

LA-SIGMA Breakout Sessions

Monte Carlo

Science Challenge

- 1) Avoid the scaling problem in Monte Carlo by developing massively parallel hybrid-MC codes
- 2) Bypass multi-scale problems
- 3) Port open source classical MC codes to massively parallel architectures.
- 4) Developing scalable codes on heterogeneous machines for 10,000 nodes and GPUs

Scientific Collaboration

- 1) Develop modular codes in collaboration with CTCL group and
- 2) Integrate MC and DFT/forcefield codes
- 3) Job submission, data analysis, visualization, distributed data storage and reuse with CTCL
- 4) Heterogeneous computing
- 5) Close coupling with and possible unification with MD team

Diversity, External Engagement, and Workforce Development

- 1) Demos of MC for the public
- 2) How parallel computers work

Teaching needs

- 1) Modules for courses both within and without LA-SIGMA
- 2) Monte Carlo course