Homework 8: Computational Physics

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1 Problem 1

Write a program that generates a random number in the interval $[1;T)$ for some T, with probablity $p(x) = 1/x$. For $T = 10$, generate 10^5 numbers using this program, and plot the distribution. In order to generate the random numbers, we use Matlab's built-in Mersenne generator. In principle the generated list is uniformly distributed with numbers from 0 to 1. Since, we want a distribution with probability $1/x$, we need to compute the cumulative probability:

$$P(r) = \int_1^r dr' \frac{1}{r'} = \ln r - \ln 1 = ln(r)$$

Now, we pick x such that $x = ln(r) \Rightarrow r = e^x$.
So, to generate a random number from 1 to 10, we to ensure that r is between 1 and 10, so x has to be between $\ln 10$ and $\ln 1$.Thus, it suffices to scale the random list by $\ln 10$. The resulting distribution is plotted in figure 1 and the generated values are plotted in figure 2. Notice, that this implies we are normalizing our probability distribution to 1. This corresponds, physically, to perform trials over the whole range from 1 to 10. Thus, notice that the plot of $1/x$ was rescaled so it fits the generated random numbers whose area below must integrate to 1, between 1 and 10.

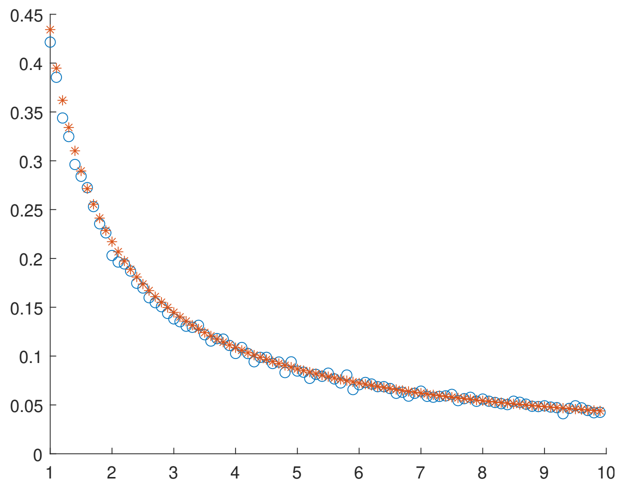
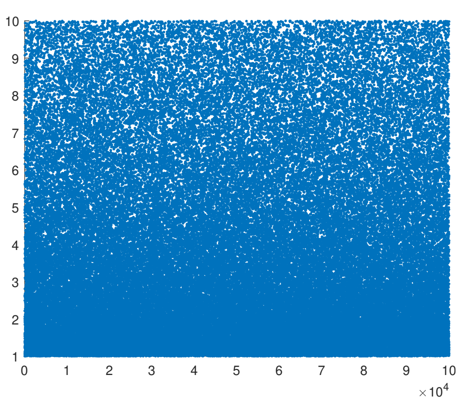


Figure 1: Distribution for a random number generator with probability of $1/x$. Numbers are from 1 to 10.



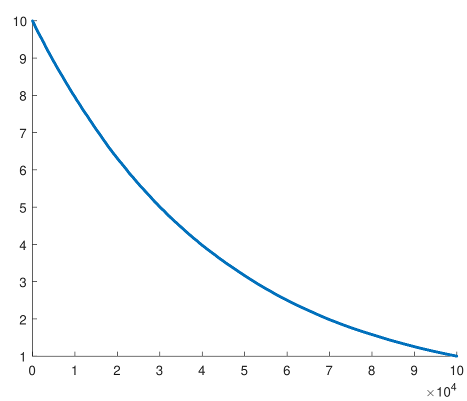


Figure 2: Generated random numbers. Left: random number vs order of generation. Right: Ordered, from largest to smallest, generated random numbers.

2 Problem 2

N identical particles in three dimensions are harmonically bound to the origin, with $Vext = \frac{k_1}{2}\sum_j \vec{r_j}^2$. They interact with each other with a central force potential $V_{int}(|r_1 - r_2|)$. The Langevin equation for each particle is $m\ddot{\vec{r_i}} = -\zeta\dot{\vec{r_i}} - \vec{\nabla}_i[V_{ext}(\vec{r_i}) + \sum_j V_{int}(|\vec{r_i} - \vec{r_j}|)] + \vec{F_i}$, where each component of all random forces are uncorrelated with zero mean: $<(F_i(t))_j>= 0$ and $<(F_i(t))_j(F_k(t))_l>= 2\zeta k_B T\delta_{ik}\delta_{jl}\delta(t-t')$.

(a) **Show that the center of mass of the particles, $\vec{R} = \frac{1}{N}\sum_i \vec{r_i}$, evolves under the effective Langevin equation $m\ddot{\vec{R}} = -\zeta\dot{\vec{R}} - k_1\vec{R} + \vec{F_c}$, with an effective random force satisfying $<F_c>= 0$ and $<(F_c(t))_i(F_c(t))_j>= 2k_BT\delta_{ij}/N$.**

We can write the Langevin equation for each one of the particles and sum all these equations together:

$$m\ddot{\vec{r_1}} = -\zeta\dot{\vec{r_1}} - \vec{\nabla}_{r1}[V_{ext}(\vec{r_1}) + \sum_j V_{int}(|\vec{r_1} - \vec{r_j}|)] + \vec{F_1}$$

$$m\ddot{\vec{r_2}} = -\zeta\dot{\vec{r_2}} - \vec{\nabla}_{r2}[V_{ext}(\vec{r_2}) + \sum_j V_{int}(|\vec{r_2} - \vec{r_j}|)] + \vec{F_2}$$

$$...$$

$$m\ddot{\vec{r_i}} = -\zeta\dot{\vec{r_i}} - \vec{\nabla}_i[V_{ext}(\vec{r_i}) + \sum_j V_{int}(|\vec{r_i} - \vec{r_j}|)] + \vec{F_i}$$

We can group similar classes of terms, so that:

$$m\ddot{\vec{r_1}} + m\ddot{\vec{r_2}} + ... + m\ddot{\vec{r_N}} = mN\ddot{\vec{R}}$$

$$-\zeta\dot{\vec{r_1}} - \zeta\dot{\vec{r_2}} + ... - \zeta\dot{\vec{r_N}} = -N\zeta\dot{\vec{R}}$$

$$\vec{F_1} + \vec{F_2} + ... + \vec{F_N} = N\vec{F_c}$$

Whereas the two remaining terms are a bit more cumbersome to work out. The V_{ext} term can be dealt with by replacing $V_{ext} = \frac{k_1}{2}\sum_j \vec{r_j}^2$. So:

$$-\vec{\nabla}_{r_1}\frac{k_1}{2}\sum_j \vec{r_j}^2 - \vec{\nabla}_{r_2}\frac{k_1}{2}\sum_j \vec{r_j}^2 + ... - \vec{\nabla}_{r_N}\frac{k_1}{2}\sum_j \vec{r_j}^2$$

$$= -\sum_s \vec{\nabla}_{r_s}\frac{k_1}{2}\sum_j \vec{r_j}^2 = -\frac{k_1}{2}\sum_s\sum_j 2\vec{r_j}\delta_{js} = -k_1\sum_s \vec{r_s} = -Nk_1\vec{R}$$

To deal with the last term, we explicitly write a few terms and make use of action-reaction law to cancel out action-reaction force pairs:

$$-\vec{\nabla}_{r_1}\sum_j V_{int}(|\vec{r_1} - \vec{r_j}|) - \vec{\nabla}_{r_2}\sum_j V_{int}(|\vec{r_2} - \vec{r_j}|) + ... - \vec{\nabla}_{r_N}\sum_j V_{int}(|\vec{r_N} - \vec{r_j}|)$$

$$-\sum_s \vec{\nabla}_{r_s}\sum_j V_{int}(|\vec{r_s} - \vec{r_j}|)$$

Notice that each the presence of two sums means there are terms like: $-\vec{\nabla}_{r_1}V_{int}(|\vec{r_1} - \vec{r_2}|)$ and $-\vec{\nabla}_{r_2}V_{int}(|\vec{r_2} - \vec{r_1}|)$, which represent the force over particle 2 due to particle 1 and the force over particle 1 due to 2.

Therefore, they are action and reaction pairs, which means they add up to zero. There will be a reaction force for any of the terms in one of the sums, thus:

$$-\sum_s \vec{\nabla}_{\vec{r_s}} \sum_j V_{int}(|\vec{r_s} - \vec{r_j}|) = 0$$

$$\therefore m\ddot{\vec{R}} = -\zeta\dot{\vec{R}} - k_1\vec{R} + \vec{F_c}$$

Now, let's prove the conditions on $\vec{F_c}$ are satisfied. The average condition is trivial, as the average for any individual force is zero itself:

$$\vec{F_c} = \frac{1}{N}(\vec{F_1} + \vec{F_2} + ... + \vec{F_N})$$

$$< \vec{F_c} >= \frac{1}{N}(< \vec{F_1} > + < \vec{F_2} > +...+ < \vec{F_N}) >$$

$$\therefore < \vec{F_c} >= 0$$

Similarly, for the correlation, we can just write the two terms carefully bookkeeping the indexes:

$$\vec{F_{ci}}\vec{F_{cj}} = \frac{1}{N^2}(\vec{F_{1i}} + \vec{F_{2i}} + ... + \vec{F_{Ni}})(\vec{F_{1j}} + \vec{F_{2j}} + ... + \vec{F_{Nj}})$$

$$< \vec{F_{ci}}\vec{F_{cj}} >= \frac{1}{N^2} < (\vec{F_{1i}} + \vec{F_{2i}} + ... + \vec{F_{Ni}})(\vec{F_{1j}} + \vec{F_{2j}} + ... + \vec{F_{Nj}}) >$$

If we recall the correlation relationship for the individual forces, $< (F_i(t))_j(F_k(t))_l >= 2\zeta k_B T\delta_{ik}\delta_{jl}\delta(t-t')$, we see that all cross terms vanish due to the δ_{jl} term.

$$< \vec{F_{ci}}\vec{F_{cj}} >= \frac{1}{N^2} < (\vec{F_{1i}} + \vec{F_{2i}} + ... + \vec{F_{Ni}})(\vec{F_{1j}} + \vec{F_{2j}} + ... + \vec{F_{Nj}}) >$$

$$= \frac{1}{N^2}(< \vec{F_{1i}}\vec{F_{1j}} > + < \vec{F_{2i}} > \vec{F_{2j}} + ...+ < \vec{F_{Ni}}\vec{F_{Nj}} >) = \frac{1}{N^2}(N)(2\zeta k_B T\delta_{ij})$$

$$\therefore < \vec{F_{ci}}\vec{F_{cj}} >= \frac{1}{N}(2\zeta k_B T\delta_{ij})$$

(b) **Solve the effective Langevin equation in (a), to show that if the initial conditions are $R(0) = 0$ and $\dot{R}(0) = 0$, that:**

$$\vec{R(t)} = \int_0^t dt' \frac{2\tau_2}{m} e^{(t-t')/2\tau_1} \sinh\left(\frac{t-t'}{2\tau_2}\right) \vec{F_c(t')}$$

Use this to determine $< R^2(t) >$. Hint: To find $R(t)$, using a Laplace Transform and the convolution theorems are likely to be helpful. Using eq. (1), the calculation of $< R^2(t) >$ does not require any special tricks (but is tedious to calculate).

We basically want to solve a second order differential equation:

$$m\ddot{\vec{R}} = -\zeta\dot{\vec{R}} - k_1\vec{R} + \vec{F_c}$$

One of our options is to use the Laplace transform, $\mathcal{L}$:

$$m\mathcal{L}(\ddot{\vec{R}}) = -\zeta\mathcal{L}(\dot{\vec{R}}) - k_1\mathcal{L}(\vec{R}) + \mathcal{L}(\vec{F_c})$$

Now recall;

$$\mathcal{L}(y) = Y(s)$$

$$\mathcal{L}(y') = sY(s) - Y(0)$$

$$\mathcal{L}(y'') = s^2 Y(s) - sY(0) - \dot{Y}(0)$$

$$\Rightarrow m(s^2\vec{R}(s) - s\vec{R}(0) - \dot{\vec{R}}(0)) = -\zeta(s\vec{R}(s) - \vec{R}(0)) - k_1\vec{R}(s) + \vec{F}(s)$$

Using the initial conditions, the expression reduces to:

$$\Rightarrow m(s^2\vec{R}(s)) = -\zeta(s\vec{R}(s)) - k_1\vec{R}(s) + \vec{F}(s)$$

$$\Leftrightarrow \vec{R}(s)(ms^2 + \zeta s + k_1) = \vec{F}(s)$$

$$\Leftrightarrow \vec{R}(s) = \frac{\vec{F}(s)}{ms^2 + \zeta s + k_1}$$

$$\Leftrightarrow \vec{R}(s) = \frac{1}{m}\frac{1}{s^2 + \frac{\zeta}{m}s + \frac{k_1}{m}}\vec{F}(s) = \vec{G}(s)\vec{F}(s)$$

Now that we have the Laplace transform, we can just use the definition for convolution to calculate the inverse transform. Recall:

$$(g * f)(t) = \int_0^t g(t-t')f(t')$$

So, the task reduces to finding the inverse Laplace transform for $G(s) = \frac{1}{m}\frac{1}{s^2+\frac{\zeta}{m}s+\frac{k_1}{m}}$. Looking at Laplace transform tables, if $G(s) = \frac{1}{(s-a)^2-b^2} = \frac{1}{s^2-2as+a^2-b^2}$, the inverse transform is given by $\frac{1}{b}e^{at}\sinh\left(b(t-t')\right)$. Thus, we can use the substitutions:

$$-2a = \frac{\zeta}{m} \Rightarrow a = -\frac{\zeta}{2m}$$

$$a^2 - b^2 = \frac{k_1}{m} \Rightarrow b = \sqrt{\frac{\zeta^2}{4m^2} - \frac{k_1}{m}}$$

So, the inverse transform is:

$$g(t) = \frac{1}{mb}e^{-t\zeta/2m}\sinh\left(\sqrt{\frac{\zeta^2 - 4m}{4m^2}}t\right)$$

'

$$\therefore R(t) = \int_0^t dt' \frac{1}{m\sqrt{\frac{\zeta^2}{4m^2} - \frac{k_1}{m}}} e^{-(t-t')\zeta/2m}\sinh\left(\sqrt{\frac{\zeta^2 - 4m}{4m^2}}(t-t')\right)\vec{F}_c(t')$$

By defining $\tau_1 = \zeta/m$ and $\tau_2 = \frac{1}{2}\sqrt{\frac{\zeta^2}{4m^2} - \frac{k_1}{m}}$, we have:

$$\therefore R(t) = \int_0^t dt' \frac{2\tau_2}{m}e^{-(t-t')/2\tau_1}\sinh\left(\frac{t-t'}{2\tau_2}\right)\vec{F}_c(t')$$

After showing this, it is straightforward to compute $< R^2(t) >$.

$$R^2(t) = \int_0^t\int_0^t dt'dt'' \frac{4\tau_2^2}{m^2}e^{-(t-t')/2\tau_1}e^{-(t-t'')/2\tau_1}\sinh\left(\frac{t-t'}{2\tau_2}\right)\sinh\left(\frac{t-t''}{2\tau_2}\right)\vec{F}_c(t')\vec{F}_c(t'')$$

$$< R^2(t) >= \int_0^t\int_0^t dt'dt'' \frac{4\tau_2^2}{m^2}e^{-(t-t')/2\tau_1}e^{-(t-t'')/2\tau_1}\sinh\left(\frac{t-t'}{2\tau_2}\right)\sinh\left(\frac{t-t''}{2\tau_2}\right)\underbrace{< \vec{F}_c(t')\vec{F}_c(t'') >}_{2\zeta k_B T\delta_{ij}\delta(t-t')/N}$$

$$< R^2(t) >= \frac{8\tau_2^2\zeta k_B T}{m^2 N}\int_0^t dt'dt'' e^{-(2t-t'-t'')/2\tau_1}\sinh\left(\frac{t-t'}{2\tau_2}\right)\sinh\left(\frac{t-t''}{2\tau_2}\right)\delta(t-t')$$

$$< R^2(t) >= \frac{8\tau_2^2\zeta k_BT}{m^2N}\int_0^t\int_0^t dt' e^{-(2t-2t')/2\tau_1}\sinh^2\left(\frac{t-t'}{2\tau_2}\right)$$

$$< R^2(t) >= \frac{8\tau_2^2\zeta k_BT}{m^2N}\int_0^t dt' e^{-(2t-2t')/2\tau_1}\frac{1}{4}\left(e^{2\frac{t-t'}{2\tau_2}}-2+e^{-2\frac{t-t'}{2\tau_2}}\right)$$

$$< R^2(t) >= \frac{2\tau_2^2\zeta k_BT}{m^2N}\int_0^t dt'\left(e^{-\frac{t-t'}{\tau_1}+\frac{t-t'}{\tau_2}}-2e^{-\frac{t-t'}{\tau_1}}+e^{-\frac{t-t'}{\tau_1}-\frac{t-t'}{\tau_2}}\right)$$

$$< R^2(t) >= \frac{2\tau_2^2\zeta k_BT}{m^2N}\int_0^t dt'\left(e^{-\frac{t-t'}{\tau_1}+\frac{t-t'}{\tau_2}}-2e^{-\frac{t-t'}{\tau_1}}+e^{-\frac{t-t'}{\tau_1}-\frac{t-t'}{\tau_2}}\right)$$

$$< R^2(t) >= \frac{2\tau_2^2\zeta k_BT}{m^2N}\int_0^t dt'\left(e^{-(t-t')(\frac{1}{\tau_1}-\frac{1}{\tau_2})}-2e^{-\frac{t-t'}{\tau_1}}+e^{-(t-t')(\frac{1}{\tau_1}+\frac{1}{\tau_2})}\right)$$

$$< R^2(t) >= \frac{2\tau_2^2\zeta k_BT}{m^2N}\left(e^{-t(\frac{1}{\tau_1}-\frac{1}{\tau_2})}\int_0^t dt' e^{t'(\frac{1}{\tau_1}-\frac{1}{\tau_2})}-2e^{-\frac{t}{\tau_1}}\int_0^t dt' e^{\frac{t'}{\tau_1}}+e^{-t(\frac{1}{\tau_1}+\frac{1}{\tau_2})}\int_0^t dt' e^{t'(\frac{1}{\tau_1}+\frac{1}{\tau_2})}\right)$$

$$< R^2(t) >= \frac{2\tau_2^2\zeta k_BT}{m^2N}\left(e^{-t(\frac{1}{\tau_1}-\frac{1}{\tau_2})}\frac{1}{\frac{1}{\tau_1}-\frac{1}{\tau_2}}(e^{t(\frac{1}{\tau_1}-\frac{1}{\tau_2})}-1)-2e^{-\frac{t}{\tau_1}}\tau_1(e^{\frac{t}{\tau_1}}-1)+e^{-t(\frac{1}{\tau_1}+\frac{1}{\tau_2})}\frac{1}{\frac{1}{\tau_1}+\frac{1}{\tau_2}}(e^{t(\frac{1}{\tau_1}+\frac{1}{\tau_2})}-1)\right)$$

$$< R^2(t) >= \frac{2\tau_2^2\zeta k_BT}{m^2N}\left(\frac{1}{\frac{1}{\tau_1}-\frac{1}{\tau_2}}(1-e^{-t(\frac{1}{\tau_1}-\frac{1}{\tau_2})})-2\tau_1(1-e^{-\frac{t}{\tau_1}})+\frac{1}{\frac{1}{\tau_1}+\frac{1}{\tau_2}}(1-e^{-t(\frac{1}{\tau_1}+\frac{1}{\tau_2})})\right)$$

$$< R^2(t) >= \frac{2\tau_2^2\zeta k_BT}{m^2N}\left(\frac{\tau_1\tau_2}{\tau_2-\tau_1}(1-e^{-t\frac{\tau_2-\tau_1}{\tau_1\tau_2}})-2\tau_1(1-e^{-\frac{t}{\tau_1}})+\frac{\tau_1\tau_2}{\tau_2+\tau_1}(1-e^{-t\frac{\tau_2+\tau_1}{\tau_1\tau_2}})\right)$$

In the thermodynamic limit $t \to \infty$:

$$< R^2(t) >= \frac{2\tau_2^2\zeta k_BT}{m^2N}\left(\frac{\tau_1\tau_2}{\tau_2-\tau_1}-2\tau_1+\frac{\tau_1\tau_2}{\tau_2+\tau_1}\right) = \frac{2\tau_2^2\zeta k_BT}{m^2N}\left(\frac{2\tau_1\tau_2^2}{\tau_2^2-\tau_1^2}-2\tau_1\right)$$

$$\therefore < R^2(t) >= \frac{4\tau_1^3\tau_2^2\zeta k_BT}{m^2N(\tau_2^2-\tau_1^2)}$$

(c) **Using the nondimensional units $m = \zeta = k_BT = 1$, and with $k1 = 0.1$ in those units, simulate the dynamics of $N = 2$ particles with a harmonic bond between them, $V_int(x) = k_2(x-a)^2/2$, with $k_2 = a = 1$ in the dimensionless units. Perform 1000 simulations starting from the initial conditions $r_1(0) = (-0.5, 0, 0)$ and $r_2(0) = (0.5, 0, 0)$, and with $\dot{\vec{r_i}}(0) = 0$ for all particles. Compute $< v^2(t) >$ (with the average taken over your 1000 simulations), and determine if your simulation agrees with the equipartition of energy. Also plot $< R^2 >$ and compare to your theoretical prediction in (b).**

We can directly apply the results in literal (a) since $\vec{R}(0) = \frac{1}{N}((0.5, 0 + (-0.5, 0))) = (0, 0)$ and the initial velocity is also 0. So, the center of mass initial position and velocity coincide with the conditions given above. Hence, we just need to modify the code given in class to account for the interaction V_{ext} and for the number of particles that enter in the calculation of averages. The code is transcribed below:

```
clear;
rng(2,'twister');

kT=1;
zeta=1;
m=1;
k1=0.1;
k2=1;
tau1=m/zeta;
```

```
tau2=sqrt(1/(zeta^2/(4*m^2)-k1/m));
dt=0.01;
nstep=100000;
nrun=1000;
N=2;

xvals=zeros(1,nstep);
xsqvals=zeros(1,nstep);
vsqvals=zeros(1,nstep);
tvals=zeros(1,nstep);

disp('predicted timescales:')
disp(tau1)
disp(tau2)
for i=1:nrun
    x=0;
    t=0;
    xold=0;
    xnew=0; %note! reinitialize!

    for i=1:nstep
        R=randn()*sqrt(2*zeta*kT/dt);
        xnew=x;
        f=force(x,k1,k2);
        xnew=xnew+(x-xold)*(1-zeta*dt/2/m)/(1+zeta*dt/2/m);
        xnew=xnew+(R+f)*dt*dt/m/(1+zeta*dt/2/m);
        v=(xnew-xold)/(2*dt);
        xold=x;
        x=xnew;
        t=t+dt;
        xvals(i)=xvals(i)+x/nrun;
        xsqvals(i)=xsqvals(i)+x*x/nrun;
        vsqvals(i)=vsqvals(i)+v*v/nrun;
        tvals(i)=t;
    end
end
xvals=xvals/N;
xsqvals=xsqvals/N;
vsqvals=vsqvals/N;

figure
hold on
plot(tvals,vsqvals,'r')
plot(tvals.*1.1,ones(1,nstep).*(kT/(m*N)),'k')
xlabel('t ')
ylabel('<v^2>' )
legend({'simulation','equipartition'},'Location','southeast')
saveas(gcf,'HW8_2velsq','epsc');
hold off

figure
hold on
plot(tvals,xsqvals,'r')
plot(tvals.*1.1,5*ones(1,nstep),'k')
xlabel('t ')
ylabel('<x^2> ')
legend({'simulation','harmonic limit'},'Location','southeast')
saveas(gcf,'HW8_2xsq','epsc');
hold off

figure
hold on
plot(tvals,xvals,'r')
xlabel('t ')
ylabel('<x> ')
```

```
saveas(gcf,'HW8_2xvals','epsc');
hold off

function f=force(x,k1,k2)
    f=-k1*(x);
end
```

The resulting plots are shown in figures 3 and 4. As it can be seen the mean position, $< x(t) >= 0$, which makes sense, since the potential is centered at zero. The central potential cancels out for the center of mass coordinates so it has no effect on its dynamics. The average position squared, $< x^2(t) >= 5$ after equilibration (after several intervals τ_1). If we replace the values for the problem parameters on the result of the previous part, $\tau_1 = 2$, $\tau_2^2 = 5/3$, $k_1 = 0,1$, $\zeta = 1 = k_B T$, we get exactly $< x^2(t) >= 5$. Finally, equipartition is indeed satisfied as expected. Notice that we have to consider the number of particles in order for our result to be consistent with equipartition. Figure 4 shows simulations over a longer period of time. However, the fluctuations are still present. In order to reduce the noise, one can increase the number of runs as shown in figure 5. **Notice that in the plots x actually stands for the coordinates of the center of mass $\vec{R}$**

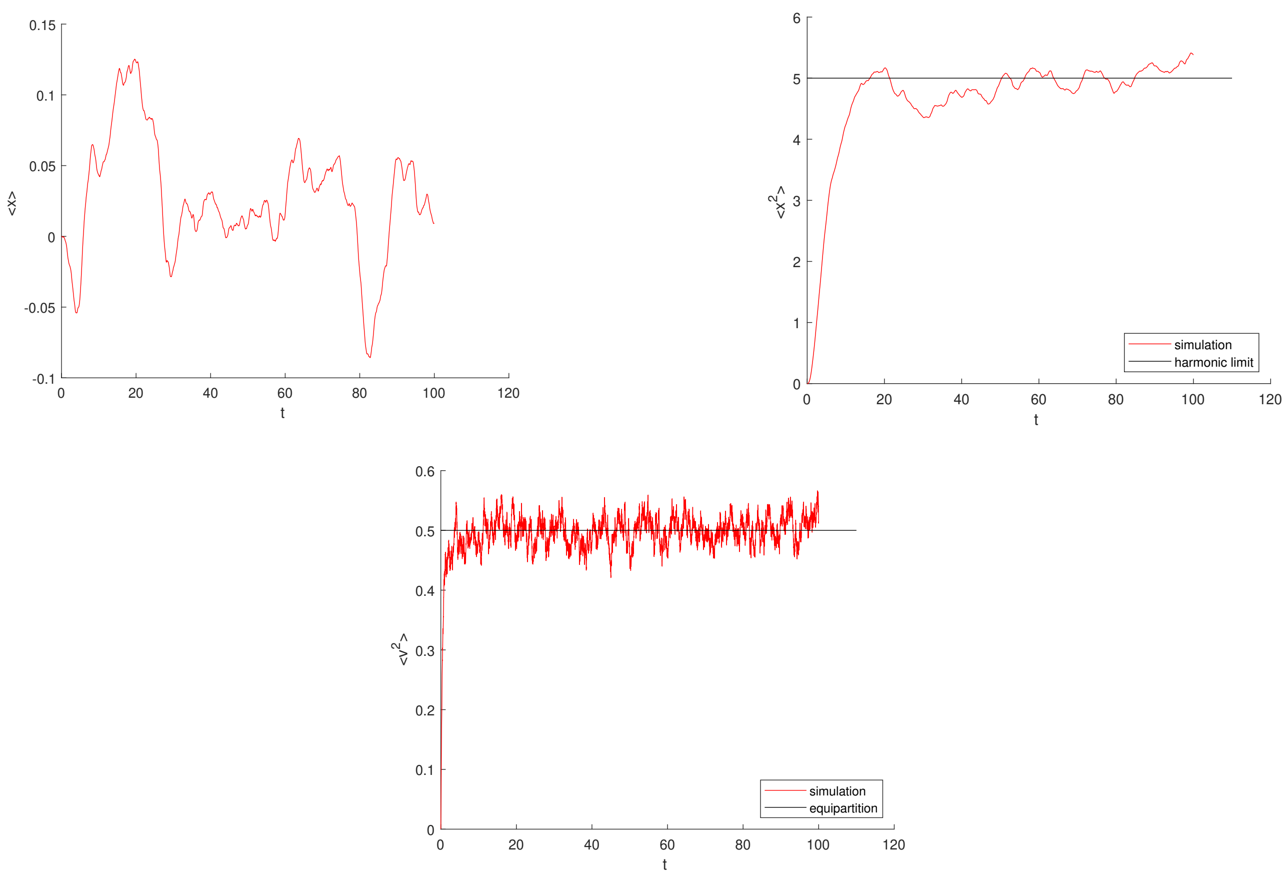


Figure 3: Averages over the 1000 simulations for $< x >$, $< x^2 >$ and $< v^2 >$

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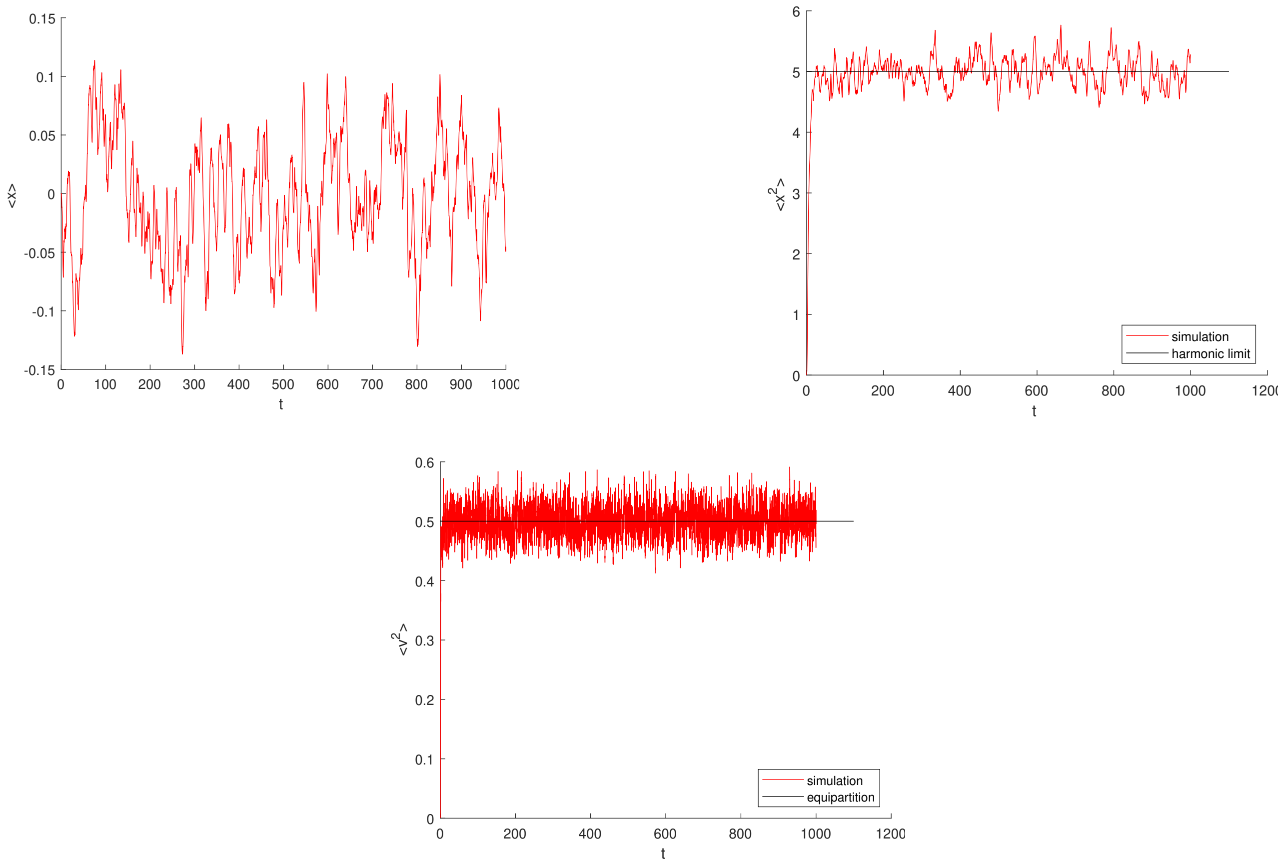

Figure 4: Averages over the 1000 simulations for $< x >$, $< x^2 >$ and $< v^2 >$ for longer times.

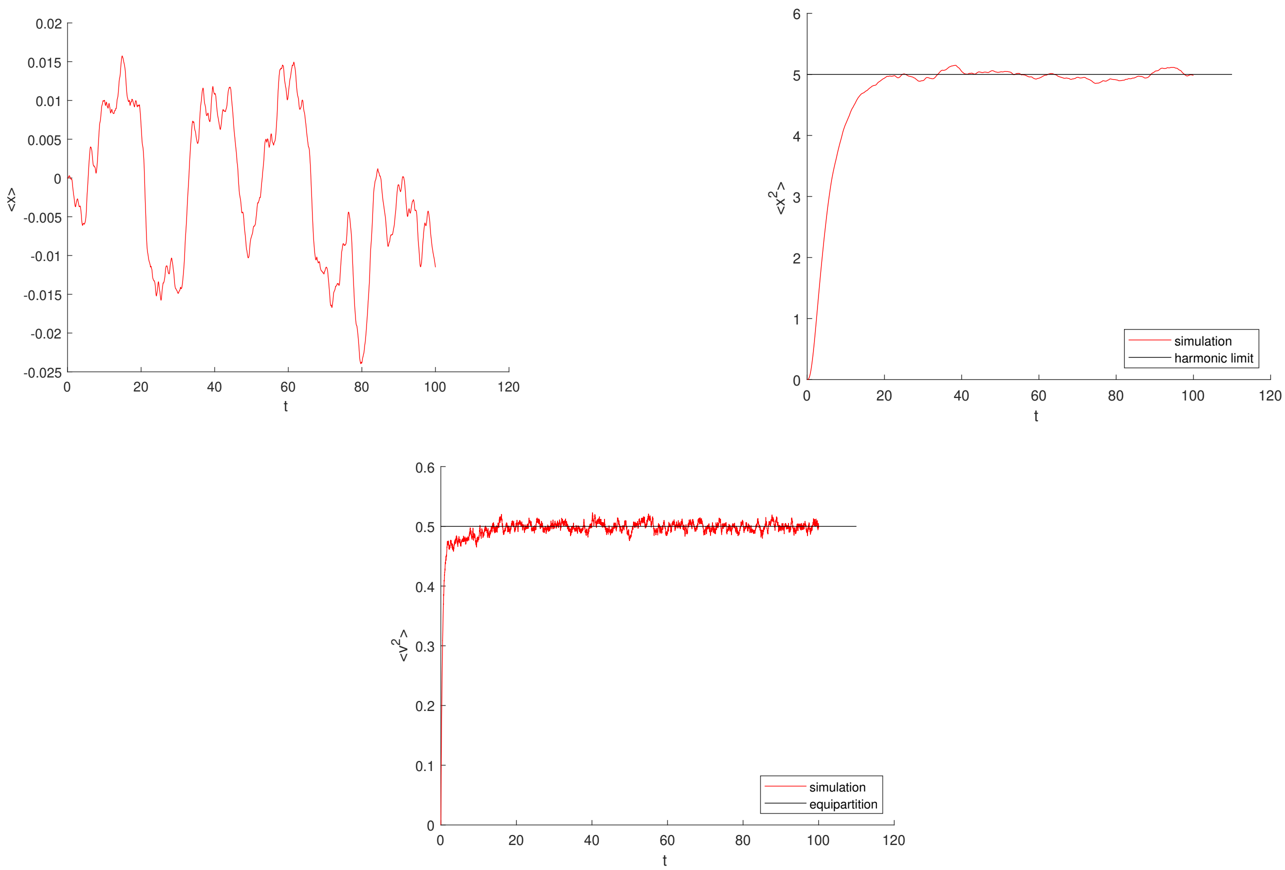

Figure 5: Averages over 10000 simulations for $< x >$, $< x^2 >$ and $< v^2 >$
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