LA-SIGMA Breakout Sessions
Biomolecular Materials

Science Challenge

- Working with experimental collaborators, provide computational insights into transport and interactions (environment/cellular milieu) of unimolecular and multimolecular drug delivery vehicles to affect targeted delivery
- Simulate large (10^6 atom) systems for long (10^-6 to 10^-3) periods time to characterize conformational barriers/uptake-release profiles/transport of delivery vehicles up to 10^6 g/mol
- Develop inter-atomic bio/non-bio potentials
- Develop accurate CG techniques to span scales and free energy methods to quantify barriers
- Develop/validate hybrid molec/continuum simulation codes for non-eq phenomena

Scientific Collaboration

- Identify expt/comp expt/comp scientist leaders in each team to serve as contact people to coordinate interdisc communication
- Contact people will coordinate weekly contact (to learn about directions each sub-group going in)/~monthly meeting
- Provide wikipages for each investigator to describe what doing in a 1 to 2 paragraph description and ~2 minute video that can be linked to RII webpage to inform what everyone doing
- Kickoff capabilities meeting (get to know you meetings)
- Write down computational challenges to make available to CTCI Make reports available up and down research hierarchy

Diversity, External Engagement, and Workforce Development

- Need to incentivize faculty to participate in open houses to engage high school URM students to meet faculty (using a stick or carrot)
- Recruit URM graduate students to speak at home institutions (UG and HS institutions) to provide actually role models to recruit
- Use the above ideas to also actively recruit teachers for RET programs
- Insure more personal contact of advisors with URM students
- Partner with local industry (like SHELL) to participate in their existing HS student recruitment programs to bring people to Louisiana

Teaching needs

- Biomaterials for Computationalists/Computational Biophysics for the Experimentalist: Series of ~40 one hour primer classes (only a UG science background assumed) to educate cross-disciplinary teams on capabilities of collaborators (what can expt or comp tell the others)