NTW Model Checks for Silica

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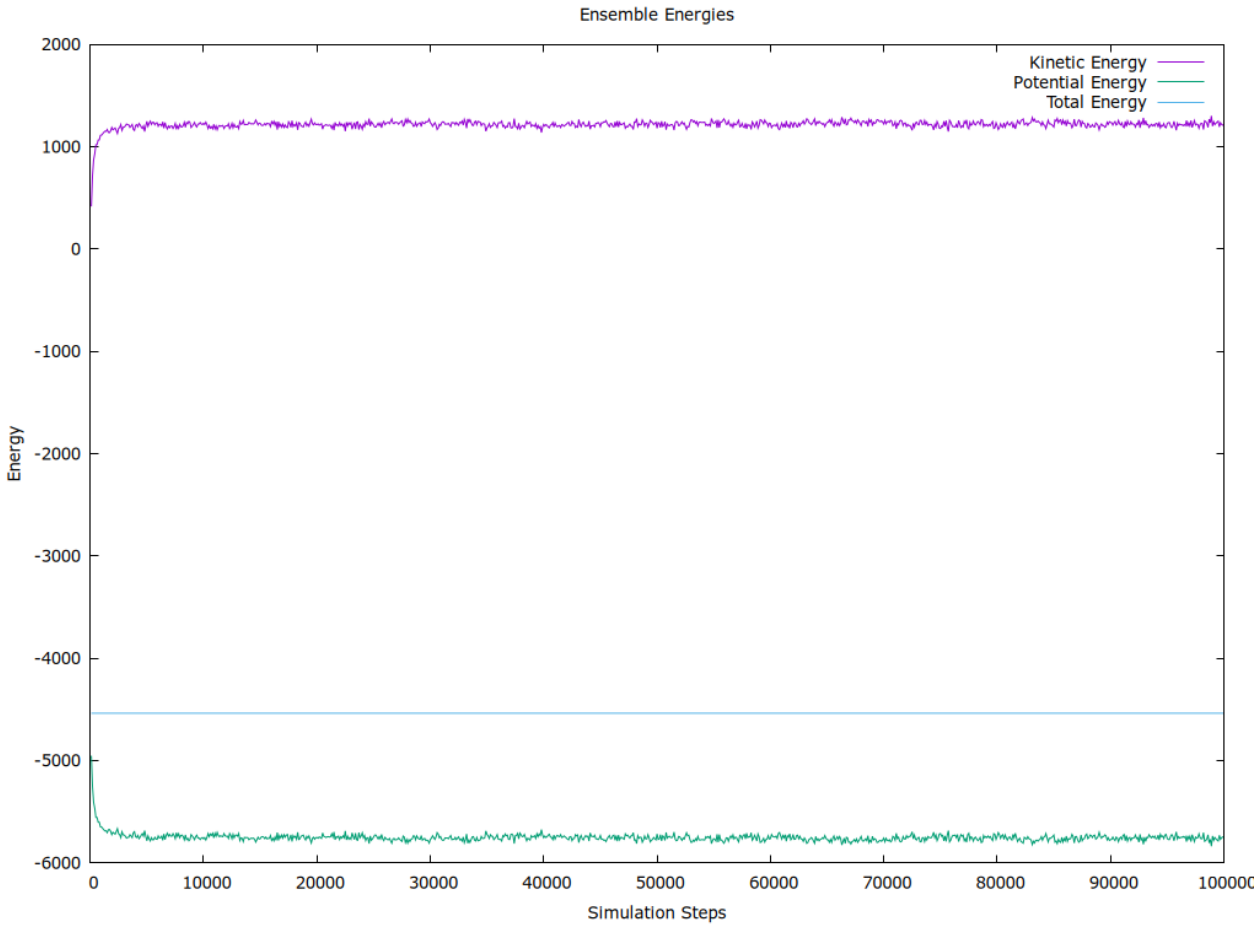
Contents

1 NVE Checks

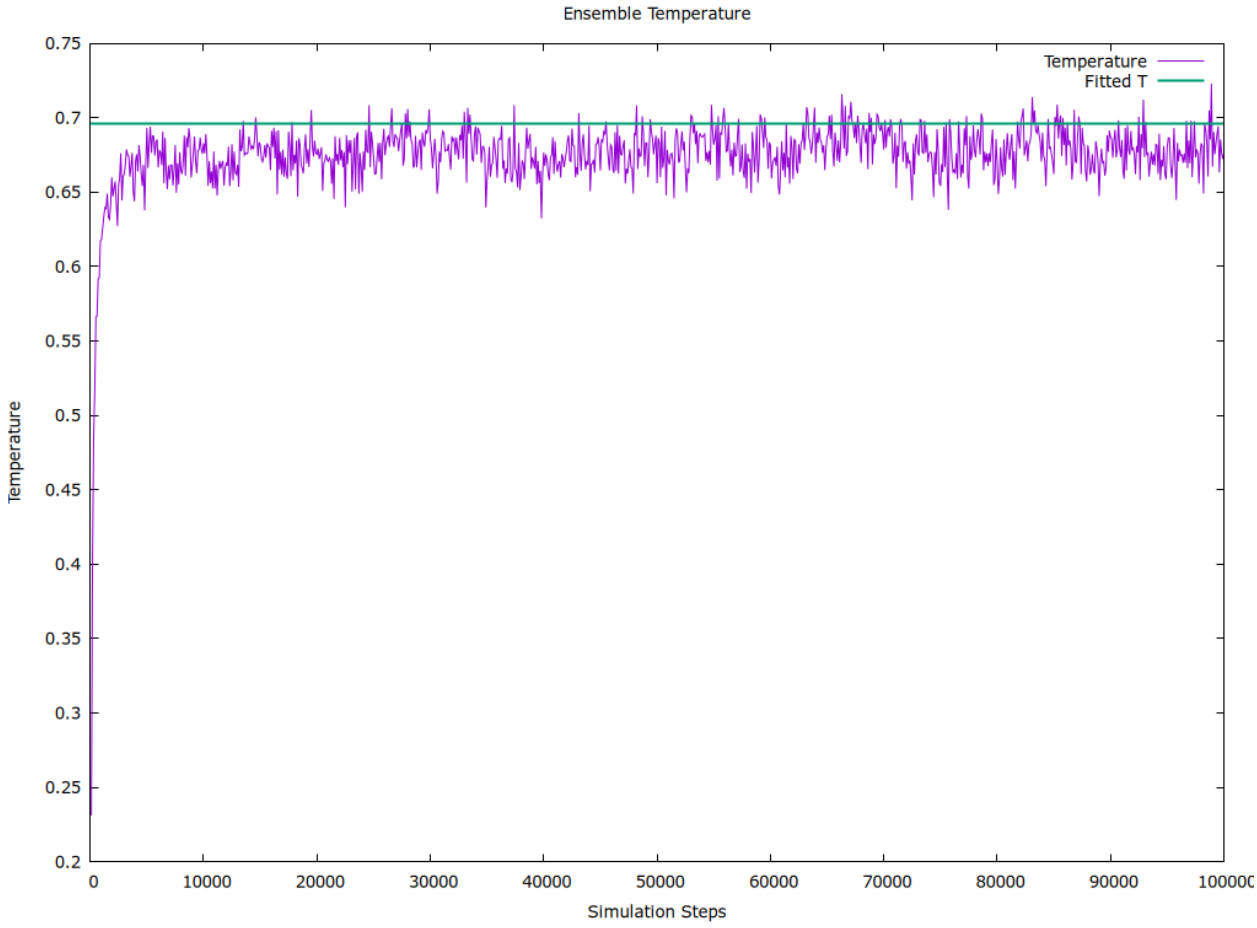
1.1 Parameters

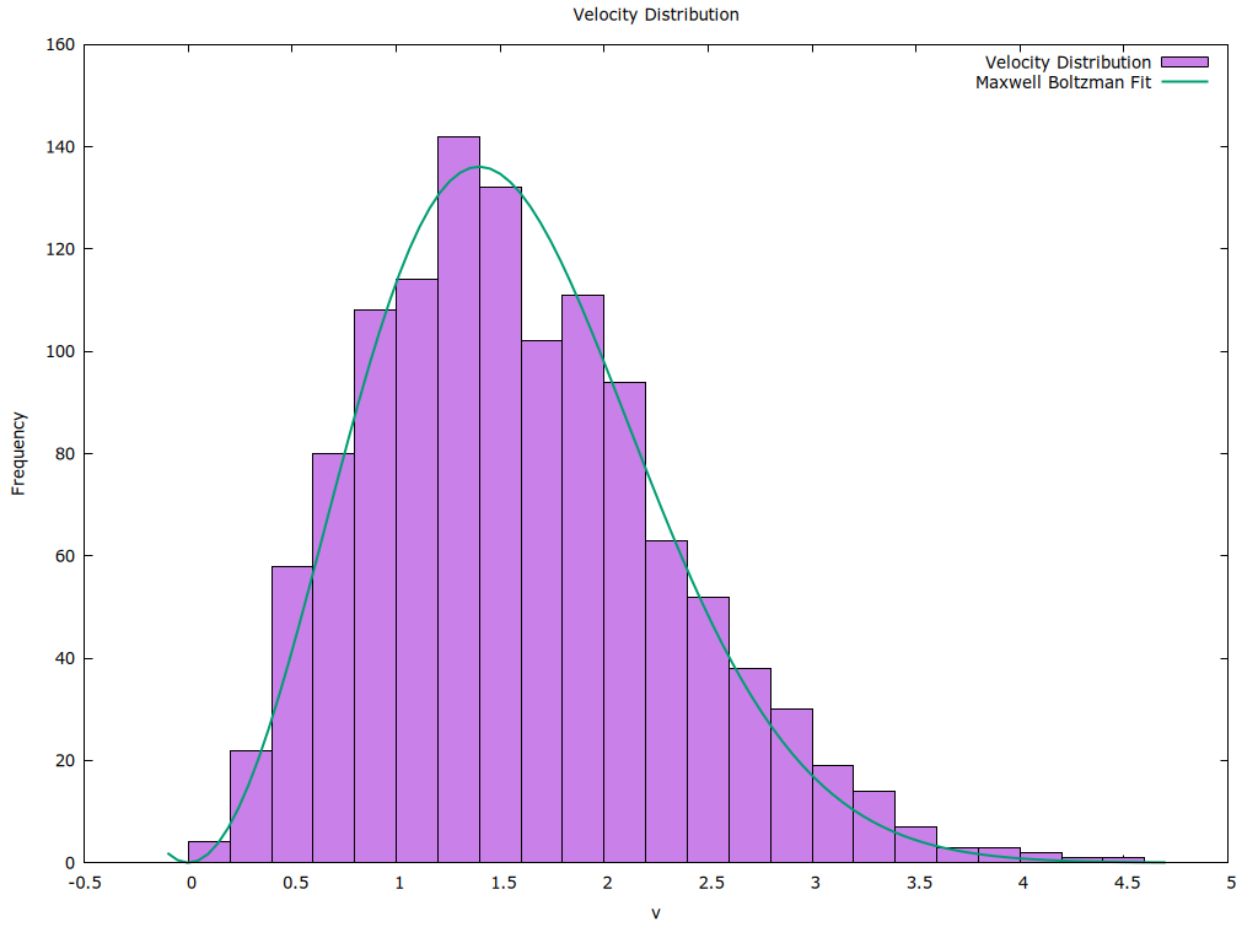
Temperature	$T_i^* = 0.28 \implies T_i = 1960K$
Density	$\rho^* = 1.655 \implies \rho = 4.475\text{g/cm}^3$
Pressure	$P^* = 2.37 \times 10^{-6} \implies P = 1$ atm
Number of Atoms	$N = 501$
	$N_{Si} = N_1 = 188$
	$N_O = N_2 = 376$

1.2 Energy

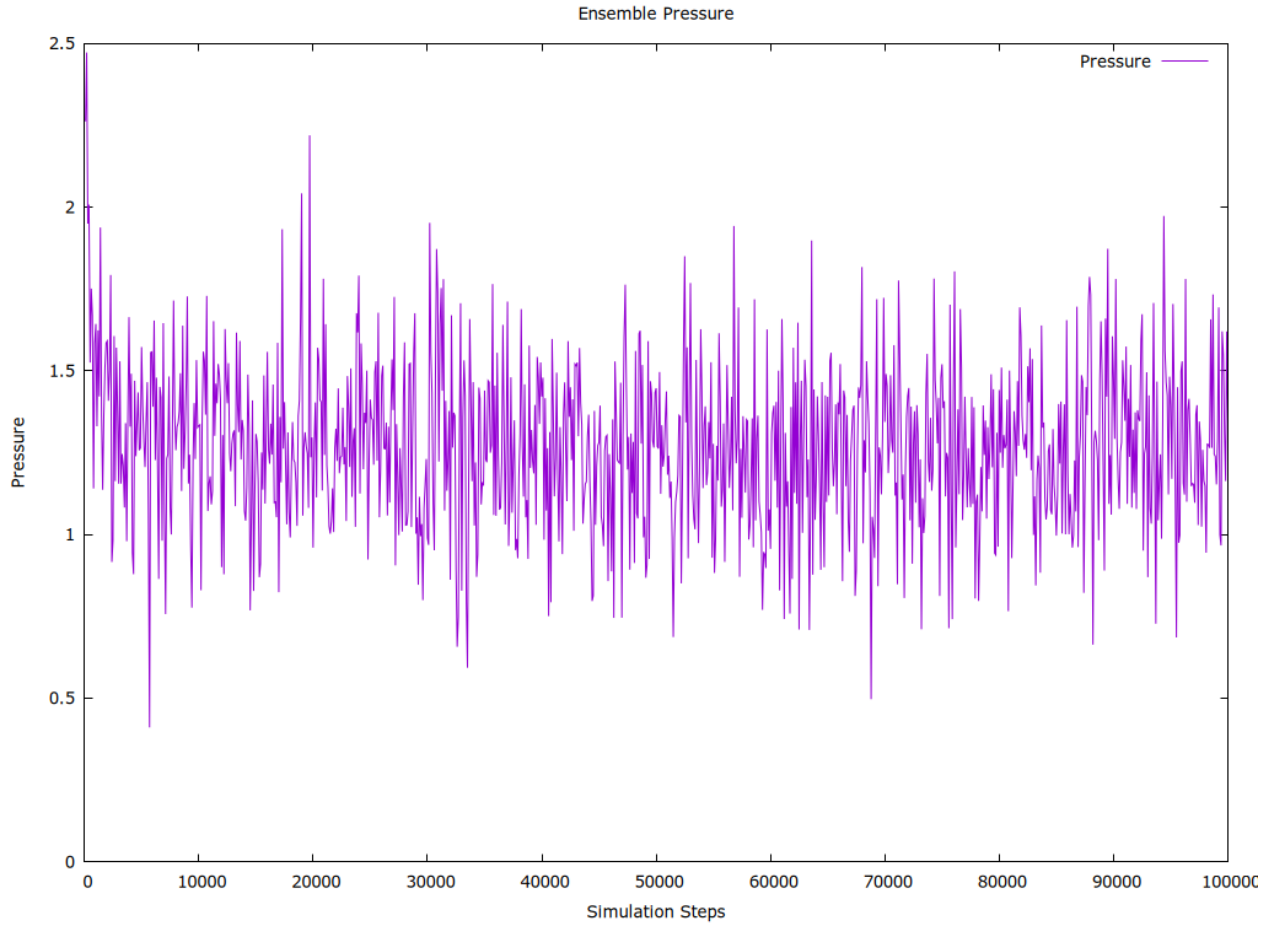


1.3 Temperature and Velocity Distribution

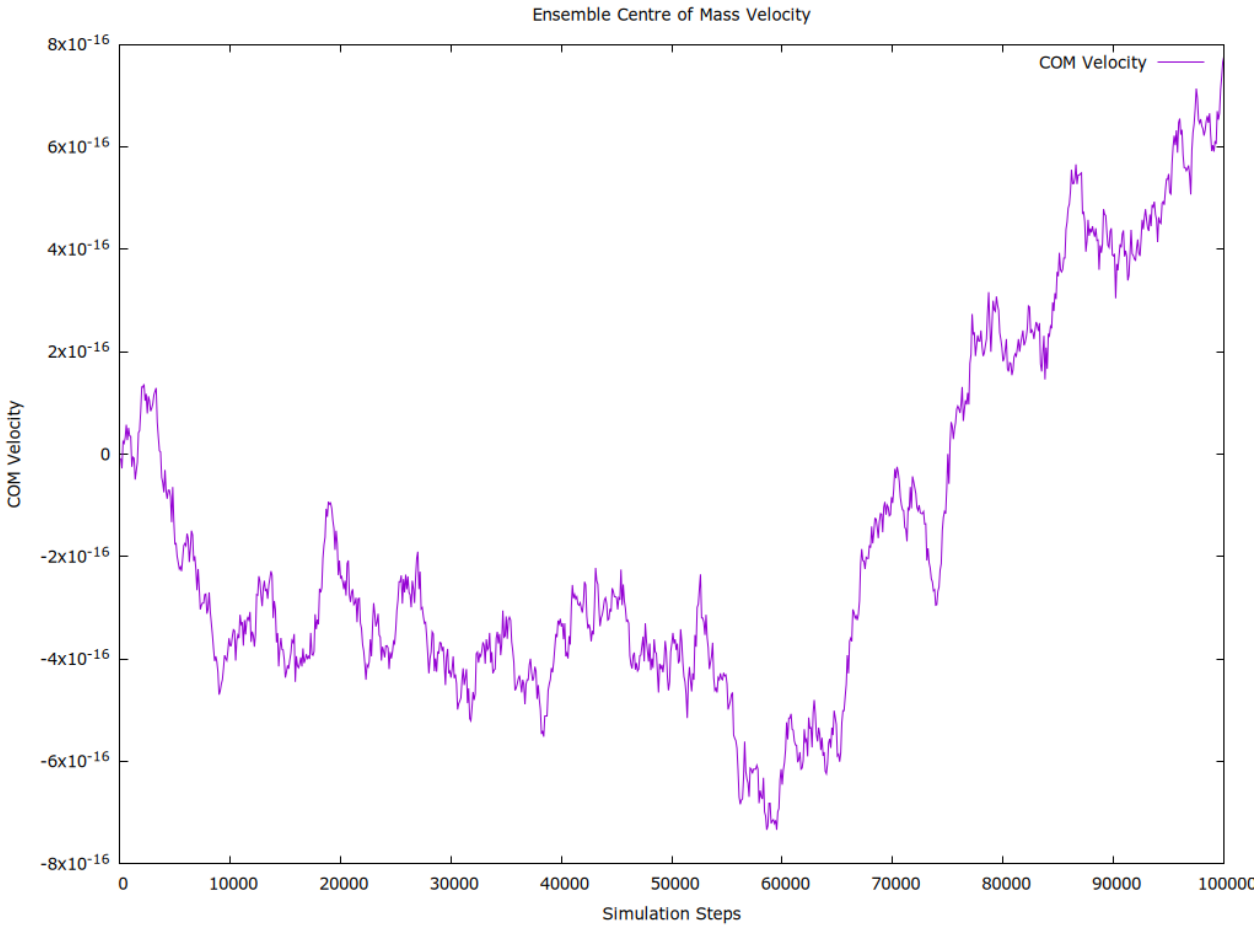


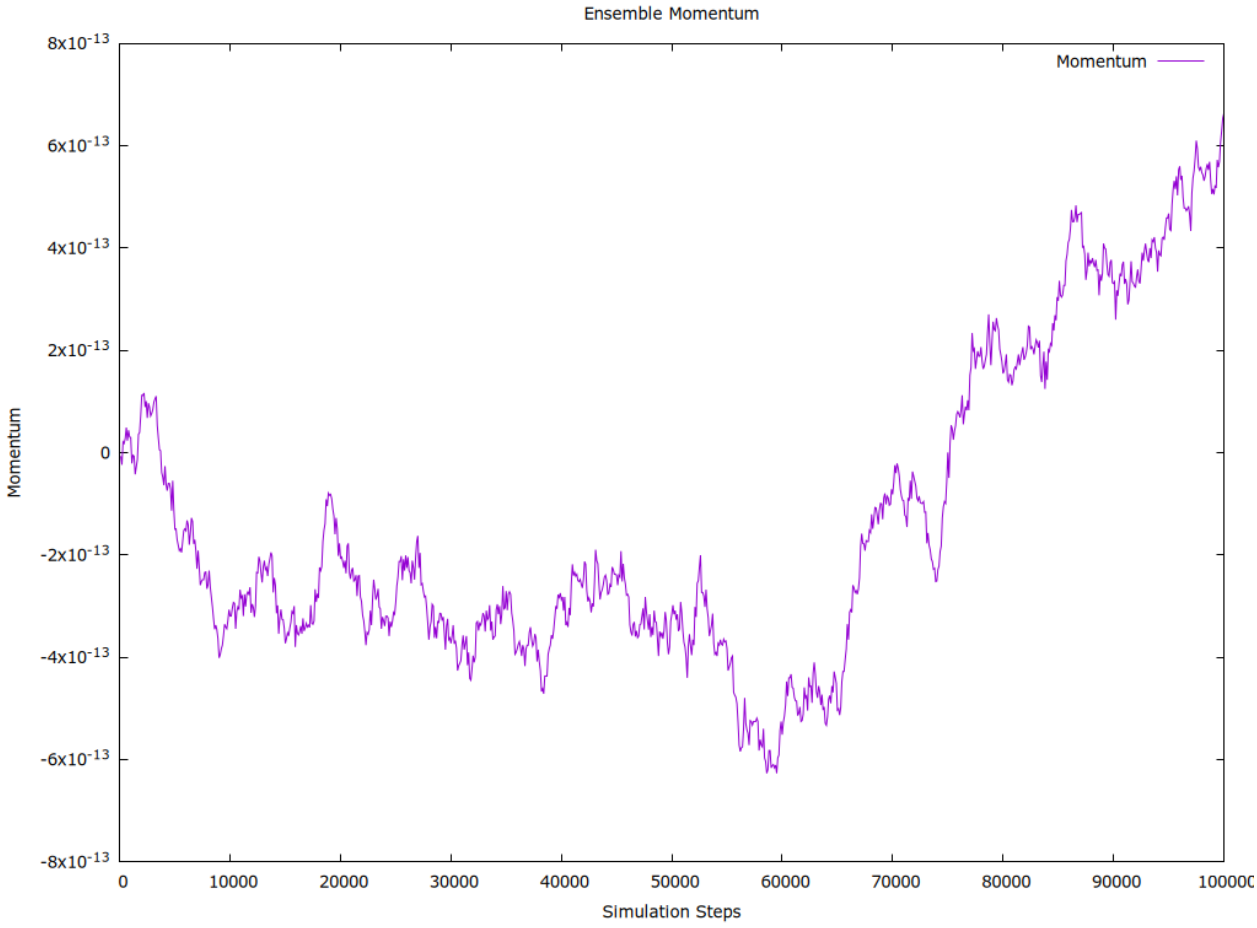

Velocity Distribution
Velocity Distribution
Maxwell Boltzman Fit
Frequency
v
160
140
120
100
80
60
40
20
0
-0.5
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5

1.4 Pressure


Ensemble Pressure
Pressure
Pressure
Simulation Steps
2.5
2
1.5
1
0.5
0
0
10000
20000
30000
40000
50000
60000
70000
80000
90000
100000

1.5 Ensemble Momentum and COM Velocity





2 Cooling Checks

2.1 Parameters

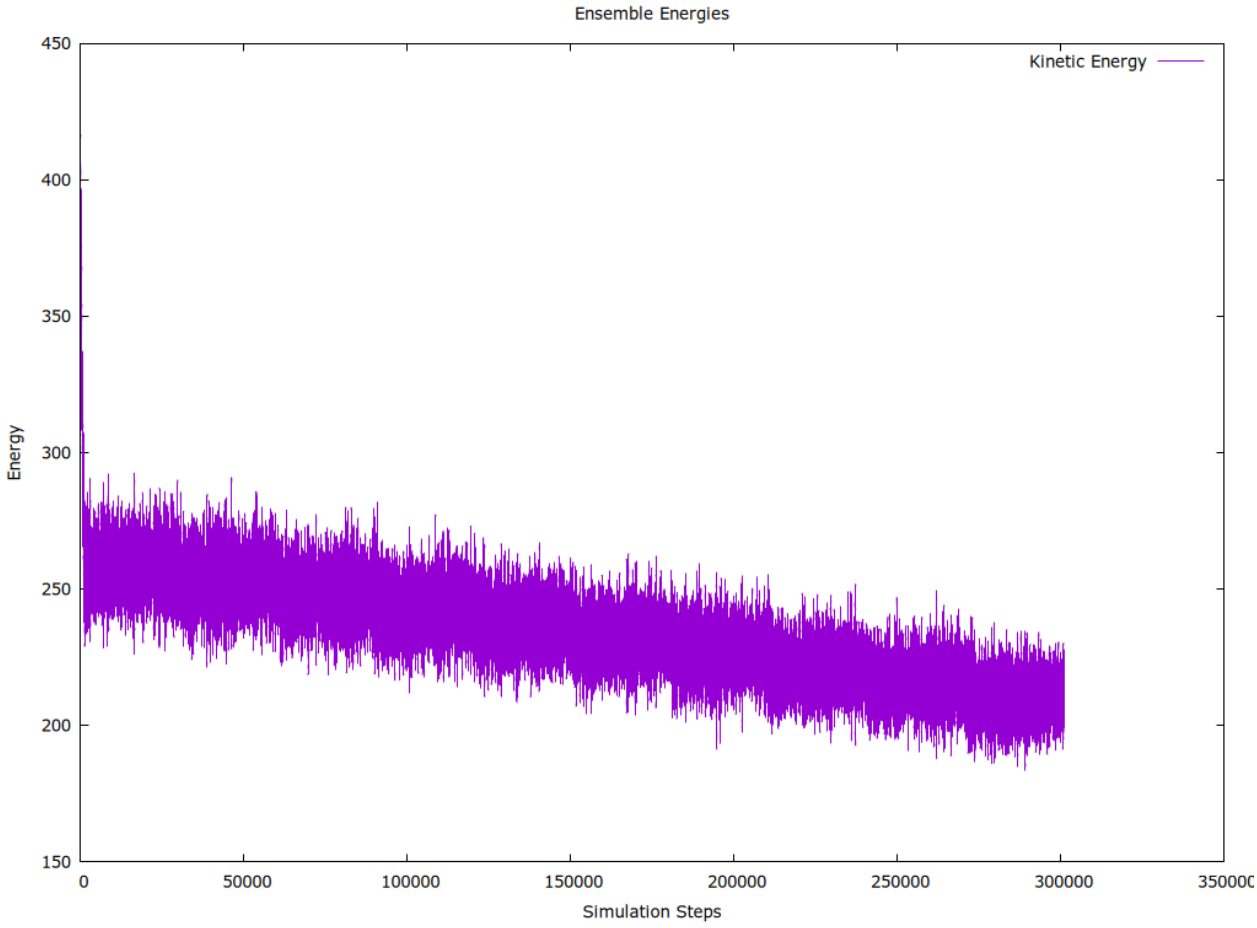
- Initial NVE Temperature T_{NVE}

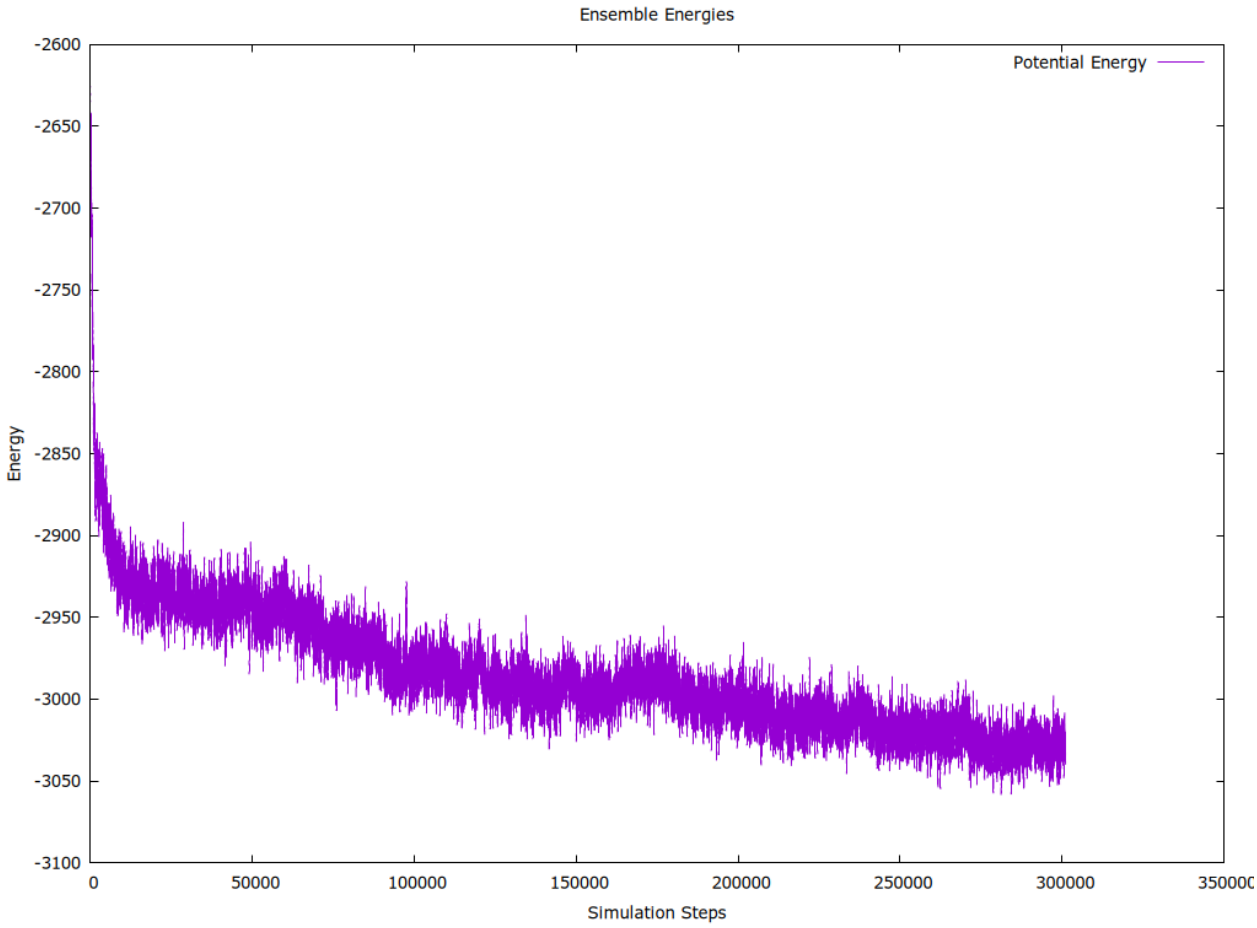
- Thermalize (Nose-Hover) to $T_f + 500K = T_f^* + 0.07$

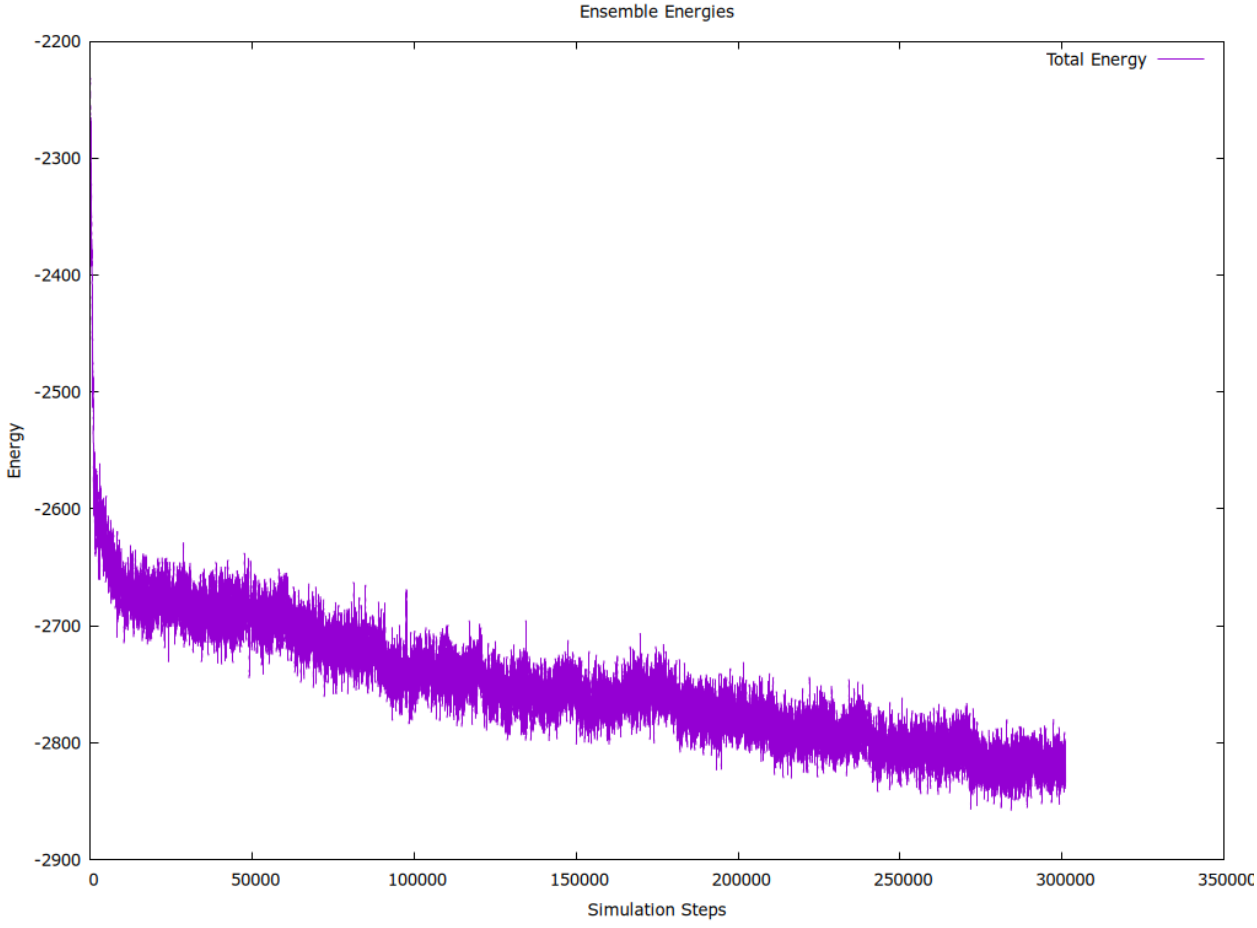
- Cooling to T_f in steps. Each cooling step involves rapid cooling for n_c, followed by thermalization (Nose-Hover) for n_t

2.2 $T_f^* = 0.28, \quad N = 501$

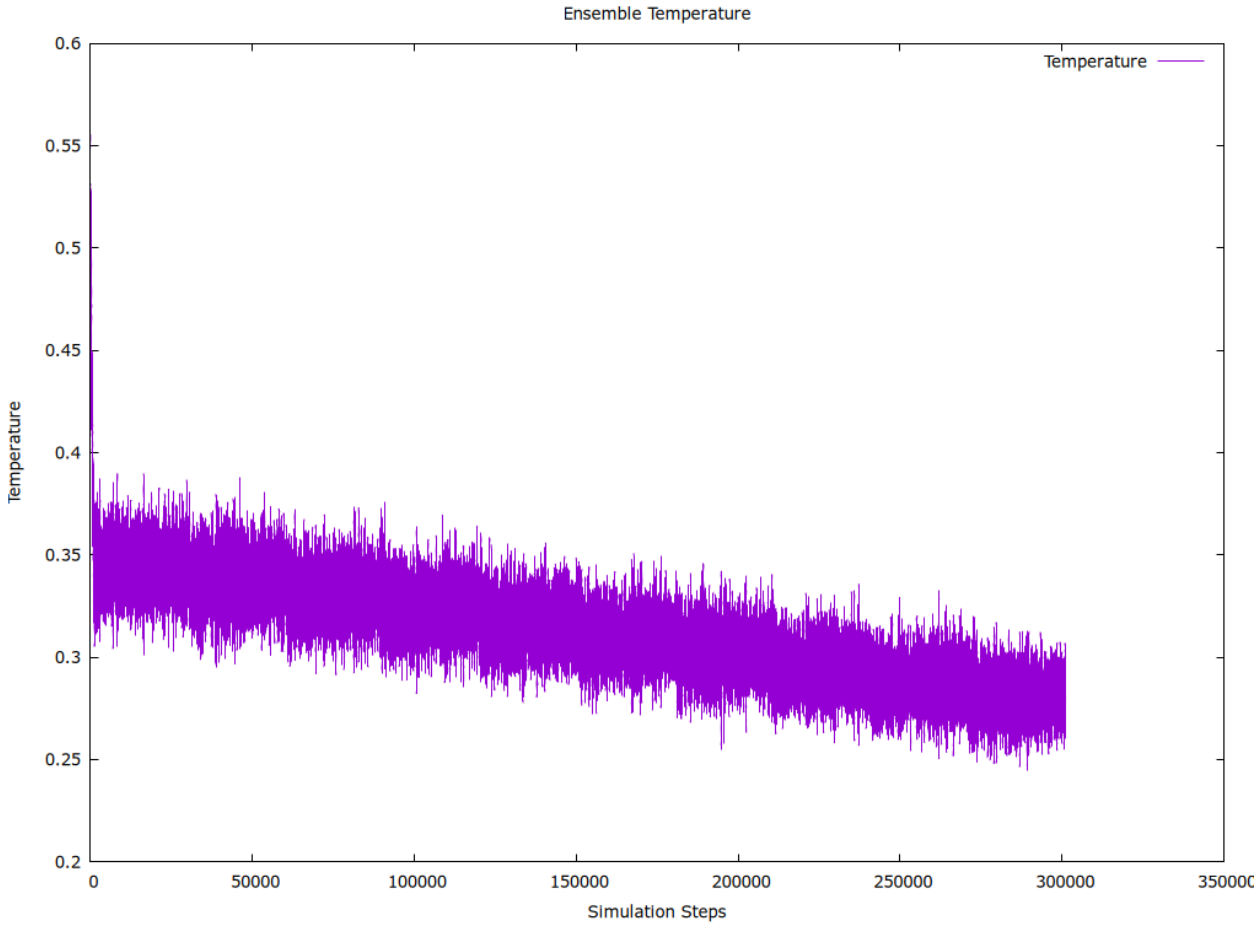
2.2.1 Energy



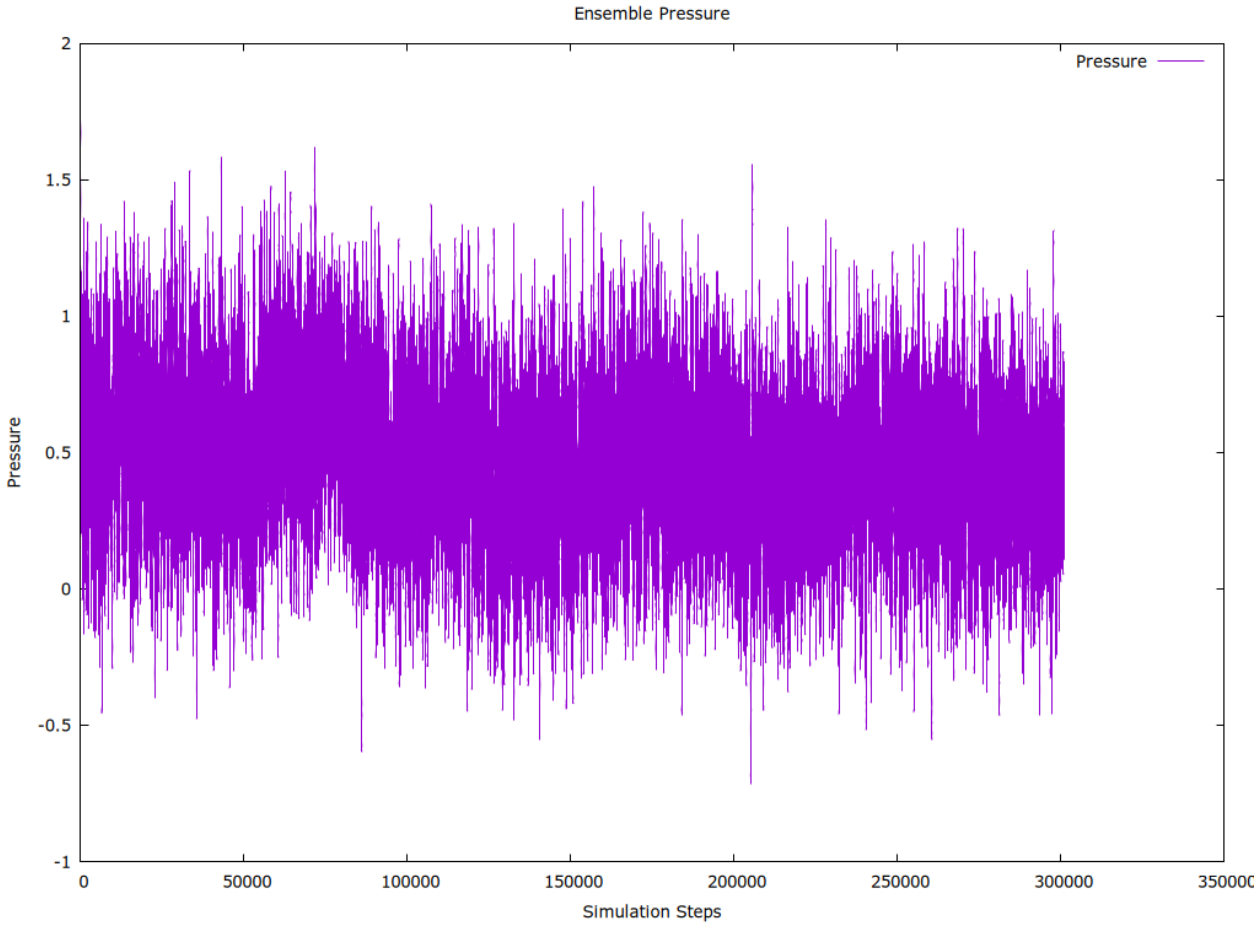

Ensemble Energies
Potential Energy
Energy
Simulation Steps
-2600
-2650
-2700
-2750
-2800
-2850
-2900
-2950
-3000
-3050
-3100
0
50000
100000
150000
200000
250000
300000
350000


Ensemble Energies
Total Energy
Energy
Simulation Steps
-2200
-2300
-2400
-2500
-2600
-2700
-2800
-2900
0
50000
100000
150000
200000
250000
300000
350000

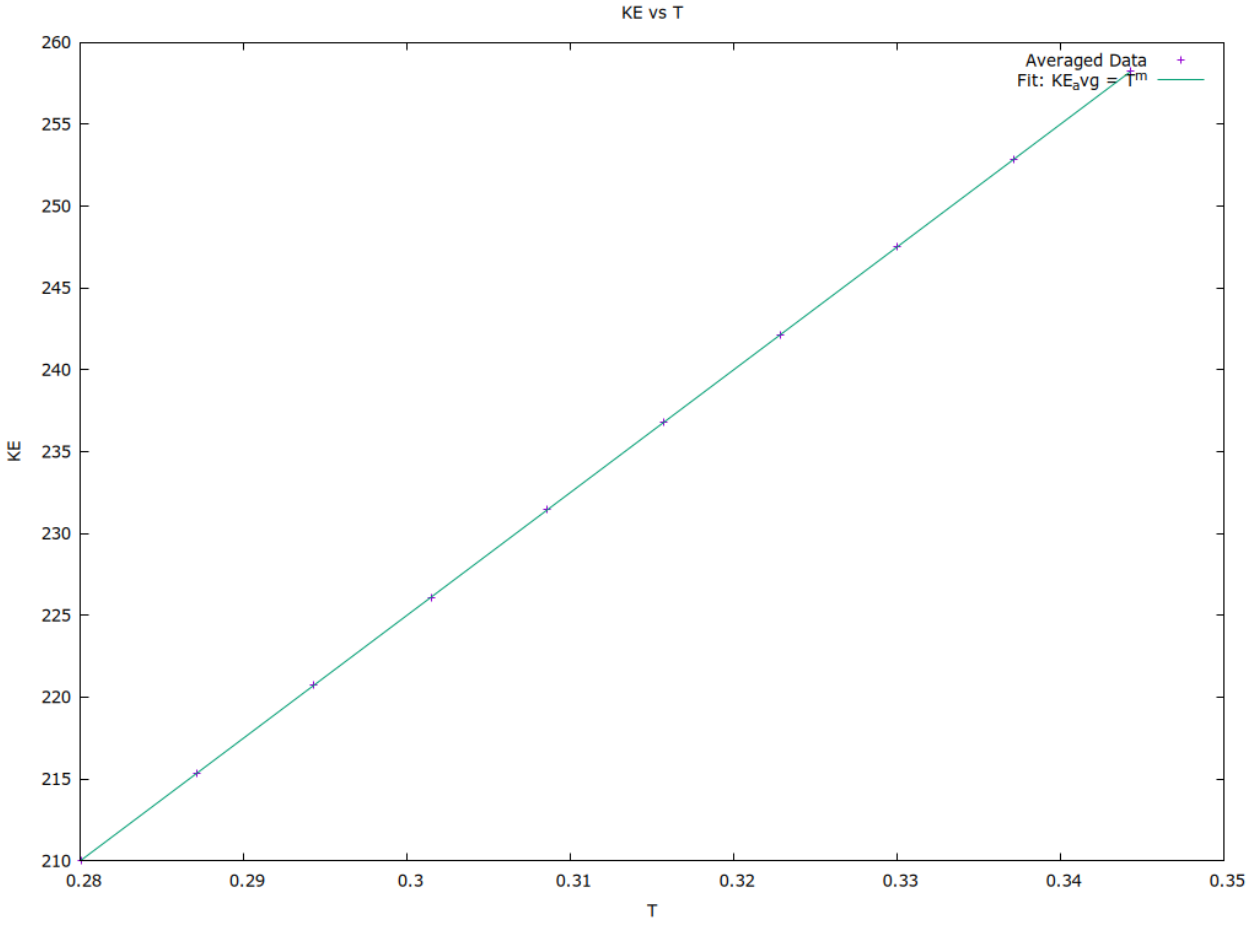
2.2.2 Temperature



2.2.3 Pressure



2.2.4 Average NVT Temperature vs KE

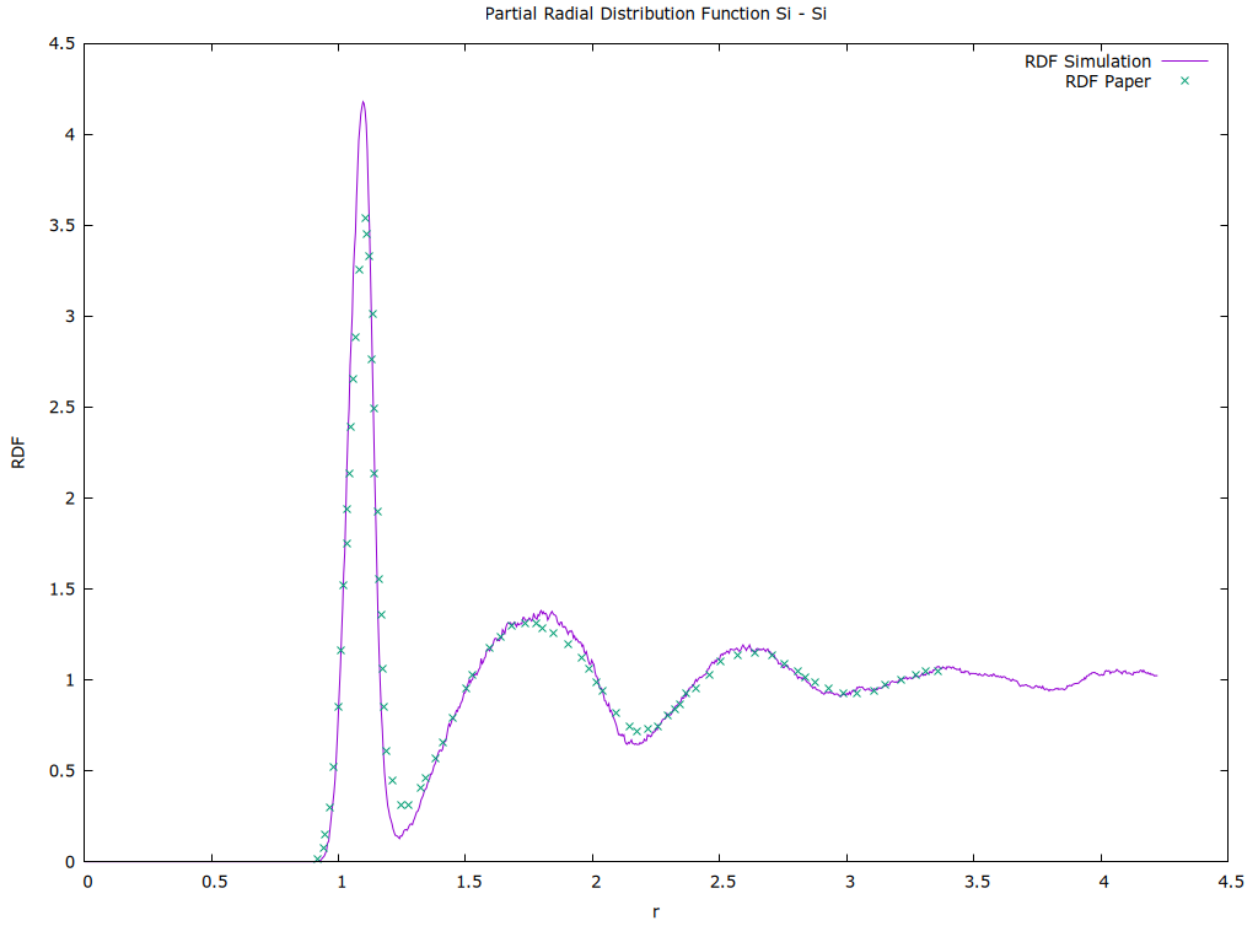


$$KE = \alpha T^m, \quad m = 0.99, \quad \alpha = 749.99$$

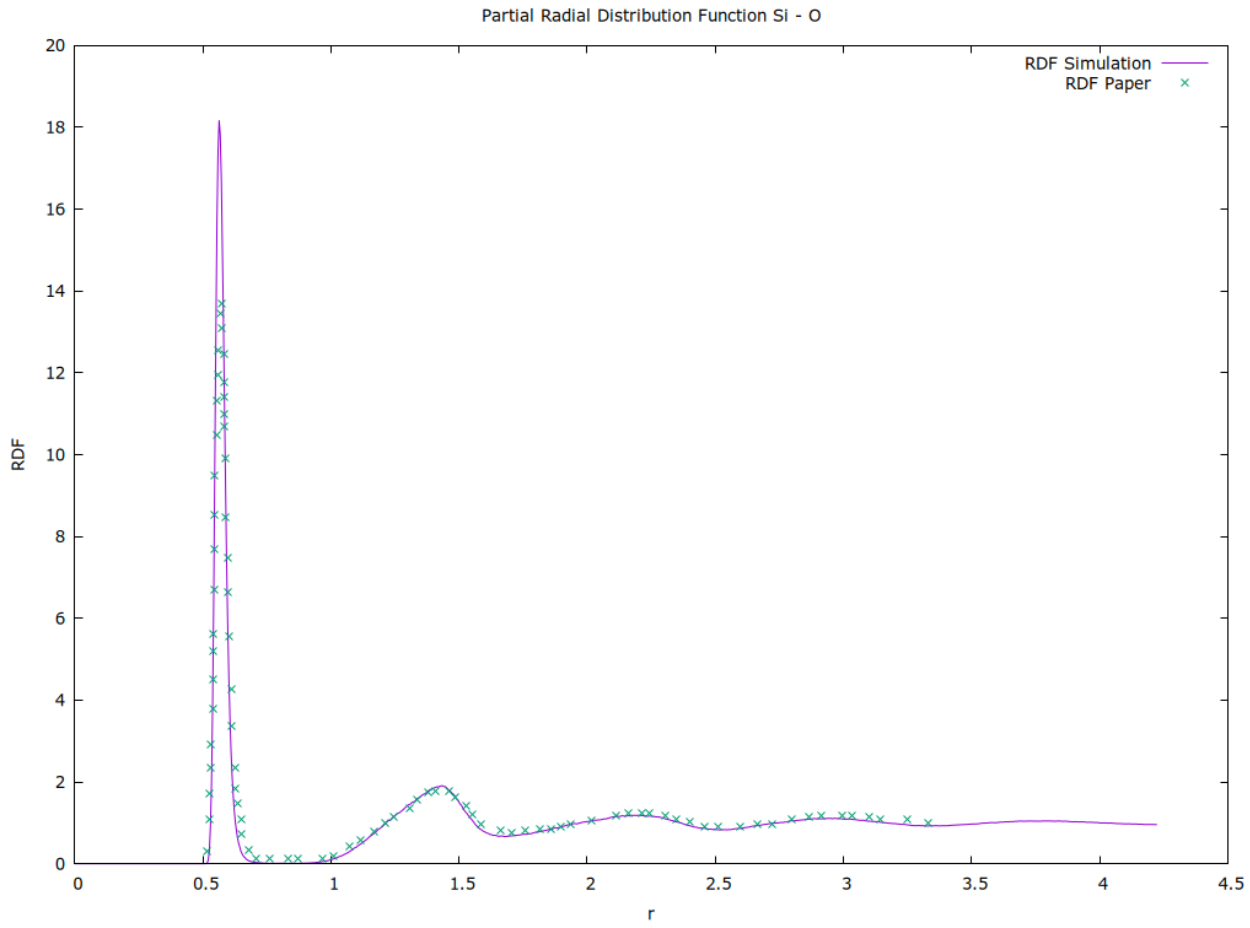
3 NVT Checks

3.1 Coslovich and Pastore RDF Check $T_f^* = 0.28, \quad N = 501, \quad \rho = 1.655$

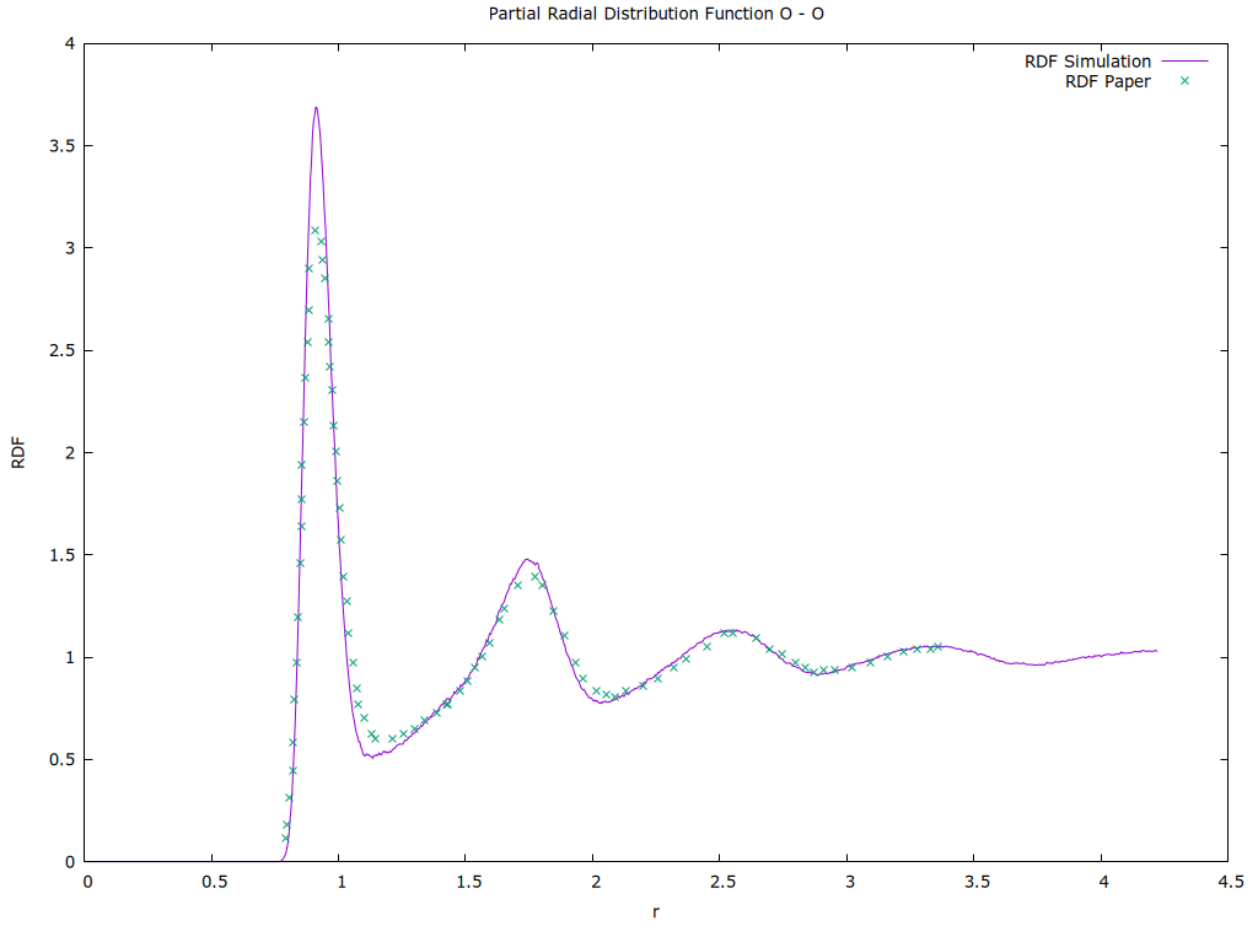
3.1.1 $g_{11}(r)$



3.1.2 $g_{12}(r)$



3.1.3 $g_{22}(r)$



3.1.4 Density Check

1. $N = 501, \quad \rho = 1.655$

$$
\begin{aligned}
z(R = 4.22113) &= 522.054 \\
R_0 = 4.22113 \implies \frac{4}{3}\pi R_0^3 &= 315.047 \\
N_{sim} = 501, \quad \rho &= 1.655 \\
\implies L = 6.71449326567 \implies L^3 &= 302.718
\end{aligned}
$$

$$
\begin{aligned}
\rho = \frac{N+1}{L^3} = \frac{z(R_0)}{\frac{4}{3}\pi R_0^3} &= 1.657 \\
\implies N + 1 = 501.7 \implies N &= 500.7 \approx 501
\end{aligned}
$$