Requested Resources

Description	# of total processors (# of nodes)	Estimated # of systems to simulate	Walltime estimate (CPU time)	Resource Units estimate
1. **Interaction strengths at various volume fractions:** Adjust polymer-nanoparticle interaction strength ε and volume fractions to test for polymer conformations around NP surfaces for homopolymers	48 (4)	32	48×32×60hr	10,000
2. **Deformation and mechanical behavior:** Test the effect of interaction strength on mechanical behavior	48 (4)	16	48×16×60hr	5,000
3. **Copolymer interaction with nanoparticle:** Change homopolymer systems to copolymer system to test the effect of interaction between copolymer and nanoparticles by changing interaction parameter ε between respective copolymer types and polymer-nanoparticle	48 (4)	64	48×64×60hr	18,000
4. **End-grafted nanoparticles:** Graft polymers to nanoparticle to see effect of polymer dynamics in FCC arrangement vs random NP arrangement at different grafting densities and compare to un-grafted systems	48(4)	40	48×40×60hr	12,000
5. **Effect of NP arrangement and volume fraction:** Study the effect of NP volume fraction and arrangement (FCC vs. random) on polymer dynamics with grafted and un-grafted nanoparticles	48(4)	52	48×52×60hr	15,000
TOTAL		**204**	**587,520**	**60,000**

These estimates are based on preliminary simulations done on Oakley cluster, which took ~60hrs; the preliminary work considered multiple un-grafted nanoparticle systems with low and high molecular weight polymers (simulation time is proportional to chain length squared). Grafted systems are expected to be the same.

We would also like to see a measure of the performance of the code - some measure of efficiency of the computational methodology.