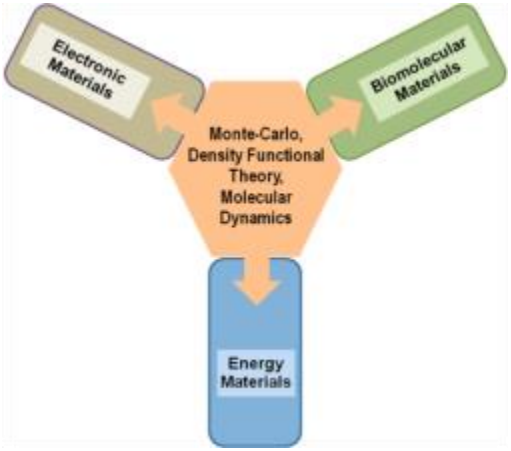
LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Computational Teams
Cybertools/Cyberinfrastructure
CTCI

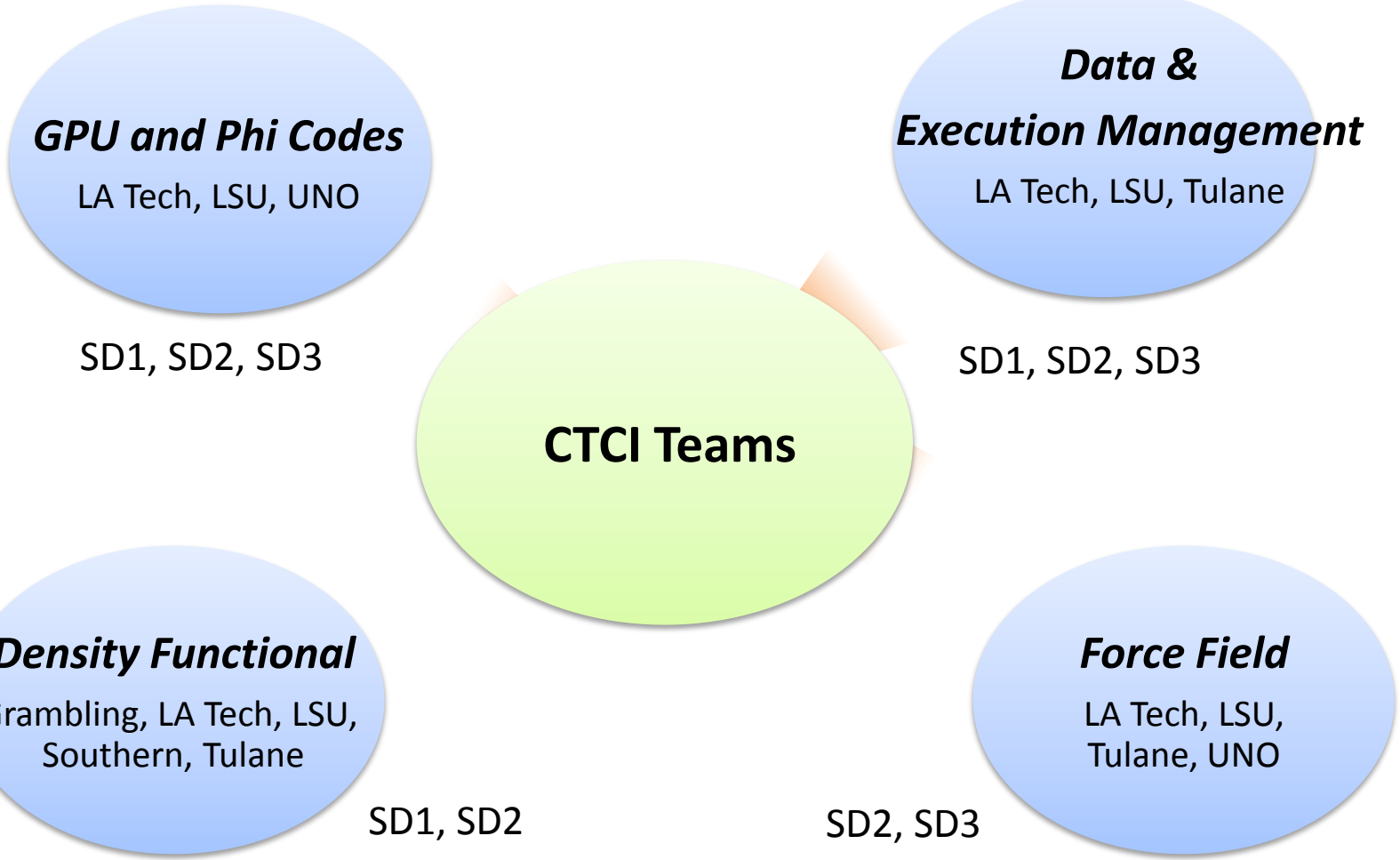


Thomas C. Bishop
Louisiana Tech University

"The glue"

Develop and experimentally validate common computational tools essential for three Science Drivers.

CTCI Research Themes



Team foci have evolved since the proposal was submitted.

CTCI Milestones

Milestones
Leverage LONI
Build on CCT/Cybertools
Migrate to Leadership Class Machines
Expand LA-SiGMA impact via codes

Heterogeneous GPU Computing:

GPU Programming Team

A ***novel collaboration*** of over 30 faculty, students, and postdocs from LSU, LA Tech, UNO, and Louisiana School for Math, Sciences and the Arts (RET/REU). Using the *Collaboratorium** at LSU.

Basis for successful MRI and CRI proposals, including a 1PFLOP PHI cluster (equivalent to the world's fastest machine, Kraken, in 2008)

LA-SiGMA GPU Team Goal

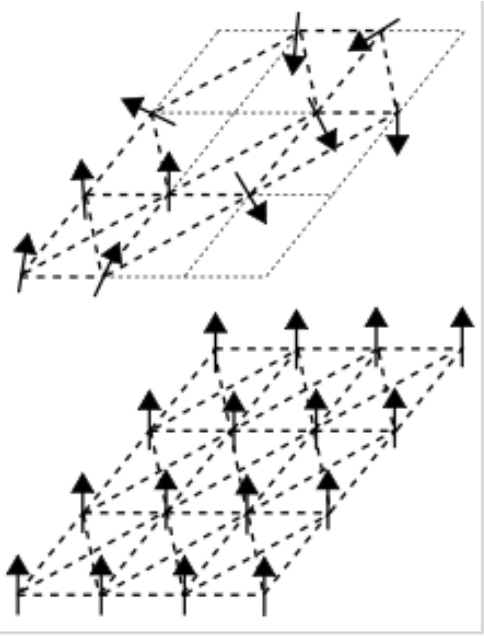
Develop efficient codes to study complex systems on next generation heterogeneous machines like BlueWaters, Stampede, and Titan.

Developing codes for quantum and classical systems and drug discovery.

*This room was initially renovated as part of an NSF-supported IGERT at CCT.

Heterogeneous GPU Computing:

GPU Simulation of Spin Glass



Many metastable structures thus many timescales to explore.

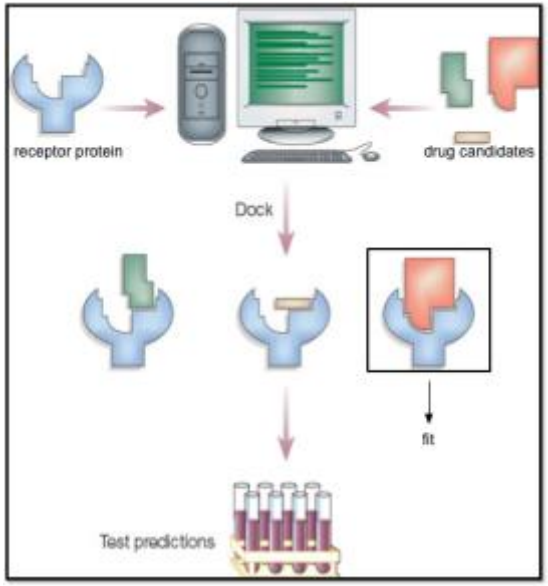
World's fastest GPU code at 35 ps/spin flip proposal for 3D Edwards-Anderson glass.

TBs of data stored in HDF5 with XML metadata

Preliminary result:

Finite size scaling shows that there is no transition.

Heterogeneous GPU Computing:

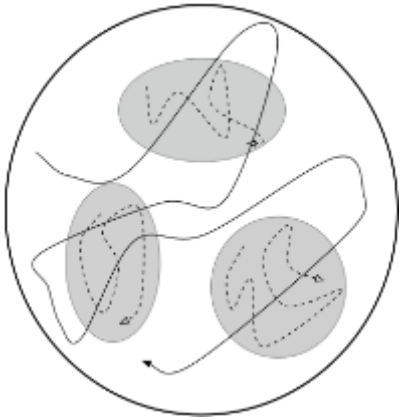


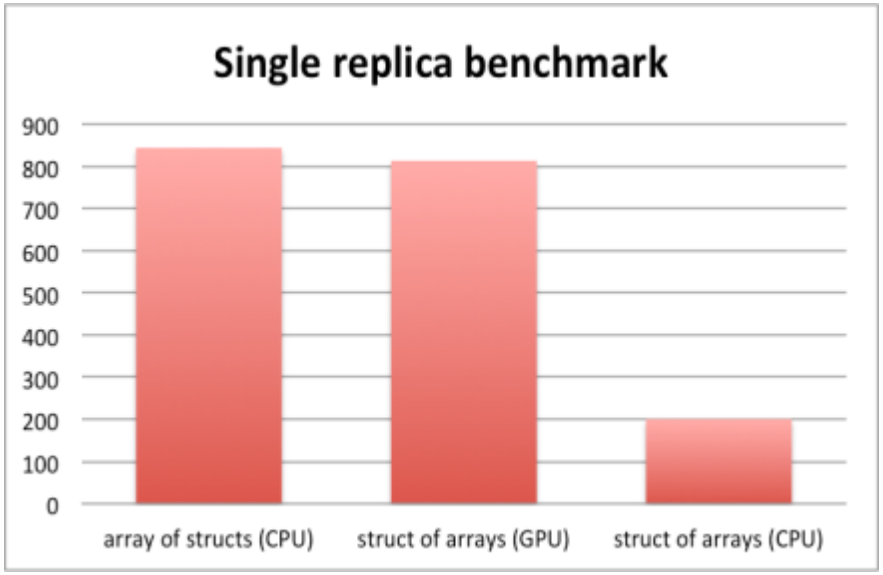
GPU drug Docking (GPUDoc)

Computer-aided drug development holds the significant promise of faster and cheaper drug discovery.

Swapping between low and high temperature systems (shaded regions) accelerates sampling.

A 4-fold speedup is obtained over CPU calculation for single replica, 50-fold for multiple replicas.



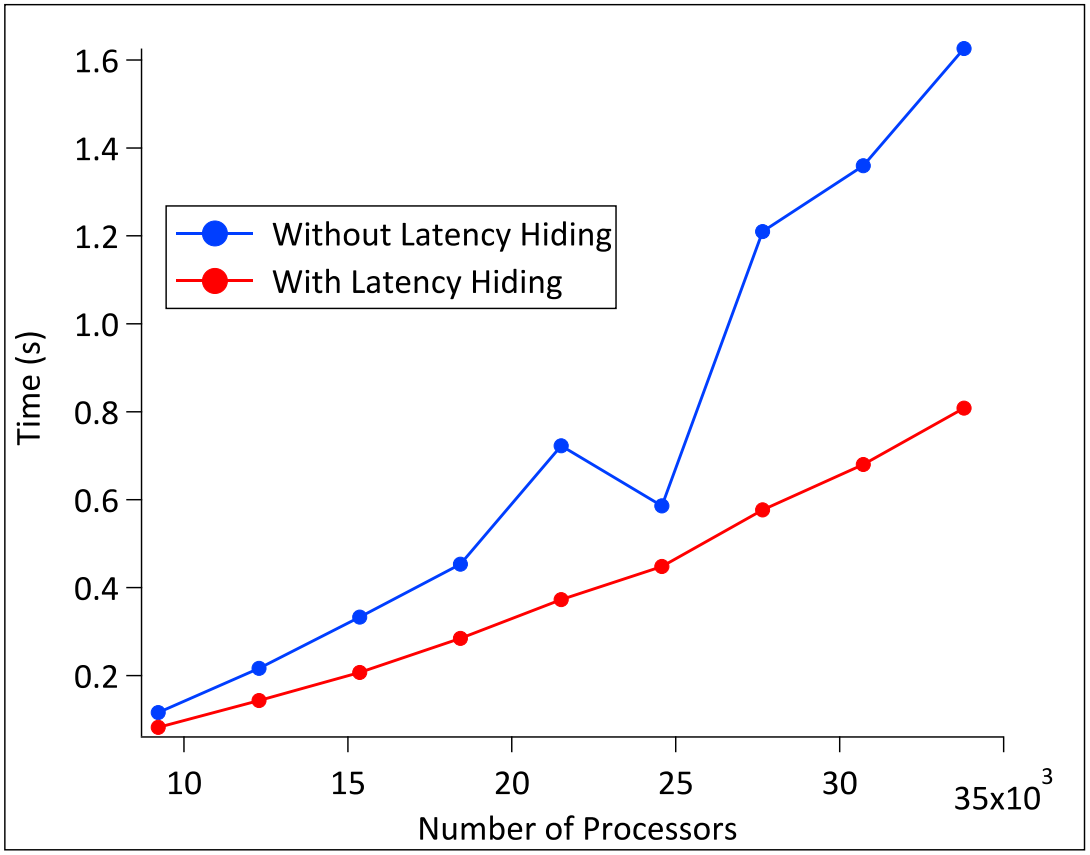


Scaling of Multi-Scale Methods to 30,000 Cores

Interdepartmental **collaboration** at LSU develops a latency hiding technique.

Kraken at the National Institute for Computational Sciences

Codes ready for National Leadership Class Machines.



Solving the Parquet Equations for the Hubbard Model beyond Weak Coupling, K. Tam, H. Fotso, S.-X. Yang, T.-W. Lee, J. Moreno, J. Ramanujam, and M. Jarrell, Phys. Rev. E 87, 013311 . Selected as *NSF Highlight*

New Algorithm for X-ray Interferometry Data Analysis

Traditional Method: FFT (not robust)

$$\widehat{counts}_{gp} = a_{1p} + a_p \sin\left[\frac{2\pi}{p_g} x_g + \phi_p\right]$$

$$\widehat{counts}_{gp} = a_{1p} + \left[\sin\left(\frac{2\pi}{p_g} x_g\right)\right] a_p \cos(\phi_p) + \left[\cos\left(\frac{2\pi}{p_g} x_g\right)\right] a_p \sin(\phi_p)$$

New and Improved: 1000-fold faster, more robust than Levenberg-Marquardt

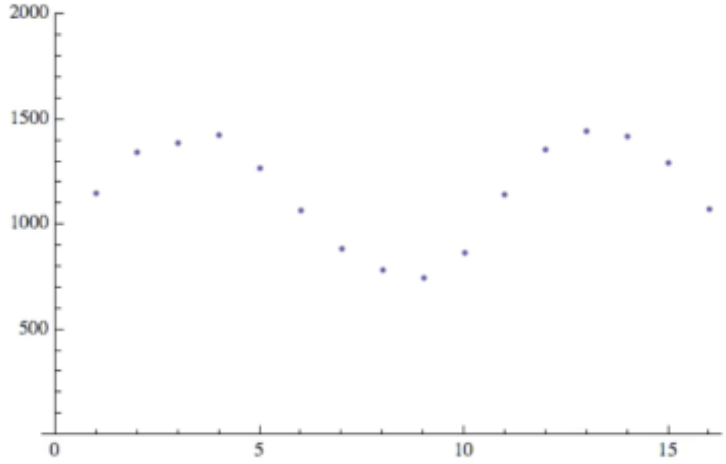
Butler (LSU) & Johnson(LIGO), Rev. Sci. Instr., Submitted

$$\widehat{counts}_{gp} = \sum_{\mu=1}^{3} B_{g\mu} a_{\mu p}$$

$$a_{2p} = a_p \cos(\phi_p), \quad a_{3p} = a_p \sin(\phi_p)$$

$$\mathbf{G} = (\mathbf{B}^T \cdot \mathbf{B})^{-1} \cdot \mathbf{B}^T$$

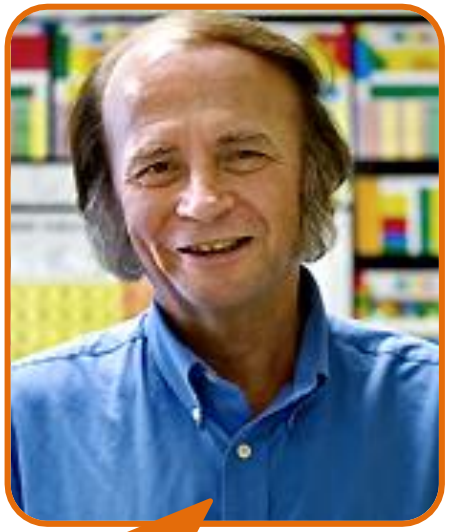
$$\mathbf{a} = \mathbf{G} \cdot \mathbf{c}$$



Density Functional Theory

- LA-SiGMA member and DFT pioneer John Perdew of Tulane University was elected to the National Academy of Sciences 2011.
- 110,000 + Google-Scholar citations for DFT Potentials. Most recently for van der Waals interactions in the semilocal meta-GGA
- Mentoring

John Perdew

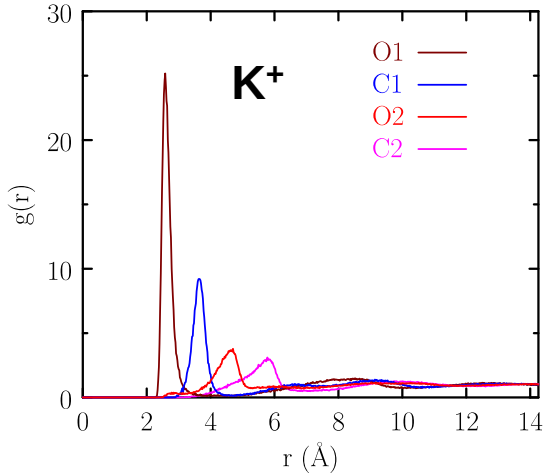


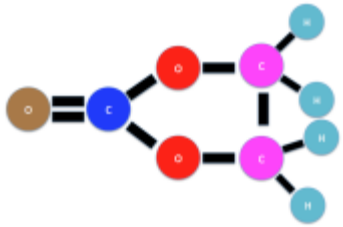
Perdew's election gives LA-SiGMA two of Louisiana's four members of the National Academies.

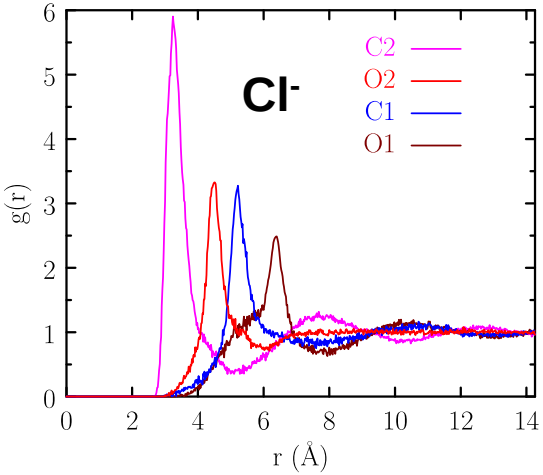
- New LA-SiGMA member and HPC pioneer William Shelton of LSU has won three Gordon Bell and a Computerworld Smithsonian awards.
- Expert in HPC, DFT, and Big Data
- Mentoring

William Shelton

Force field development for ethylene carbonate/ion solutions

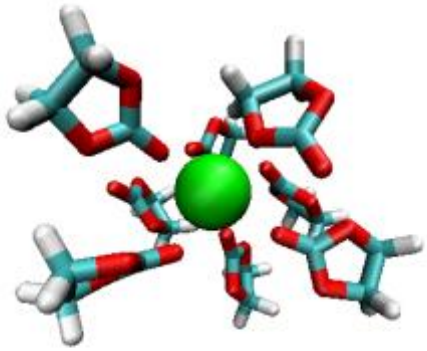


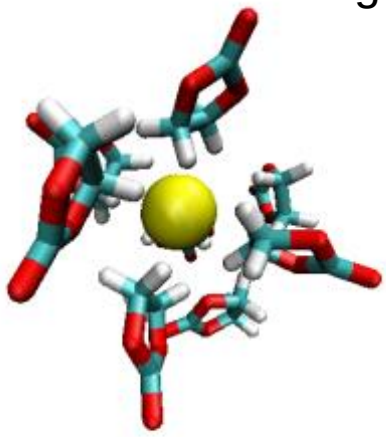




Used Thermodynamic Integration (TI) to calculate solvation free energies of ions and determine parameters that agreed with experiment for five ions K+,F-,Cl-,Br-, and I-..

Pair correlations show that the ethylene carbonate binds the ions edge on to ethylene carbonate. Only K+ and Cl- are shown



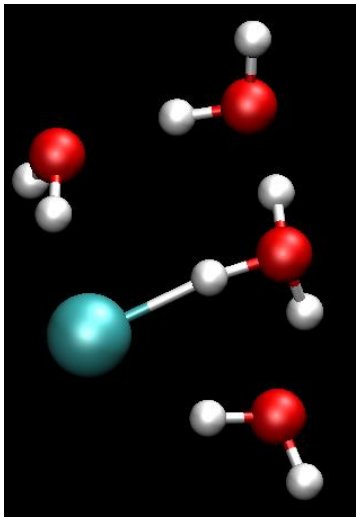


Victoria Bishop, Dexter Taylor, Steve Rick, UNO Chemistry, Summer REU program

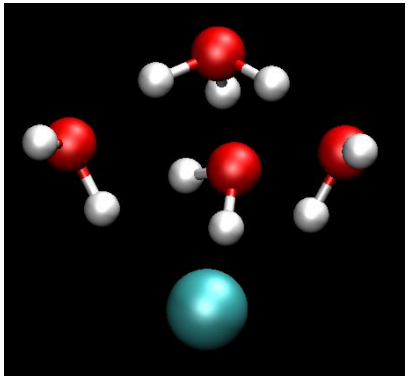
Reactive Model to Investigate HCl Dissociation at the Surface of Water

- Relevant to acid catalysis in biofuel generation, hydrolysis and transesterification.
- Calculated pKa of HCl compares favorably with experiment 5.5 (calc) vs 7.0 (exp)
- Three step mechanism:
  1. HCl makes oriented contact with water
  2. Dissociation into a contact ion pair
  3. Further dissociation to solvent separated ion pair
- Hydronium's greater propensity for the interface makes the surface of water more positively charged.

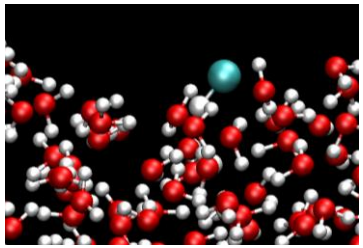
Contact Ion Pair



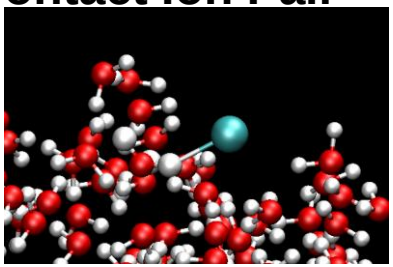
Solvent Separated Ion Pair



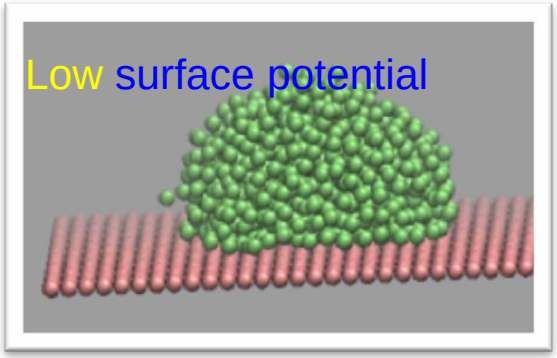
Molecular HCl

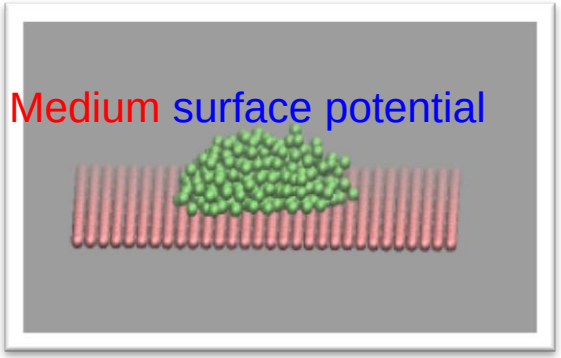


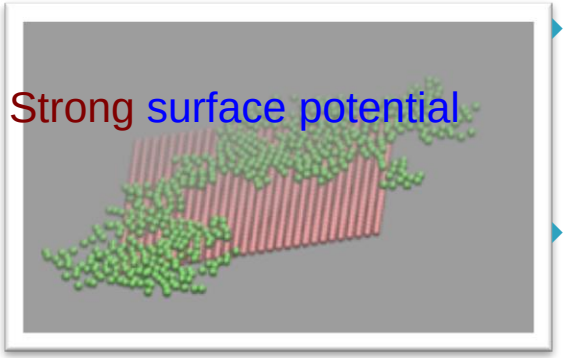
Contact Ion Pair

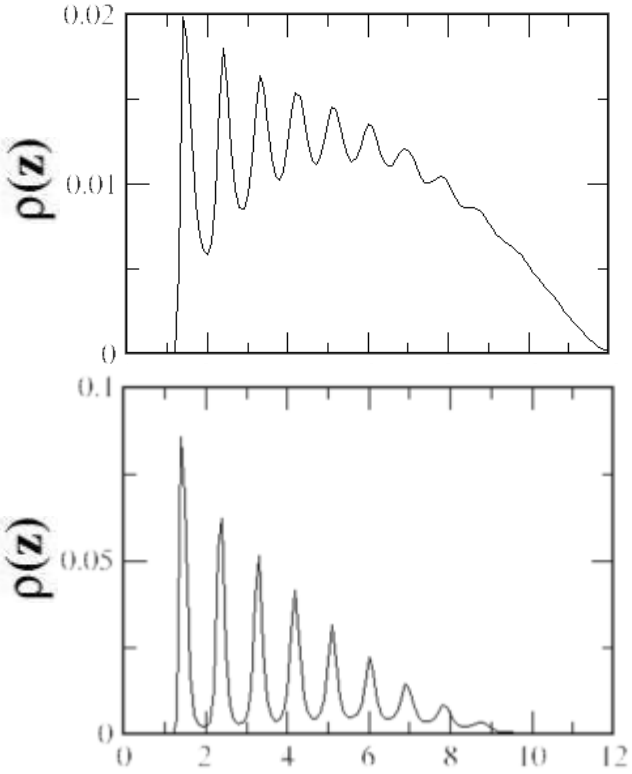


Surface-Induced Nucleation



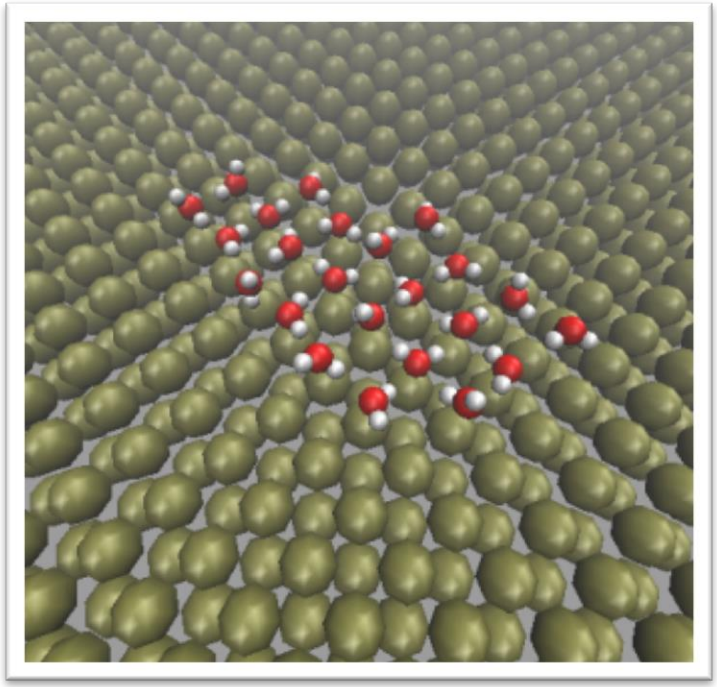


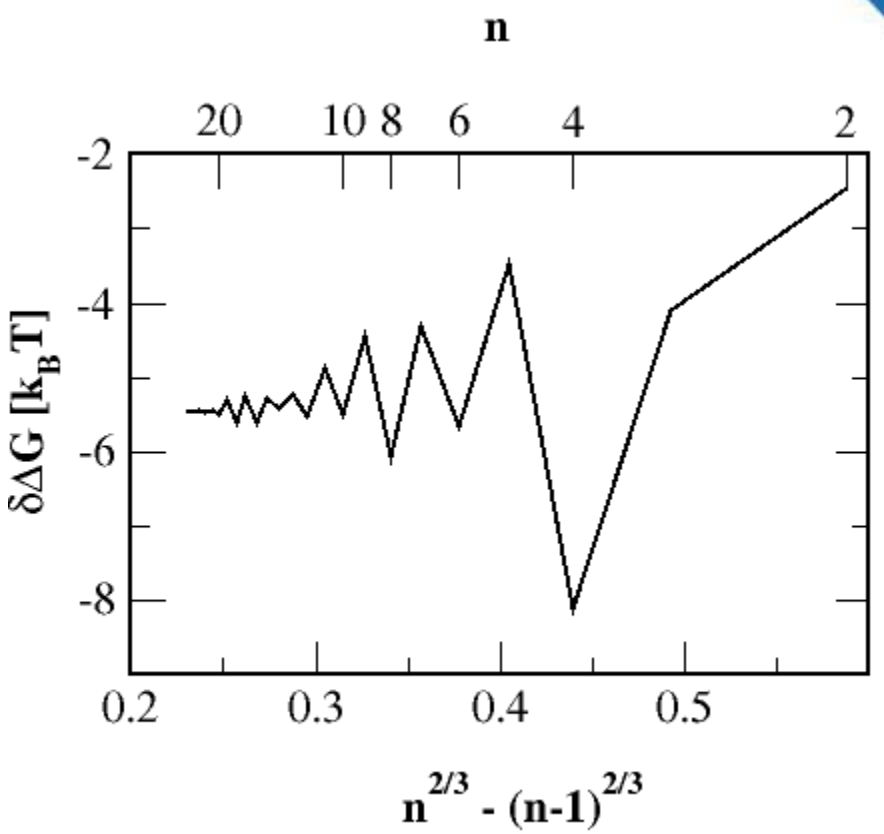




- Surface catalyzes not only the formation of the droplets but also the transition of these droplets into crystal structures due to the surface-induced layering effects (see density profiles plots).
- When surface attraction is too strong, crystallization may be inhibited due to the spreading of the particles on the surface and the corresponding formation of two-dimensional clusters (see snapshots on the left).

Nucleation of Water Clusters on a Platinum Surface





- Water clusters on a platinum surface display unconventional hydrogen bonding structures compared to the bulk liquid water.
- The free energy data (plotted on the right) show unusual odd-even effects that persist for even very large cluster sizes, consistent with the preferred 4-membered ring structures shown on the left.

Water-Platinum potential is borrowed from Heinzinger, Spohr, *Electrochimica* ***34*** *(12)*, 1849-1856 (1989)

Leveraging and Extending LONI Facilities

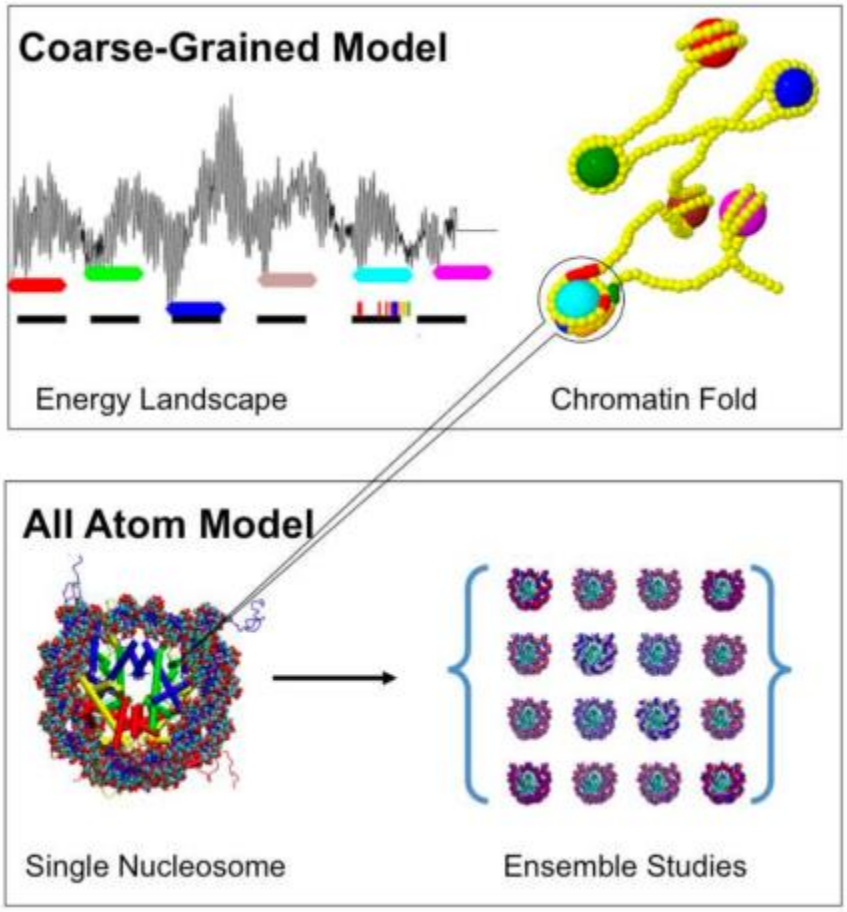
LA-SiGMA REU panel

LA-SiGMA graduate courses

LA-SiGMA **collaborative** (LONI, BoR) solutions for ***HD*** synchronous video, lecture/seminar ***capture, and sharing. In installation.***

Builds upon State LONI investments to bring HD video to each campus.

Leveraging and Extending LONI Cybertools to Investigate Genomic Biomaterials



LA Tech (Bishop), LSU (Jha), Jack Smith (WVU, XSEDE Fellow)

Nucleosomal DNA: Kinked, Not Kinked or Self-Healing Material?, R. Mukherjee and T. Bishop, Frontiers in Nucleic Acids Chapter 5, pp 69–92. ACS Symposium Series, Vol. 1082, 2012

Refines and extends tools developed by Cybertools to produce publicly available execution management tools.

Millions of simulation and analysis tasks to study folding of DNA managed using **collaboratively** developed "**ManyJobs**" and "**BigJobs**" software.

Running Many MD Simulations on Many Supercomputers.

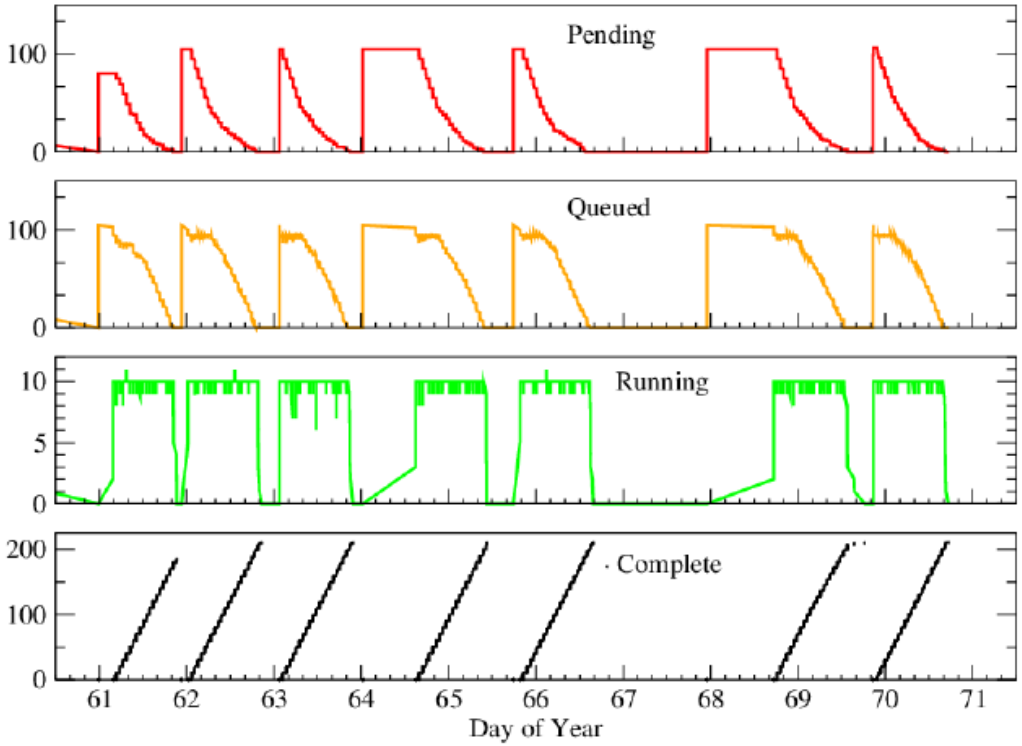
The anatomy of successful ECSS projects: lessons of supporting high-throughput high-performance ensembles on XSEDE.

Proceedings of the 1st Conference of the XSEDE '12.

Execution Management Across XSEDE Resources

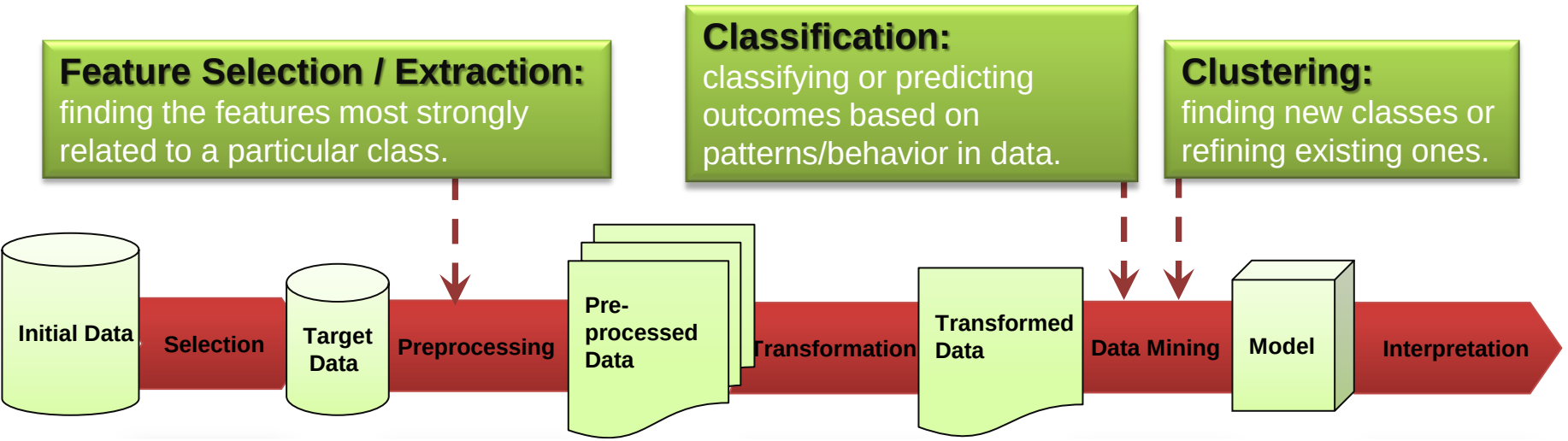
BigJobs on LONESTAR

- 2100 Simulation tasks
- 240 CPU/simulation
- 100 Sims/BigJob
- 2400 CPU/BigJob
- 500,000 SU in 10 days
- 2.1μs of simulation
- 8.2 TB of DCD data
- 2.1M snapshots analyzed -> 370GB



Scalable Online Comparative Genomics of Mononucleosomes: A BigJob.
Proceedings of 2nd Conference of XSEDE '13 .

Knowledge Discovery and Data Mining (KDD)



Unsupervised Learning: Clustering, Association Rule Discovery

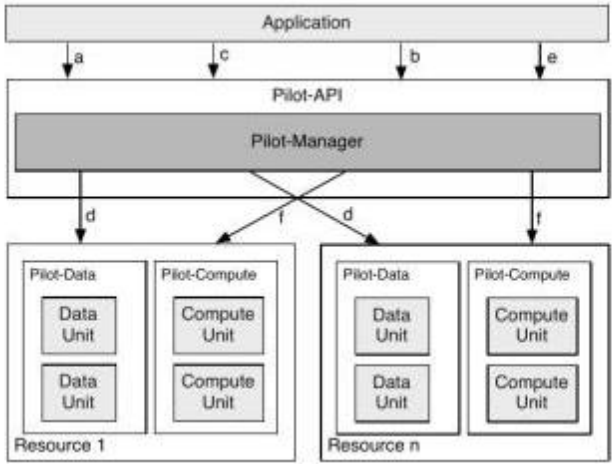
Supervised Learning: Predictive Classification models

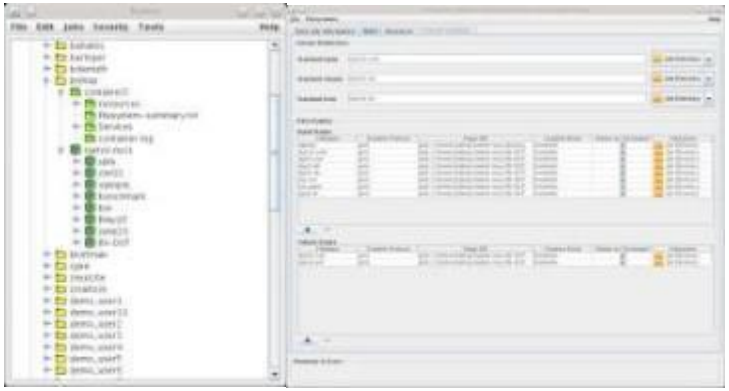
Algorithm Design in Distributed Environment:

Scalability, Reliability, Availability, Evolution

Workflow Management & Data Enabling Technologies

Pilot Jobs with SAGA & BigJobs

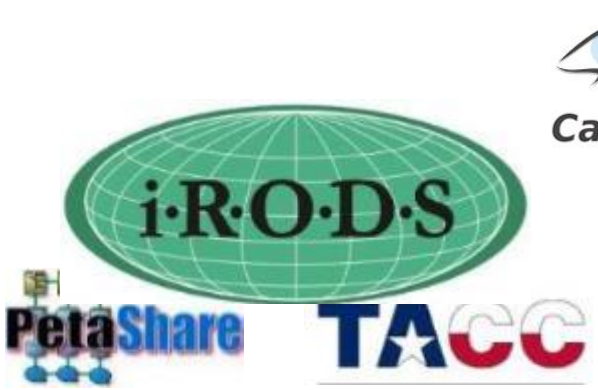




Global Federated File System (GFFS):

Data and Queue Management

XSEDE Campus Bridging Pilot Project



Data Management

TACC

TEXAS ADVANCED COMPUTING CENTER

2013 Data Workshop

June 7-8, 2013

- *"Connecting data with semantics and ontologies"*.
- LA-SiGMA data plan and advisory team
- Long term visit
- 8 invited experts in data management and semantics
- Data sharing through website
- Data sharing pilot project with members on all campuses
- Pilot projects
  - HDF5 + CML/XML
- Partnership with TACC

LA-SiGMA is helping to guide LONI's efforts.

CTCI Milestones

Milestones	Y1	Y2	Y3	Y4	Y5	
Leverage LONI	X	X	X	X	X	*On Track*
Build on CCT/Cybertools	X	X	X	X	X	*On Track*
Migrate to Leadership Class Machines			X	X	X	*Ahead*
Expand LA-SiGMA impact via codes			X	X	X	*On Track*

Challenges/Barriers: More GPU, data use/reuse, 3 CTCI faculty depart.

Mitigation plan: Added a GPU and a data use/reuse expert. Succession plans for departing faculty.