Validation of Diblock Coploymer MC moves

In order to validate the various Monte Carlo moves contained within Simpatico, a test was performed to compare equilibrated systems. The systems of diblock copolymers were brought to equilibrium using four separate sets of simulation techniques.

The main objective of this validation was to ensure the correctness of the mc EndSwap and the mc Reptation moves specifically for diblock simulations.

The systems that were simulated were 588 molecules of length 32. The diblocks were each of length 16 within the molecules of 32.

For these simulations a k for the Harmonic Bond constant was taken to be 400 and the average bond length was taken as one. In order to acccount for more realistic repulsion, epsilon values were set at 1.00 and 1.10 for the diblock. Sigma for these simulations remained at 1.00.

In order to determine adequate equilibration, the Auto correlation function was exained for each of the cases. Whenever possible, the data gathering simulations were run for roughly double the amount of time that it took the systems correlation function to decay to zero.

The MD simulation was performed in a constant NVT ensemble in order to compare to the MC moves tested. Since the MD simulation has been thoroughly validated, it serves as a good model to test the recently changed MC moves.

Alone, HybridMd did not seem to be the most effective simulation tool. However, when paired with the EndSwap or Reptation moves, equilibration proceeded more rapidly.

As shown in the table below, it seems as though the Endsawp move resulted in a better equilibration than any of the other methods.

The next step for these Monte Carlo moves will be to combine them in order to find an effective mix of moves in order to equilibrate larger, more comlex systems in a reasonable amount of CPU time.

Move/Simulation	steps	acceptance	Potential Energy		Radius of Gyration	
			average	standard deviation	average	standard deviation
mdNVT	5.00000E+06	NA	1.40928E+04	1.23031E+02	9.77513E+00	1.41325E-01
mc HybridMd	3.00000E+05	NA	1.40770E+04	9.97240E+01	9.52845E-01	1.91781E-01
mc EndSwap	4.00000E+06	0.1040	1.40084E+04	1.46233E+02	9.49169E+00	5.60263E-02
mc Reptation	3.00000E+06	0.8376	1.40879E+04	1.19463E+02	9.89246E+00	1.20102E-01

Table 1-Validation data for diblock simulations (all at dt = 0.001)