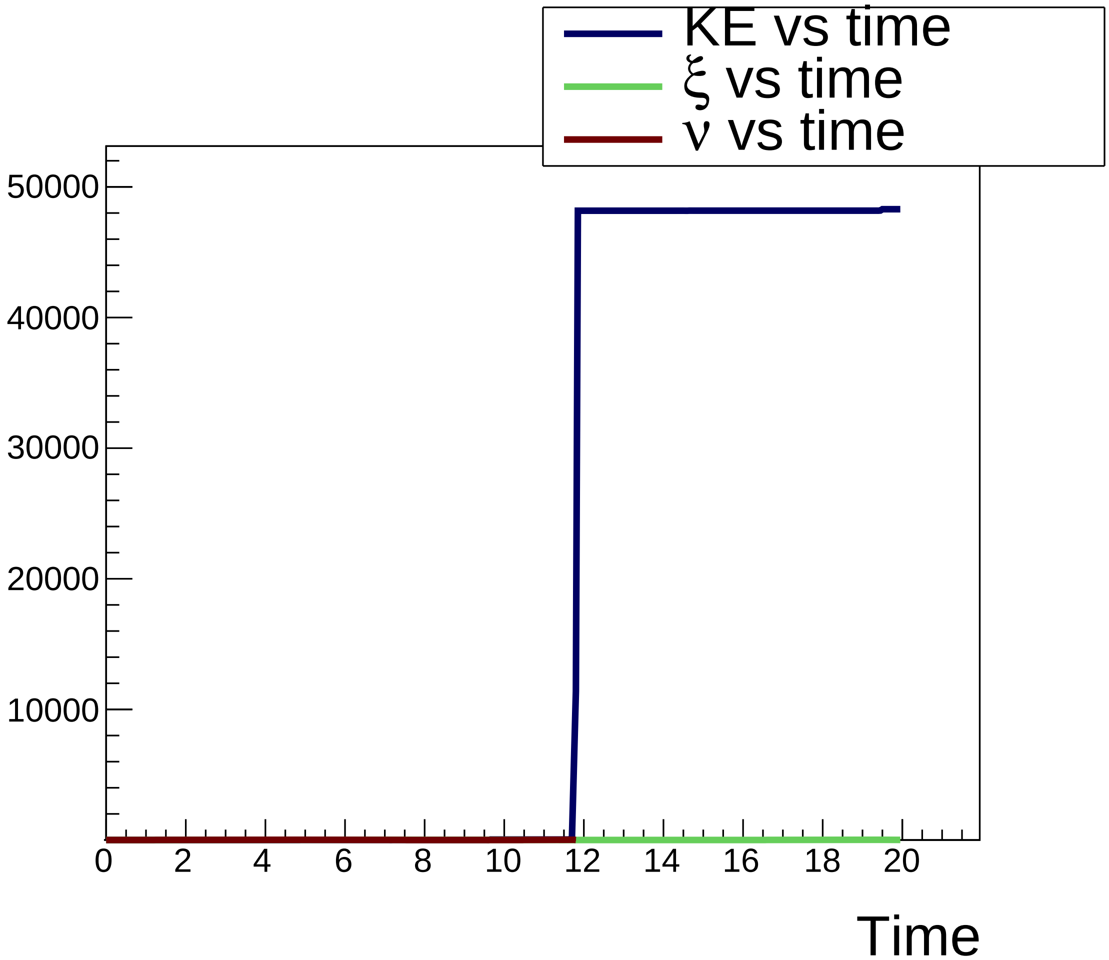

Figure 7: Different initial conditions

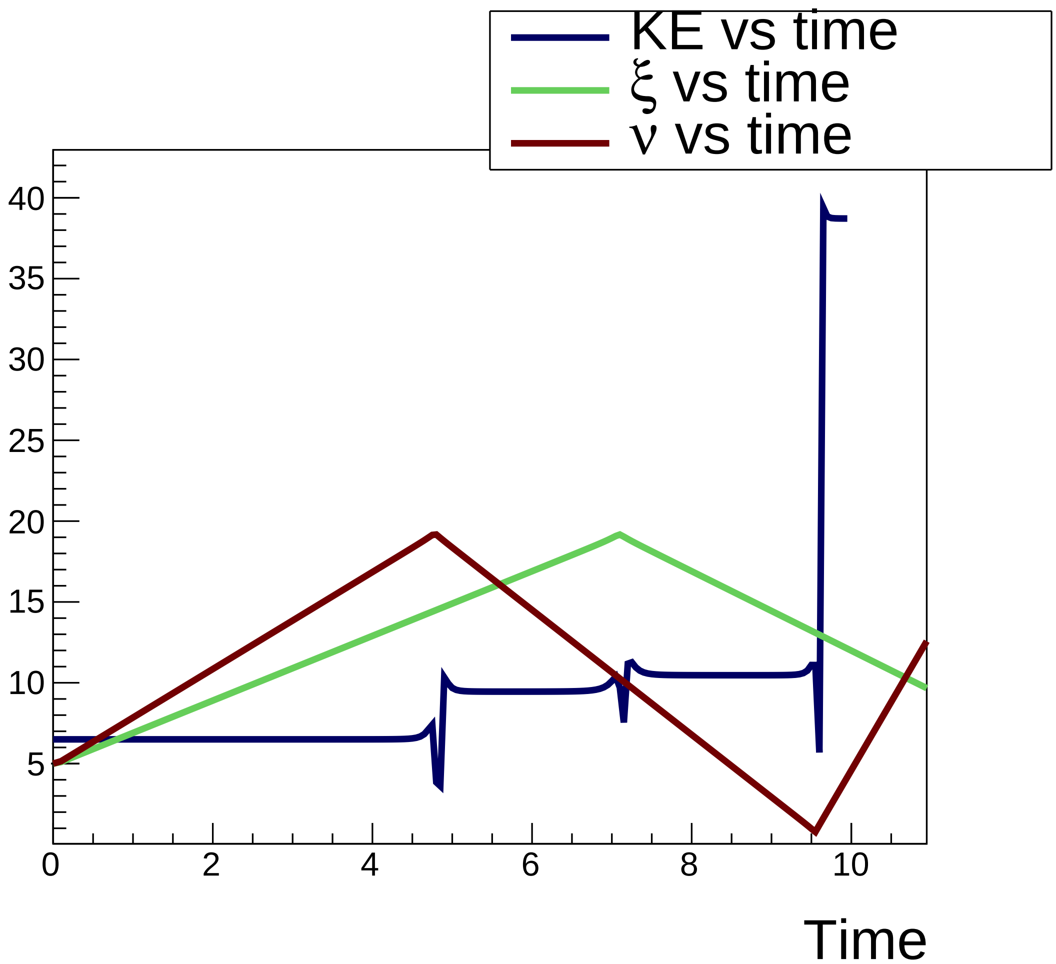

Figure 8: Different initial conditions

4.1.2 Wall-Potential

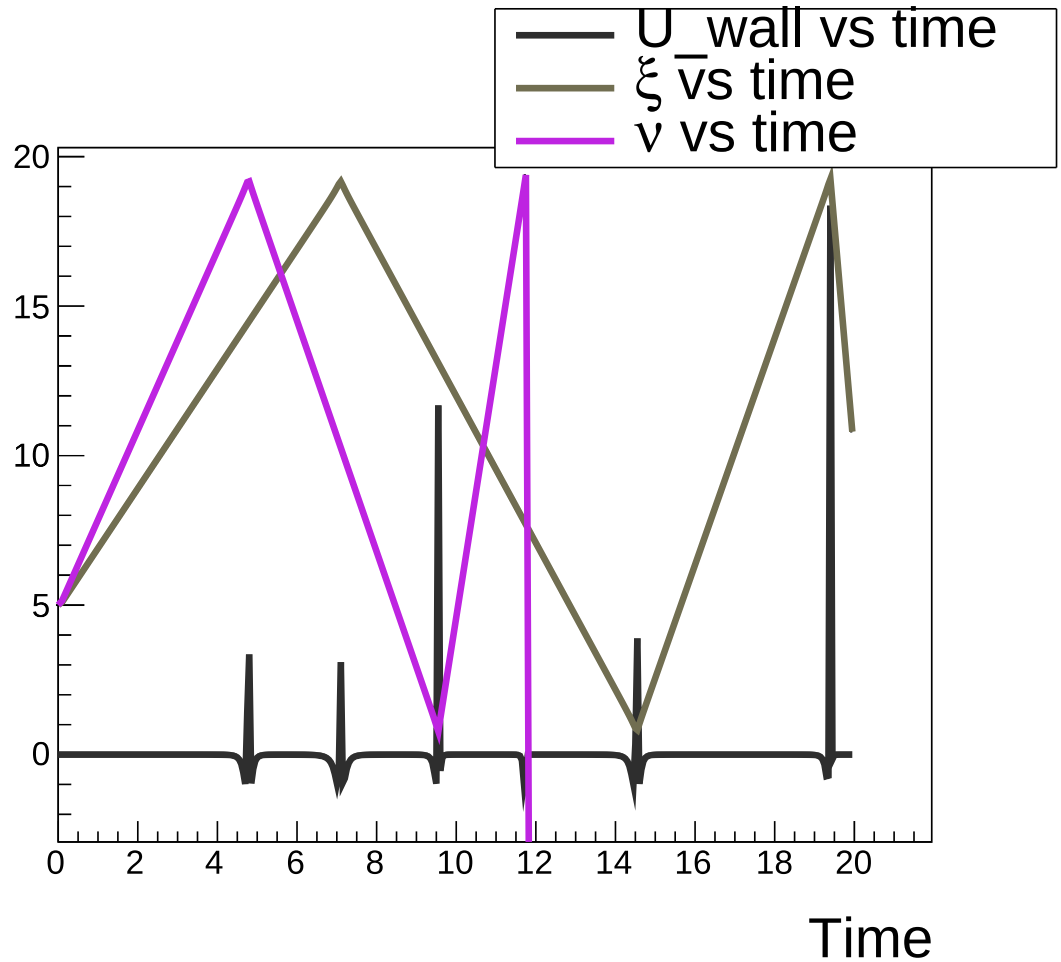

Figure 9: Different initial conditions

4.1.3 Lenard-Jones Potential

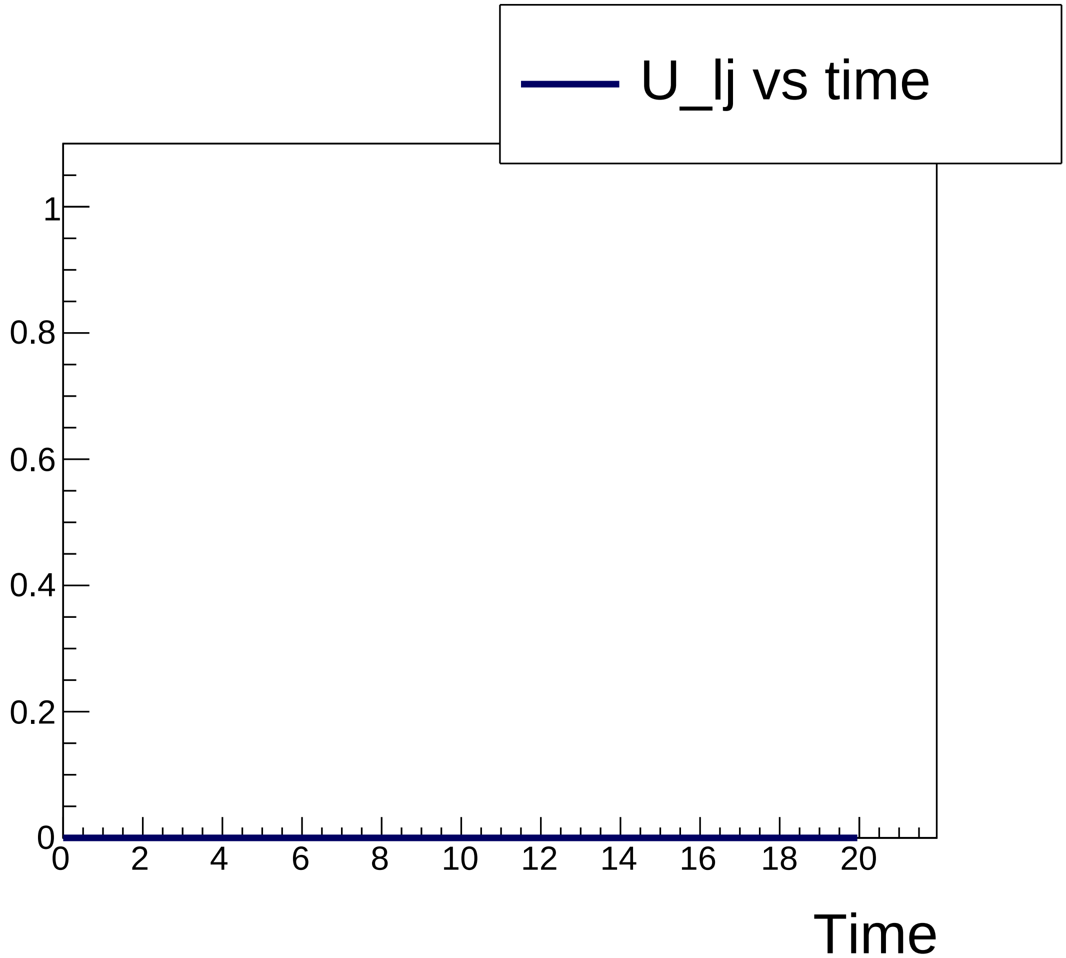

Figure 10: Different initial conditions