Tutorial

Descriptors

* Molecular Dynamics
* Solvated Polymer-Grafted Nanoparticles
* Implicit Solvent
* Fixed Distance
* Obtainment of Force versus Distance Profiles

Instructions

1. Determine the values of interest for ${nanoparticle\_radius}, ${length\_grafted\_chains}, ${target\_grafting\_density}, and ${epsilon\_mon\_mon\_attractive}
2. On Finder, navigate to  
   /Users/felipe.pace.evaristo/Library/CloudStorage/Dropbox/Mac/Desktop/Projects/Solvated Polymer-Grafted Nanoparticles/Molecular Dynamics/Implicit Solvent/Fixed Distance/
3. On <https://ondemand.osc.edu/>, log in and open a second OnDemand tab
4. On the first tab, go to Active Jobs
5. On the second tab, go to Files and navigate to  
   /fs/scratch/PAS2029/felipepacci/Projects/Solvated\_Polymer\_Grafted\_Nanoparticles/Molecular\_Dynamics/Implicit\_Solvent/Fixed\_Distance/
6. Upload 18 relevant files in  
   /Users/felipe.pace.evaristo/Library/CloudStorage/Dropbox/Mac/Desktop/Projects/Solvated Polymer-Grafted Nanoparticles/Molecular Dynamics/Implicit Solvent/Fixed Distance/   
   to  
   /fs/scratch/PAS2029/felipepacci/Projects/Solvated\_Polymer\_Grafted\_Nanoparticles/Molecular\_Dynamics/Implicit\_Solvent/Fixed\_Distance/
7. On the Files tab of OnDemand, edit params.sh to set the values of ${nanoparticle\_radius}, ${length\_grafted\_chains}, ${target\_grafting\_density}, and ${epsilon\_mon\_mon\_attractive} in params.sh to the desired values
8. On Terminal, enter  
   ssh -X -Y [felipepacci@cardinal.osc.edu](mailto:felipepacci@pitzer.osc.edu)
9. On Terminal, enter  
   cd /fs/scratch/PAS2029/felipepacci/Projects/Solvated\_Polymer\_Grafted\_Nanoparticles/Molecular\_Dynamics/Implicit\_Solvent/Fixed\_Distance/
10. On Terminal, enter  
    chmod u+x \*.sh

and

chmod u+x \*.py

1. On Terminal, enter  
   ./job\_setup\_PGNs\_implicit\_solvent\_fixed\_distance\_soft\_pushoff.sh
2. On the Files tab of OnDemand, navigate to /fs/scratch/PAS2029/felipepacci/Projects/Solvated\_Polymer\_Grafted\_Nanoparticles/Molecular\_Dynamics/Implicit\_Solvent/Fixed\_Distance/${nanoparticle\_radius}/${length\_grafted\_chains}/${target\_grafting\_density}/${epsilon\_mon\_mon\_attractive}/
3. On Terminal, enter  
   cd /fs/scratch/PAS2029/felipepacci/Projects/Solvated\_Polymer\_Grafted\_Nanoparticles/Molecular\_Dynamics/Implicit\_Solvent/Fixed\_Distance/${nanoparticle\_radius}/${length\_grafted\_chains}/${target\_grafting\_density}/${epsilon\_mon\_mon\_attractive}/
4. On Terminal, enter  
   ./warning\_error\_dangerous\_builds\_verification.sh
5. On Terminal, enter  
   ./job\_setup\_PGNs\_implicit\_solvent\_fixed\_distance\_equilibration\_nvt.sh
6. On Terminal, enter  
   ./warning\_error\_dangerous\_builds\_verification.sh
7. On Terminal, enter  
   exit
8. On Terminal, enter  
   cd "/Users/felipe.pace.evaristo/Library/CloudStorage/Dropbox/Mac/Desktop/Projects/Solvated Polymer-Grafted Nanoparticles/Molecular Dynamics/Implicit Solvent/Fixed Distance/"
9. On Terminal, enter  
   ./data\_retrieval\_pgns\_implicit\_solvent\_fixed\_distance.sh
10. On Finder, navigate to  
    /Users/felipe.pace.evaristo/Library/CloudStorage/Dropbox/Mac/Desktop/Projects/Solvated Polymer-Grafted Nanoparticles/Molecular Dynamics/Implicit Solvent/Fixed Distance/${length\_grafted\_chains}/${target\_grafting\_density}/${epsilon\_mon\_mon\_attractive}/
11. On MATLAB, run PGNs\_implicit\_solvent.m
12. On line 119 of PGNs\_implicit\_solvent.m, adjust number\_values\_hyperaverage\_radii\_of\_gyration\_equilibrium
13. Ensure that reference\_radius\_of\_gyration\_equilibrium.txt contains the proper values of reference\_radius\_of\_gyration\_equilibrium and standard\_deviation\_radius\_of\_gyration\_equilibrium