MD-Assignment 3

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May 2019

1 Assignment

Generate 10^{10} random Gaussian numbers from two uniformly distributed variables.

1.1 Box-Muller Algorithm

The Box-Muller Algorithm (1 and 2) relies on two numbers (ξ_1 and ξ_2) that are taken from a uniform distribution.

$$\eta_1 = \sqrt{-2\ln(\xi_1)}\cos(2\pi\xi_2) \tag{1}$$

$$\eta_2 = \sqrt{-2\ln(\xi_1)}\sin(2\pi\xi_2) \tag{2}$$

We can then use these two numbers (ξ_1 and ξ_2) to compute a Gaussian distributed value (η_1 or η_2). If we plot the distribution, by creating a histogram, of (1) and (2) we should see a Gaussian distribution. Regardless of the quality of random number generator, the distribution should look Gaussian, a study of the HMO's response will provide a better view of the pseudo-random number generator's quality.

$$g(\eta_1,\eta_2) = -\frac{1}{2\pi}e^{-\frac{\eta_1^2}{2}}e^{-\frac{\eta_2^2}{2}} \tag{3}$$

$$= -\frac{1}{2\pi}e^{-\left(\frac{\eta_1^2+\eta_2^2}{2}\right)} \tag{4}$$

$$= -\frac{1}{2\pi}e^{-\frac{1}{2}\left(\eta_1^2+\eta_2^2\right)} \tag{5}$$

$$= -\frac{1}{2\pi}e^{-\frac{1}{2}\left(-2\ln(\xi_1)\cos^2(2\pi\xi_2)+-2\ln(\xi_1)\sin^2(2\pi\xi_2)\right)} \tag{6}$$

$$= -\frac{1}{2\pi}e^{\ln\xi_1\left[\cos^2(2\pi\xi_2)+\sin^2(2\pi\xi_2)\right]} \tag{7}$$

$$= -\frac{1}{2\pi}e^{\ln\xi_1} \tag{8}$$

$$= -\frac{1}{2\pi}\xi_1 \tag{9}$$

What does (9) actually mean? I do not know. But in the meantime, lets take a look at the produced data for the ξ_1, ξ_2, ν_1, and ν_2 distributions (Figure 1 and 2). Figures 1 and 2) demonstrate n=10^4; meanwhile, n=10^8 are demonstrated in Figures (3 and 4). Generating 10^8 uniformally distributed samples (Figures 3 and 4) took approximately ten hours, even with the sampling within four sigma's or four standard deviations method.

We then use our choice of η_1 or η_2 to determine $\beta^{n+1} = \sqrt{2\alpha kT}\eta$.

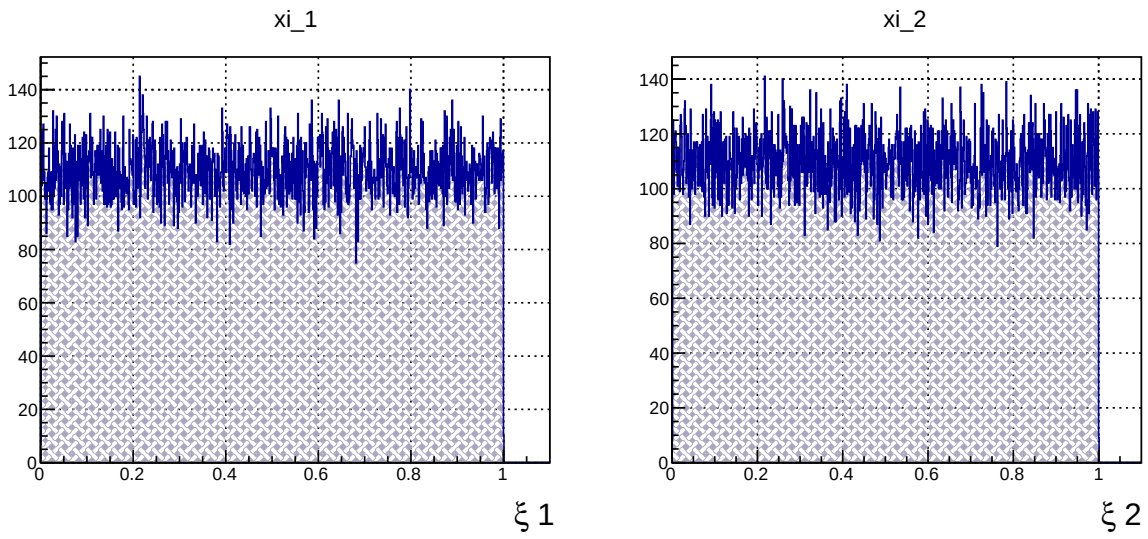

Figure 1: Uniform ξ_1 and ξ_2 Distribution with n=10^4

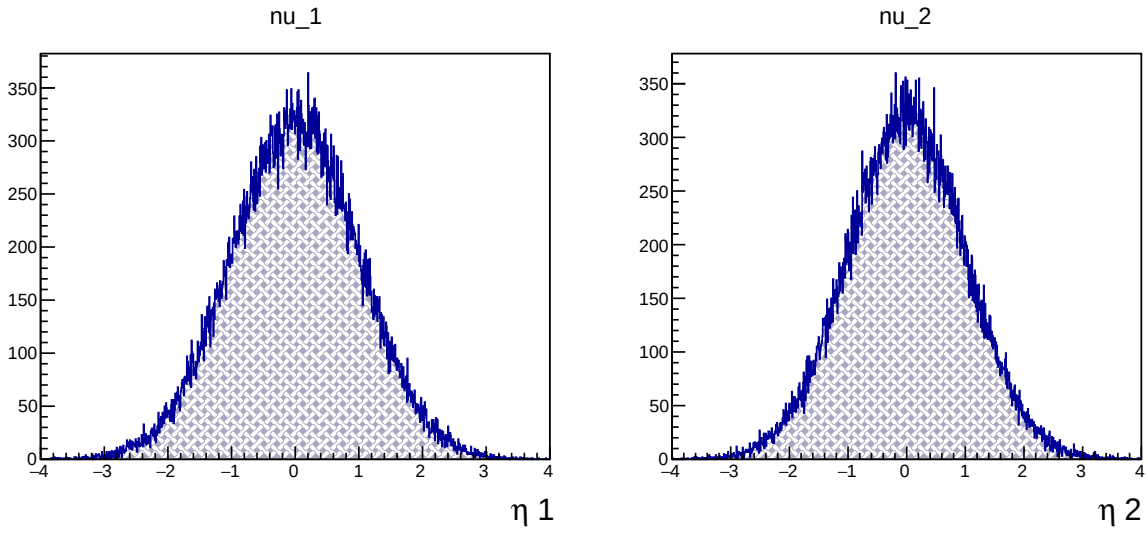

Figure 2: Gauss η_1 and η_2 Distribution with n=10^4

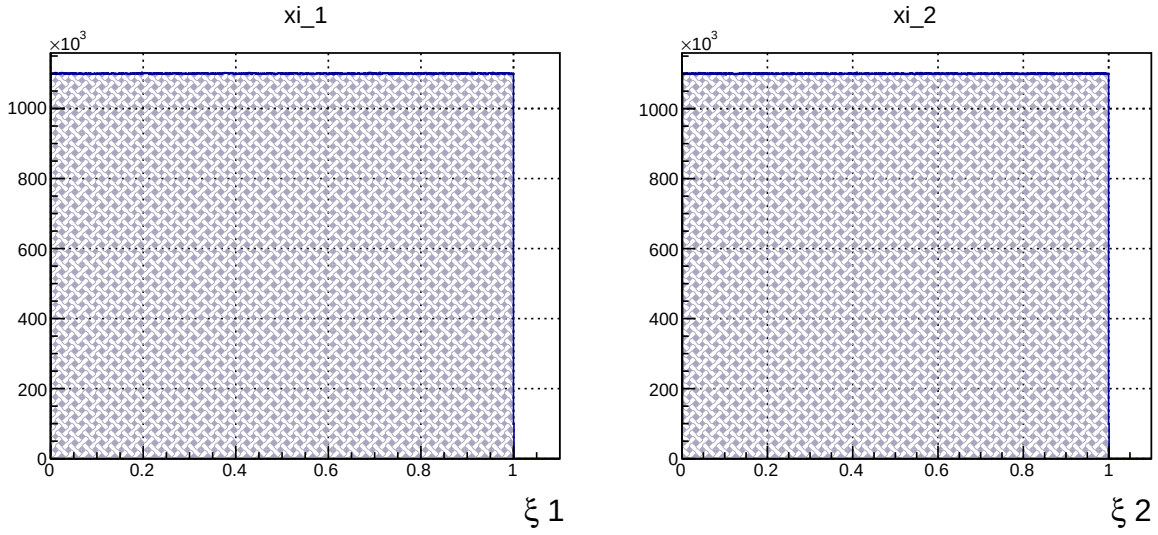

Figure 3: Uniform ξ_1 and ξ_2 Distribution with n=10^8

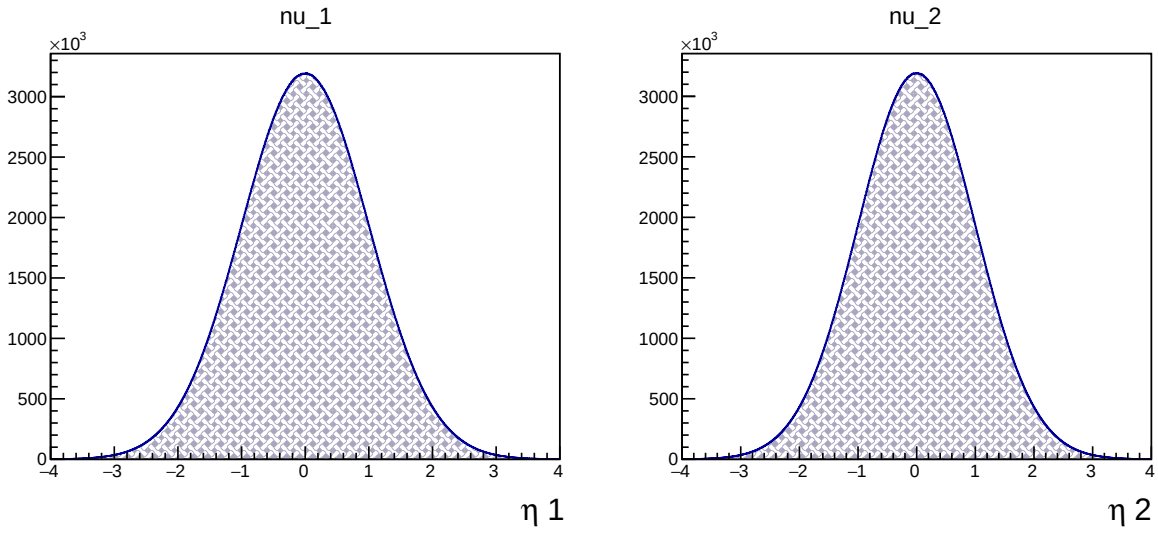

Figure 4: Gauss η_1 and η_2 Distribution with n=10^8

1.2 Modeling a HMO with Noise

We shall now try to model a harmonic oscillator (HMO) with friction and stochastic noise. We start with the Langevin equation, which we will discretize in the following steps.

$$m\ddot{r} + \alpha\dot{r} = f + \beta$$

Let us rewrite the Langevin equation in a more convenient fashion.

$$m\ddot{r} = f + \beta - \alpha\dot{r}$$

Now we begin to discretize by taking the integral.

$$m\int_{t_n}^{t_{n+1}} \dot{v}dt = \int_{t_n}^{t_{n+1}} f dt + \int_{t_n}^{t_{n+1}} \beta(\xi)dt - \alpha\int_{t_n}^{t_{n+1}} \dot{r}dt \tag{10}$$

Our goal is to determine $(r^{n+1} - r^n)$ and $(v^{n-1} - v^n)$. In order to do this we utilize the trapezoidal approximation shown below (11 and 12), let us define some things that will help us find $(r^{n+1} - r^n)$ and $(v^{n-1} - v^n)$.

$$\int_{t_n}^{t_{n+1}} \dot{r}dt \approx \frac{dt}{2}\left(v^{n+1} + v^n\right) \qquad \int_{t_n}^{t_{n+1}} \dot{r}dt \Rightarrow r^{n+1} - r^n \tag{11}$$

$$\int_{t_n}^{t_{n+1}} f dt \approx \frac{dt}{2}\left(f^{n+1} + f^n\right) \tag{12}$$

Let us write the langevin equation (10) in discrete form.

$$m\left[v^{n+1} - v^n\right] = \int_{t_n}^{t_{n+1}} f dt + \beta_{n+1} - \alpha\left[r^{n+1} - r^n\right] \tag{13}$$

$$\left[v^{n+1} - v^n\right] = \frac{1}{m}\left[\int_{t_n}^{t_{n+1}} f dt + \beta_{n+1} - \alpha\left[r^{n+1} - r^n\right]\right] \tag{14}$$

To find $(r^{n+1} - r^n)$ we remember 11 so basically:

$$\begin{aligned} r^{n+1} - r^n &\approx \frac{dt}{2}\left(v^{n+1} + v^n\right) \\ &\approx \frac{dt}{2}\left(v^{n+1} - v^n + 2v^n\right) \end{aligned}$$

We can then replace $v^{n+1} - v^n$ with our equation 14.

$$r^{n+1} - r^n \approx \frac{dt}{2}\left(\frac{1}{m}\left[\int_{t_n}^{t_{n+1}} f dt + \beta_{n+1} - \alpha\left[r^{n+1} - r^n\right]\right] + 2v^n\right) \tag{15}$$

Do more simplifications to the equation above and define $b = \frac{1}{1+\frac{\alpha dt}{2m}}$. We end up with equation 16.

$$\boxed{r^{n+1} = r^n + b\left[dtv^n + \frac{dt^2}{2m}f^n + \frac{dt}{2m}\beta^{n+1}\right]} \tag{16}$$

Similarly to get $v^{n+1} - v^n$ we go back to the Langevin equation (10) and write it discretely.

$$m\left(v^{n+1} - v^n\right) = \int_{t_n}^{t_{n+1}} f dt + \beta^{n+1} - \alpha\left(r^{n+1} - r^n\right)$$
$$m\left(v^{n+1} - v^n\right) = \frac{dt}{2}\left(f^{n+1} - f^n\right) + \beta^{n+1} - \alpha b\left[dtv^n + \frac{dt^2}{2m}f^n + \frac{dt}{2m}\beta^{n+1}\right]$$

yada yada...

Then we do more simplification and arrive at equation 17.

$$\boxed{v^{n+1} = av^n + \frac{dt}{2m}\left(f^{n+1} + af^n\right) + \frac{b}{m}\beta^{n+1}} \tag{17}$$

We can do further simplifications and rewrite (r^{n+1}) and (v^{n-1}) with the half step velocity, which I have not formally derive myself. But here's the algorithm produced by Dr. Niels Jensen.

$$\begin{aligned}
u^{n+1} &= \sqrt{b}\left[v^n + \frac{dt}{2m}f^n + \frac{1}{2m}\beta^{n+1}\right] \\
r^{n+1} &= r^n + \sqrt{b}dtu^{n+1/2} \\
v^{n+1} &= \frac{a}{\sqrt{b}}u^{n+1/2} + \frac{dt}{2m}f^{n+1} + \frac{1}{2m}\beta^{n+1} \\
\beta^{n+1} &= \sqrt{2\alpha kT}\sigma^{n+1} \\
&= \sqrt{2\alpha kT}\eta
\end{aligned}$$

don't forget that we will be modeling a HMO so:

$$f = -kr^n$$

and

$$\Omega_0 dt = \sqrt{\frac{k}{m}}dt$$

1.2.1 Tasks

1. "Calculate averages (over integer number of periods) for Potential, Kinetic (U,V), and total energies as a function of normalized time-step" - So basically sum both kinetic and potential energies each time step and divide by the total number of time steps at the end, then switch the friction coefficient.

2. visualize displacement r(t) for fun

Simple simulations of a HMO with damping were conducted by solving the discretized Langevin equation. Figures 1.2.1 and 1.2.1 represent averaged energies with 10^3 time steps. Additional time steps did not seem to improve nor change the time averaged energies, Figure 1.2.1

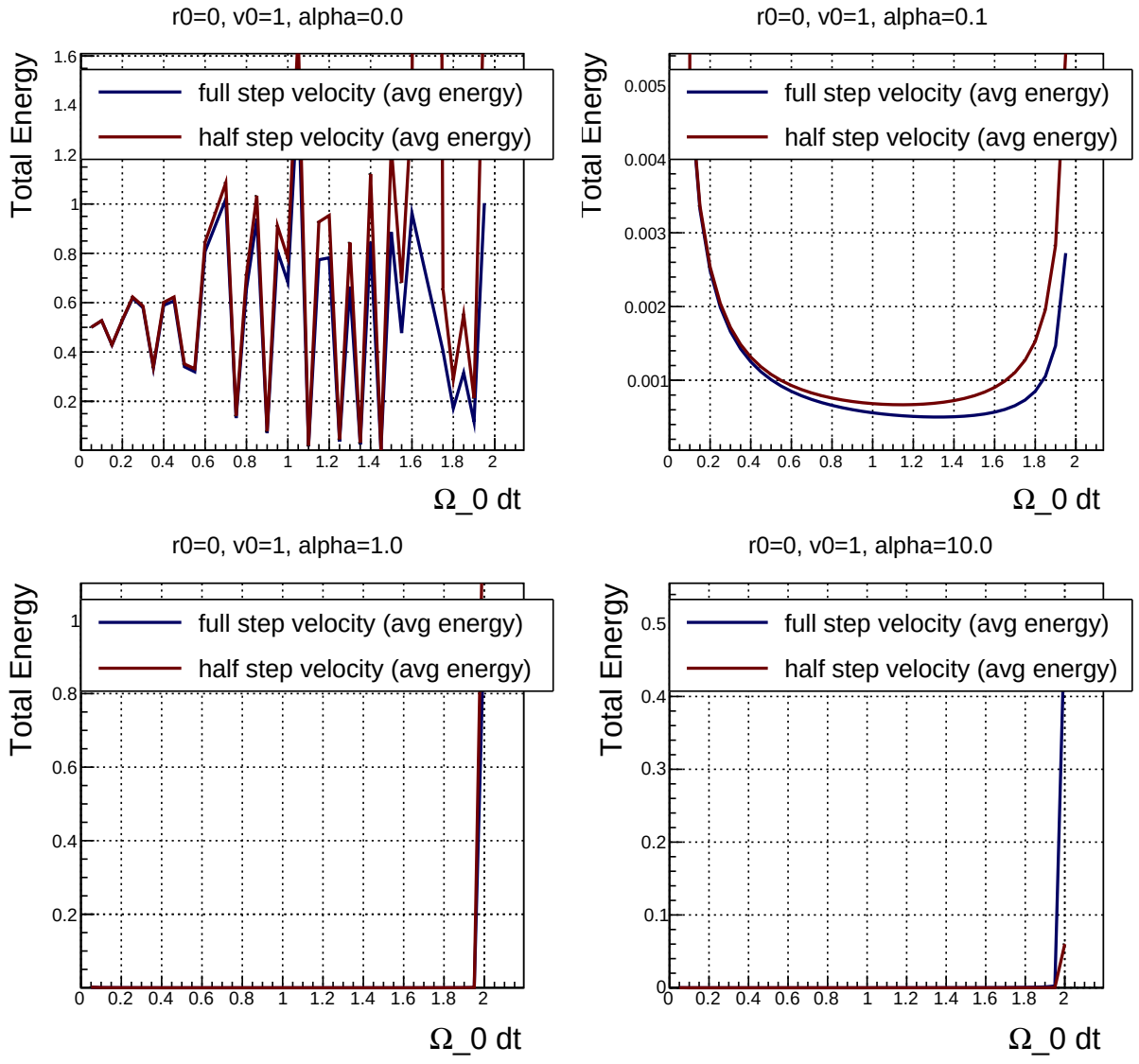

Figure 5: Average total energy (10^3 steps) at various friction coefficients and initial conditions r_0=0 v_0=1

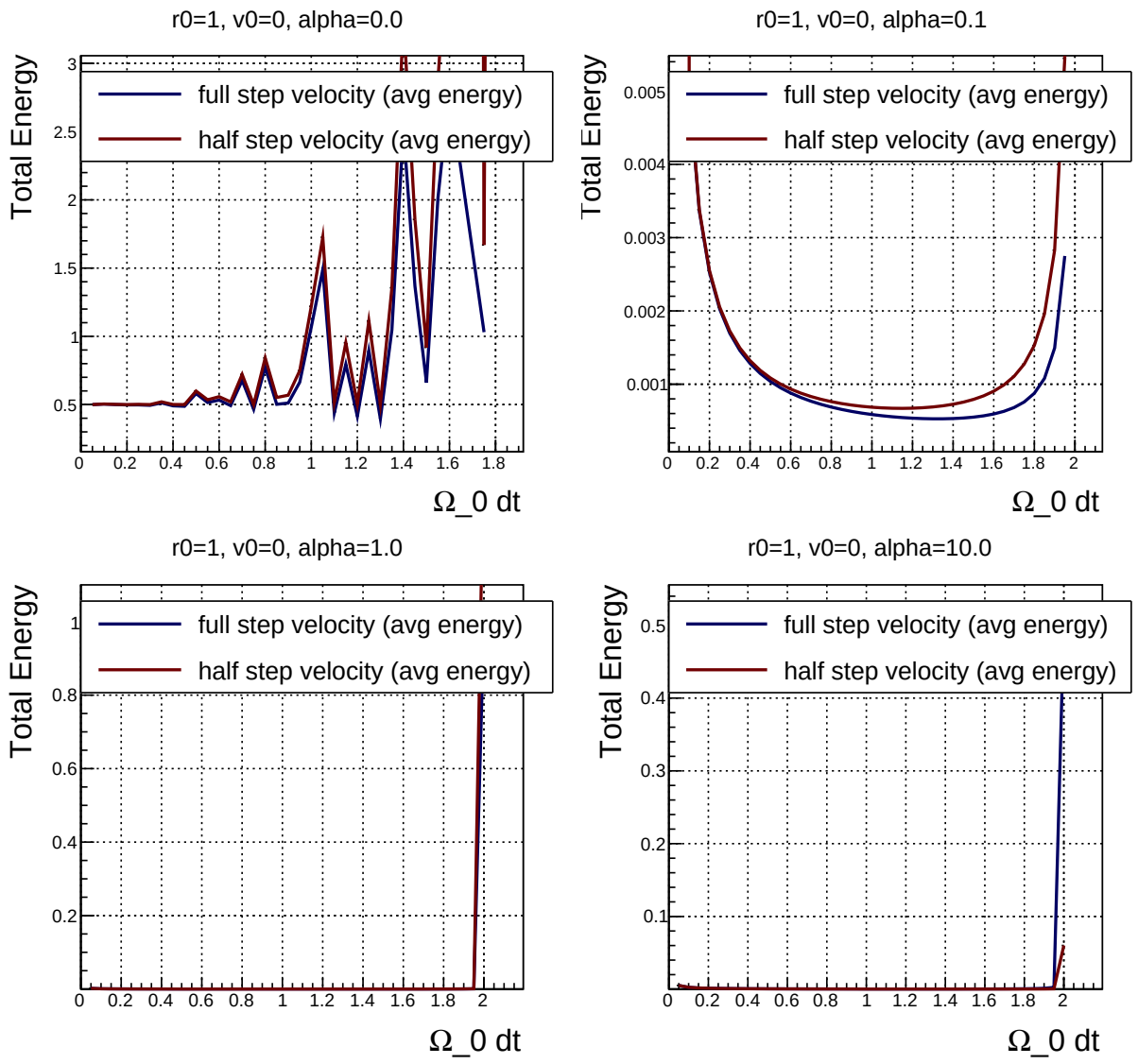

Figure 6: Average total energy (10^3 steps) at various friction coefficients and initial conditions r_0=1 v_0=0

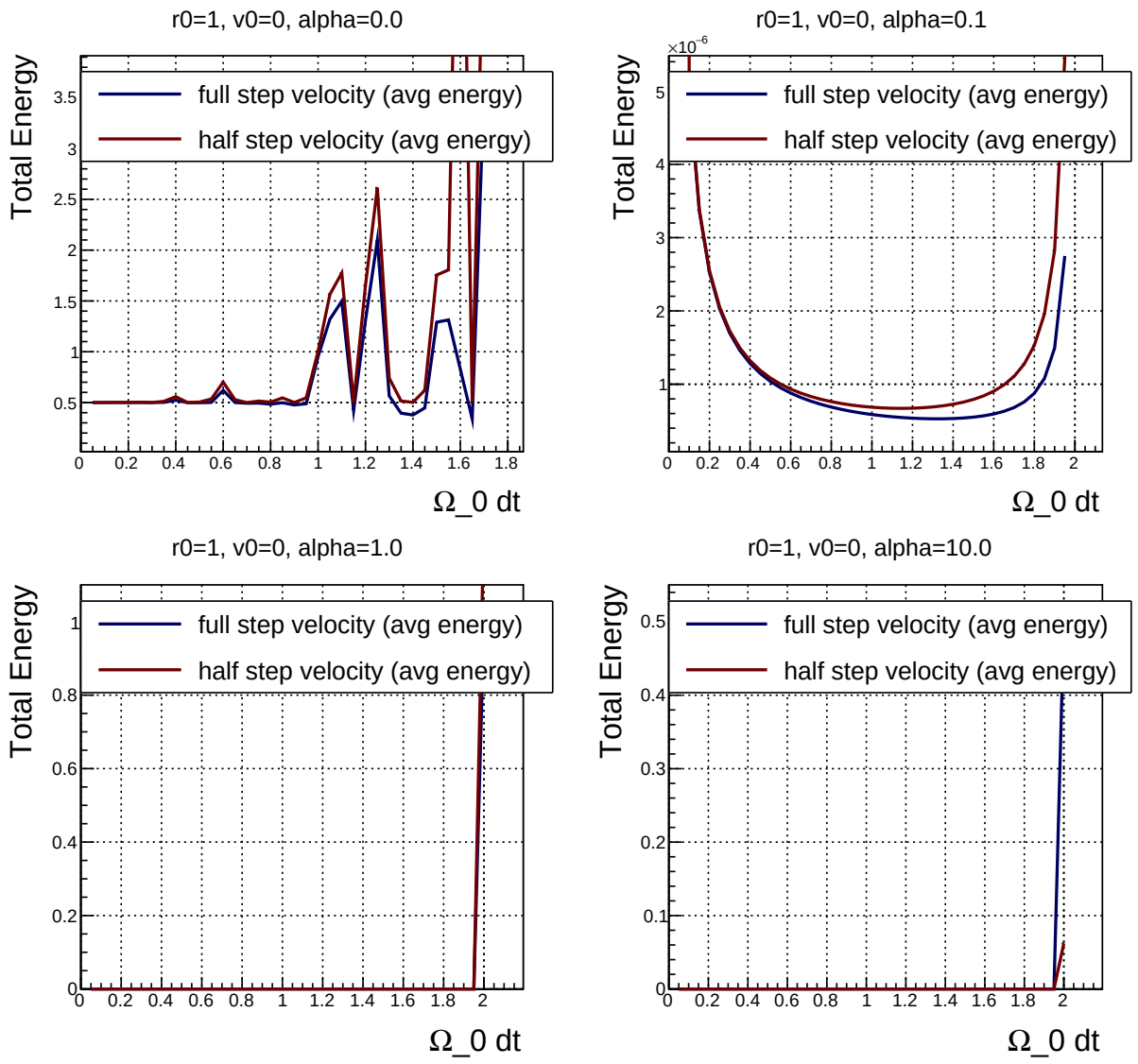

Figure 7: Average total energy (10^6 steps) at various friction coefficients and initial conditions r_0=1 v_0=0

1.2.2 Discussion of Energy Results

So to make sense of Figures 1.2.1 to 1.2.1 let us look at the first plot of any of the grouped plots, or **lets look at the plot of** $r_0 = 1$ $v_0 = 0$ and 'alpha'=0. Without friction essentially we have a perfect oscillator, where no energy is dissipated. So at very fine time steps ($\Omega_0 dt \approx 0.05 to 0.8$) total energy for both the half step velocity, U, and the full step velocity, V, hover around 0.5. This result makes sense because the total energy should be $1/2mv^2$, where m=1 and v=1. Velocity should be 1 because we set the spring constant k=1, additionally potential energy is $1/2kx^2$.

Since the system is conserved the total energy should not deviate from 0.5, unless there's energy loss or our simulation becomes unstable due to insufficient dt parameter. We see that total energy resides at 0.5, which is good, however as we increase friction there's clear energy losses. It is apparent that total energy approaches zero as alpha increases. But why is this?

Physically we can see damping occur with higher frictional values (Figures 8). Of course with damping motion will be decreased, thereby decreasing kinetic energy, so time averaged kinetic and potential energy should approach zero as time goes to infinity. With higher damping coefficients the displacement settles at equilibrium, Figure 8, which means energy approaches zero, likewise.

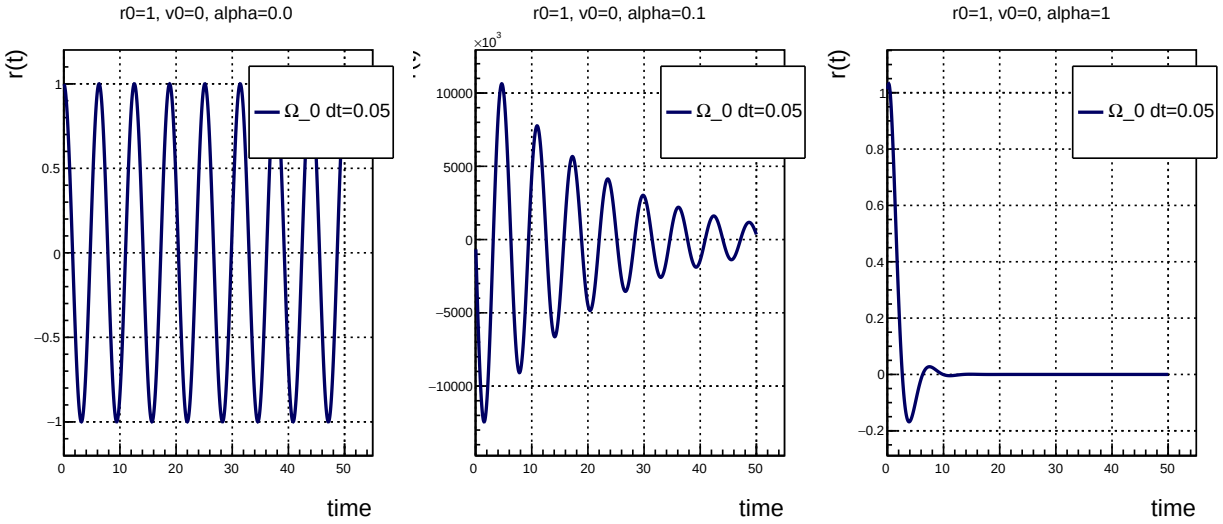

Figure 8: Damping visualization, initial conditions r_0=1 v_0=0

No damping on the first figure due to alpha being set to zero.