

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

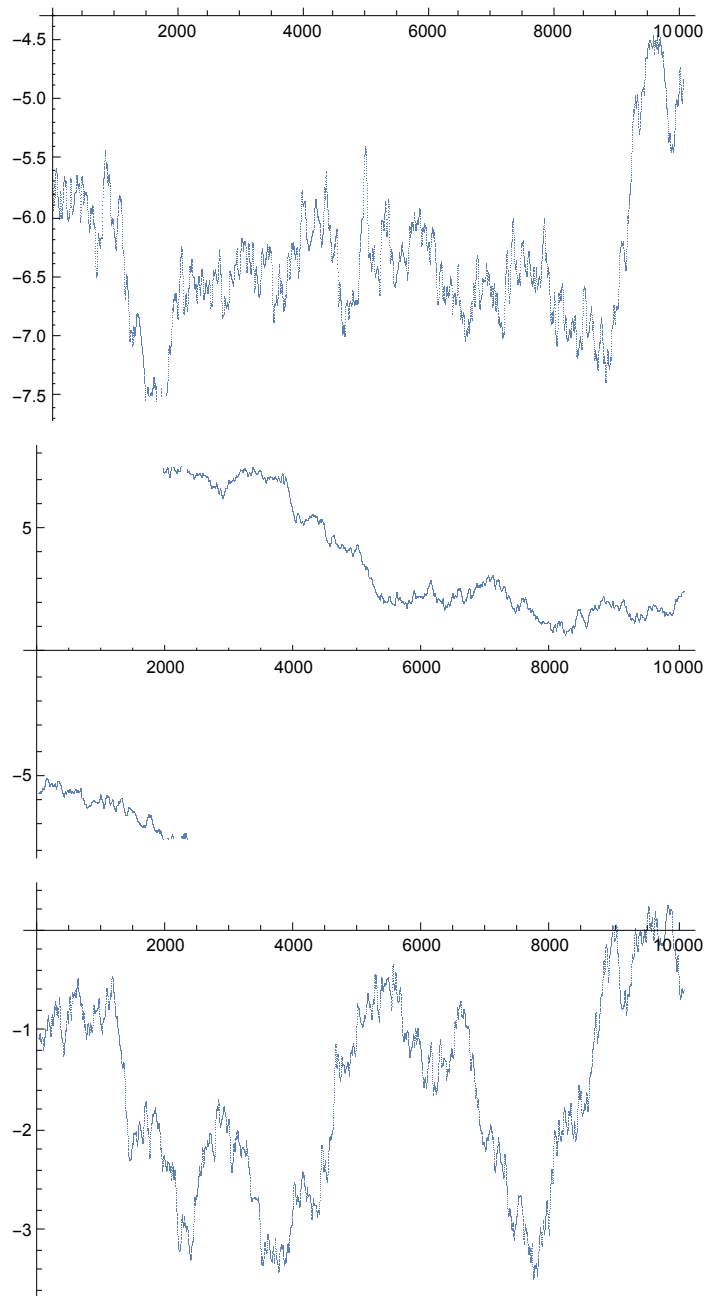
```
SetDirectory[  
  "/Users/kofke/Documents/Teaching/CE\ 530/Homework/2016/Assignment\ 6"]  
fileData = Import["rv_data2.csv", "CSV"];  
(*fileData=Drop[fileData,1];*)  
/Users/kofke/Documents/Teaching/CE 530/Homework/2016/Assignment 6
```

```
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)

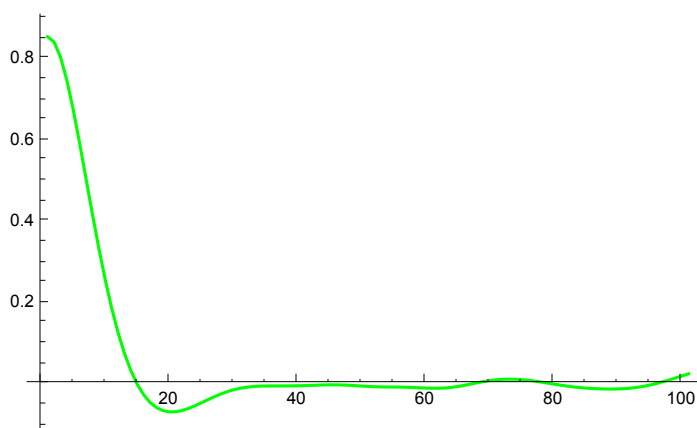
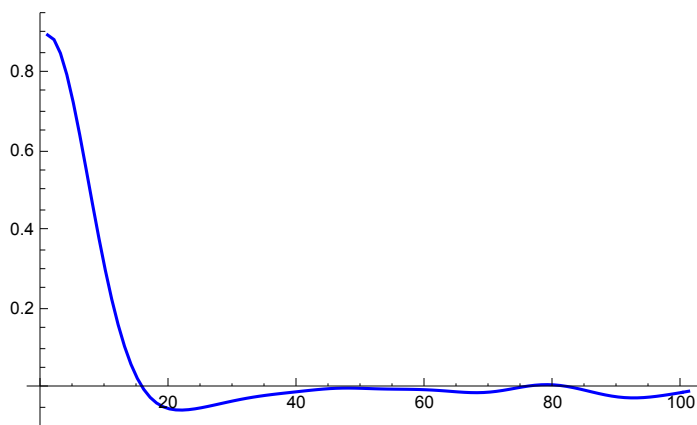
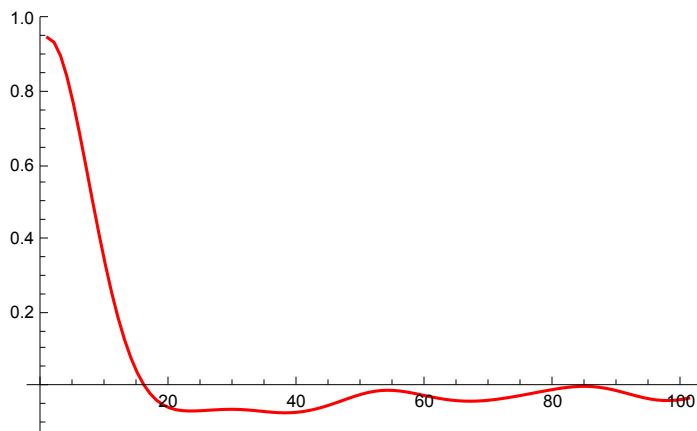
```

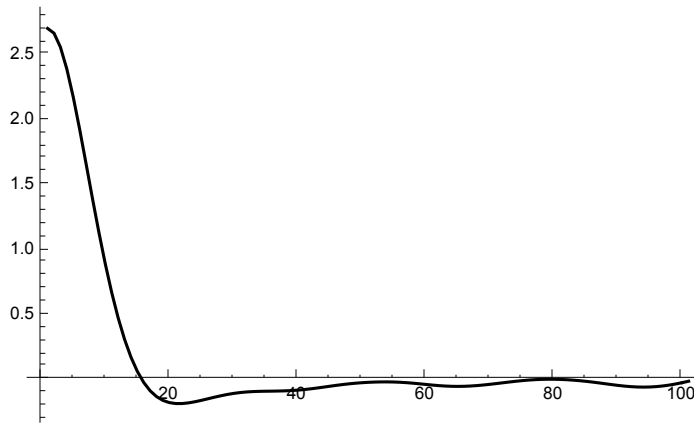
```

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).