Institute for Advanced Simulation
Jülich Supercomputing Centre

IAS Seminar

Topic: **UltraScan - a Science Gateway for Macromolecular Characterization**

Speaker: Borries Demeler, University of Texas Health Science Center at San Antonio

Contents: UltraScan is a HPC-enabled modeling software for analytical ultracentrifugation experiments (AUC). Using the Apache Airavata framework (developed under the NSF SciGaP initiative), we have built a global science gateway which not only enables users to perform sophisticated hydrodynamic modeling on remote HPC resources available in the US and Germany, but also fosters worldwide collaboration using the UltraScan Laboratory Information Management System, a web-based, centrally-stored data warehouse enabling multiple satellite gateways. The Ultrascan science gateway serves over 70 institutions worldwide, and has the ability to communicate using GRAM and Unicore middleware. It is firmly established on national resources at the Texas Advanced Computing Center (TACC), San Diego Supercomputing Center (SDSC), at the University of Texas Health Science Center at San Antonio, and on the Juropa infrastructure at the Juelich Supercomputing Center.

AUC is a technique that is primarily used in biophysics, structural and molecular biology, biomedical, and polymer science to study proteins, nucleic acids, carbohydrates and synthetic polymers. Recently, material scientists have expanded its use to the broad field of nanoparticles, quantum dots, graphene and nanotubes, and many other nanomaterials. AUC makes it possible to study these molecules in the solution phase, where they are unaffected by crystal packing and EM drying artifacts, and dynamic interactions can be followed.

In this talk I will provide an overview of the UltraScan project, its integration into the SciGaP initiative, and I will be discussing the types of experiments and analyses that can be performed with AUC, and provide examples of what can be learned. I will illustrate the challenges that need to be overcome, and explain how the SciGaP approach used with UltraScan and other SciGaP gateways can be a model for the integration of many other gateways. I will close out by highlighting some results obtained recently by our laboratory using the UltraScan software.

Time: Wednesday, 15 October 2014, 15:00

Venue: Jlich Supercomputing Centre , building 16.3, room 107 (Besprechungsraum 1)

Anyone interested is cordially invited to participate in this seminar.

sgd Prof. Dr. Dr. Thomas Lippert