

Correlation

```
DCorr[T_, p_] := 10^(0.05 + 0.07 p - (1.04 + 0.1 p) / T)
```

```
DCorr[.9247, .6590]
```

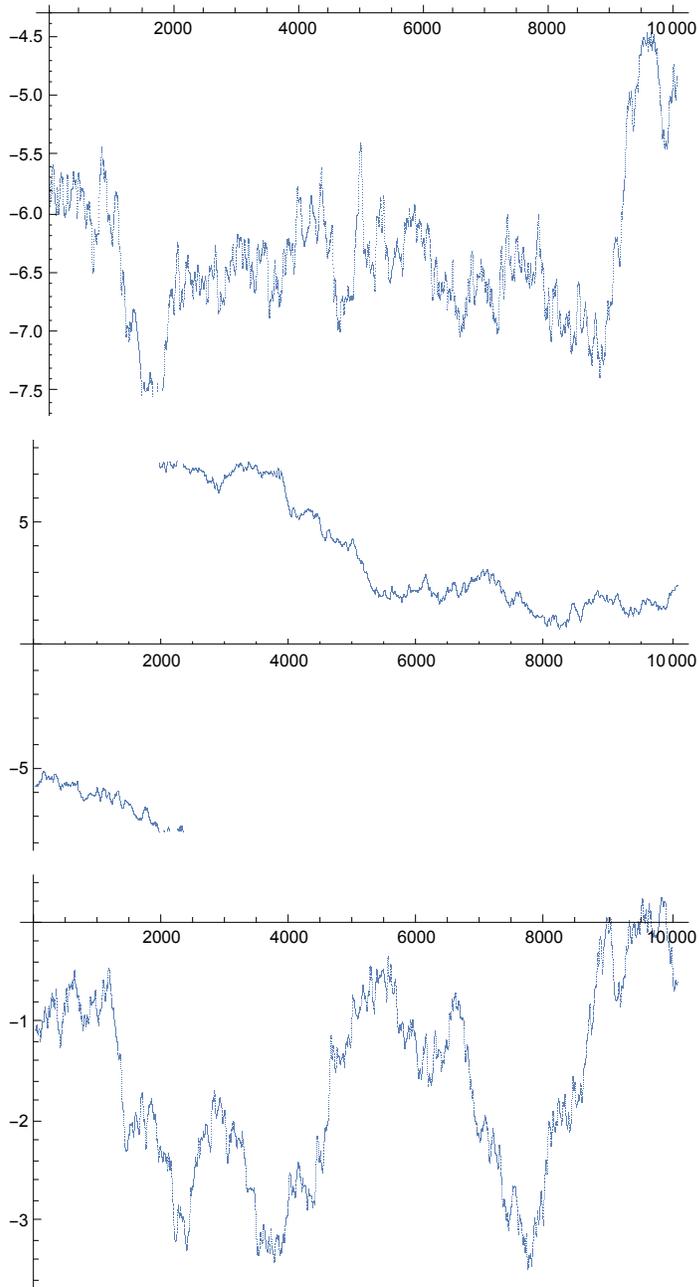
```
0.0794648
```

Read data and set up variables

```
SetDirectory[  
  "/Users/kofke/Documents/Teaching/CE\ 530/Homework/2016/Assignment\ 6"]  
fileData = Import["rv_data2.csv", "CSV"];  
(*fileData=Drop[fileData,1];*)  
/Users/kofke/Documents/Teaching/CE 530/Homework/2016/Assignment 6
```

```
timeStep = 0.01;  
r = Take[#, 3] & /@ fileData;  
rx = #[[1]] & /@ fileData;  
ry = #[[2]] & /@ fileData;  
rz = #[[3]] & /@ fileData;  
vy = #[[5]] & /@ fileData;  
vz = #[[6]] & /@ fileData;  
vx = #[[4]] & /@ fileData;  
vy = #[[5]] & /@ fileData;  
vz = #[[6]] & /@ fileData;
```

```
ListPlot[rx]
ListPlot[ry] (* one can see the discontinuity caused by PBC *)
ListPlot[rz]
```

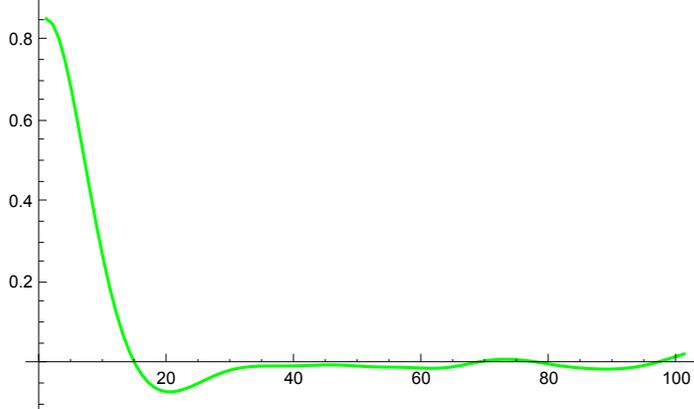
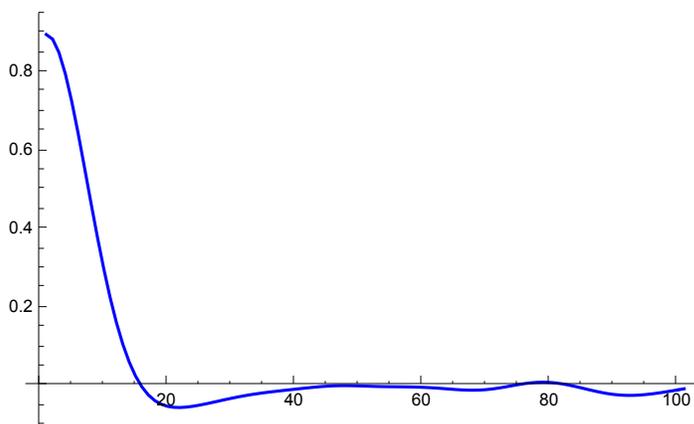
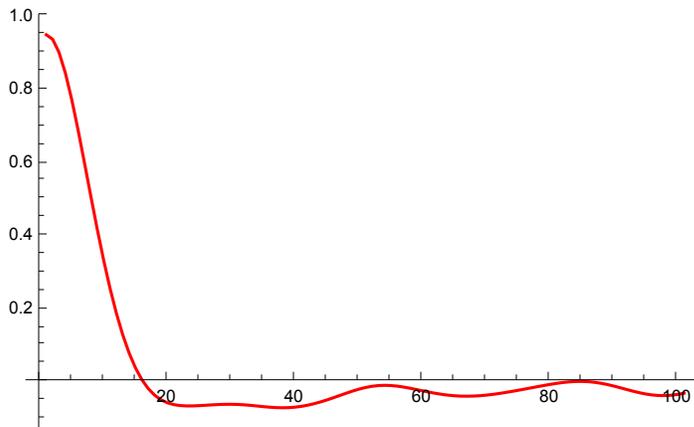


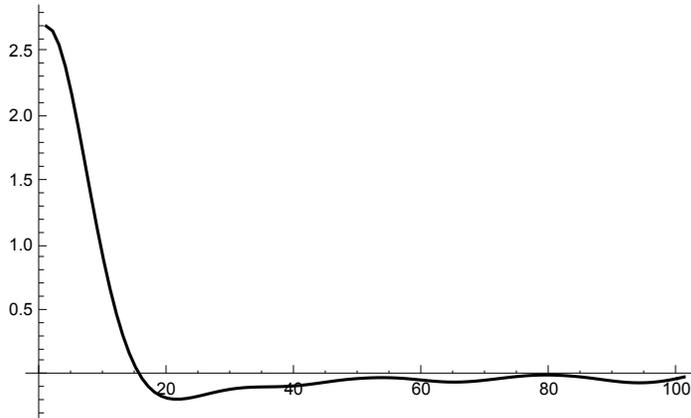
Velocity autocorrelation function

```
vacf[v_List, n_] := Sum[v[[k]] v[[k+n]], {k, Length[v] - n}] / (Length[v] - n)
```

```
vacfx = vacf[vx, #] & /@ Range[0, 100];  
vacfy = vacf[vy, #] & /@ Range[0, 100];  
vacfz = vacf[vz, #] & /@ Range[0, 100];  
vacfTot = (vacfx + vacfy + vacfz);
```

```
ListPlot[vacfx, PlotRange -> All, Joined -> True, PlotStyle -> Red]  
ListPlot[vacfy, PlotRange -> All, Joined -> True, PlotStyle -> Blue]  
ListPlot[vacfz, PlotRange -> All, Joined -> True, PlotStyle -> Green]  
ListPlot[vacfTot, PlotRange -> All, Joined -> True, PlotStyle -> Black]
```





VACF as a function of range of integral

```
Integrate[Interpolation[vacfTot, InterpolationOrder -> 2][x], {x, 0, 40}] / 3 / 100  
Integrate[Interpolation[vacfTot, InterpolationOrder -> 2][x], {x, 0, 60}] / 3 / 100  
Integrate[Interpolation[vacfTot, InterpolationOrder -> 2][x], {x, 0, 80}] / 3 / 100  
Integrate[Interpolation[vacfTot, InterpolationOrder -> 2][x], {x, 0, 100}] / 3 / 100
```

0.0650282

0.0624222

0.060377

0.0580903

Value seems to settle in at 0.060 (in LJ units).