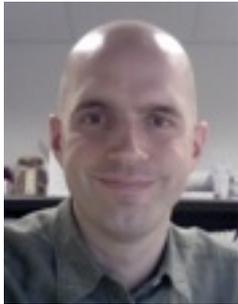
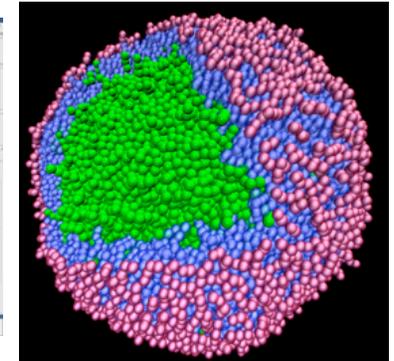
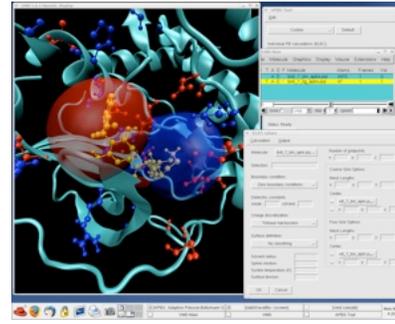


Macromolecular Proteins and Protein Complexes



Nathan A. Baker
Associate Professor
Center for Computational Biology,
Dept. of Biochemistry and
Molecular Biophysics
Washington University in St. Louis



Current Area of Research Interest

- Numerical methods and software for biomolecular solvation and electrostatics
- Theory and modeling of protein allostery
- Simulations of nanomaterials for cancer diagnosis and therapy

Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- Transferable adaptive multiscale and/or hybrid simulation methods
- On-the-fly titration state sampling in molecular simulation
- Common frameworks for algorithm development and validation in biomolecular simulation

DOE/Office of Science Graphic

Name of Workshop

Date

Macromolecular Proteins and Protein Complexes

Analysis and validation of very large scale and non-equilibrium simulations

David A. C. Beck
Sr. Research Scientist
eScience Institute
University of Washington, Seattle



Current Area of Research Interest

- HPC simulation methods (parallelism, algorithms)
- HPC analytics (data mining, clustering, algorithms)
- Molecular mechanics methods development

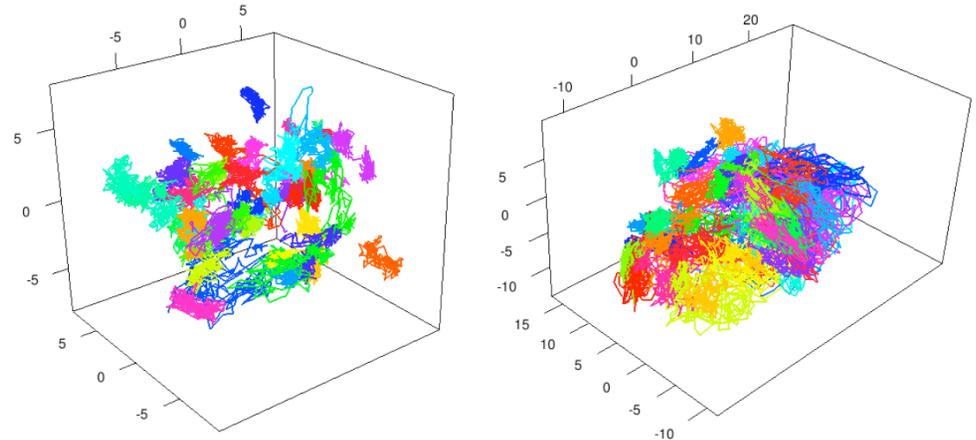
Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- Working with petabyte scale simulation databases (e.g. Dyanameomics)
 - Storing, sharing, provenance management
 - Data mining, analysis, informatics at scale

Quantitative Analysis of Disorder in Protein Dynamics

Analysis and validation of very large scale and non-equilibrium simulations

Mike Colvin
Professor
School of Natural Sciences
University of California, Merced



Current Area of Research Interest

- MD simulations of intrinsically disordered proteins
- Dynamics of biomolecules in nanostructures
- Simulations of modified DNA
- Statistical modeling of stem cell lineages

Figure: Reduced dimensional representations of 40 replicate MD trajectories of two intrinsically disordered proteins

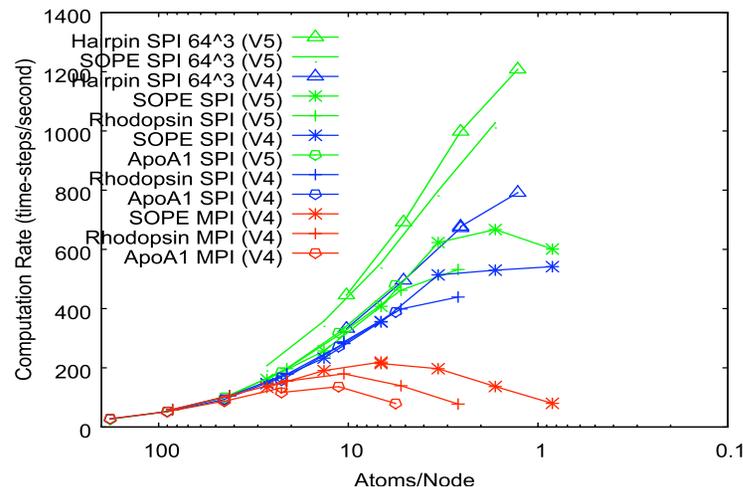
Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- Machine-learning algorithms for analyzing protein ensembles
- Quantitative metrics of polymer disorder
- Automated annotation of large scale biomolecular simulations

Computational Challenges in Macromolecular Proteins and Protein Complexes



Robert S. Germain
Manager Biomolecular
Dynamics & Scalable
Modeling
IBM T.J. Watson Res.



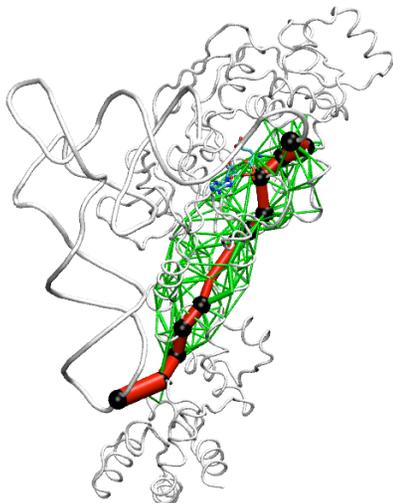
Current Area of Research Interest:

- Parallel decompositions/algorithms for molecular dynamics
- Understanding the tradeoffs between approximations for speed and “correctness” (e.g. effects of time step size and other integrator choices, effects of thermostats/barostats)
- Data intensive computing and data management (storage & analysis of trajectories)

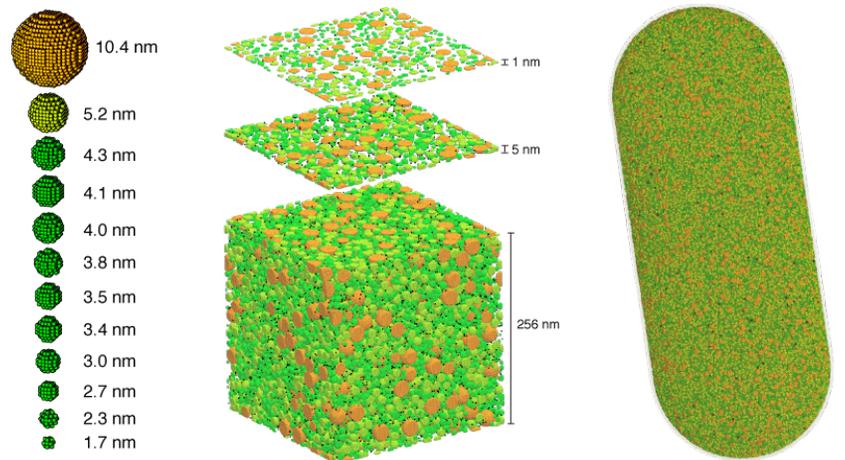
Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- Increasing time scales accessible through simulation to provide insights (e.g. hypotheses to be tested by experiment) into complex biological systems such as membrane bound proteins.

Macromolecular Proteins & Protein Complexes



Name: Zan Luthey-Schulten
Title: Professor of Chemistry
University of Illinois, Urbana



Current Area of Research Interest

- Whole cell simulations of *in vivo* processes using GPU hardware
- MD simulations of signaling networks in RNA:protein complexes
- Evolution of translational machinery

Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- Long timescale whole cell simulations of *in vivo* processes/networks
- tRNA migration in translation and ribosomal assembly
- Long timescale simulations of protein and RNA folding

Computational Challenges in Macromolecular Proteins and Protein Complexes

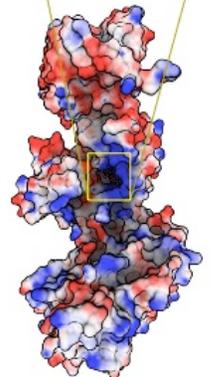
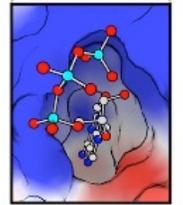
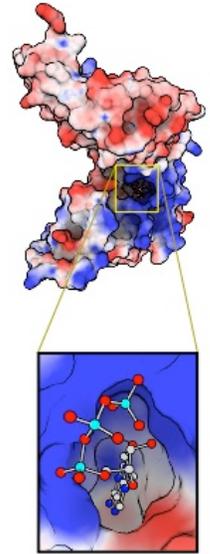


Julie C Mitchell

Associate Professor

Mathematics and Biochemistry

University of Wisconsin - Madison



Current Area of Research Interest

- Protein-Protein and Protein-DNA Complexes
- GPU-enabled Computing for Molecular Simulations

Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

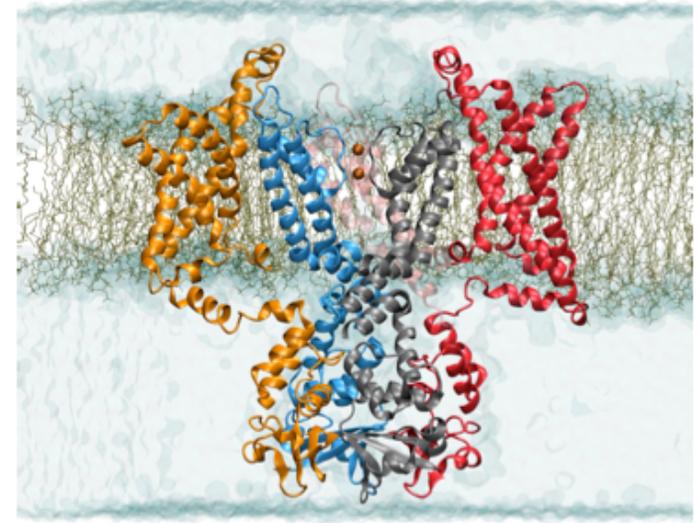
- Rigorous Classification of Functional Surfaces of Proteins
- Search for Functional Surface Homology Within Large Databases
- Discovery of Unknown Protein Functions



Protein/Complexes



Benoît Roux
Professor, Dept Biochemistry
University of Chicago

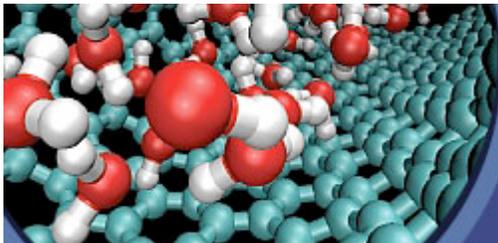


Current Area of Research Interest

- Development of polarizable force field
- Large conformational changes related to function
- Transition rates
- Ligand binding free energy

Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- Quantitative validation of atomistic models
- Effective algorithms to treat electrostatics in large systems
- Sampling issues, novel strategies, statistical mechanics, etc...



Opportunities in Biology at the
Extreme Scale of Computing

August 17 - August 19, 2009 - Chicago, IL

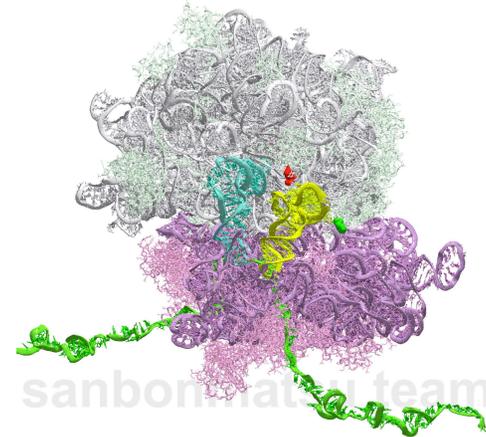
08/11/09



U.S. DEPARTMENT OF
ENERGY

Protein Complexes

Kevin Y. Sanbonmatsu
Principal Investigator
LANL



Current Area of Research Interest [Include graphic]

- Large-scale all-atom molecular dynamics simulation of biological systems
- Mechanism of molecular machines and biomolecular complexes
- **Non-coding RNA**

Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- Simulating the ribosome at physiological time scales (milliseconds-seconds)
- Secondary and tertiary structure prediction of non-coding RNA
- Micron-sized systems (billion atom simulation)

DOE/Office of Science Graphic

Name of Workshop

Date

Macromolecular Proteins and Complexes



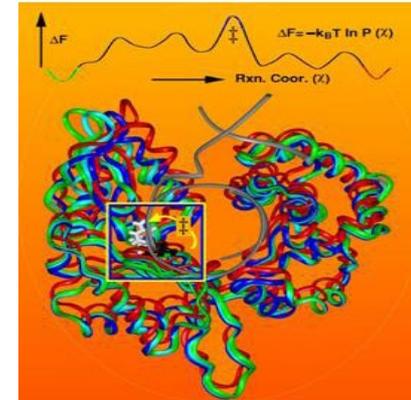
Tamar Schlick

Professor of Chemistry, Mathematics,
and Computer Science

Department of Chemistry and Courant Institute of
Mathematical Sciences, New York University

Current Research Interests

- Unraveling DNA polymerase replication and repair mechanisms
- Developing novel mesoscale models for protein/DNA complexes
- Modeling chromatin organization dynamics
- Using graph theory and innovative tools to catalog, analyze, and predict RNA structure
- Simulate *in vitro* selection of RNA aptamers



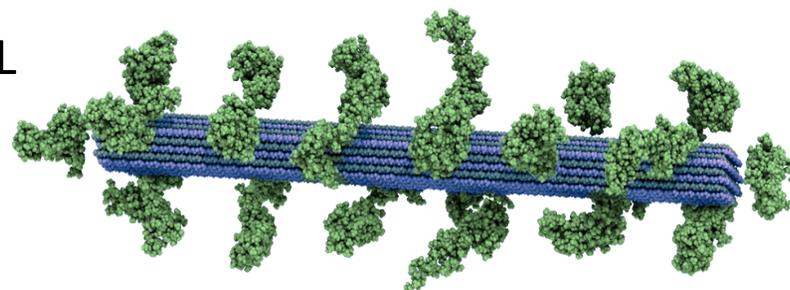
Challenges to Address with Advanced Computing and Modeling

- Systematic development of hierarchical models for spatial and temporal resolution of biomolecules
- Large-scale, long-time simulations of protein/DNA and protein/RNA complexes for understanding structure and function (regulation)
- Improved QM/MM dynamics and reaction rate approaches for capturing transition states and reactions for biomolecular systems
- New conceptual frameworks for predicting RNA 3D interactions and folding

Imaging, Computing and the Loop



Jeremy C Smith
Professor and UT/ORNL
Governor's Chair and
Director Center for
Molecular Biophysics



Current Area of Research Interest [Include graphic]

- Petascale and Multiscale Biomolecular Simulation
- Neutron Scattering in Biology
- Bioenergy: Cellulosic Ethanol Production
- Mercury Bioremediation
- Protein Dynamics/Enzyme Reaction Mechanisms/Theoretical Biophysics

Challenges that May be Addressed with Advanced Computing and Mathematics Capabilities

- Simulation of one tenth of a living cell at atomic detail for one microsecond
- Protein Folding and Ligand Binding: Biological Structures, Drug Design.
- The workings of biomolecular machines.

DOE/Office of Science Graphic

Name of Workshop

Date