Supporting information for: Efficient Computation of Entropy and Other Thermodynamic Properties for Two-Dimensional Systems Using Two-Phase Thermodynamic Model

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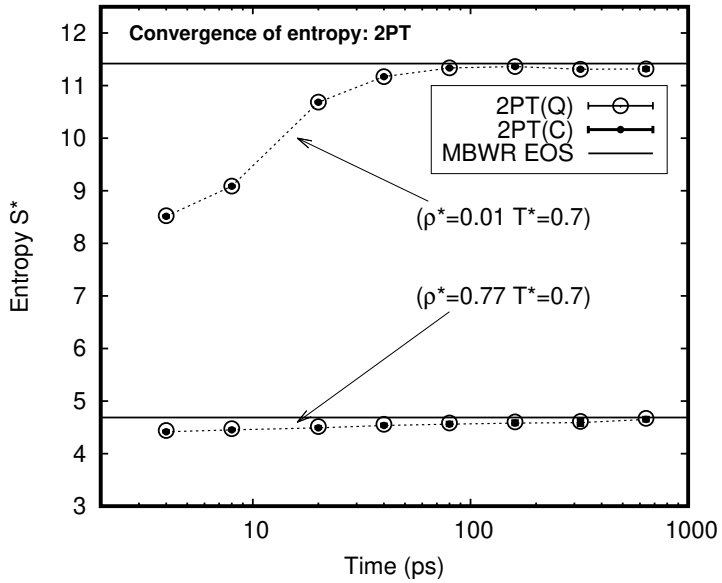


Figure S1: Convergence of entropy(per particle) with length of MD run for 2PT(2D) method. Integration time step of 8fs was used for MD simulations. The solid lines represent the MBWR EOS results for entropy of (ρ*=0.77, T*=0.7) and (ρ*=0.01, T*=0.7).

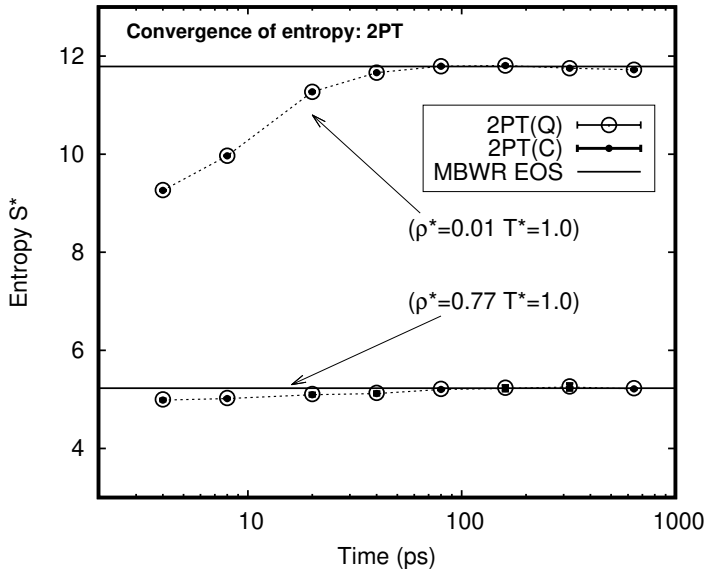
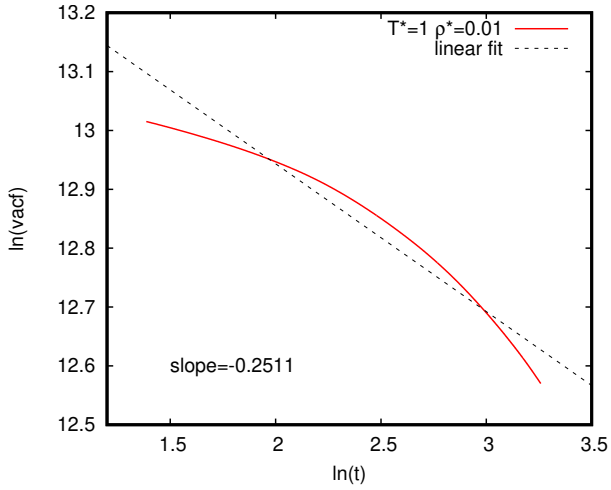
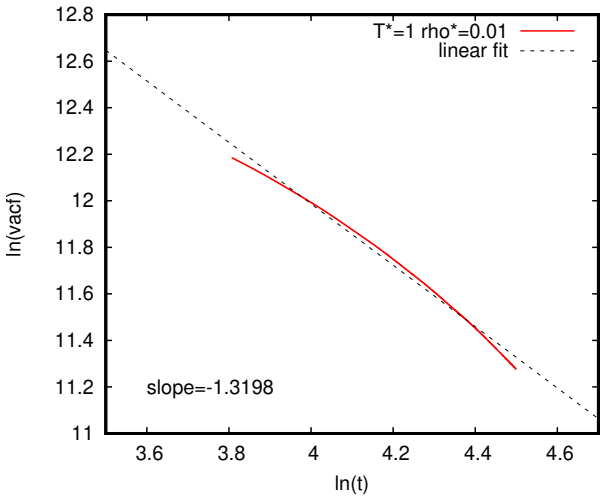


Figure S2: Convergence of entropy(per particle) with length of MD run for 2PT(2D) method. Integration time step of 8fs was used for MD simulations. The solid lines represent the MBWR EOS results for entropy of (ρ*=0.77, T*=1.0) and (ρ*=0.01, T*=1.0).

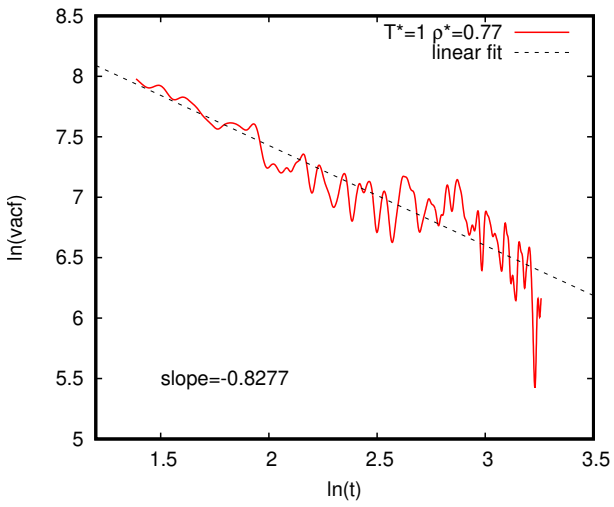


(a) Time 4 ps to 26 ps

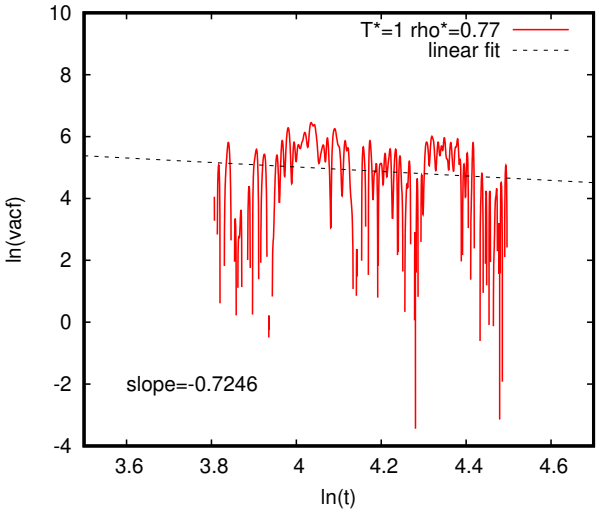


(b) Time 45 ps to 90 ps

Figure S3: The above figures are the log-log plot of the velocity autocorrelation function (VACF) and time at $T^* = 1$, $\rho^* = 0.01$. Slope of the log-log plot shows that at later times (45 ps to 90 ps), the VACF decays faster than t^{-1} for $T^* = 1$, $\rho^* = 0.01$.

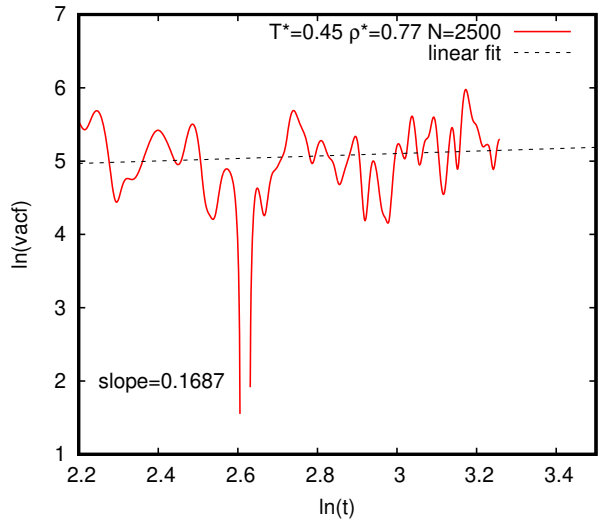


(a) Time 4 ps to 26 ps

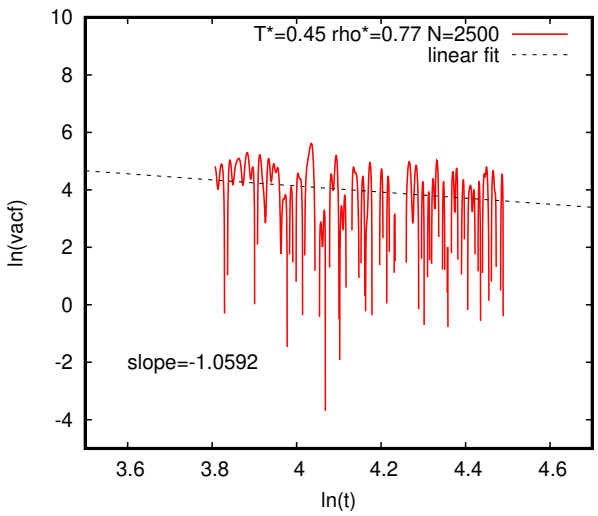


(b) Time 45 ps to 90 ps

Figure S4: The above figures are the log-log plot of the velocity autocorrelation function (VACF) and time at $T^* = 1$, $\rho^* = 0.77$. Unlike the $\rho^* = 0.01$ case, the velocity autocorrelation function for $T^* = 1$, $\rho^* = 0.77$ decays slower than t^{-1} till 90 ps. Analysis of times greater than 90 ps for $T^* = 1$, $\rho^* = 0.77$ are examined Figure S7

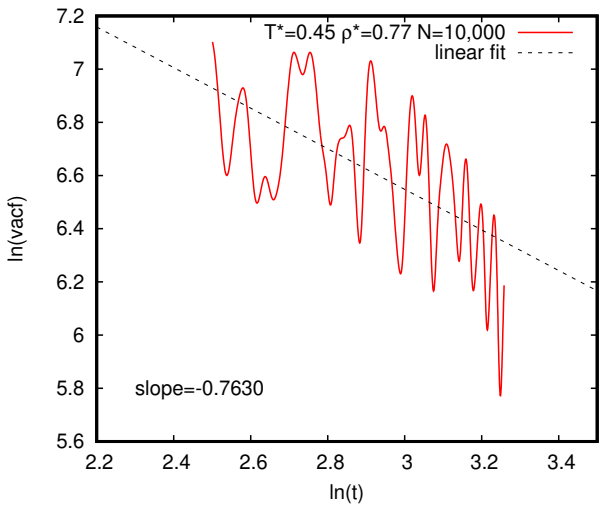


(a) Time 12 ps to 26 ps

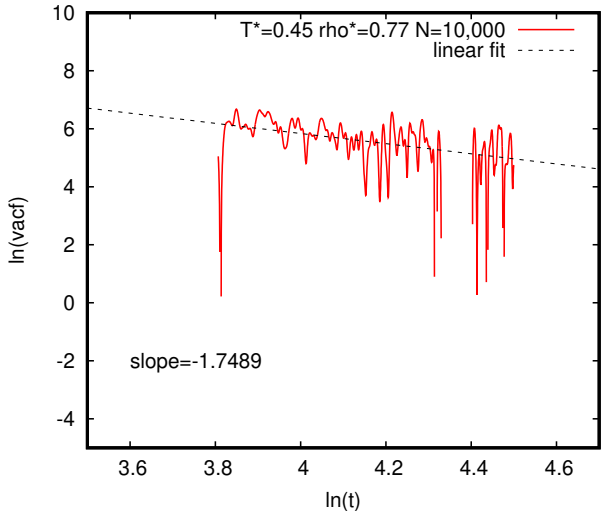


(b) Time 45 ps to 90 ps

Figure S5: The above figures are the log-log plot of the velocity autocorrelation function (VACF) and time at $T^* = 0.45$, $\rho^* = 0.77$ and number of particles N=2500. Slope of the log-log plot shows that at later times (45 ps to 90 ps), the VACF decays faster than t^{-1} for $T^* = 0.45$, $\rho^* = 0.77$.



(a) Time 12 ps to 26 ps



(b) Time 45 ps to 90 ps

Figure S6: The above figures are the log-log plot of the velocity autocorrelation function (VACF) and time at $T^* = 0.45$, $\rho^* = 0.77$ and number of particles N=10,000 (System size of N=2500 was used for all other simulations). Slope of the log-log plot shows that at later times (45 ps to 90 ps), the VACF decays faster than t^{-1} for $T^* = 0.45$, $\rho^* = 0.77$.

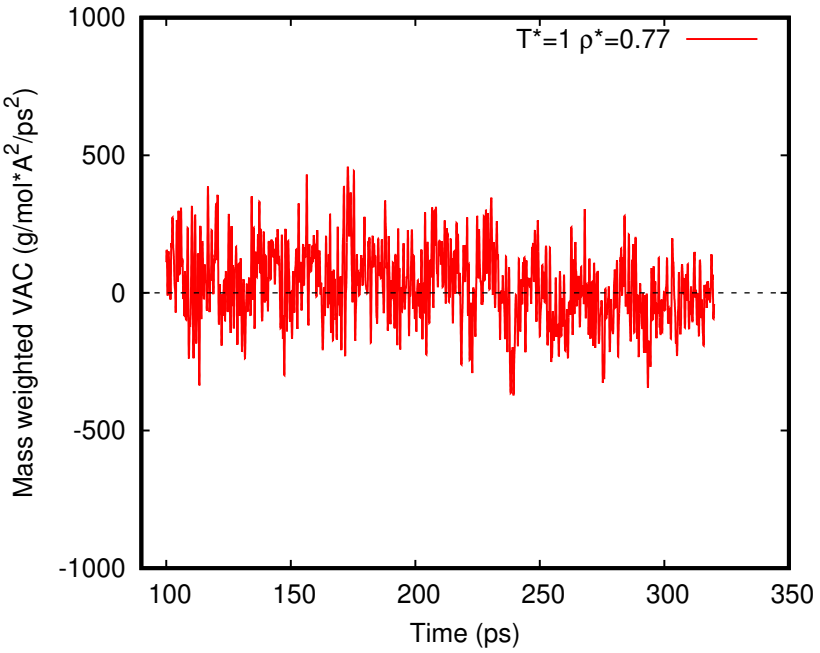


Figure S7: Velocity autocorrelation function (VACF) plotted against time from 100 ps to 320 ps for $T^* = 1$, $\rho^* = 0.77$.

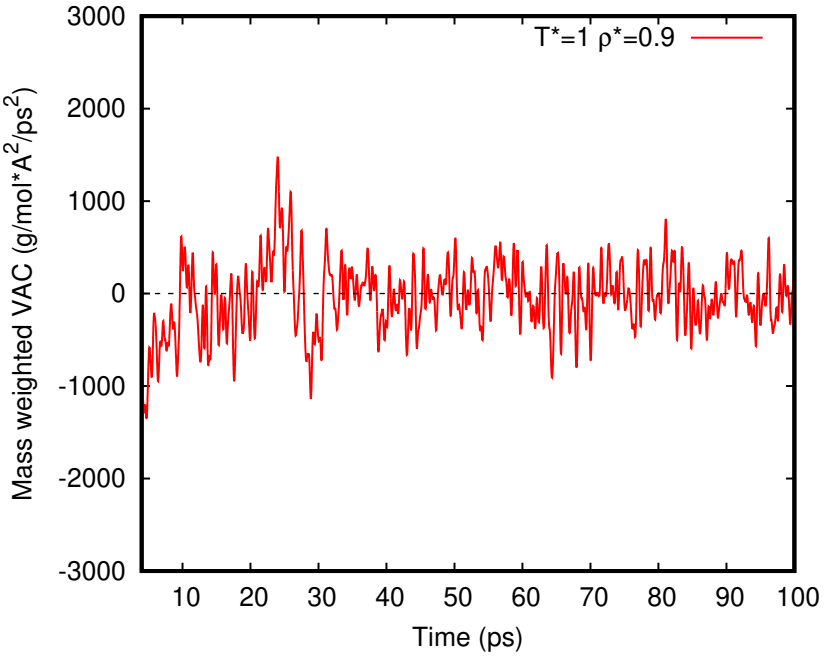


Figure S8: Velocity autocorrelation function (VACF) plotted against time from 10 ps to 100 ps for $T^* = 1.0$, $\rho^* = 0.9$.

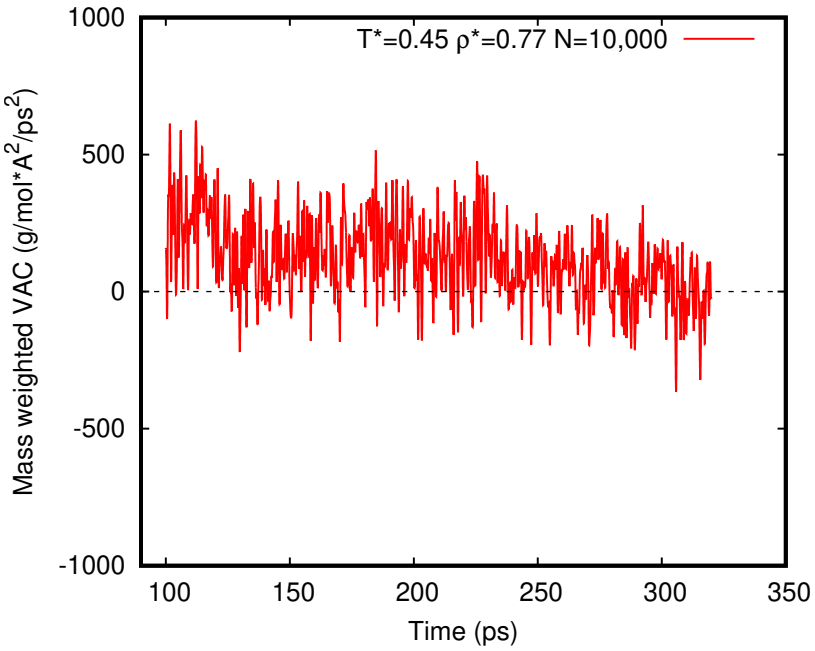


Figure S9: Velocity autocorrelation function (VACF) plotted against time from 100 ps to 320 ps for $T^* = 0.45$, $\rho^* = 0.77$ and N=10,000.