Graduate School of Biomedical Sciences, Dept. of Biochemistry
UT HEALTH SCIENCE CENTER™
San Antonio

Borries Demeler, Ph.D.

INTERNATIONAL
SUPERCOMPUTING CONFERENCE

HPC Applications in Biophysics, Material Science and Biomedicine - enabled by UNICORE
The UltraScan XSEDE Science Gateway

A Science Gateway for Biophysical Analysis

Task

Model data from hydrodynamic experiments to describe molecules under dynamic solution conditions

Challenges

Computationally expensive inverse problems, many users

Biophysical applications used

- **Analytical Ultracentrifugation (AUC)**
- **Molecular Dynamics (MD)**
- **Bead Modeling**
- **Small angle X-ray and neutron scattering (SAXS/SANS)**

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AUC Background

What is Analytical Ultracentrifugation (AUC)?

A technique to separate macromolecules dissolved in solution in a centrifugal force field. AUC can “watch” the molecules *while* they are separating and identify and differentiate them by their hydrodynamic properties and partial concentration. AUC is a “first Principle” method, which does NOT require standards.

How does AUC work?

By applying a very large centrifugal force, molecules are separated based on their molar mass and their shape. The molecules are observed using different optical systems that detect different properties of the molecules, such as refractive index, UV or visible absorbance, or fluorescent light emission.

What molecules can be studied?

Virtually any molecule, colloid or particle that can be dissolved in a liquid can be measured by AUC, as long as it does not sediment by gravity alone. The molecule or particle can be as small as a salt ion, or as large as an entire virus particle.

The ultracentrifuge can spin at 60,000 rpm, generating forces close to 300,000 x g. Even small molecules like salt ions will sediment in such a force.

AUC Background

- Molecules can be studied in a physiological environment

- Very large size range (10^2 – 10^8 Dalton, complements cryo-EM and NMR)

- Dynamic processes can be studied
    - reversible self/hetero-association (ex.: oligomerization states)
    - binding strengths (ex.: protein/protein, protein/DNA, drug binding)
    - slow kinetics
    - Response to changes in pH, ionic strength, ligands, small molecules

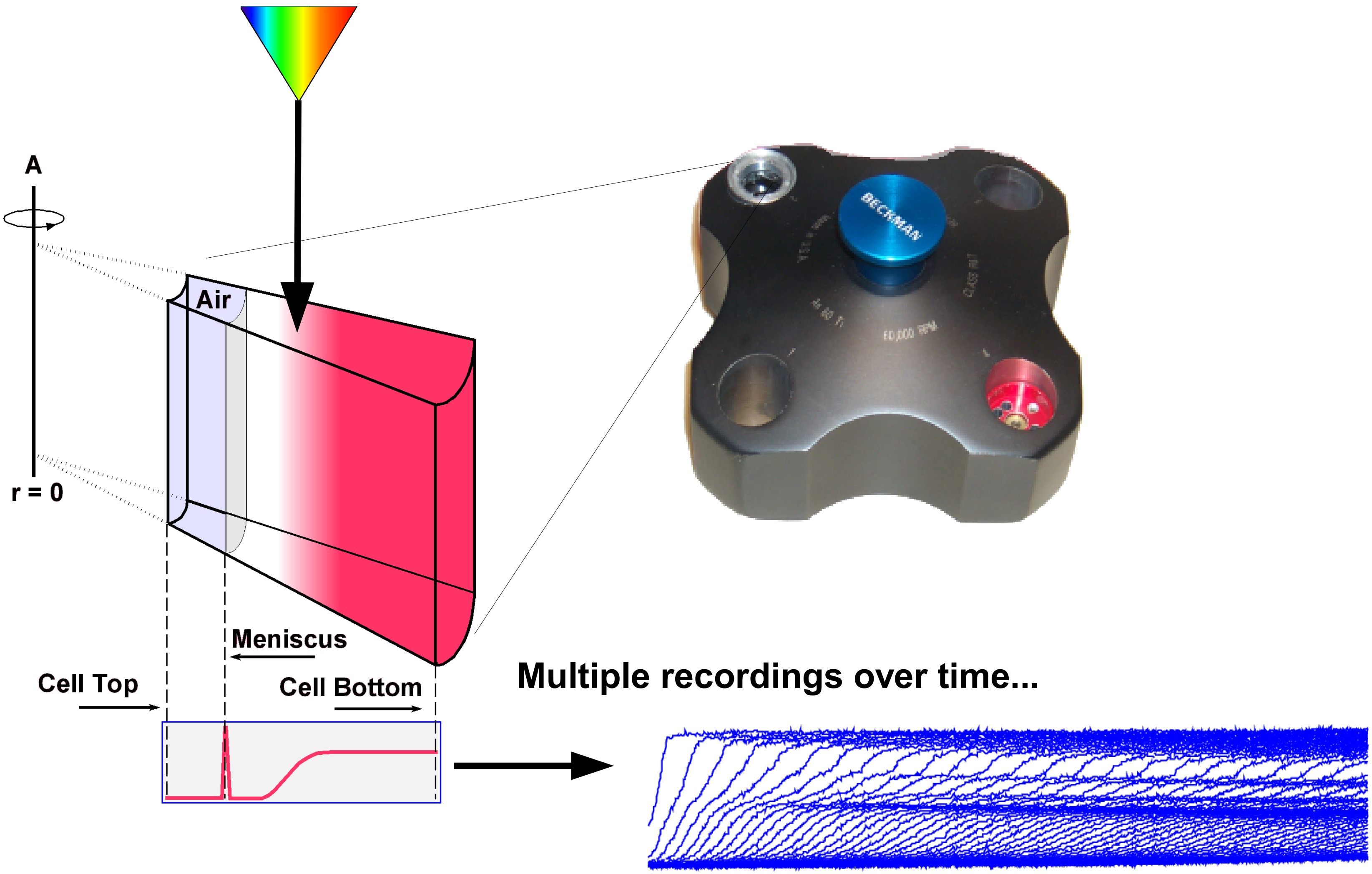
- Composition analysis
    - Formulation properties, purity, aggregation, stoichiometry
    - Partial concentration, molecular weight, shape

- Conformational studies
    - protein folding, denaturation, anisotropy studies

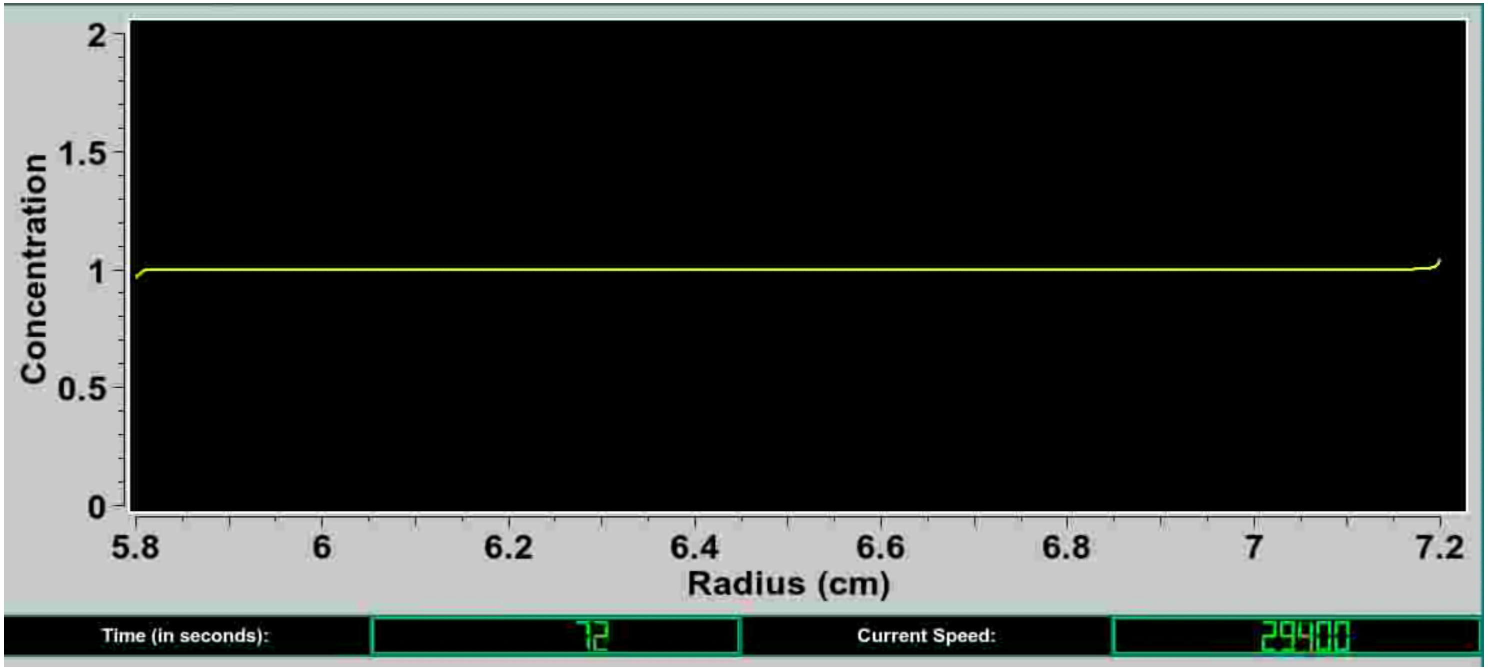
- Mutational studies
    - functional studies, oligomerization, binding strength

- *First Principles approach!*

A Science Gateway for Biophysical Analysis



Multiple recordings over time...



The experiment is described by the Lamm equation, which is solved with FEM

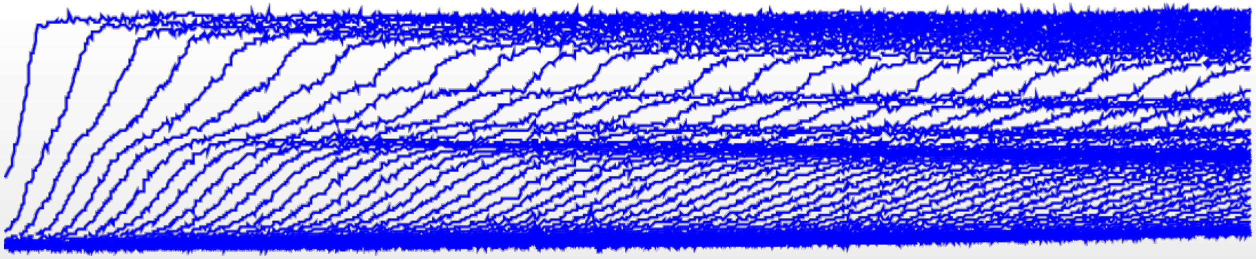
Cao W and Demeler B. Modeling analytical ultracentrifugation experiments with an adaptive space-time finite element solution of the Lamm equation. (2005) Biophys J. 89(3):1589-602.

Cao, W and Demeler B. Modeling Analytical Ultracentrifugation Experiments with an Adaptive Space-Time Finite Element Solution for Multi-Component Reacting Systems. Biophys. J. (2008) 95(1):54-65

$$L(s,D):\quad \left(\frac{\partial C}{\partial t}\right)_r = \frac{-1}{r}\frac{\partial}{\partial r}\left[s\,\omega^2 r^2 C - D\,r\,\frac{\partial C}{\partial r}\right]_t$$

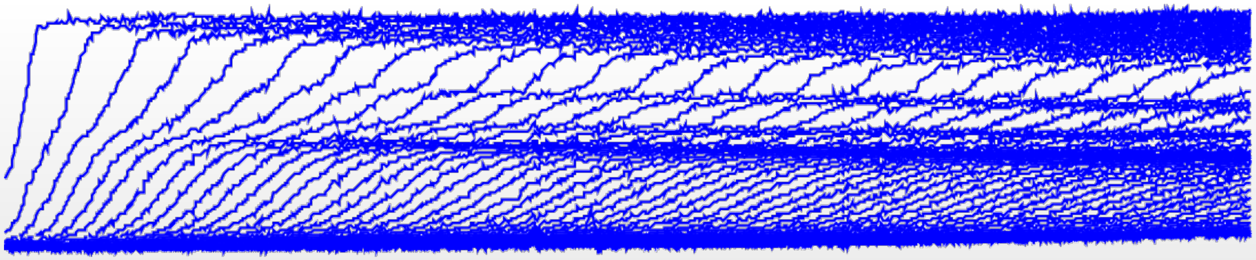
$$MIN:\ \sum_{i=1,j=1}^{r,t}\left[Y_{i,j}-\sum_{k=1}^{n}\left(L_k(s_k,D_k)_{i,j}\right)\right]^2$$

Sedimentation Velocity



Sedimentation velocity profile of a mixture of macromolecules over time

Sedimentation Velocity

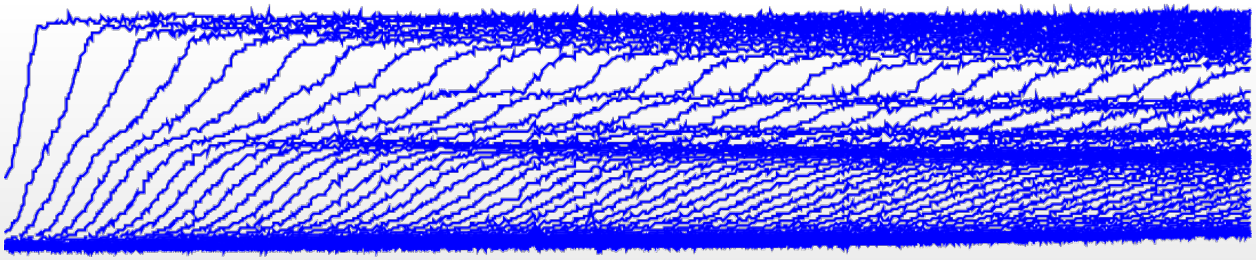


Composition Analysis

We can answer these questions:

How many components?

Sedimentation Velocity



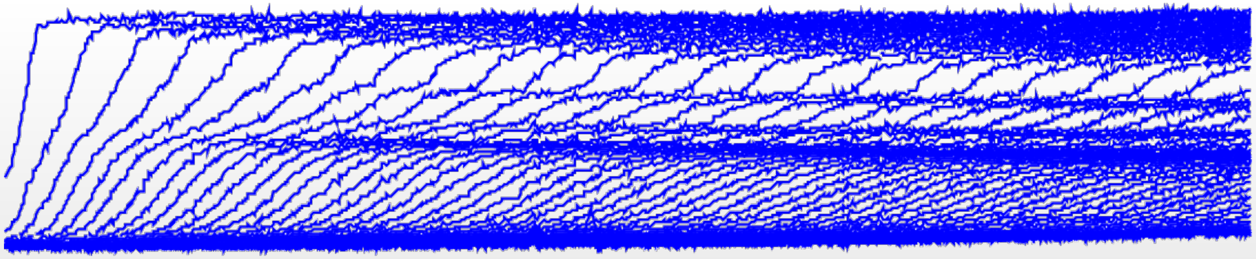
Composition Analysis

We can answer these questions:

How many components?

What are their molecular weights?

Sedimentation Velocity



Composition Analysis

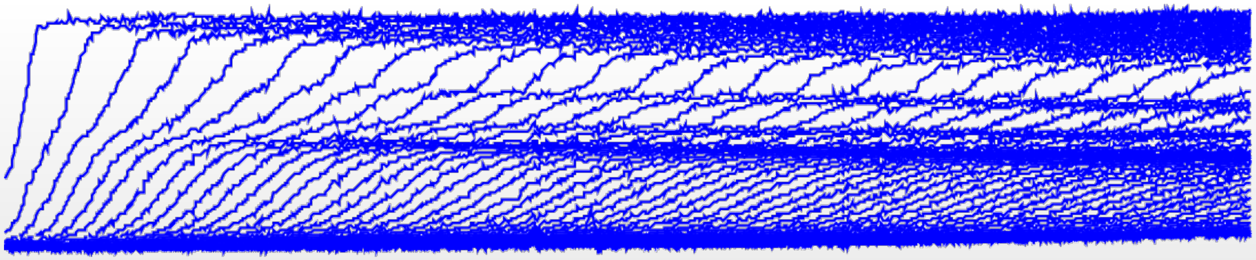
We can answer these questions:

How many components?

What are their molecular weights?

What are their shapes?

Sedimentation Velocity



Composition Analysis

We can answer these questions:

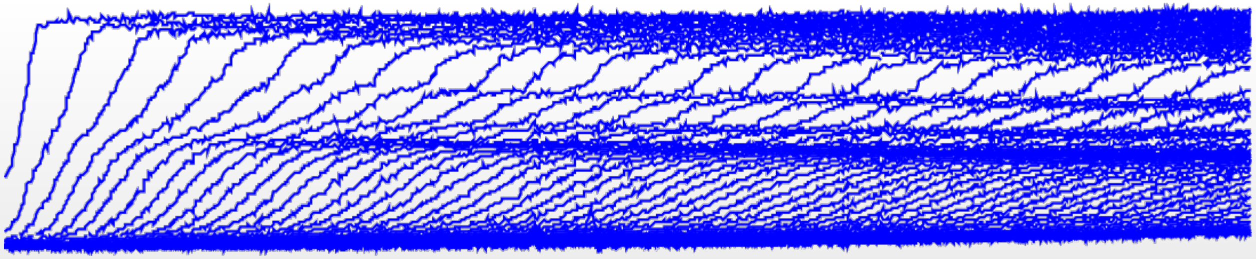
How many components?

What are their molecular weights?

What are their shapes?

What is the partial concentration of each component?

Sedimentation Velocity



Composition Analysis

We can answer these questions:

How many components?

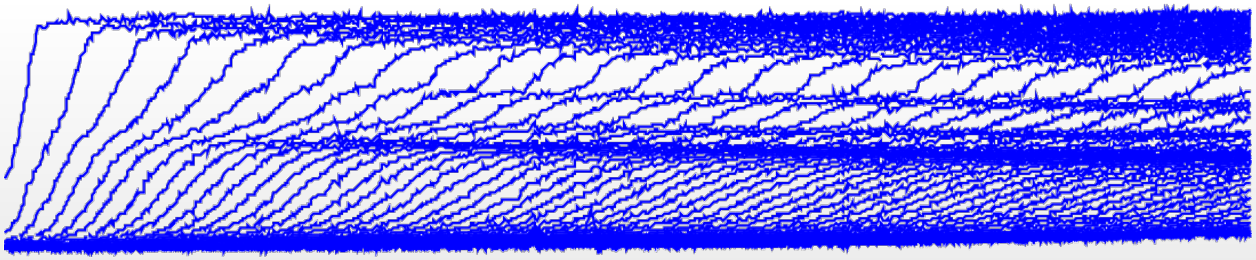
What are their molecular weights?

What are their shapes?

What is the partial concentration of each component?

Do the components interact (how fast, strong)?

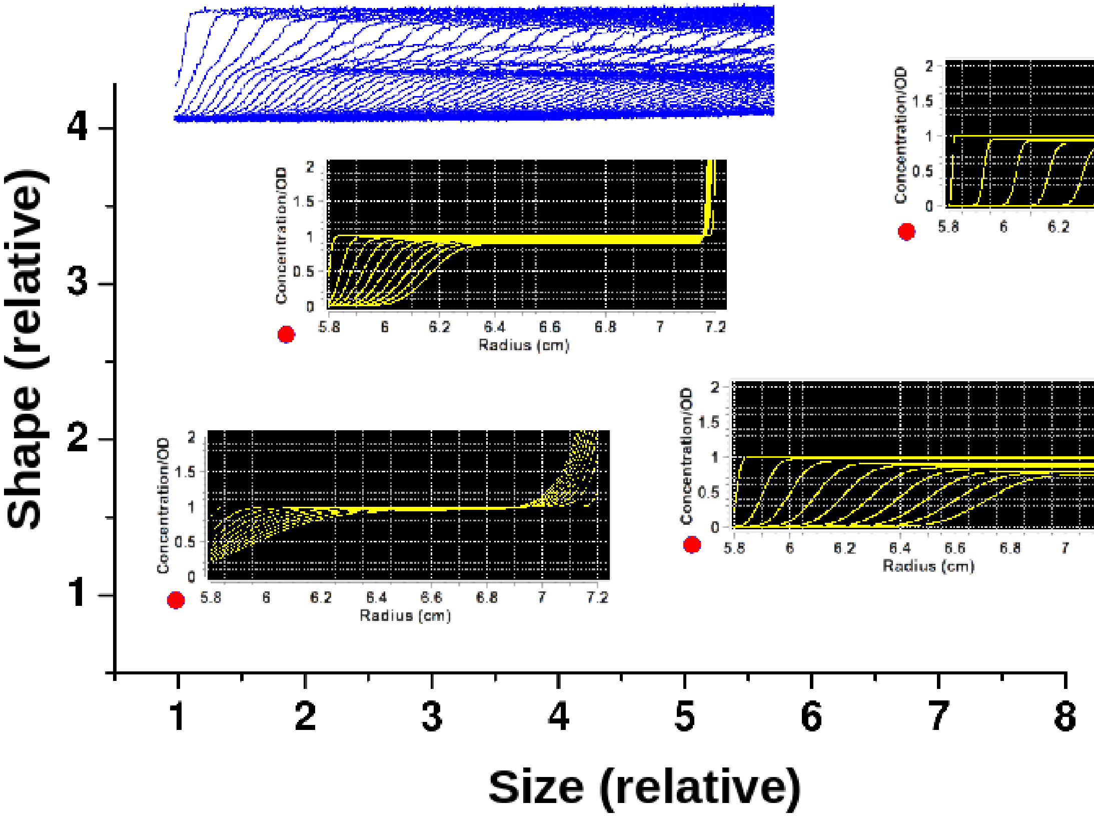
Sedimentation Velocity

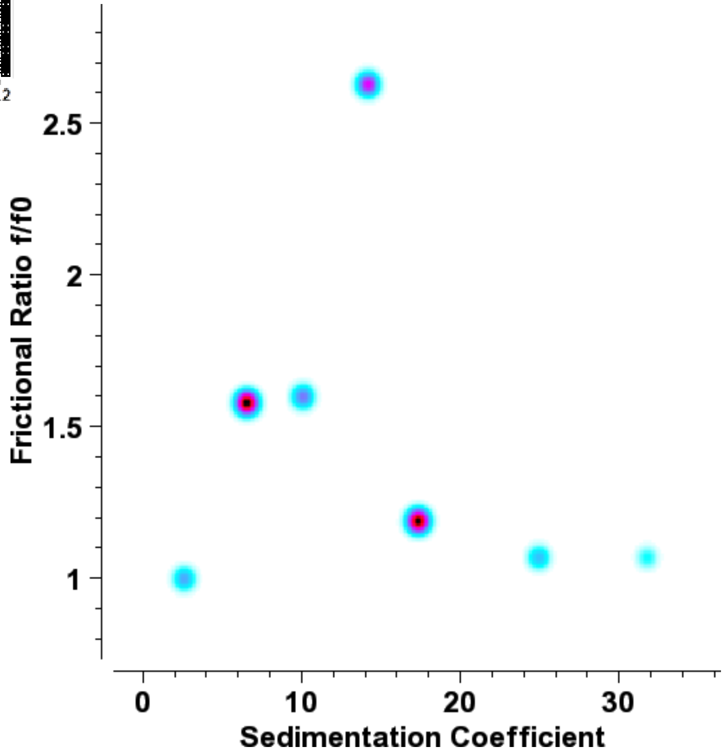


Composition Analysis

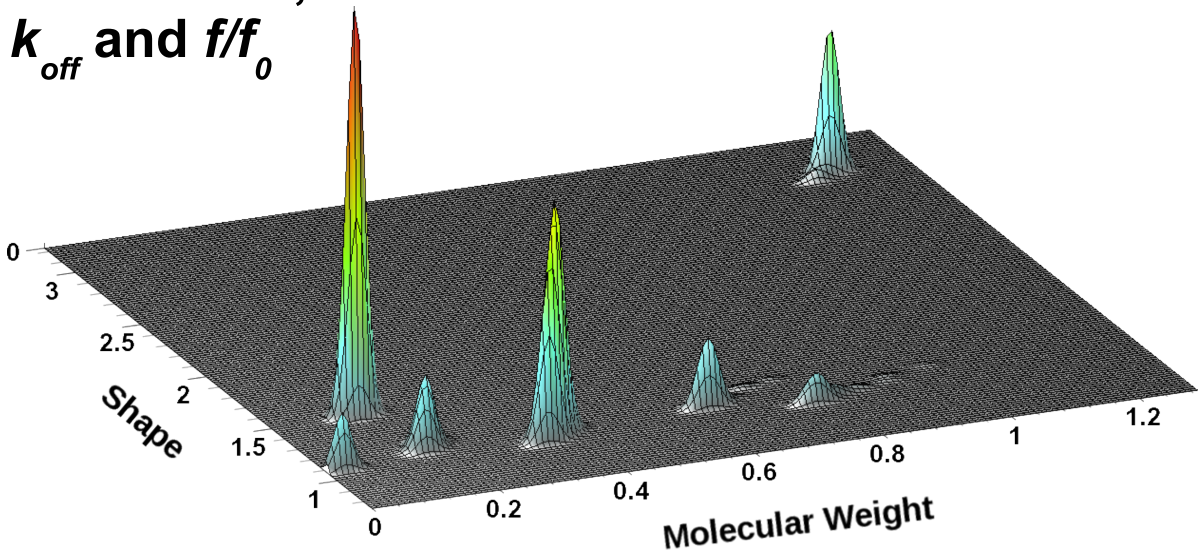
We can answer these questions:

How many components?
What are their molecular weights?
What are their shapes?
What is the partial concentration of each component?
Do the components interact (how fast, strong)?
What is the reliability of our measurement?





Find: partial concentration,
***s, D, MW, Kd, k*$_{off}$ and *f/f*$_0$**



Optimization:

2D-Spectrum Analysis
Genetic Algorithms
Monte Carlo Analysis

A Science Gateway for Biophysical Analysis

We needed an HPC interface for UltraScan to support analysis of AUC experiments on molecules in the solution environment

Goals:

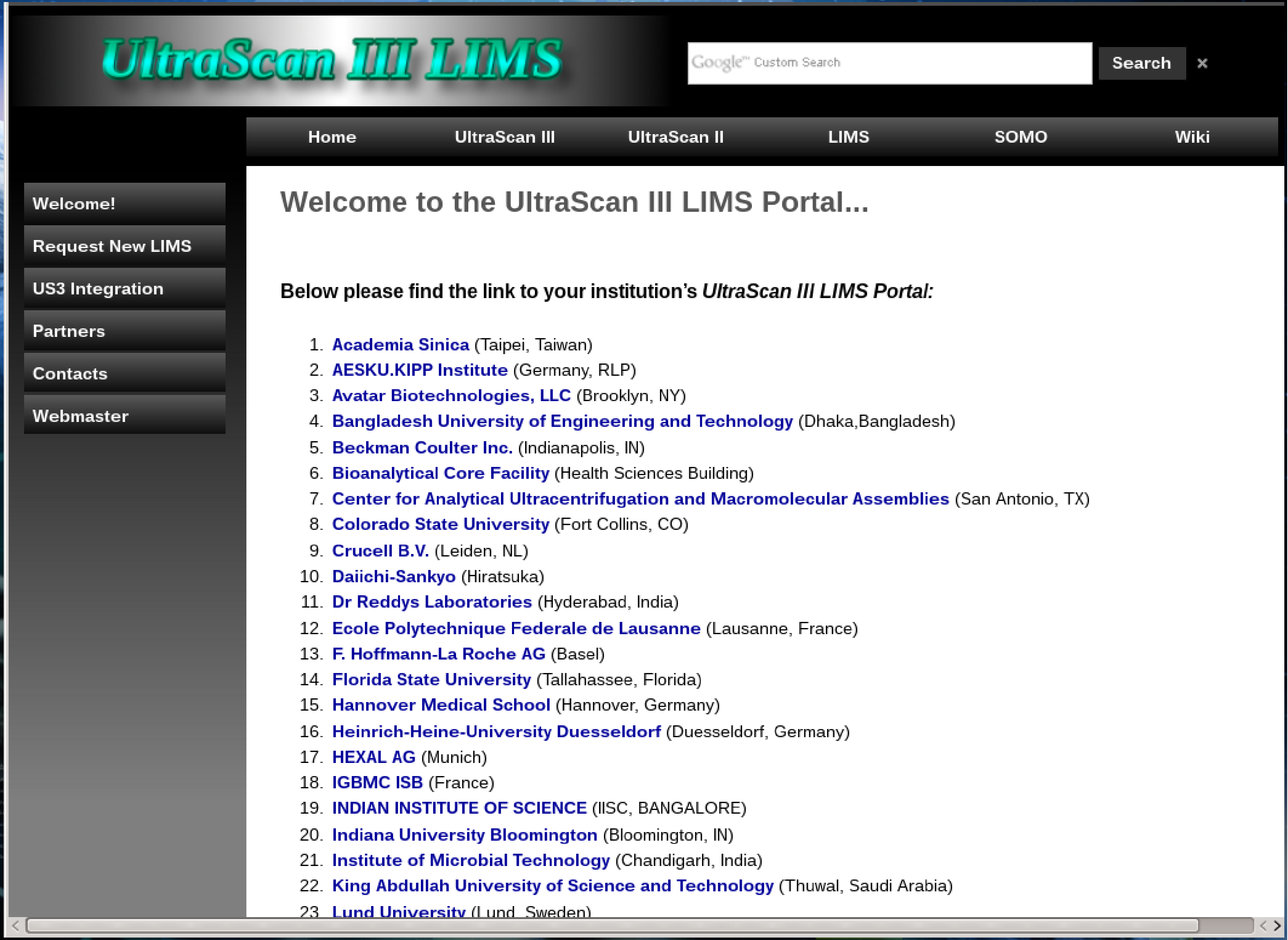
- ***Provide highest possible resolution in the analysis – requires HPC***
- ***Offer a flexible approach for multiple optimization methods***
- ***Integrate a variety of HPC environments into a uniform submission framework***
- ***Must be easy to learn and use – users should not have to be HPC experts***
- ***Support a large number of users and analysis instances simultaneously***
- ***Support data sharing and collaborations***
- ***Easy installation, easy maintenance***
- ***Robust and secure multi-user/multi-role framework***
- ***Provide check-pointing and easy to understand error messages***
- ***Support for multiple grid middleware (UNICORE, GRAM5)***
- ***Fast turnaround to support serial workflows (model refinement)***

XSEDE

Science Gateways

Apache Airavata

UNICORE GRAM5



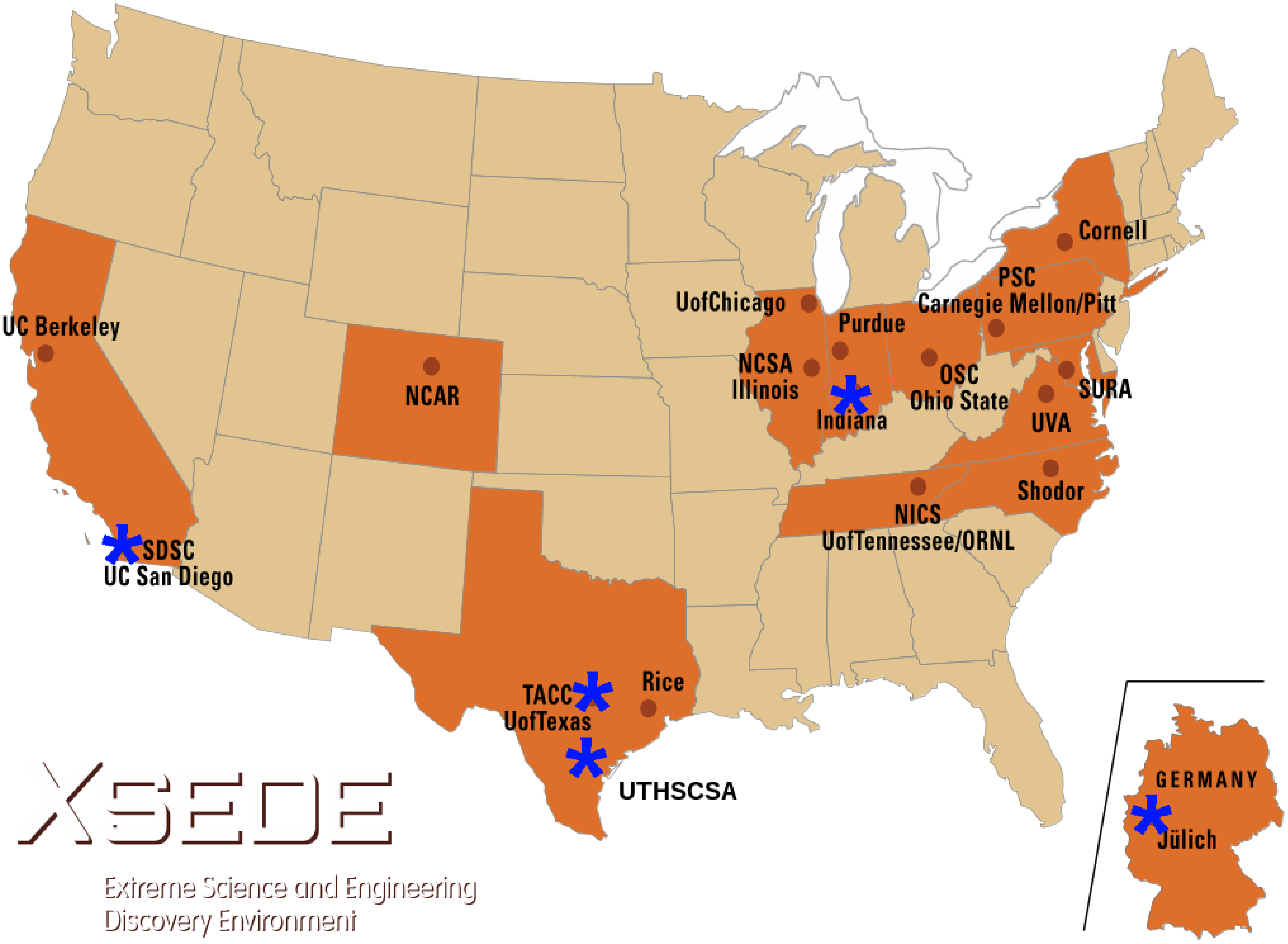
Welcome to the UltraScan III LIMS Portal...

Below please find the link to your institution's *UltraScan III LIMS Portal:*

1. **Academia Sinica** (Taipei, Taiwan)
2. **AESKU.KIPP Institute** (Germany, RLP)
3. **Avatar Biotechnologies, LLC** (Brooklyn, NY)
4. **Bangladesh University of Engineering and Technology** (Dhaka,Bangladesh)
5. **Beckman Coulter Inc.** (Indianapolis, IN)
6. **Bioanalytical Core Facility** (Health Sciences Building)
7. **Center for Analytical Ultracentrifugation and Macromolecular Assemblies** (San Antonio, TX)
8. **Colorado State University** (Fort Collins, CO)
9. **Crucell B.V.** (Leiden, NL)
10. **Daiichi-Sankyo** (Hiratsuka)
11. **Dr Reddys Laboratories** (Hyderabad, India)
12. **Ecole Polytechnique Federale de Lausanne** (Lausanne, France)
13. **F. Hoffmann-La Roche AG** (Basel)
14. **Florida State University** (Tallahassee, Florida)
15. **Hannover Medical School** (Hannover, Germany)
16. **Heinrich-Heine-University Duesseldorf** (Duesseldorf, Germany)
17. **HEXAL AG** (Munich)
18. **IGBMC ISB** (France)
19. **INDIAN INSTITUTE OF SCIENCE** (IISC, BANGALORE)
20. **Indiana University Bloomington** (Bloomington, IN)
21. **Institute of Microbial Technology** (Chandigarh, India)
22. **King Abdullah University of Science and Technology** (Thuwal, Saudi Arabia)
23. **Lund University** (Lund, Sweden)

XSEDE

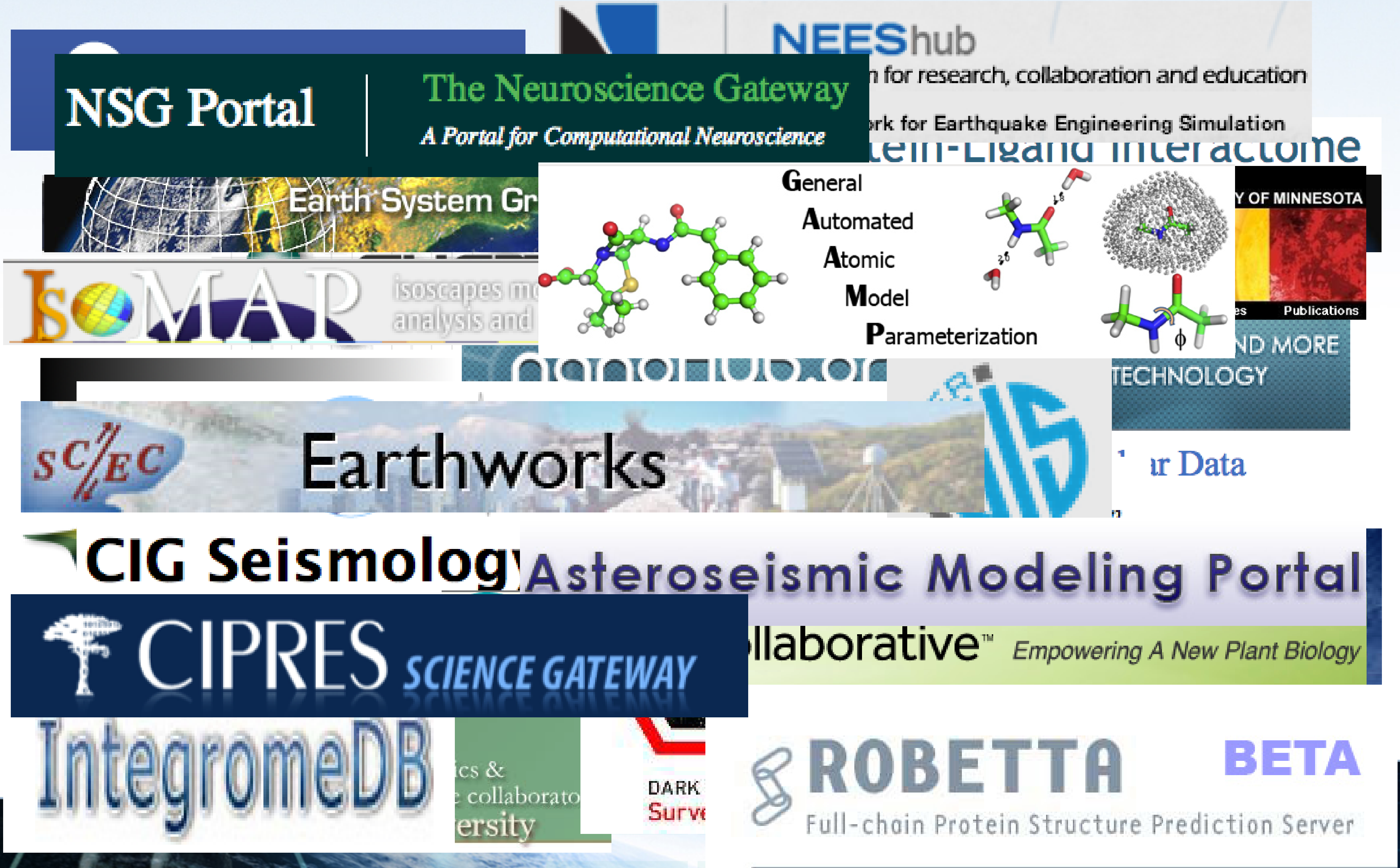
Extreme Science and Engineering
Discovery Environment



XSEDE

Extreme Science and Engineering Discovery Environment

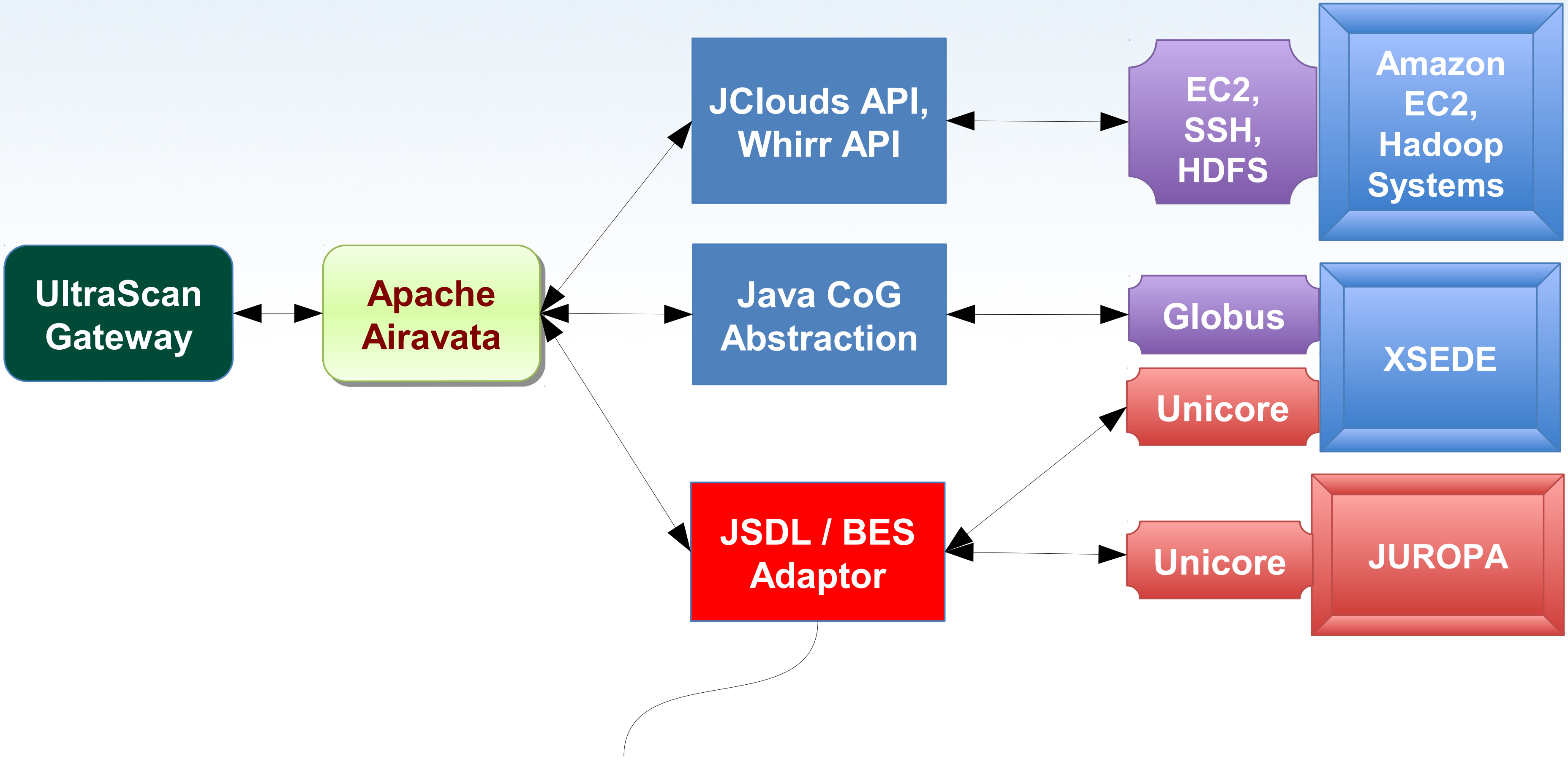
Today, there are over 30 gateways using XSEDE



What Is Apache Airavata?

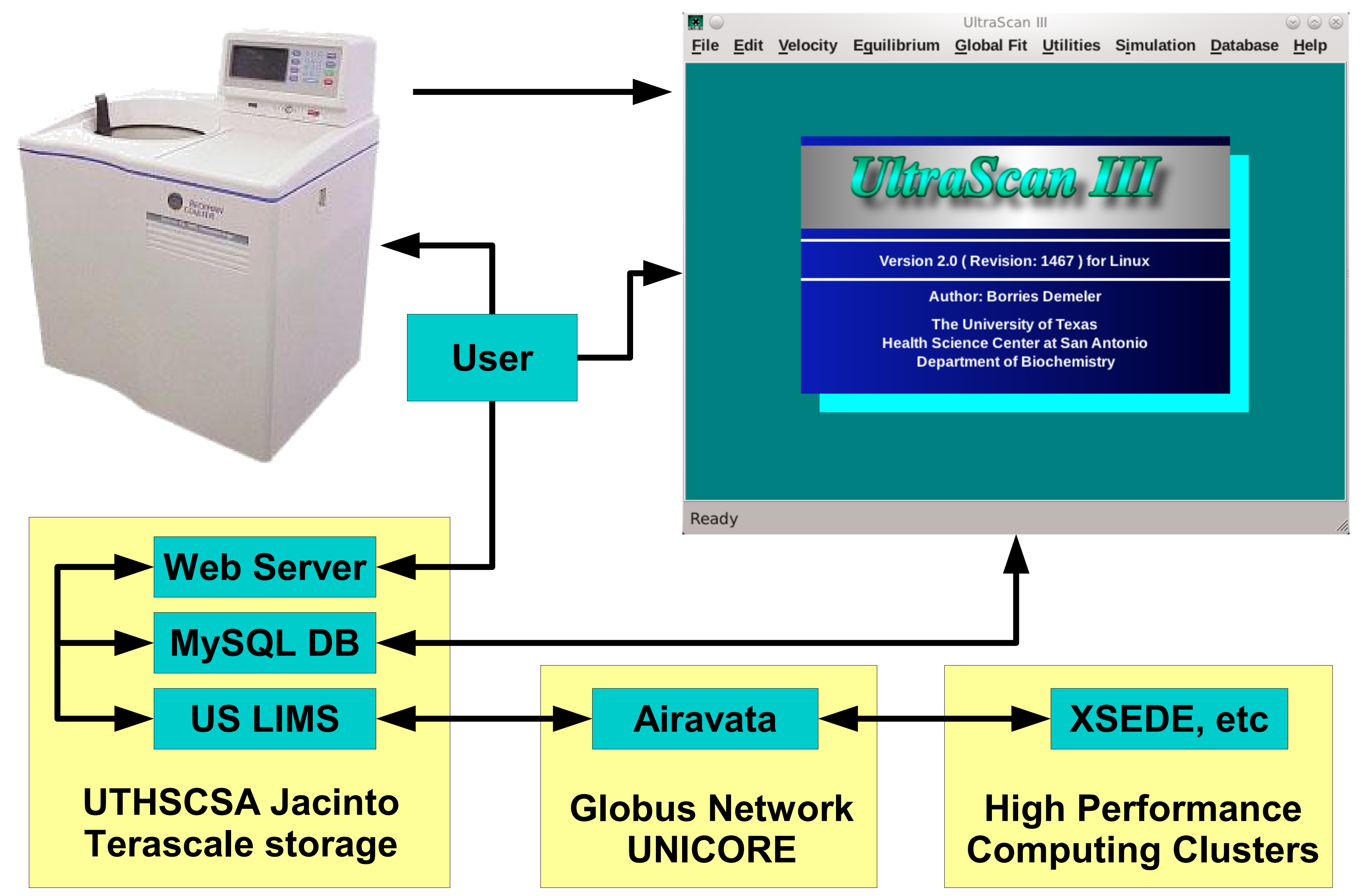
- Science Gateway software system to
  - Compose, manage, execute, and monitor distributed, computational workflows
  - Wrap legacy command line scientific applications with Web services.
  - Abstract job submission and provide uniform API for all resources
  - Run jobs on computational resources ranging from local resources to computational grids and clouds
- Airavata software is largely derived from NSF-funded academic research.

Jülich Contributions to Airavata



Contributed by Shahbaz Memon, JSC

UltraScan Organization (open source, multi-platform)



Version 2.0 (Revision: 1467) for Linux

Author: Borries Demeler

The University of Texas
Health Science Center at San Antonio
Department of Biochemistry

User

Web Server

MySQL DB

US LIMS

UTHSCSA Jacinto
Terascale storage

Airavata

Globus Network
UNICORE

XSEDE, etc

High Performance
Computing Clusters

A Science Gateway for Biophysical Analysis

UltraScan (US) components and 3rd party software:

US-GUI: (Linux, Mac, Windows): used for data processing, editing, uploading, visualization, report generation (C++/Qt).

US-LIMS: web-based interface to the MySQL database. Gives the user web-based access to their data, visualizations and analysis reports (PHP).

US-HPC: includes finite element solver for multiple models and performs all optimization algorithms (2DSA, GA, Monte Carlo)

US-Gridcontrol: PHP daemon to manage job submission, communications and reporting from US-HPC,

MySQL: houses all LIMS data, a separate Airavata DB holds job status info. Each institution has a separate database and separate US-LIMS instance. All interactions with MySQL are performed through stored procedure calls.

Airavata: accepts job requests and brokers them over the appropriate grid middleware to the requested supercomputer, controls job status in Airavata DB.

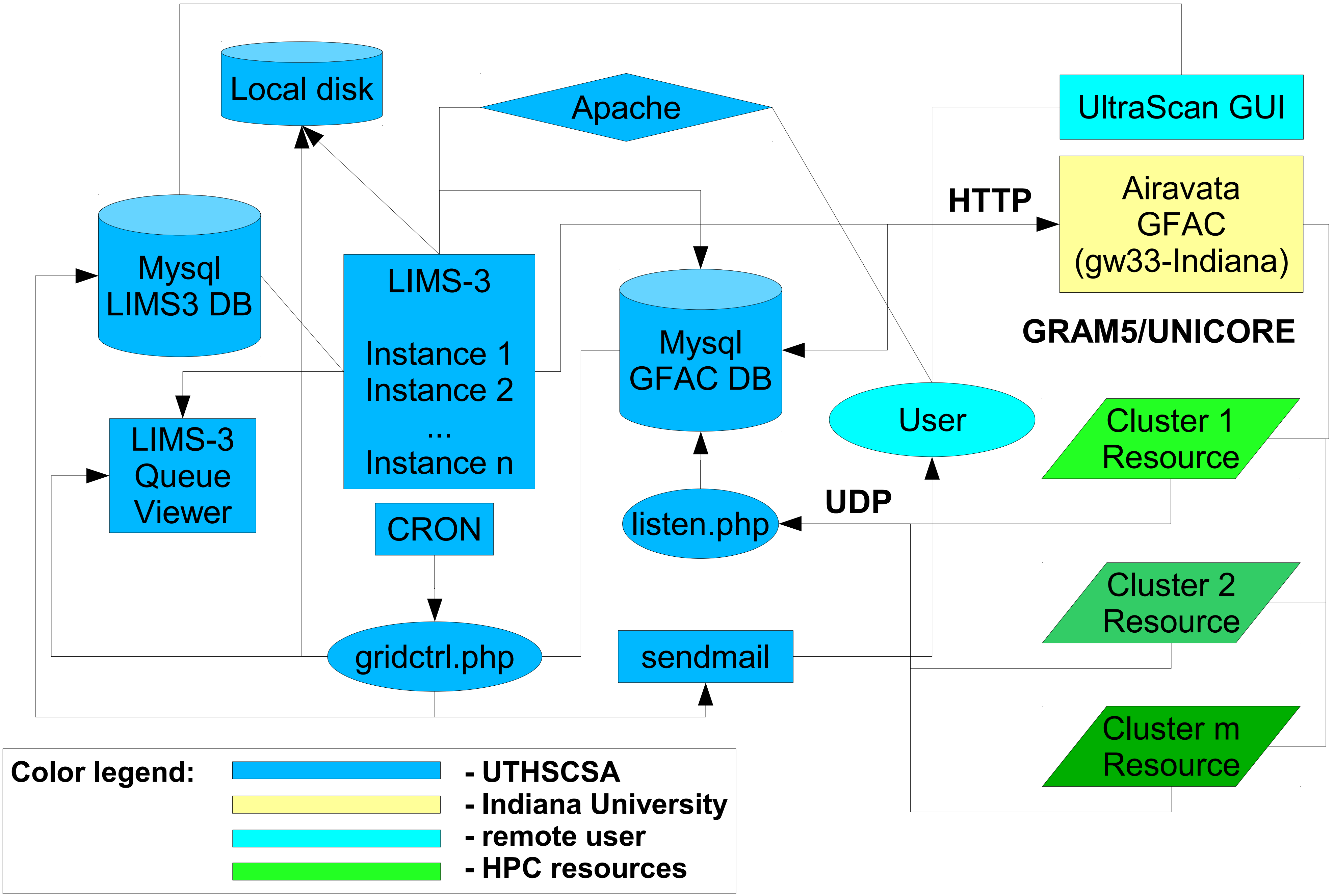
GRAM/UNICORE grid middleware

SSL communications: All communications and data transfers are SSL encrypted. All database access and LIMS access requires authentication.

Statistic scripts: queries database and reports usage and provides details for XSEDE reporting.

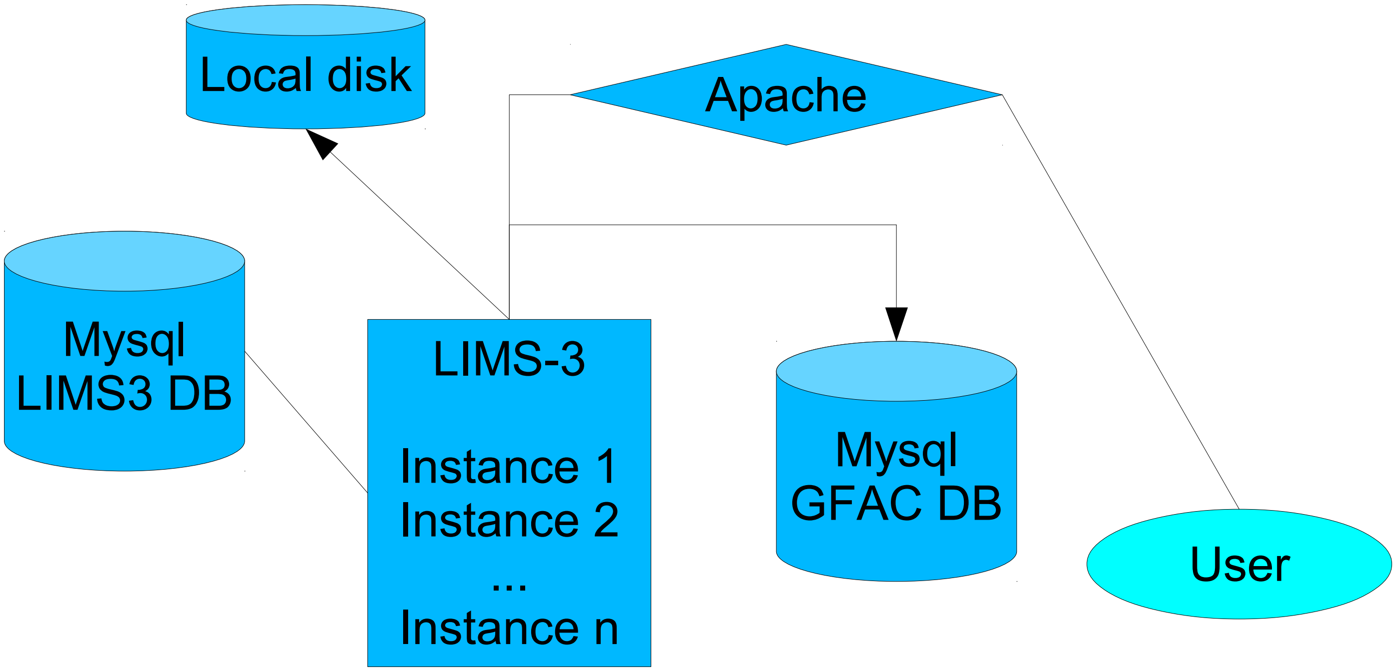
UltraScan LIMS3/GFAC Workflow Overview

(GFAC = Generic Factory Component of Apache Airavata)



UltraScan LIMS3/GFAC Workflow Overview

(Step 1: User logs into LIMS and requests their data, sets analysis parameters, job is retrieved from DB and packaged for submission, job request gets stored in GFAC DB)



Local disk

Apache

Mysql
LIMS3 DB

LIMS-3

Instance 1
Instance 2
...
Instance n

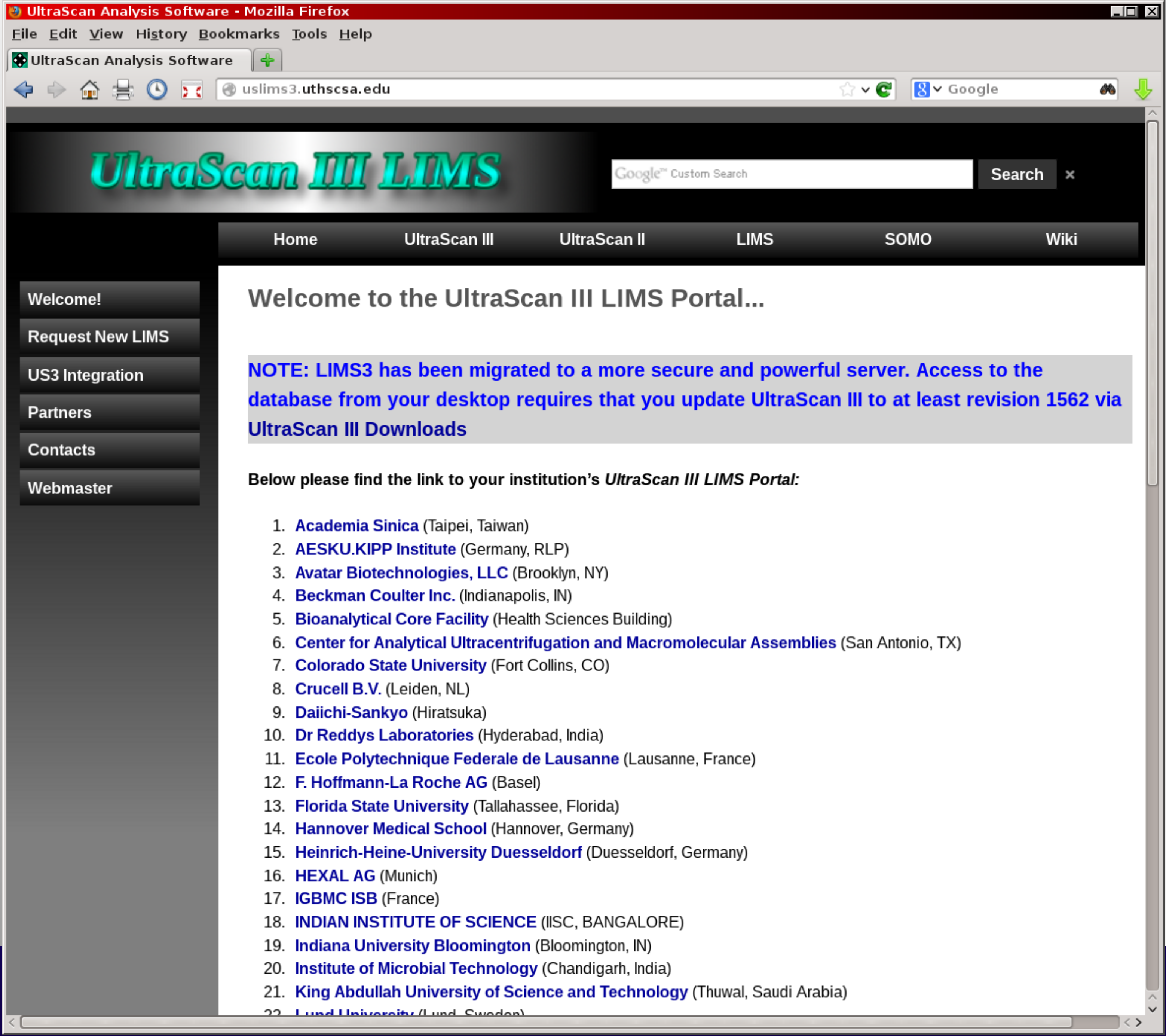
Mysql
GFAC DB

User

Color legend:

🟦	**- UTHSCSA**
🟨	**- Indiana University**
🟦	**- remote user**
🟩	**- HPC resources**

3. Selecting Gateway Instance



Welcome to the UltraScan III LIMS Portal...

NOTE: LIMS3 has been migrated to a more secure and powerful server. Access to the database from your desktop requires that you update UltraScan III to at least revision 1562 via UltraScan III Downloads

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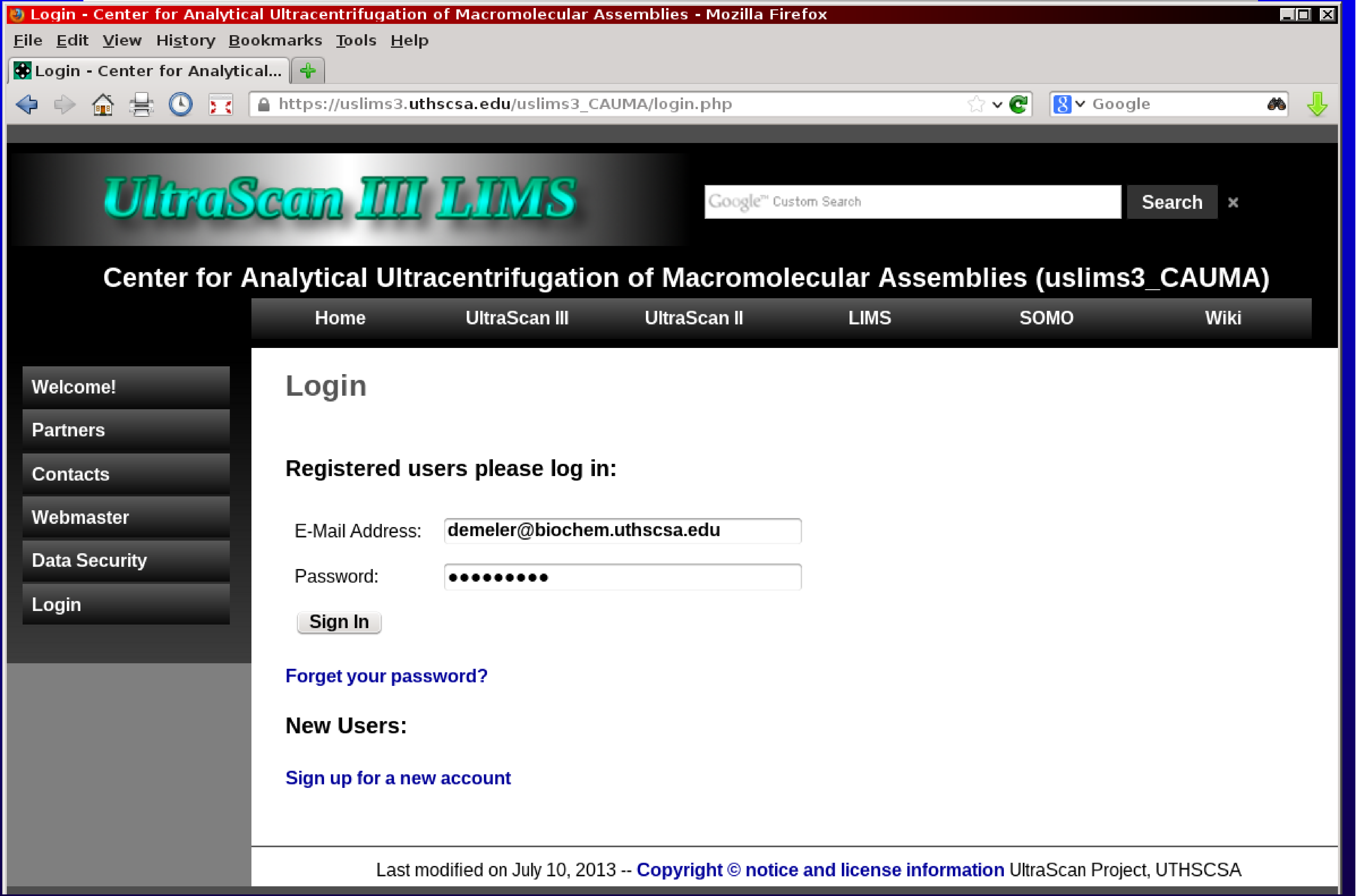
4. Authentication...



Center for Analytical Ultracentrifugation of Macromolecular Assemblies (uslims3_CAUMA)

Login

Registered users please log in:

E-Mail Address: demeler@biochem.uthscsa.edu

Password: ●●●●●●●●●

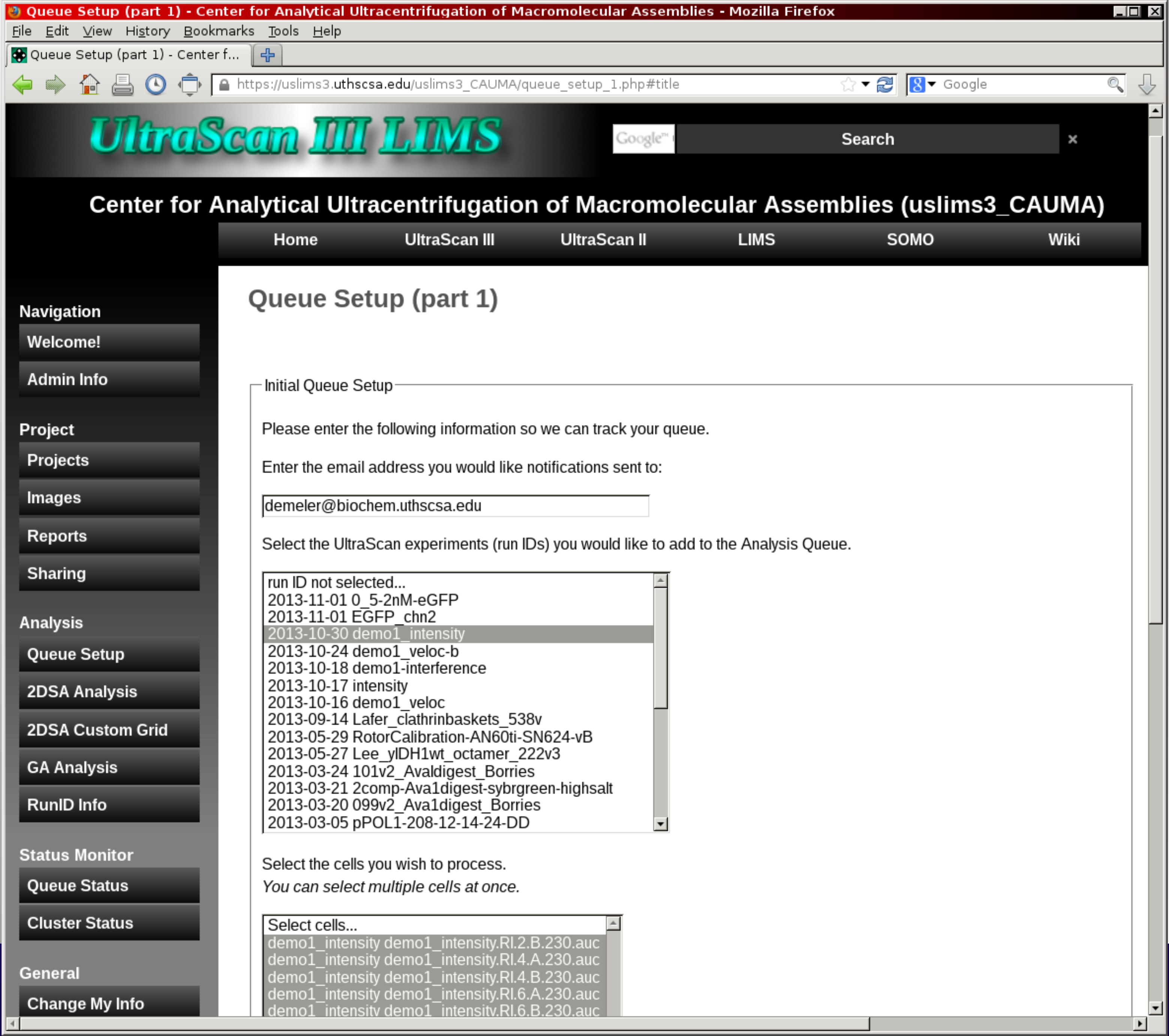
Forget your password?

New Users:

Sign up for a new account

Last modified on July 10, 2013 -- Copyright © notice and license information UltraScan Project, UTHSCSA

5. Data Selection



Center for Analytical Ultracentrifugation of Macromolecular Assemblies (uslims3_CAUMA)

Queue Setup (part 1)

Initial Queue Setup

Please enter the following information so we can track your queue.

Enter the email address you would like notifications sent to:

demeler@biochem.uthscsa.edu

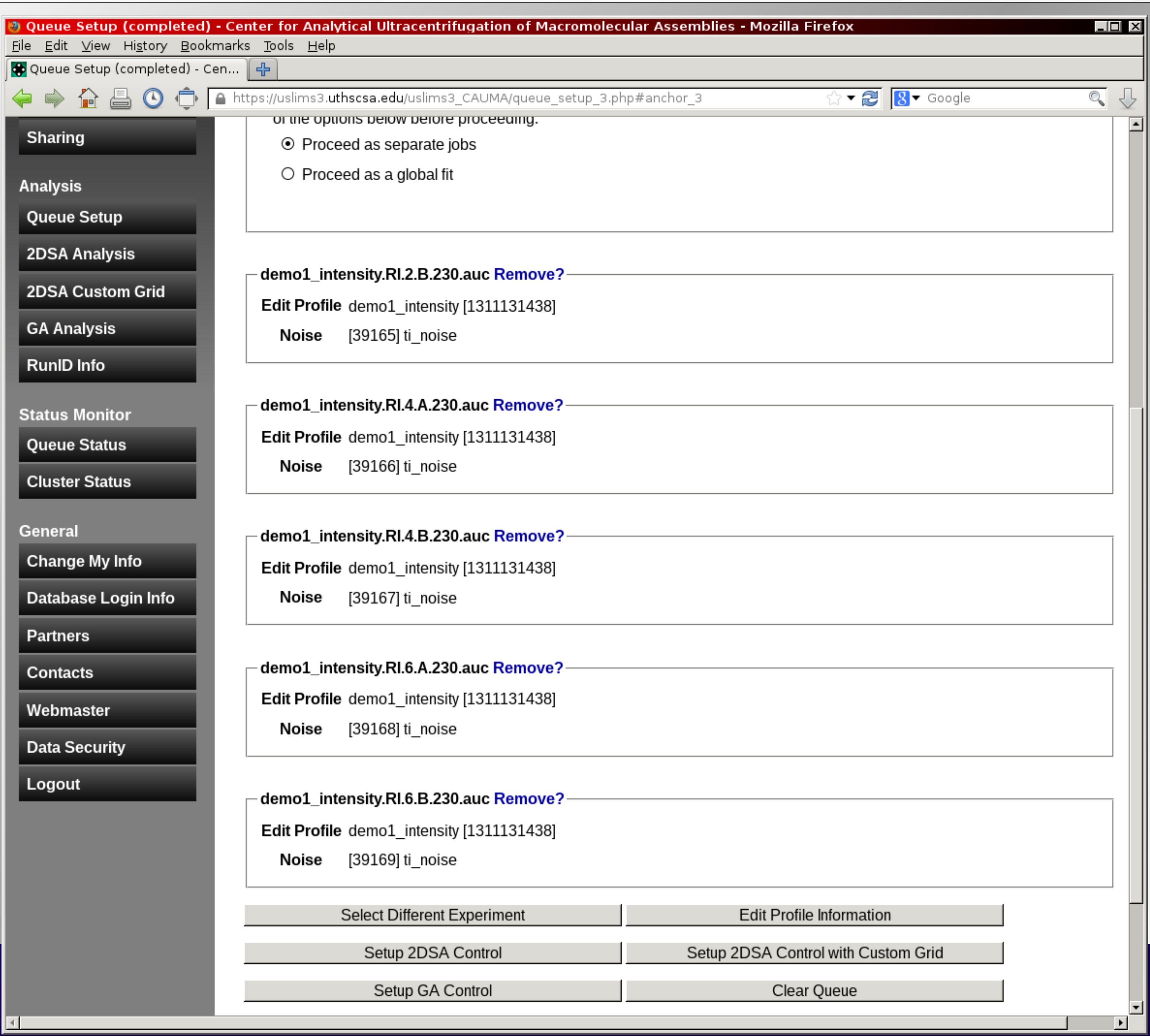
Select the UltraScan experiments (run IDs) you would like to add to the Analysis Queue.

run ID not selected...
2013-11-01 0_5-2nM-eGFP
2013-11-01 EGFP_chn2
2013-10-30 demo1_intensity
2013-10-24 demo1_veloc-b
2013-10-18 demo1-interference
2013-10-17 intensity
2013-10-16 demo1_veloc
2013-09-14 Lafer_clathrinbaskets_538v
2013-05-29 RotorCalibration-AN60ti-SN624-vB
2013-05-27 Lee_ylDH1wt_octamer_222v3
2013-03-24 101v2_Avaldigest_Borries
2013-03-21 2comp-Ava1digest-sybrgreen-highsalt
2013-03-20 099v2_Ava1digest_Borries
2013-03-05 pPOL1-208-12-14-24-DD

Select the cells you wish to process.
You can select multiple cells at once.

Select cells...
demo1_intensity demo1_intensity.RI.2.B.230.auc
demo1_intensity demo1_intensity.RI.4.A.230.auc
demo1_intensity demo1_intensity.RI.4.B.230.auc
demo1_intensity demo1_intensity.RI.6.A.230.auc
demo1_intensity demo1_intensity.RI.6.B.230.auc

6. Analysis Method Selection



of the options below before proceeding.

● Proceed as separate jobs

○ Proceed as a global fit

demo1_intensity.RI.2.B.230.auc Remove?

Edit Profile demo1_intensity [1311131438]

Noise [39165] ti_noise

demo1_intensity.RI.4.A.230.auc Remove?

Edit Profile demo1_intensity [1311131438]

Noise [39166] ti_noise

demo1_intensity.RI.4.B.230.auc Remove?

Edit Profile demo1_intensity [1311131438]

Noise [39167] ti_noise

demo1_intensity.RI.6.A.230.auc Remove?

Edit Profile demo1_intensity [1311131438]

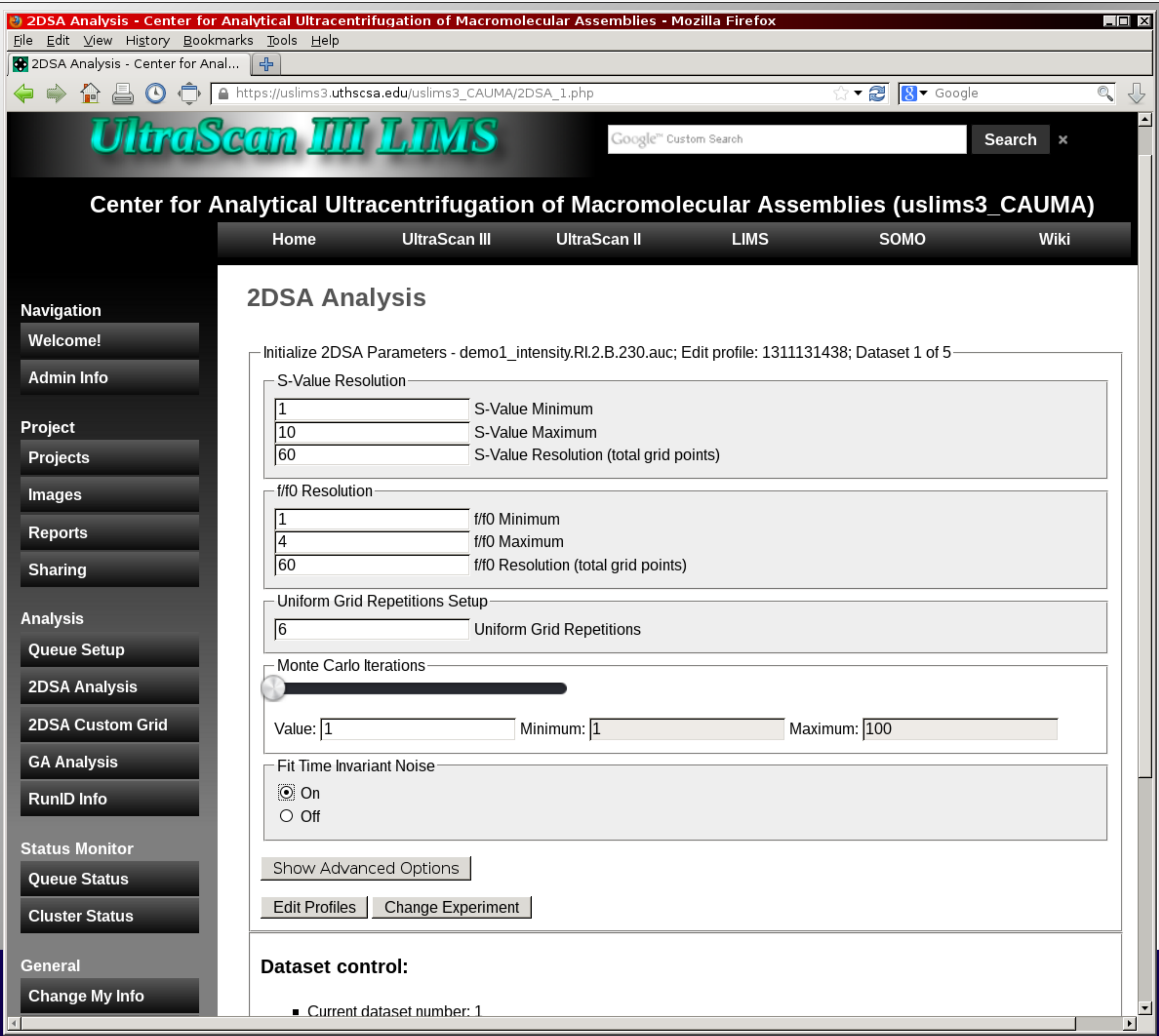
Noise [39168] ti_noise

demo1_intensity.RI.6.B.230.auc Remove?

Edit Profile demo1_intensity [1311131438]

Noise [39169] ti_noise

7. Analysis Method Parameter Selection



Center for Analytical Ultracentrifugation of Macromolecular Assemblies (uslims3_CAUMA)

2DSA Analysis

Initialize 2DSA Parameters - demo1_intensity.RI.2.B.230.auc; Edit profile: 1311131438; Dataset 1 of 5

S-Value Resolution
- S-Value Minimum: 1
- S-Value Maximum: 10
- S-Value Resolution (total grid points): 60

f/f0 Resolution
- f/f0 Minimum: 1
- f/f0 Maximum: 4
- f/f0 Resolution (total grid points): 60

Uniform Grid Repetitions Setup
- Uniform Grid Repetitions: 6

Monte Carlo Iterations

Value: 1 Minimum: 1 Maximum: 100

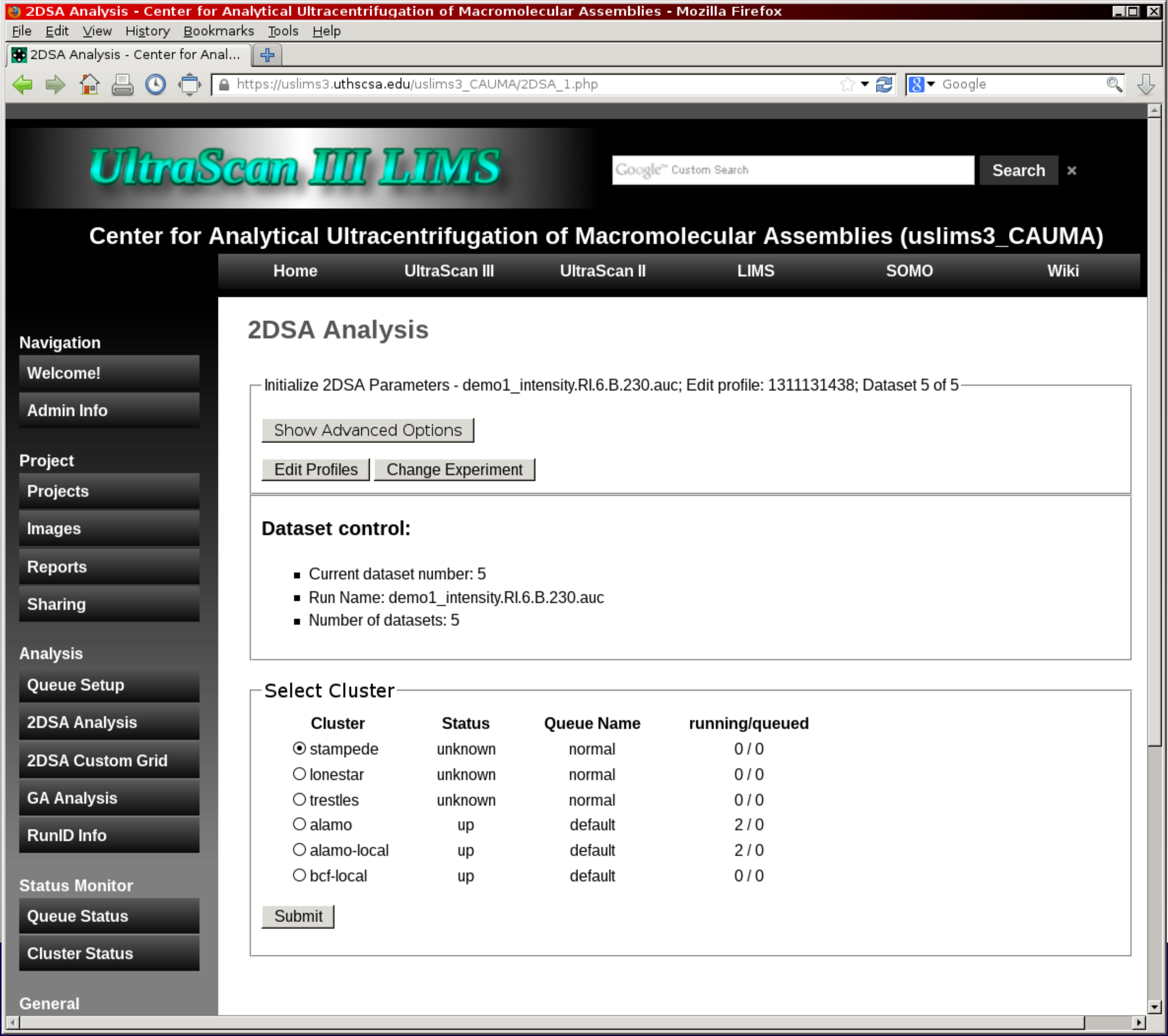
Fit Time Invariant Noise

● On
○ Off

Dataset control:

- Current dataset number: 1

9. Cluster Resource Selection



Center for Analytical Ultracentrifugation of Macromolecular Assemblies (uslims3_CAUMA)

2DSA Analysis

Initialize 2DSA Parameters - demo1_intensity.RI.6.B.230.auc; Edit profile: 1311131438; Dataset 5 of 5

Dataset control:

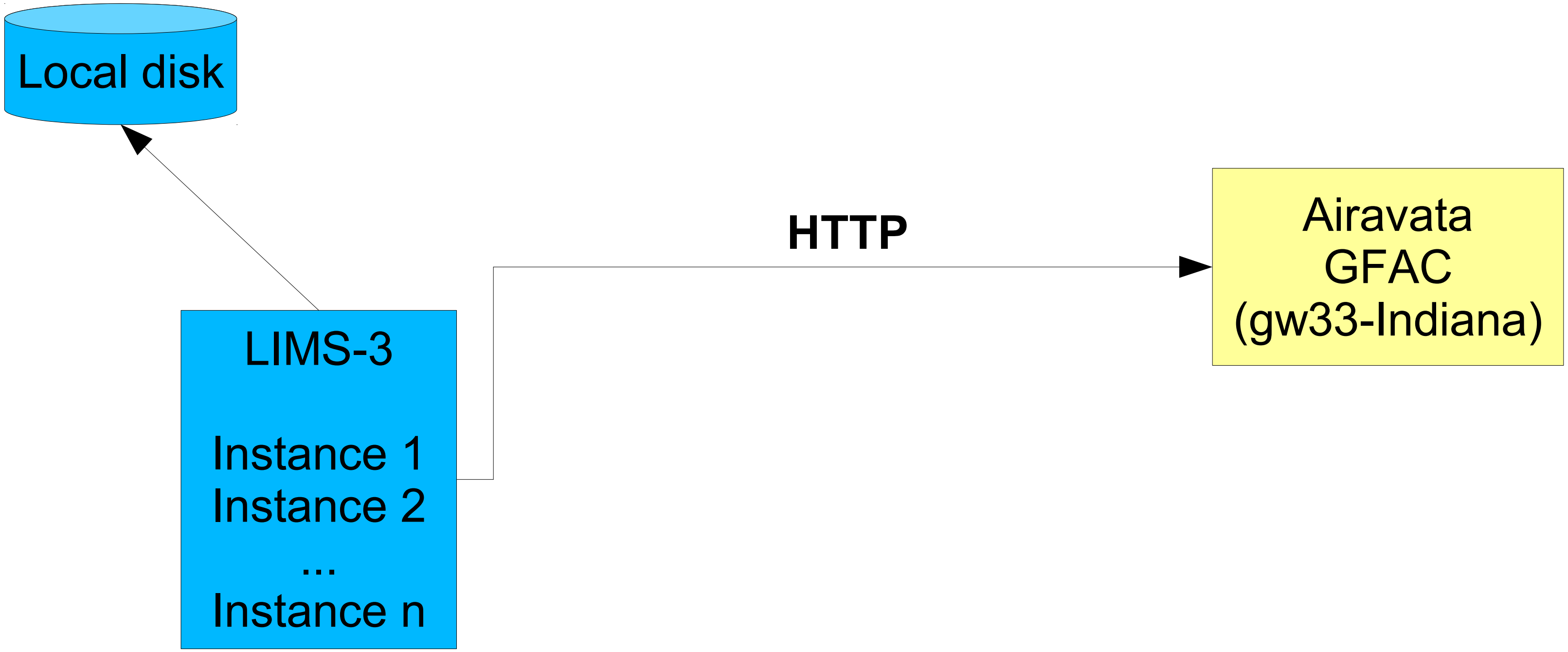
- Current dataset number: 5
- Run Name: demo1_intensity.RI.6.B.230.auc
- Number of datasets: 5

Select Cluster

Cluster	Status	Queue Name	running/queued
● stampede	unknown	normal	0 / 0
○ lonestar	unknown	normal	0 / 0
○ trestles	unknown	normal	0 / 0
○ alamo	up	default	2 / 0
○ alamo-local	up	default	2 / 0
○ bcf-local	up	default	0 / 0

UltraScan LIMS3/GFAC Workflow Overview

(Step 2: LIMS packages data and job parameter on the local storage and sends notification of pending job to GFAC)

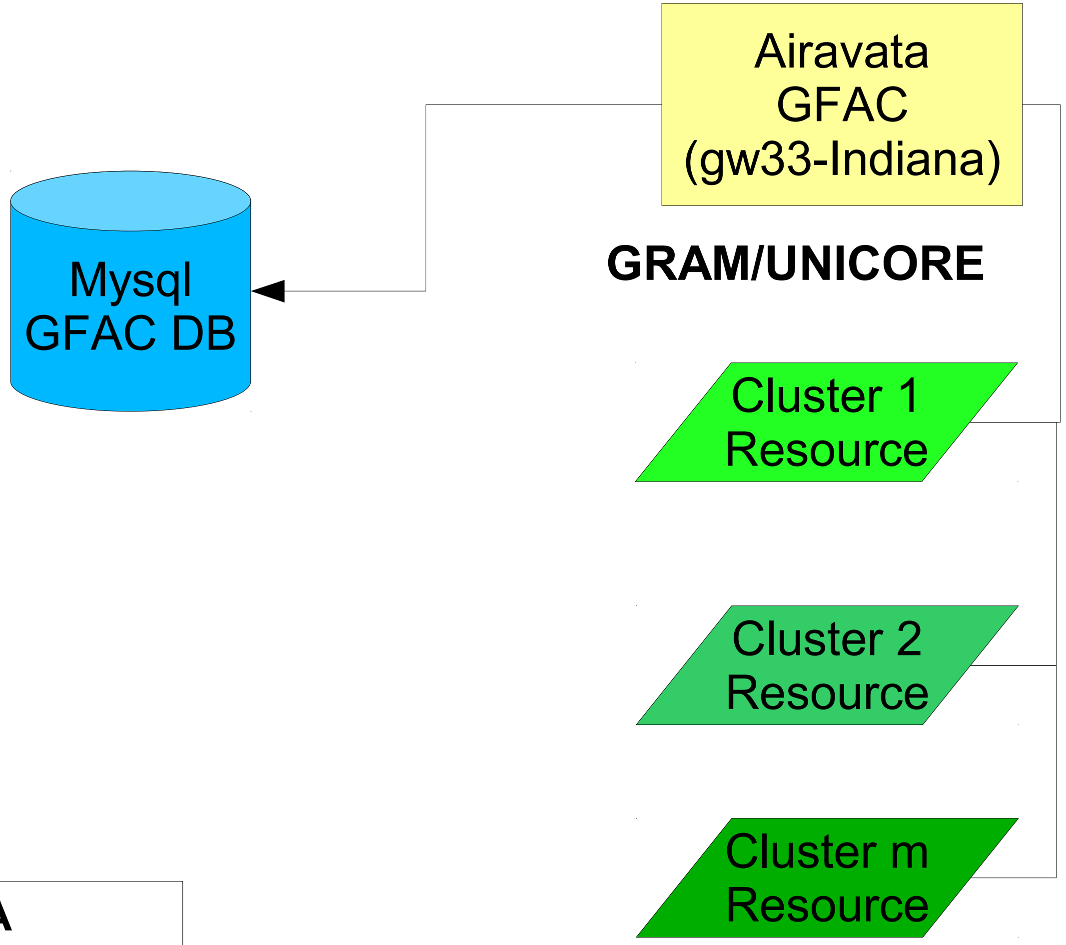


Color legend:

🟦 - UTHSCSA
🟨 - Indiana University
🟦 - remote user
🟩 - HPC resources

UltraScan LIMS3/GFAC Workflow Overview

(Step 3: GFAC grabs data from GFAC DB, and queues the job on the requested resource)



Airavata GFAC (gw33-Indiana)

Mysql GFAC DB

GRAM/UNICORE

Cluster 1 Resource

Cluster 2 Resource

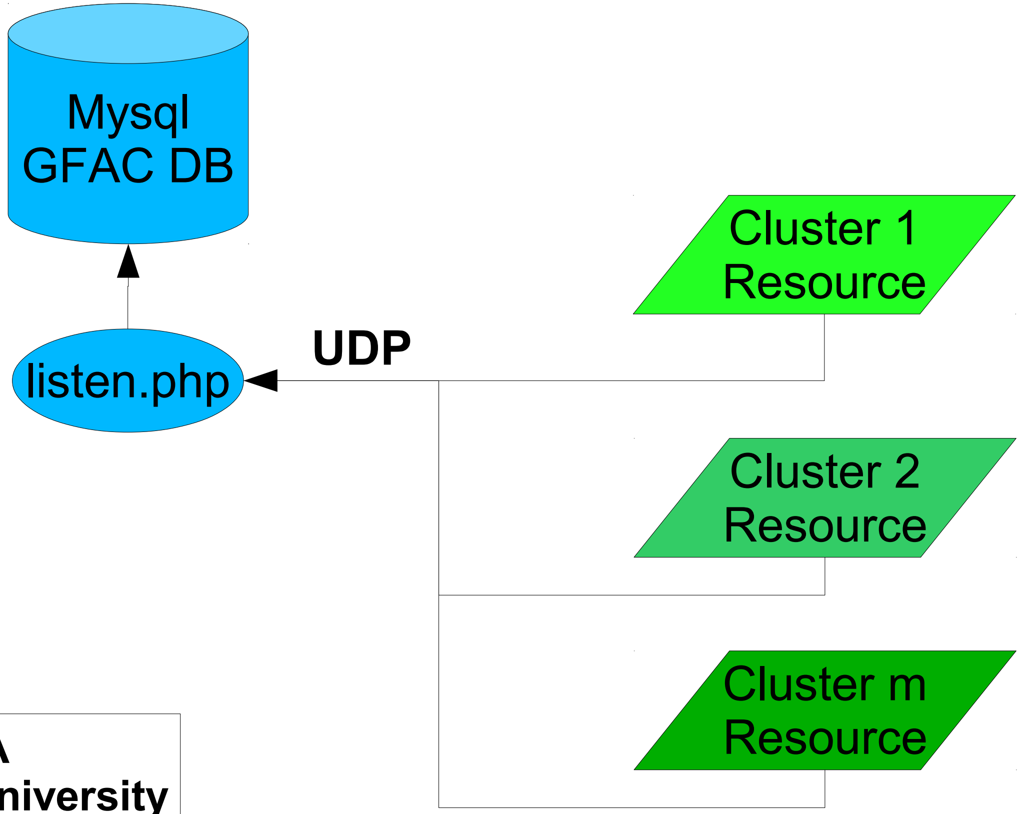
Cluster m Resource

Color legend:

- 🟦 **- UTHSCSA**
- 🟨 **- Indiana University**
- 🟦 **- remote user**
- 🟩 **- HPC resources**

UltraScan LIMS3/GFAC Workflow Overview

(Step 4: US-HPC sends job status over UDP to a daemon which updates GFAC DB)


Mysql
GFAC DB

listen.php

UDP

Cluster 1
Resource

Cluster 2
Resource

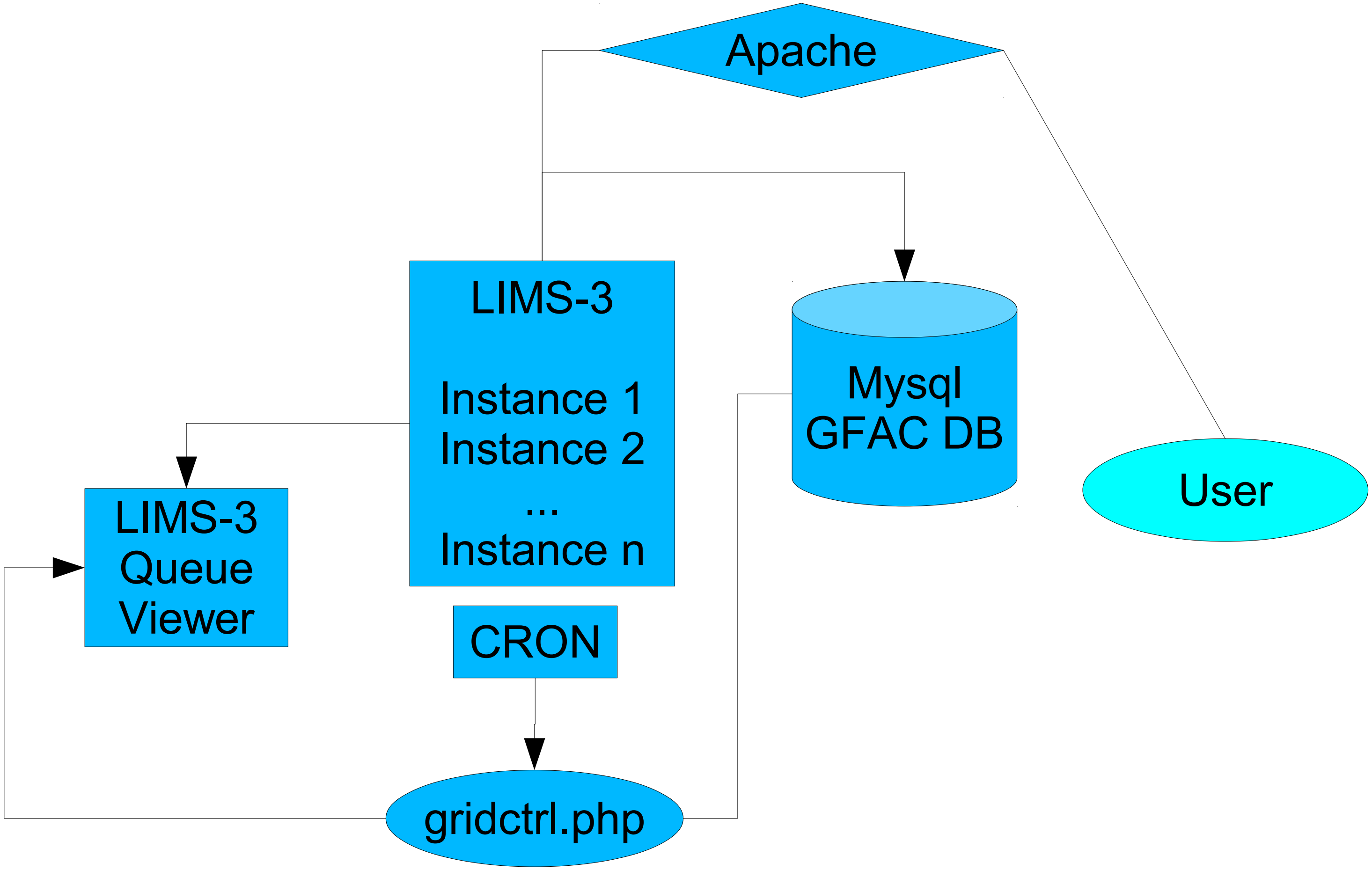
Cluster m
Resource

Color legend:

🟦 **- UTHSCSA**
🟨 **- Indiana University**
🟦 **- remote user**
🟩 **- HPC resources**

UltraScan LIMS3/GFAC Workflow Overview

(Step 5: cron triggers gridcontrol script periodically to check each job status in the GFAC DB, updates the Queue Viewer. User checks queue viewer through LIMS)



Apache

LIMS-3

Instance 1
Instance 2
...
Instance n

Mysql
GFAC DB

User

LIMS-3
Queue
Viewer

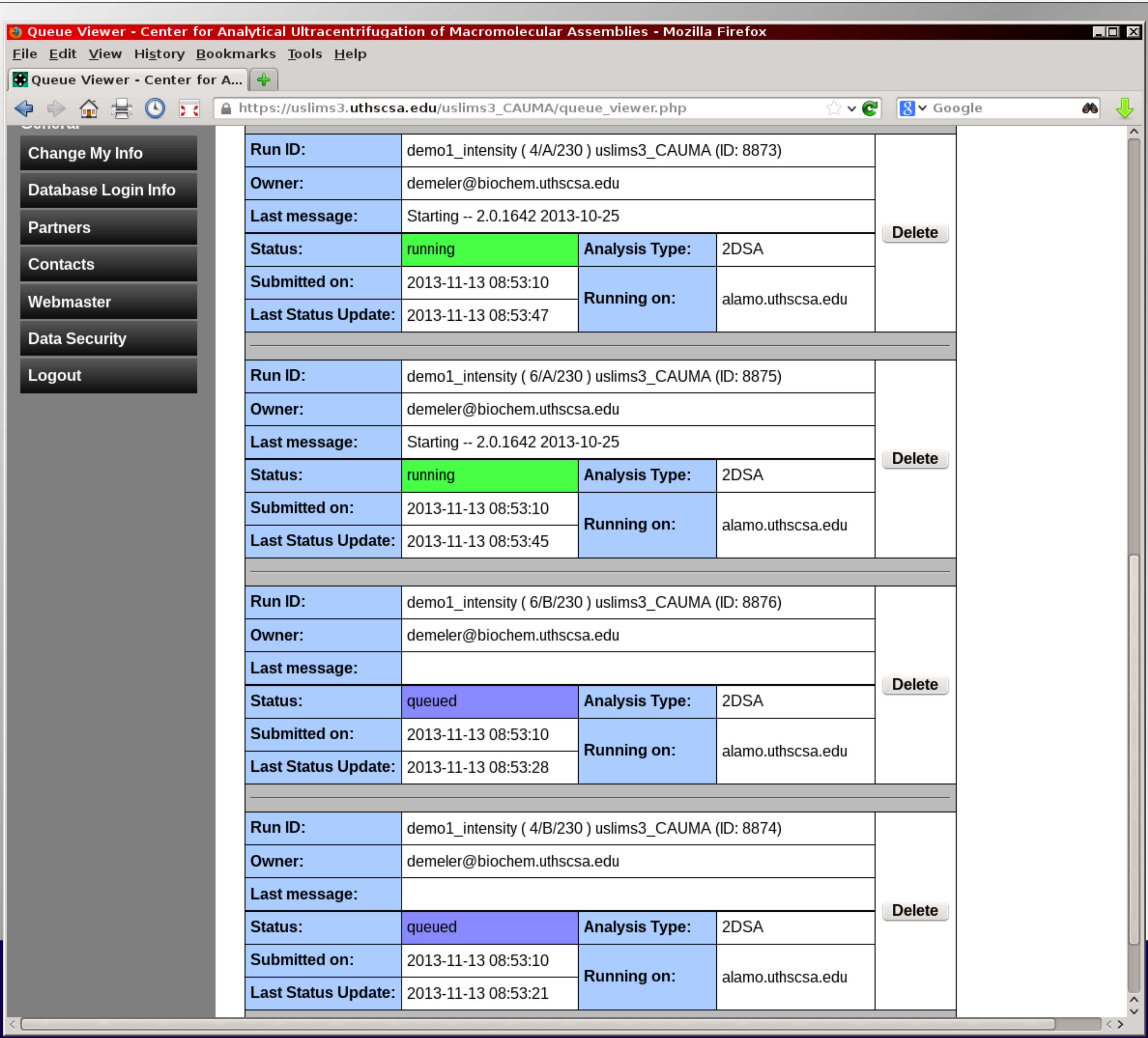
CRON

gridctrl.php

Color legend:

- 🟦 **- UTHSCSA**
- 🟨 **- Indiana University**
- 🟦 **- remote user**
- 🟩 **- HPC resources**

10. Queue Monitor



Run ID:	demo1_intensity (4/A/230) uslims3_CAUMA (ID: 8873)		
Owner:	demeler@biochem.uthscsa.edu		
Last message:	Starting -- 2.0.1642 2013-10-25		
Status:	running	**Analysis Type:**	2DSA
Submitted on:	2013-11-13 08:53:10	**Running on:**	alamo.uthscsa.edu
Last Status Update:	2013-11-13 08:53:47		

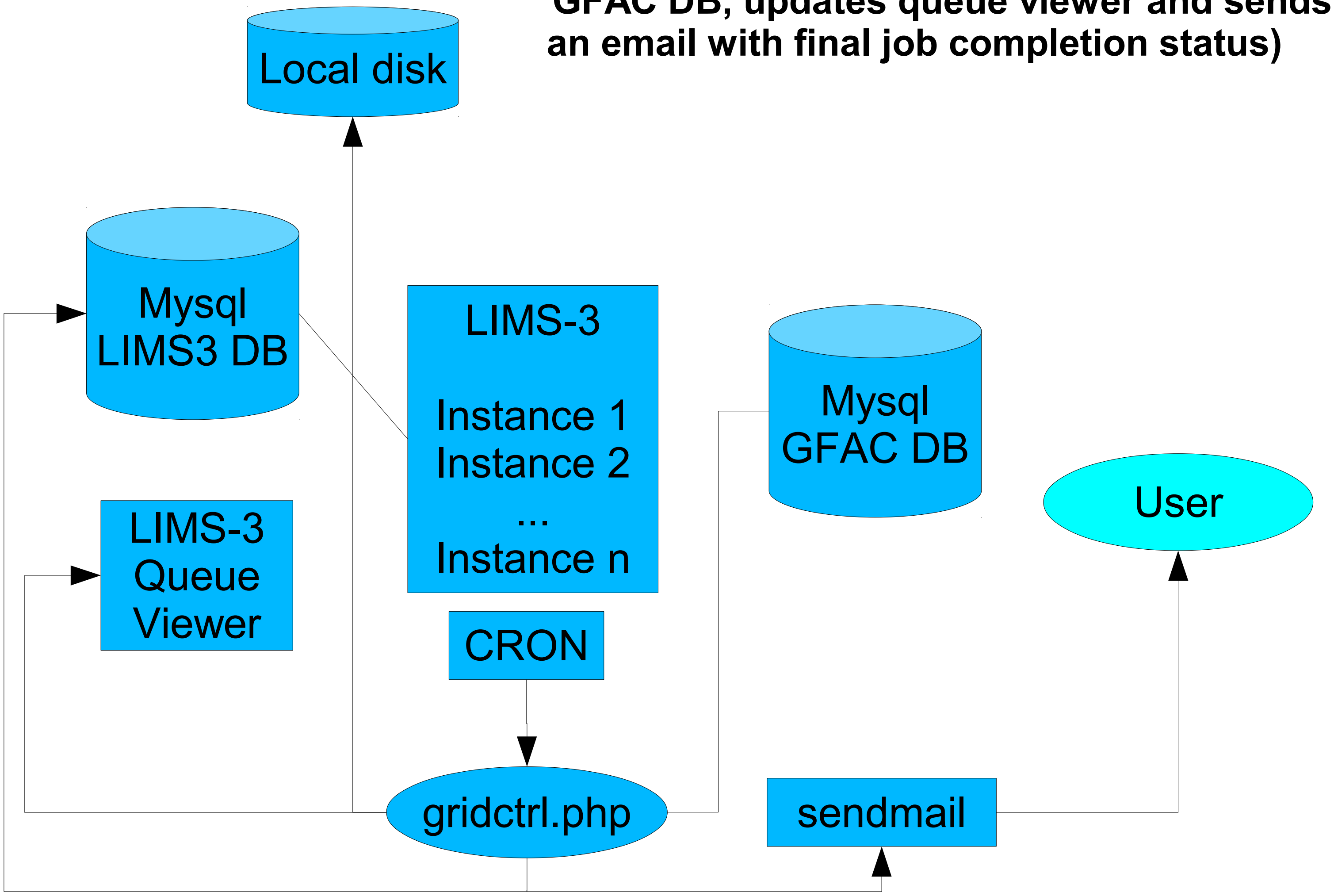
Run ID:	demo1_intensity (6/A/230) uslims3_CAUMA (ID: 8875)		
Owner:	demeler@biochem.uthscsa.edu		
Last message:	Starting -- 2.0.1642 2013-10-25		
Status:	running	**Analysis Type:**	2DSA
Submitted on:	2013-11-13 08:53:10	**Running on:**	alamo.uthscsa.edu
Last Status Update:	2013-11-13 08:53:45		

Run ID:	demo1_intensity (6/B/230) uslims3_CAUMA (ID: 8876)		
Owner:	demeler@biochem.uthscsa.edu		
Last message:			
Status:	queued	**Analysis Type:**	2DSA
Submitted on:	2013-11-13 08:53:10	**Running on:**	alamo.uthscsa.edu
Last Status Update:	2013-11-13 08:53:28		

Run ID:	demo1_intensity (4/B/230) uslims3_CAUMA (ID: 8874)		
Owner:	demeler@biochem.uthscsa.edu		
Last message:			
Status:	queued	**Analysis Type:**	2DSA
Submitted on:	2013-11-13 08:53:10	**Running on:**	alamo.uthscsa.edu
Last Status Update:	2013-11-13 08:53:21		

UltraScan LIMS3/GFAC Workflow Overview

(Step 6: cron triggers gridcontrol to check job list on GFAC DB for completed jobs, moves results to LIMS DB, copies stderr/out results to local disk, deletes completed jobs from GFAC DB, updates queue viewer and sends user an email with final job completion status)

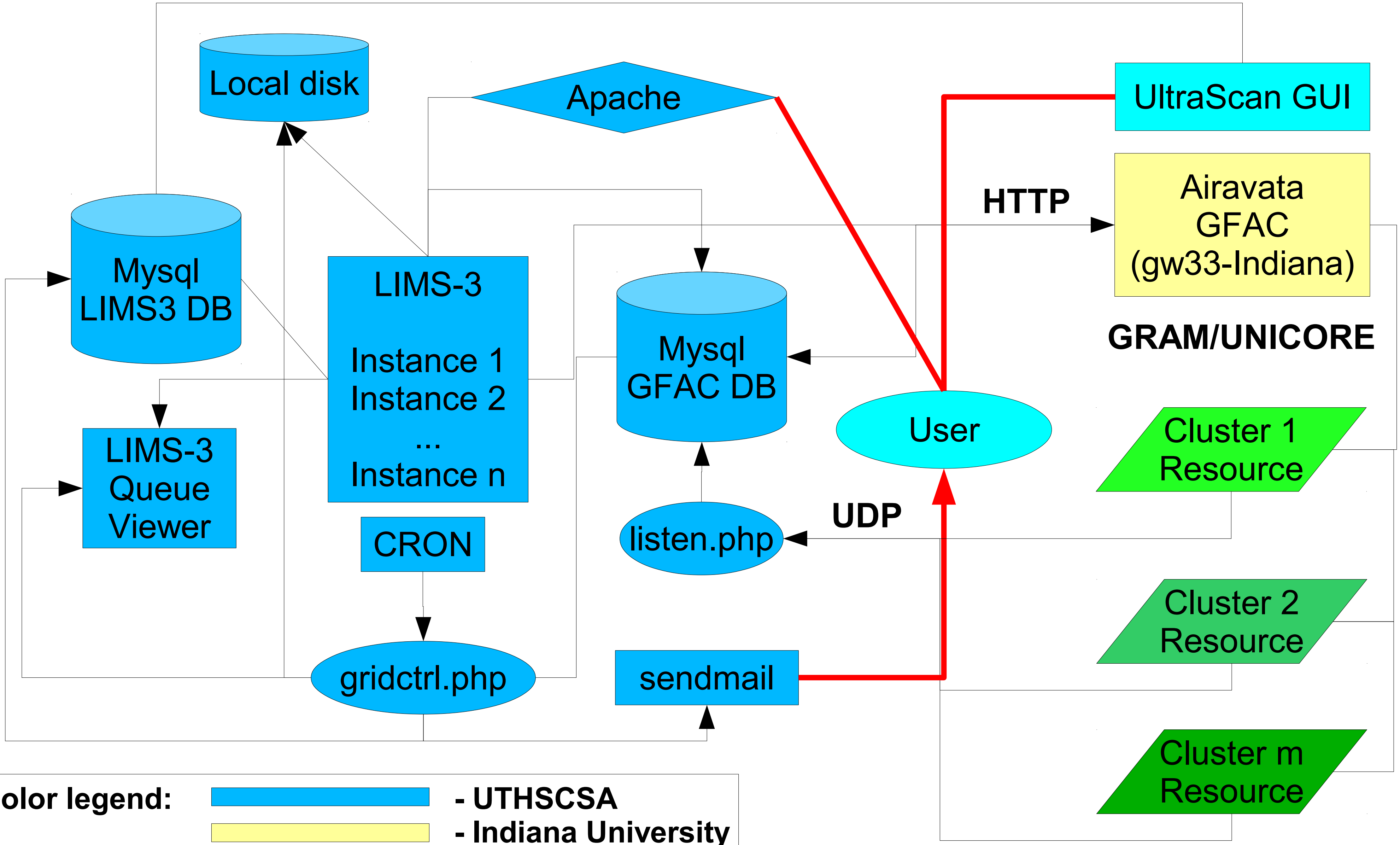


Color legend:

🟦 - UTHSCSA
🟨 - Indiana University
▨ - remote user
🟩 - HPC resources

UltraScan LIMS3/GFAC Workflow Overview

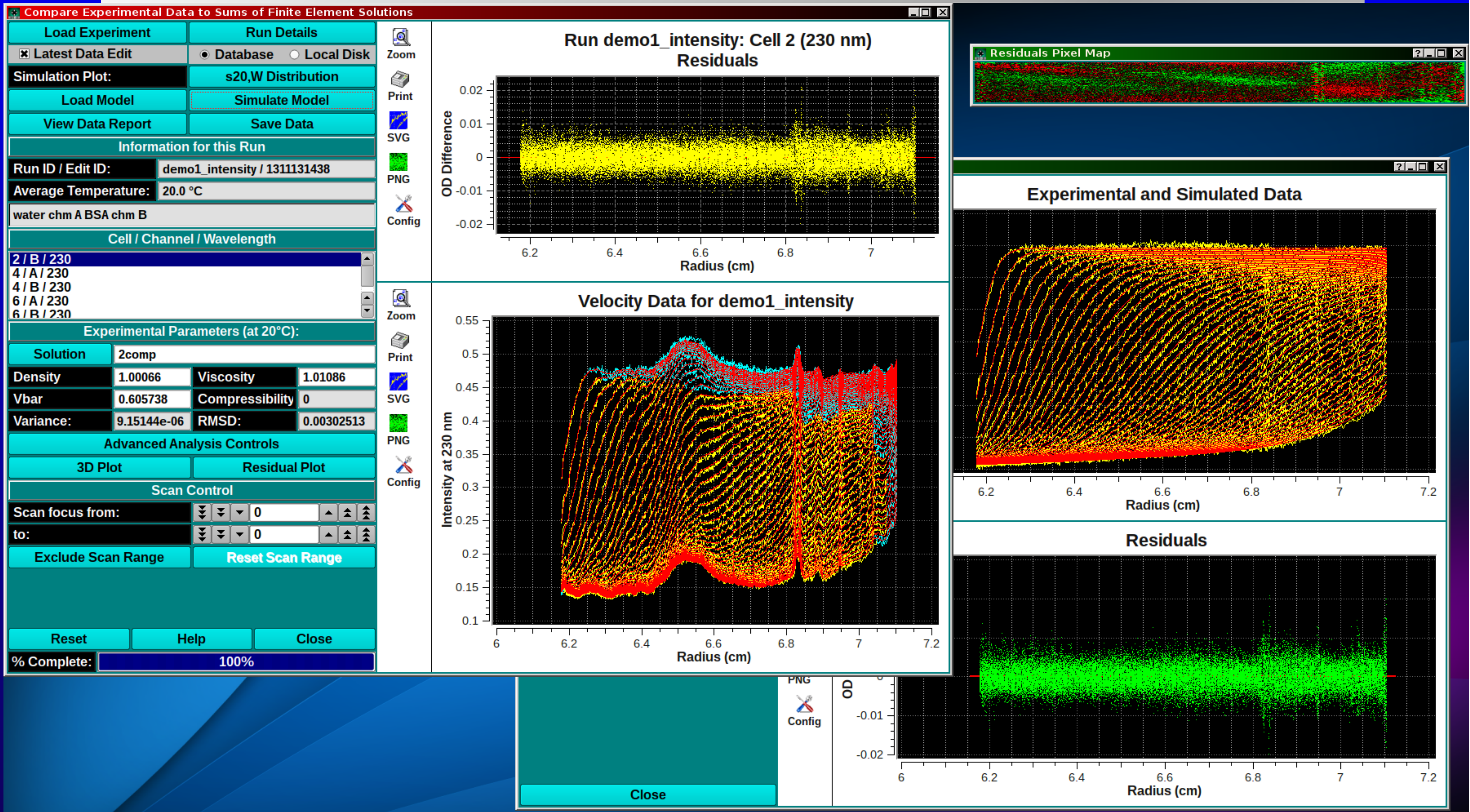
(User only interacts with web service or uses US-GUI to visualize final results)



Color legend:

🟦 **- UTHSCSA**
🟨 **- Indiana University**
🟦 **- remote user**
🟩 **- HPC resources**

11. Result Visualization



Compare Experimental Data to Sums of Finite Element Solutions

☒ Latest Data Edit

● Database ○ Local Disk

Simulation Plot: s20,W Distribution

Information for this Run

Run ID / Edit ID: demo1_intensity / 1311131438

Average Temperature: 20.0 °C

water chm A BSA chm B

Cell / Channel / Wavelength

- 2 / B / 230
- 4 / A / 230
- 4 / B / 230
- 6 / A / 230
- 6 / B / 230

Experimental Parameters (at 20°C):

Solution: 2comp

Density: 1.00066

Viscosity: 1.01086

Vbar: 0.605738

Compressibility: 0

Variance: 9.15144e-06

RMSD: 0.00302513

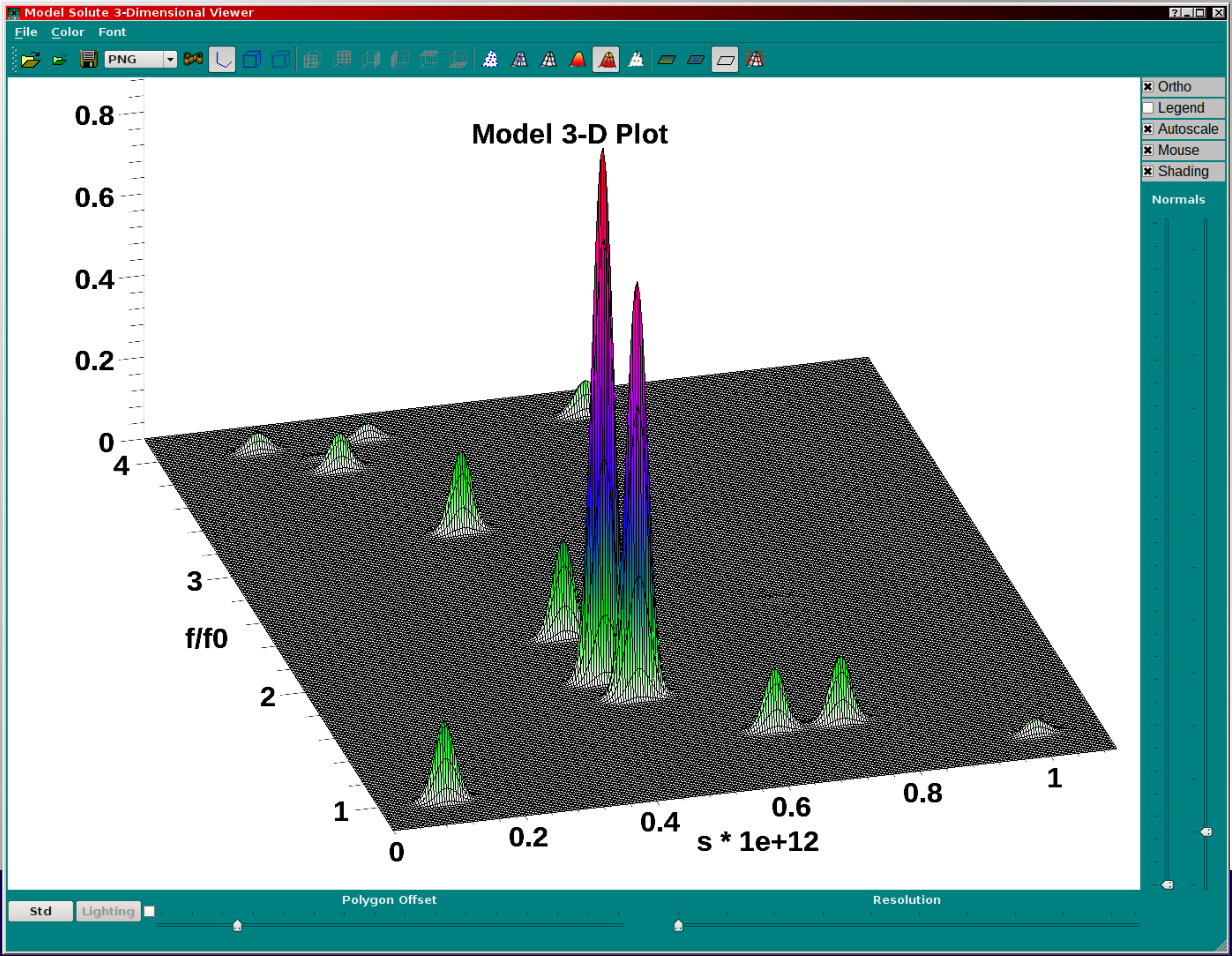
Scan Control

Scan focus from: 0

to: 0

% Complete: 100%

12. Result Metadata analysis



- ☒ Ortho
- ☐ Legend
- ☒ Autoscale
- ☒ Mouse
- ☒ Shading

A Science Gateway for Biophysical Analysis

Usage statistics (in SUs) for the UltraScan Gateway Jan-Dec 2013

Alamo (UTHSCSA)	BCF (UTHSCSA)	Ranger (TACC)	Juropa (Jülich)	Lonestar (TACC)	Stampede (TACC)	Trestles (SDSC)	Number of Investigators	Analyses
153,375	2,295	1,466	24,147	411,574	593,338	381,935	127	39,191

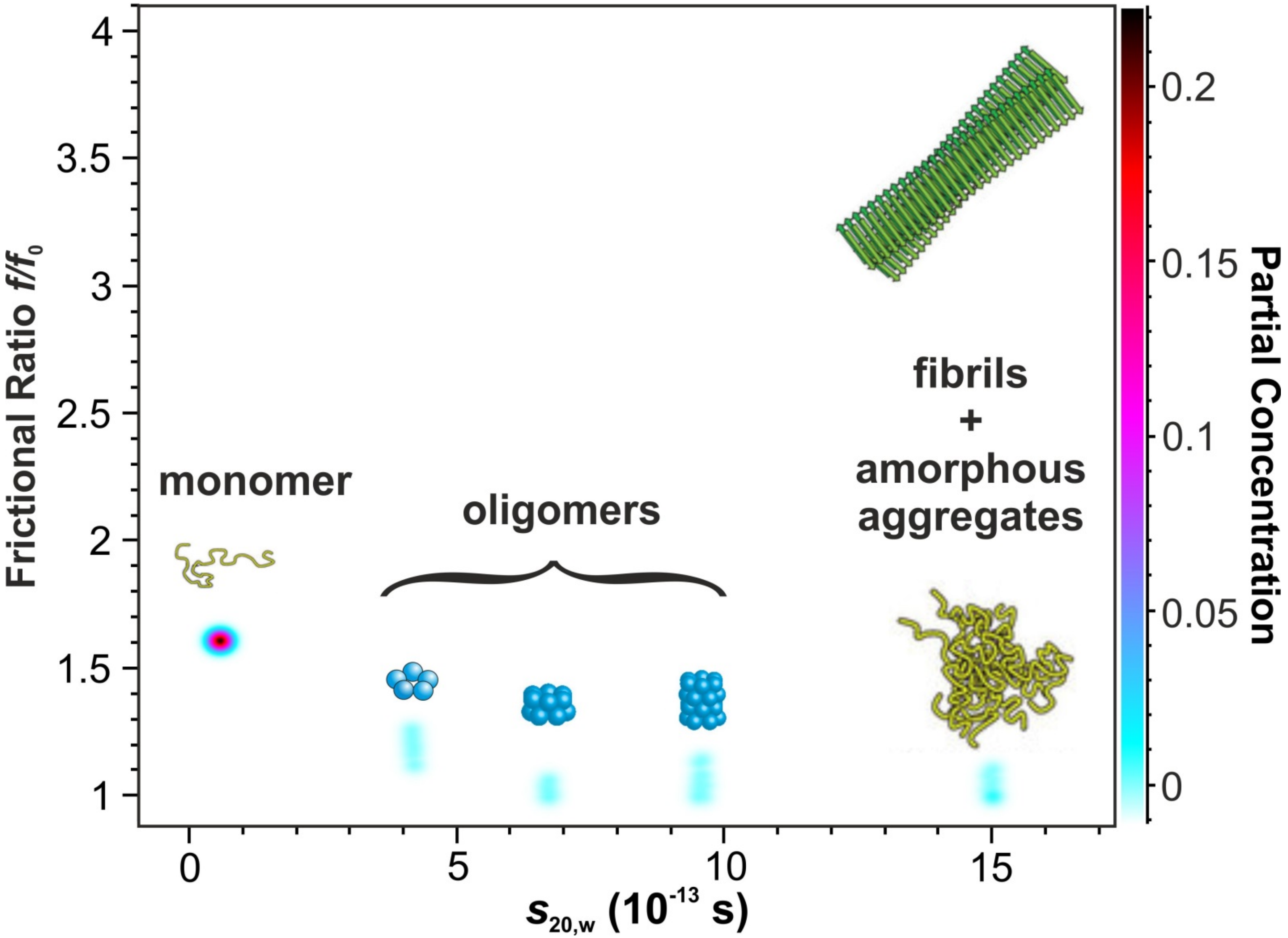
There are over 70 institutions in 18 countries actively using UltraScan/LIMS Implemented currently on 7 HPC platforms, including one commercial installation (non-public). In 2013 over 1.5 Million service units provided by XSEDE, Jülich and UTHSCSA.

Ongoing Projects:

Integration of SAXS/SANS modeling
Integration of Molecular Dynamics (DMD)
Integration of SDSC Gordon Supercomputer with GRAM5 and UNICORE
Integration of Multi-wavelength optics (500-1000 fold higher data density)
Development of Performance Prediction algorithms through datamining
Development of a meta scheduler for mass submissions (of MW data)

Amyloid-β Aggregation studied by Sedimentation Velocity Analytical Ultracentrifugation

L. Nagel-Steger at the Dept. of Physical Biology, Heinrich-Heine-University Düsseldorf
& ICS-6, RC-Jülich, Germany

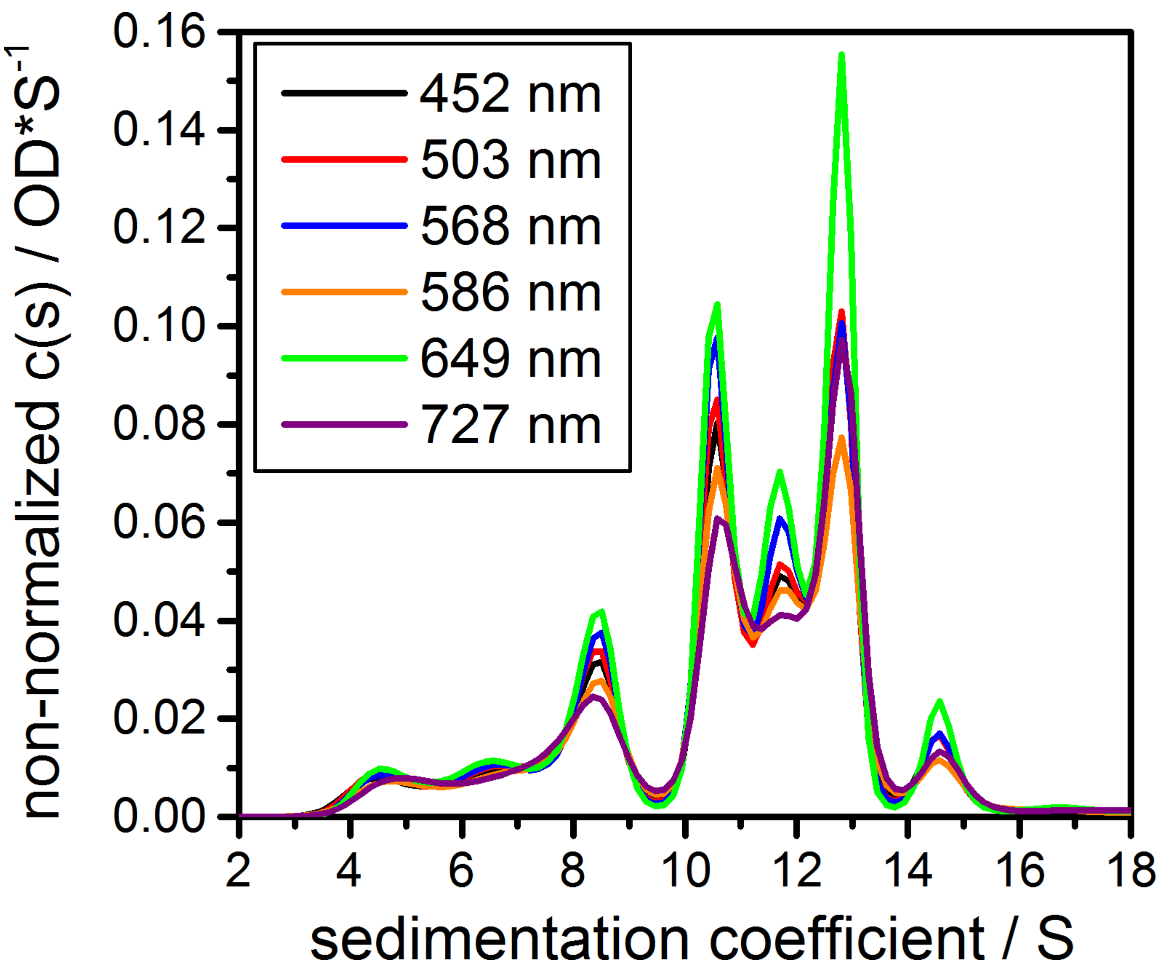


"Our application for high resolution data analysis with USIII is the investigation of amyloid formation by disease associated proteins.

The existence of differently sized and shaped species in such protein solutions provides the primary motivation to use high-resolution AUC analysis which delivers individual shape parameters in addition to s-values and partial concentrations for all species."

Sedimentation analysis of single-walled carbon nanotube composition with a multi-wavelength AUC detector.

Walter, J. and W. Peukert, Dept. of Feststoff- und Grenzflächenverfahrenstechnik, Friedrich-Alexander-Universität Erlangen-Nürnberg.



1. Analysis of quantum dots

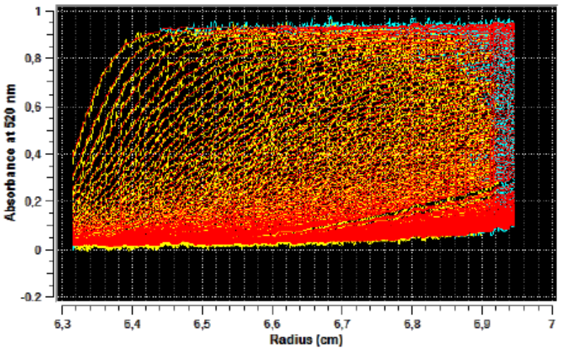
We want to study the size dependent optical properties by means of multi-wavelength AUC analysis. Hydrodynamic analysis will be complemented by simultaneous spectral analysis. We are also interested in the effect of surface modifications using different surfactants. AUC allows us to study surface properties and stabilizer interactions of particles in the lower nanoscale.

2. Analysis of carbon nanotubes
The evaluation of carbon nanotubes using AUC allows us to distinguish between different species of tubes in even complex mixtures exploiting their unique optical and hydrodynamic properties.

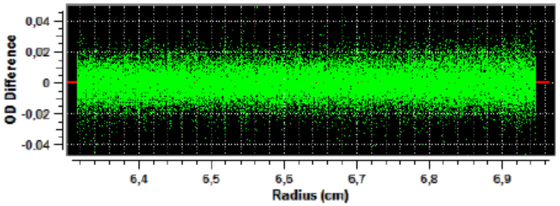
Synthesis and Characterization of DNA-Metal Hybrid Materials

Urban, M. and H. Cölfen, Dept. of Chemistry and biofunctional Materials
University of Konstanz

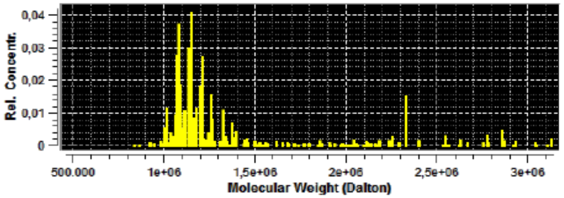
Velocity Data for 5078_r

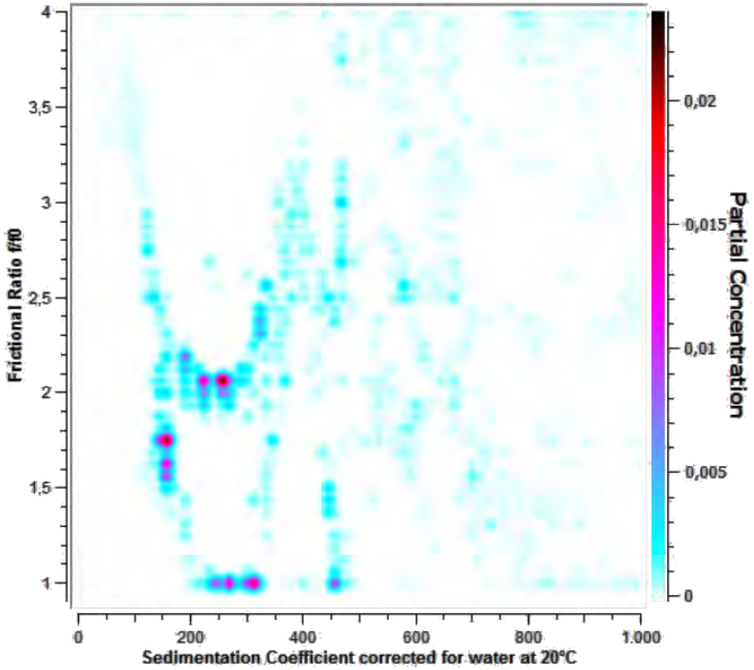


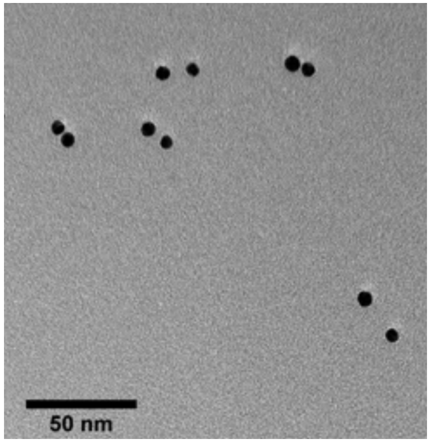
Residuals



Run 5078_r: Cell 2 (520 nm)
MW Distribution







Development of new plasmonic devices.

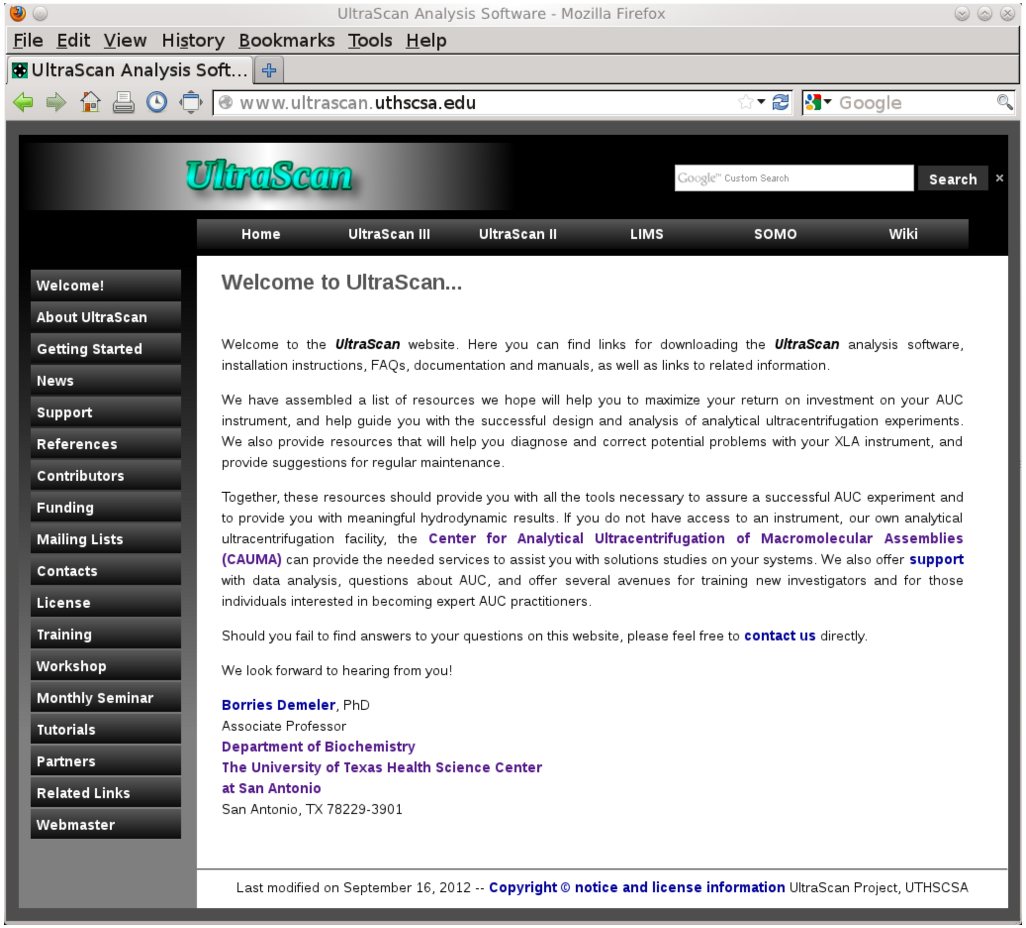
We want to develop DNA-Metal hybrid materials by linking two gold nanoparticles by DNA single- and double-stranded oligomers. The number of bases in the oligomer allows us to precisely control the distances between the metal cores to optimize plasmon resonance and fluorescence properties.

AUC provides the necessary size and shape characterization of DNA-Metal hybrid particles to allow us to bulk-characterize mixtures of nanoparticles and their assemblies with DNA.

Links:

UltraScan-III:
http://www.ultrascan.uthscsa.edu
XSEDE Science Gateway:
https://portal.xsede.org/science-gateways

SciGaP Project:
http://www.scigap.org
Airavata Project:
http://airavata.apache.org/



Welcome to UltraScan...

Welcome to the ***UltraScan*** website. Here you can find links for downloading the ***UltraScan*** analysis software, installation instructions, FAQs, documentation and manuals, as well as links to related information.

We have assembled a list of resources we hope will help you to maximize your return on investment on your AUC instrument, and help guide you with the successful design and analysis of analytical ultracentrifugation experiments. We also provide resources that will help you diagnose and correct potential problems with your XLA instrument, and provide suggestions for regular maintenance.

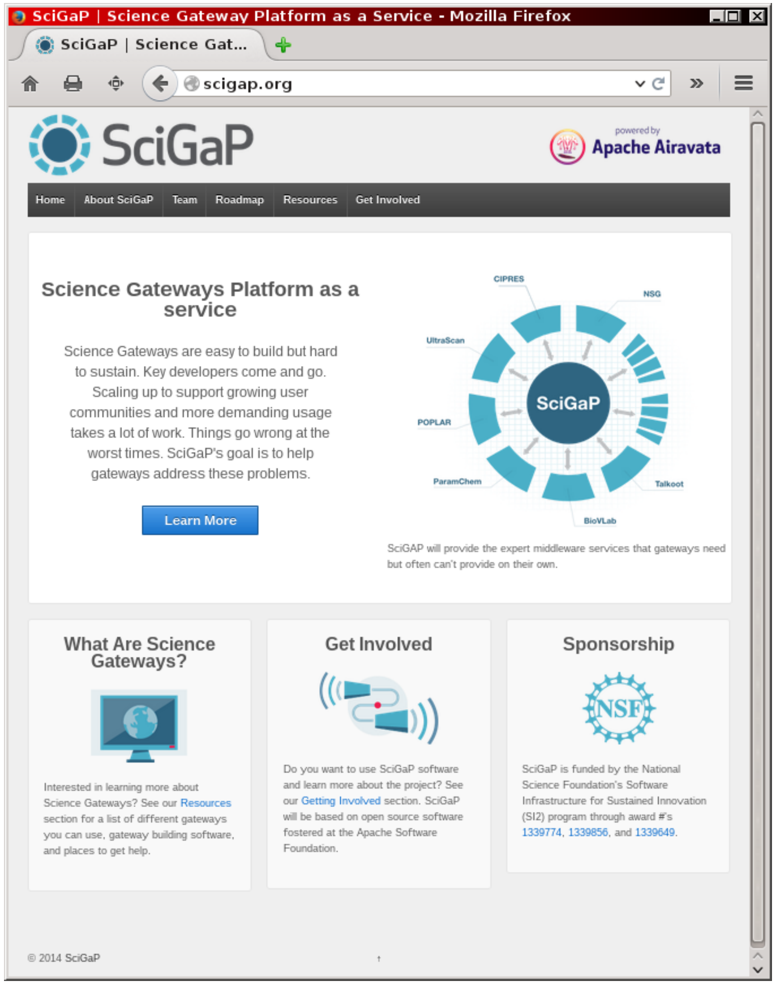
Together, these resources should provide you with all the tools necessary to assure a successful AUC experiment and to provide you with meaningful hydrodynamic results. If you do not have access to an instrument, our own analytical ultracentrifugation facility, the **Center for Analytical Ultracentrifugation of Macromolecular Assemblies (CAUMA)** can provide the needed services to assist you with solutions studies on your systems. We also offer **support** with data analysis, questions about AUC, and offer several avenues for training new investigators and for those individuals interested in becoming expert AUC practitioners.

Should you fail to find answers to your questions on this website, please feel free to **contact us** directly.

We look forward to hearing from you!

Borries Demeler, PhD
Associate Professor
Department of Biochemistry
The University of Texas Health Science Center
at San Antonio
San Antonio, TX 78229-3901

Last modified on September 16, 2012 -- **Copyright © notice and license information** UltraScan Project, UTHSCSA



Science Gateways Platform as a service

Science Gateways are easy to build but hard to sustain. Key developers come and go. Scaling up to support growing user communities and more demanding usage takes a lot of work. Things go wrong at the worst times. SciGaP's goal is to help gateways address these problems.

SciGAP will provide the expert middleware services that gateways need but often can't provide on their own.

What Are Science Gateways?

Interested in learning more about Science Gateways? See our Resources section for a list of different gateways you can use, gateway building software, and places to get help.

Get Involved

Do you want to use SciGaP software and learn more about the project? See our Getting Involved section. SciGaP will be based on open source software fostered at the Apache Software Foundation.

Sponsorship

SciGaP is funded by the National Science Foundation's Software Infrastructure for Sustained Innovation (SI2) program through award #'s 1339774, 1339856, and 1339649.

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A copy of this presentation:

http://www.demeler.uthscsa.edu/unicore-2014.pdf

Acknowledgements:

Thanks to the UNICORE Summit Organizers!

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Indiana University

Marlon Pierce
Suresh Marru
Raminder Singh

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Demeler Lab:

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Virgil Schirf
Gary Gorbet
Dan Zollars

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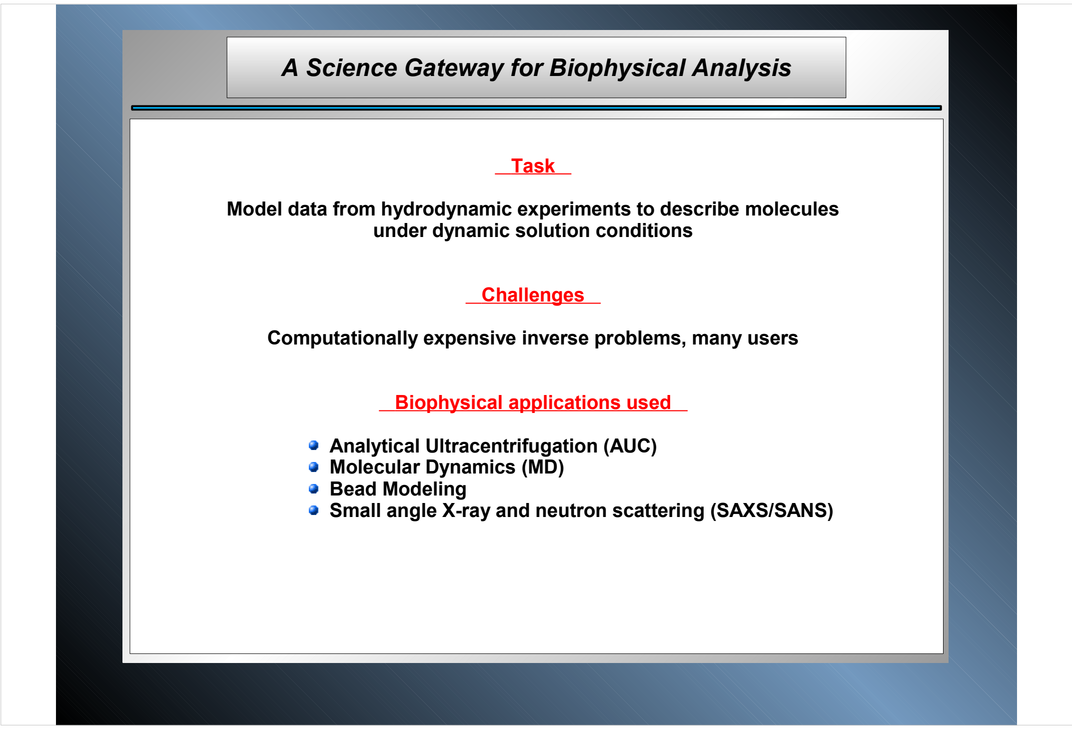
SACI (NCI)
National Science Foundation
NSF Teragrid (XSEDE)
San Antonio Life Science Institute
Howard Hughes Medical Institute
UT Permanent University Fund

Graduate School of Biomedical Sciences, Dept. of Biochemistry
UT HEALTH SCIENCE CENTER™
San Antonio

Borries Demeler, Ph.D.

INTERNATIONAL
SUPERCOMPUTING CONFERENCE

HPC Applications in Biophysics, Material Science and Biomedicine - enabled by UNICORE
The UltraScan XSEDE Science Gateway



A Science Gateway for Biophysical Analysis

Task

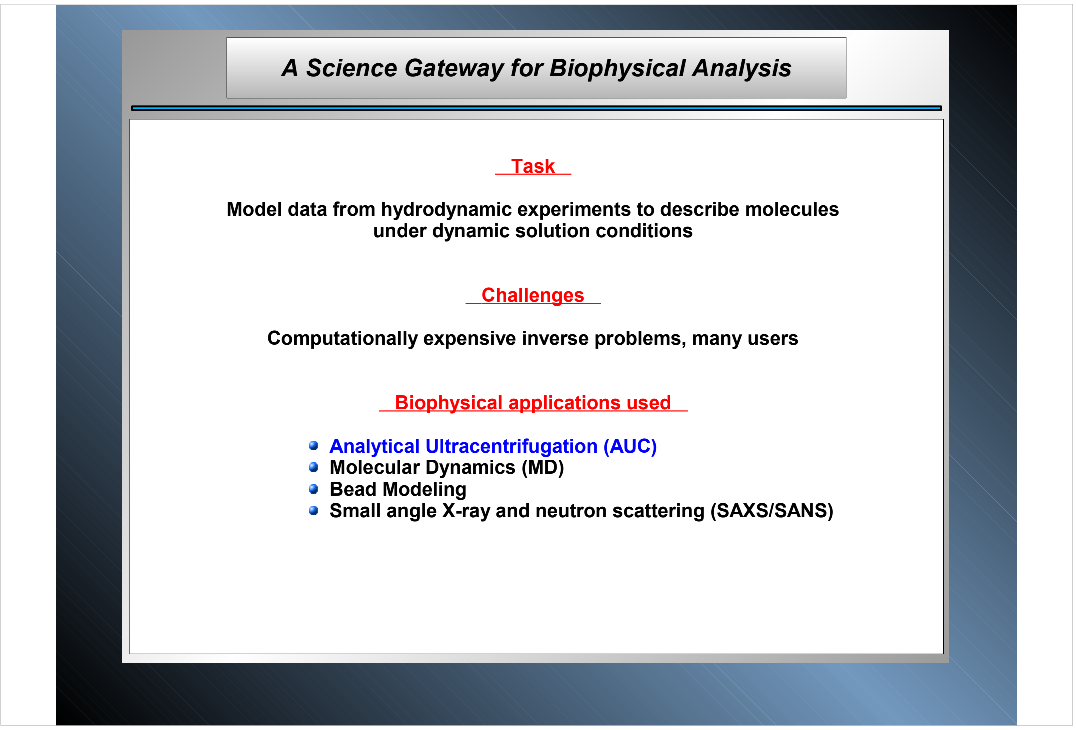
Model data from hydrodynamic experiments to describe molecules under dynamic solution conditions

Challenges

Computationally expensive inverse problems, many users

Biophysical applications used

- **Analytical Ultracentrifugation (AUC)**
- **Molecular Dynamics (MD)**
- **Bead Modeling**
- **Small angle X-ray and neutron scattering (SAXS/SANS)**



A Science Gateway for Biophysical Analysis

Task

Model data from hydrodynamic experiments to describe molecules
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Challenges

Computationally expensive inverse problems, many users

Biophysical applications used

- Analytical Ultracentrifugation (AUC)
- Molecular Dynamics (MD)
- Bead Modeling
- Small angle X-ray and neutron scattering (SAXS/SANS)

AUC Background

What is Analytical Ultracentrifugation (AUC)?

A technique to separate macromolecules dissolved in solution in a centrifugal force field. AUC can “watch” the molecules *while* they are separating and identify and differentiate them by their hydrodynamic properties and partial concentration. AUC is a “first Principle” method, which does NOT require standards.

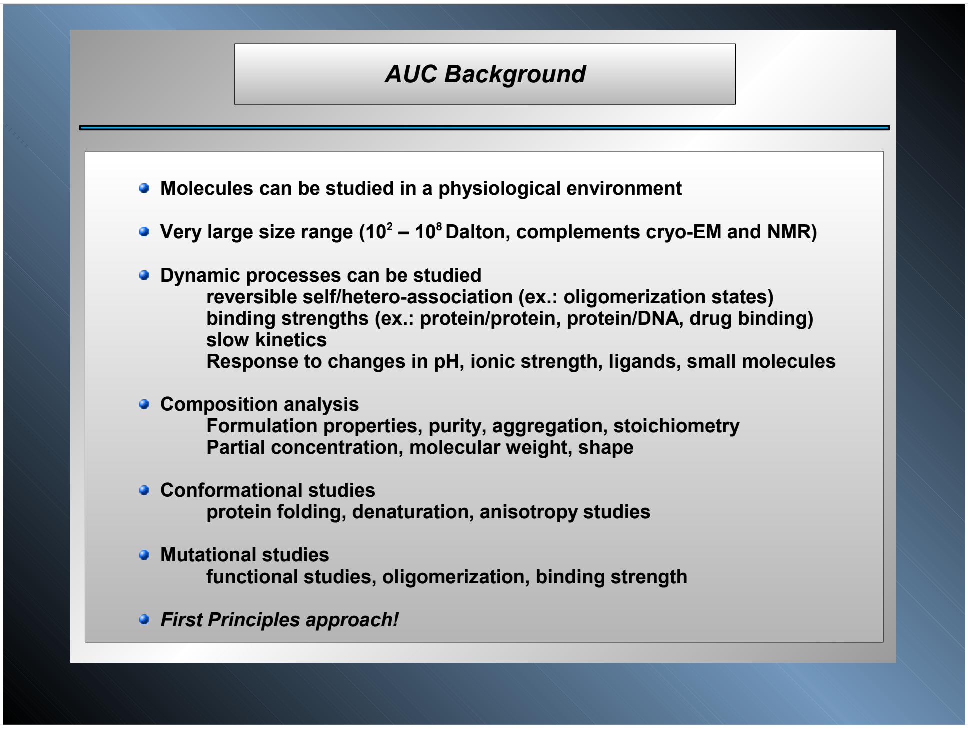
How does AUC work?

By applying a very large centrifugal force, molecules are separated based on their molar mass and their shape. The molecules are observed using different optical systems that detect different properties of the molecules, such as refractive index, UV or visible absorbance, or fluorescent light emission.

What molecules can be studied?

Virtually any molecule, colloid or particle that can be dissolved in a liquid can be measured by AUC, as long as it does not sediment by gravity alone. The molecule or particle can be as small as a salt ion, or as large as an entire virus particle.

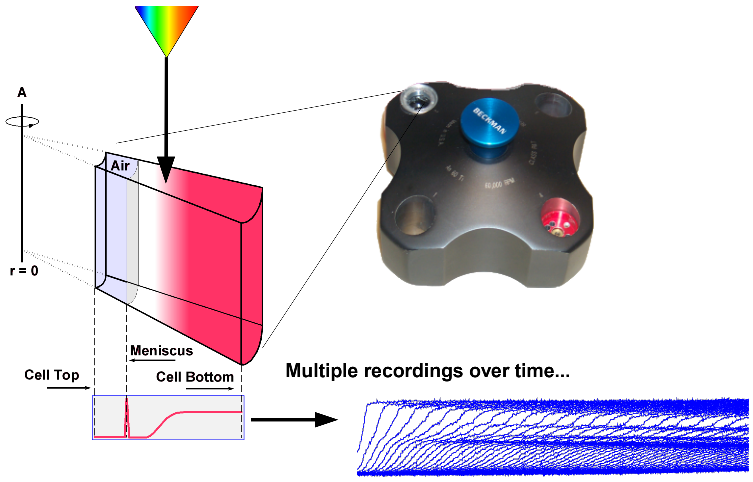
The ultracentrifuge can spin at 60,000 rpm, generating forces close to 300,000 x g. Even small molecules like salt ions will sediment in such a force.



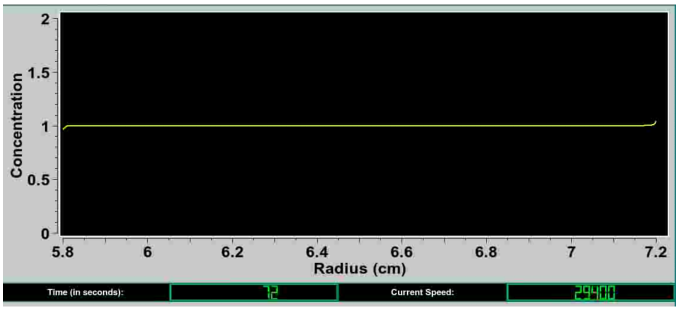
AUC Background

- Molecules can be studied in a physiological environment
- Very large size range (10^2 – 10^8 Dalton, complements cryo-EM and NMR)
- Dynamic processes can be studied
    - reversible self/hetero-association (ex.: oligomerization states)
    - binding strengths (ex.: protein/protein, protein/DNA, drug binding)
    - slow kinetics
    - Response to changes in pH, ionic strength, ligands, small molecules
- Composition analysis
    - Formulation properties, purity, aggregation, stoichiometry
    - Partial concentration, molecular weight, shape
- Conformational studies
    - protein folding, denaturation, anisotropy studies
- Mutational studies
    - functional studies, oligomerization, binding strength
- *First Principles approach!*

A Science Gateway for Biophysical Analysis



Multiple recordings over time...



Time (in seconds): 72

Current Speed: 29400

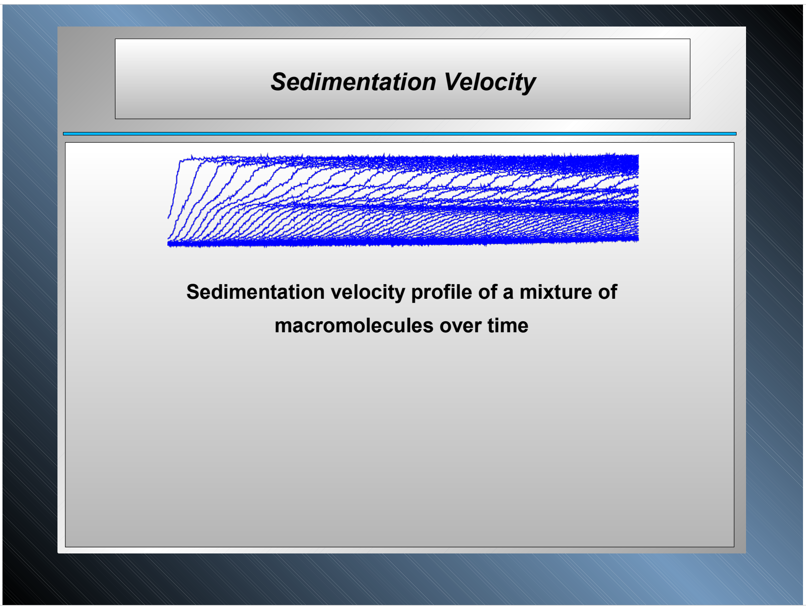
The experiment is described by the Lamm equation, which is solved with FEM

Cao W and Demeler B. Modeling analytical ultracentrifugation experiments with an adaptive space-time finite element solution of the Lamm equation. (2005) Biophys J. 89(3):1589-602.

Cao, W and Demeler B. Modeling Analytical Ultracentrifugation Experiments with an Adaptive Space-Time Finite Element Solution for Multi-Component Reacting Systems. Biophys. J. (2008) 95(1):54-65

$$L(s, D): \quad \left(\frac{\partial C}{\partial t}\right)_r = \frac{-1}{r}\frac{\partial}{\partial r}\left[s\,\omega^2 r^2 C - D r\,\frac{\partial C}{\partial r}\right]_t$$

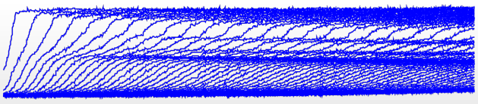
$$MIN: \sum_{i=1, j=1}^{r, t} \left[Y_{i,j} - \sum_{k=1}^{n} \left(L_k(s_k, D_k)_{i,j}\right)\right]^2$$



Sedimentation Velocity

Sedimentation velocity profile of a mixture of macromolecules over time

Sedimentation Velocity

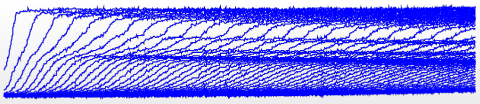


Composition Analysis

We can answer these questions:

How many components?

Sedimentation Velocity

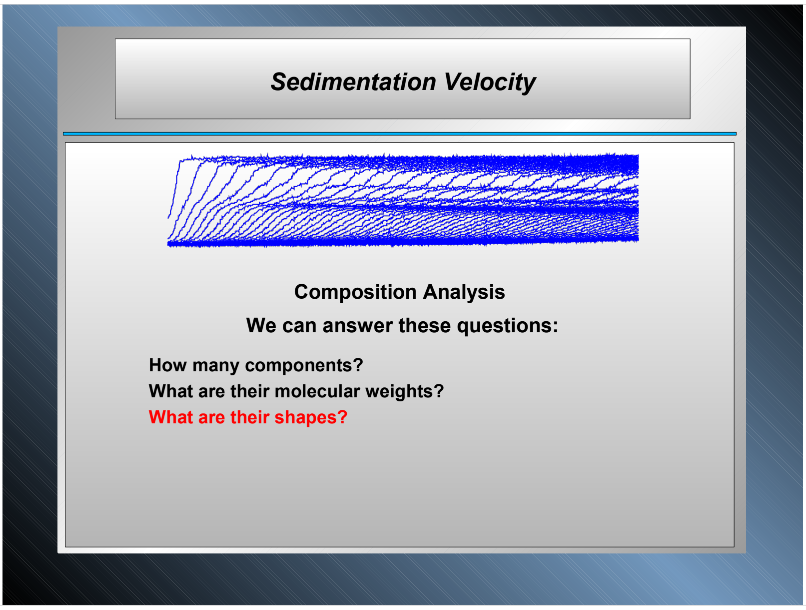


Composition Analysis

We can answer these questions:

How many components?

What are their molecular weights?

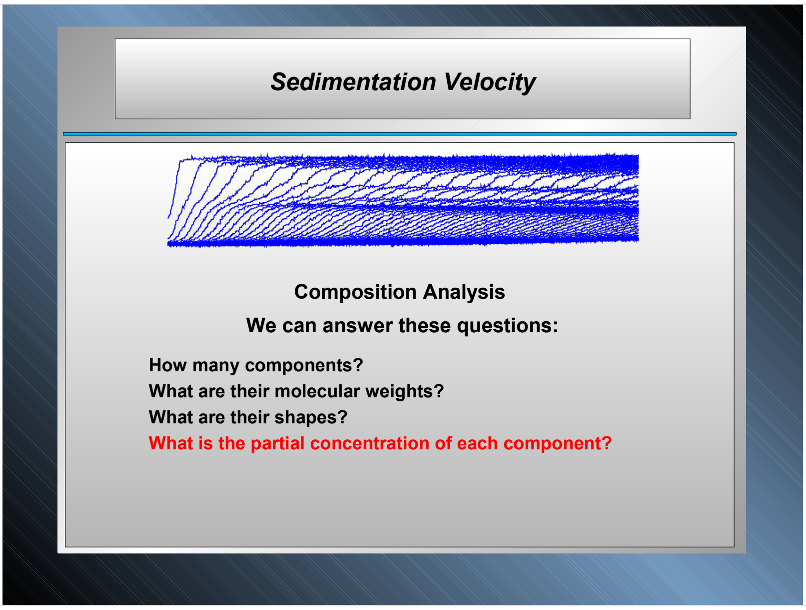


Sedimentation Velocity

Composition Analysis

We can answer these questions:

How many components?
What are their molecular weights?
What are their shapes?

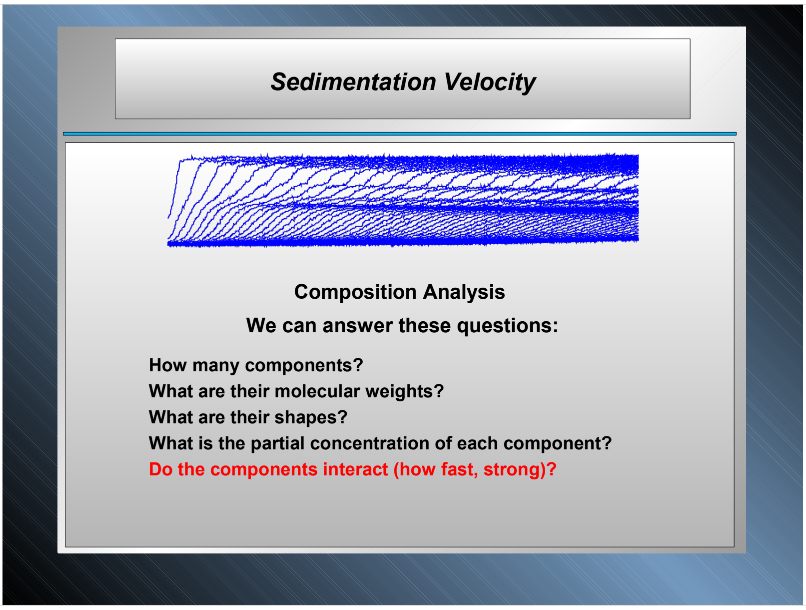


Sedimentation Velocity

Composition Analysis

We can answer these questions:

How many components?
What are their molecular weights?
What are their shapes?
What is the partial concentration of each component?

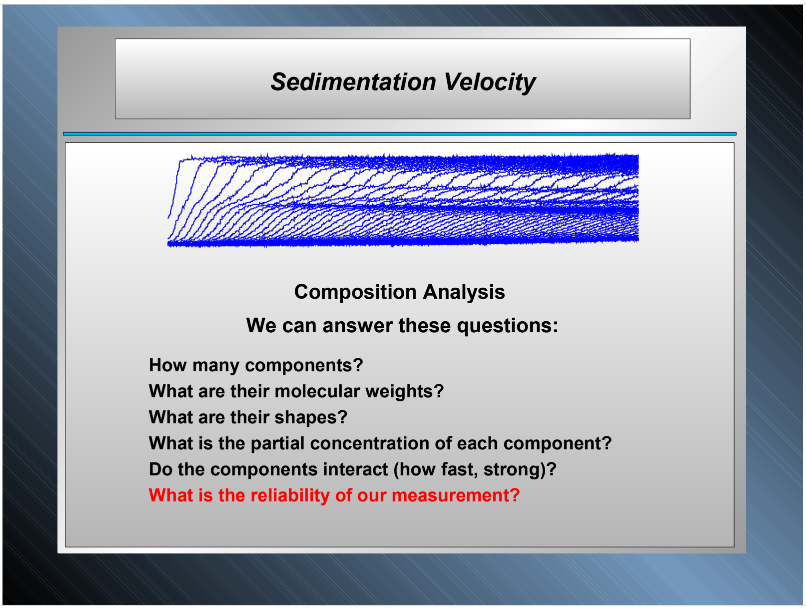


Sedimentation Velocity

Composition Analysis

We can answer these questions:

How many components?
What are their molecular weights?
What are their shapes?
What is the partial concentration of each component?
Do the components interact (how fast, strong)?

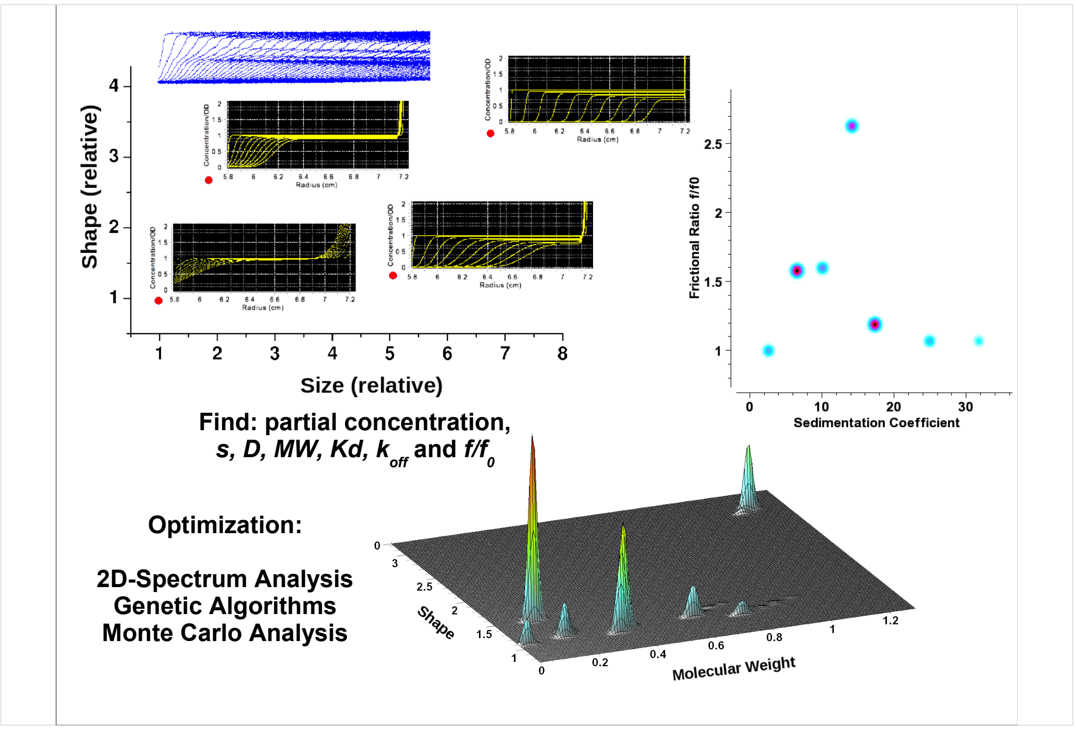


Sedimentation Velocity

Composition Analysis

We can answer these questions:

How many components?
What are their molecular weights?
What are their shapes?
What is the partial concentration of each component?
Do the components interact (how fast, strong)?
What is the reliability of our measurement?

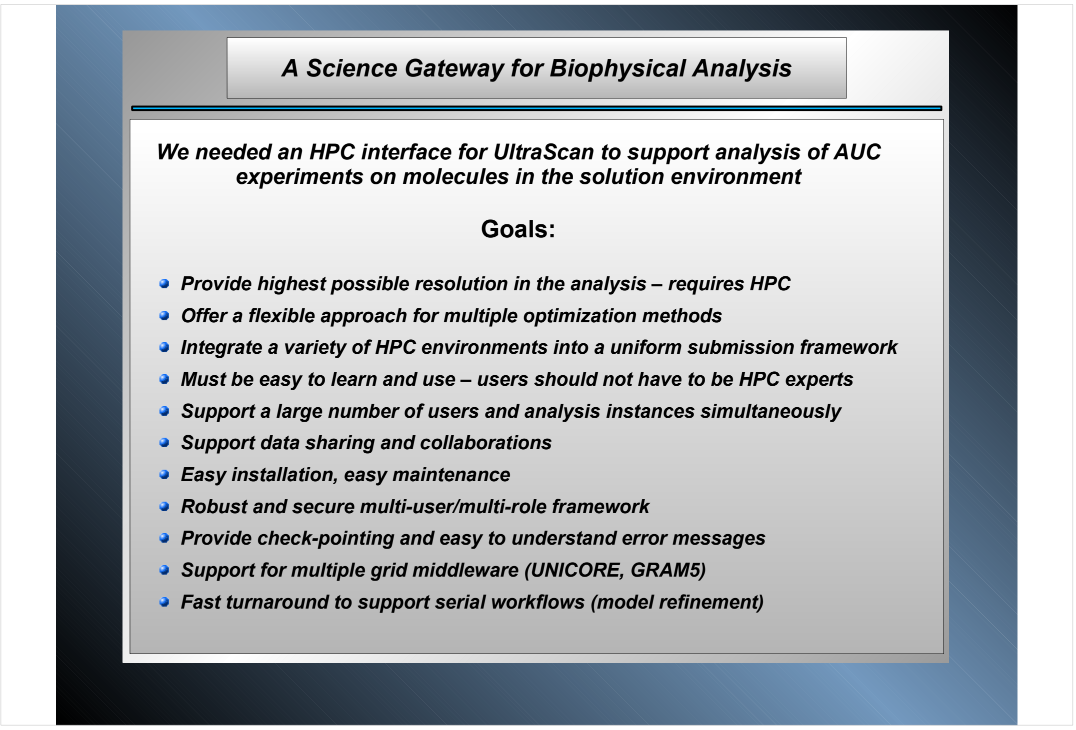


Find: partial concentration,
s, D, MW, Kd, k_{off} **and** f/f_0

Optimization:

2D-Spectrum Analysis
Genetic Algorithms
Monte Carlo Analysis

We can represent the sedimentation problem as a 2-dimensional parameter space (s and f/f0, or s and MW, or MW and f/f0, or s and D, or D and MW, or D and f/f0, etc.). Each one of these representations is valid and provides the entire information necessary to describe completely the solution properties of individual solutes. The problem is then to identify the solutes (blue dots in the plane), and their relative concentration that when combined make up the experimental data shown as a blue concentration traces for differen time and radius values.



A Science Gateway for Biophysical Analysis

We needed an HPC interface for UltraScan to support analysis of AUC experiments on molecules in the solution environment

Goals:

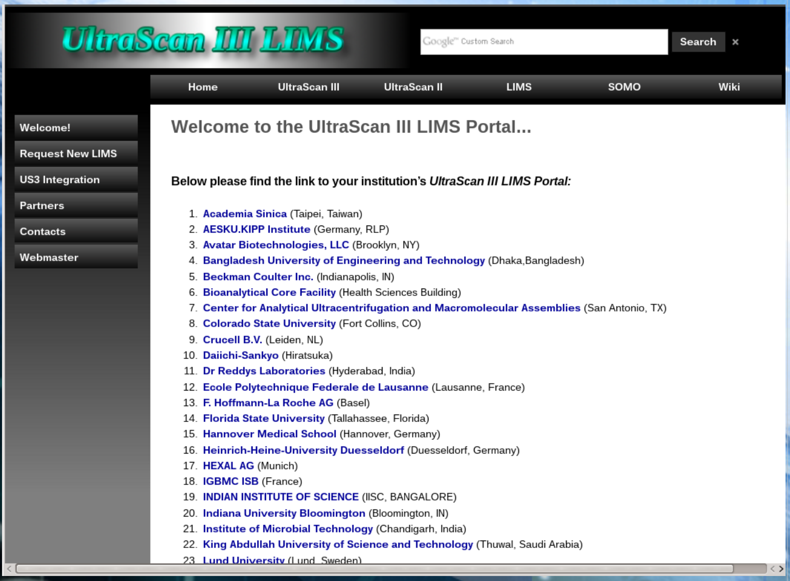
- ***Provide highest possible resolution in the analysis – requires HPC***
- ***Offer a flexible approach for multiple optimization methods***
- ***Integrate a variety of HPC environments into a uniform submission framework***
- ***Must be easy to learn and use – users should not have to be HPC experts***
- ***Support a large number of users and analysis instances simultaneously***
- ***Support data sharing and collaborations***
- ***Easy installation, easy maintenance***
- ***Robust and secure multi-user/multi-role framework***
- ***Provide check-pointing and easy to understand error messages***
- ***Support for multiple grid middleware (UNICORE, GRAM5)***
- ***Fast turnaround to support serial workflows (model refinement)***

XSEDE

Science Gateways

Apache Airavata

UNICORE GRAM5



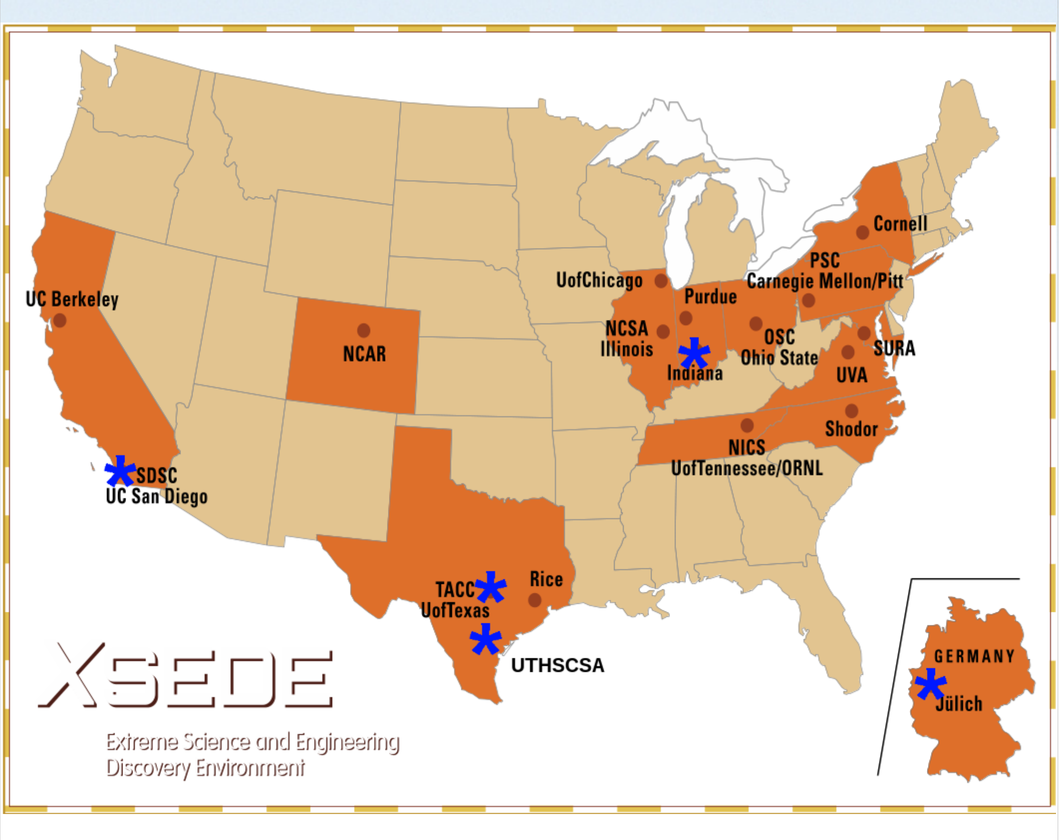
Welcome to the UltraScan III LIMS Portal...

Below please find the link to your institution's *UltraScan III LIMS Portal:*

1. **Academia Sinica** (Taipei, Taiwan)
2. **AESKU.KIPP Institute** (Germany, RLP)
3. **Avatar Biotechnologies, LLC** (Brooklyn, NY)
4. **Bangladesh University of Engineering and Technology** (Dhaka,Bangladesh)
5. **Beckman Coulter Inc.** (Indianapolis, IN)
6. **Bioanalytical Core Facility** (Health Sciences Building)
7. **Center for Analytical Ultracentrifugation and Macromolecular Assemblies** (San Antonio, TX)
8. **Colorado State University** (Fort Collins, CO)
9. **Crucell B.V.** (Leiden, NL)
10. **Daiichi-Sankyo** (Hiratsuka)
11. **Dr Reddys Laboratories** (Hyderabad, India)
12. **Ecole Polytechnique Federale de Lausanne** (Lausanne, France)
13. **F. Hoffmann-La Roche AG** (Basel)
14. **Florida State University** (Tallahassee, Florida)
15. **Hannover Medical School** (Hannover, Germany)
16. **Heinrich-Heine-University Duesseldorf** (Duesseldorf, Germany)
17. **HEXAL AG** (Munich)
18. **IGBMC ISB** (France)
19. **INDIAN INSTITUTE OF SCIENCE** (IISC, BANGALORE)
20. **Indiana University Bloomington** (Bloomington, IN)
21. **Institute of Microbial Technology** (Chandigarh, India)
22. **King Abdullah University of Science and Technology** (Thuwal, Saudi Arabia)
23. **Lund University** (Lund, Sweden)

XSEDE

Extreme Science and Engineering Discovery Environment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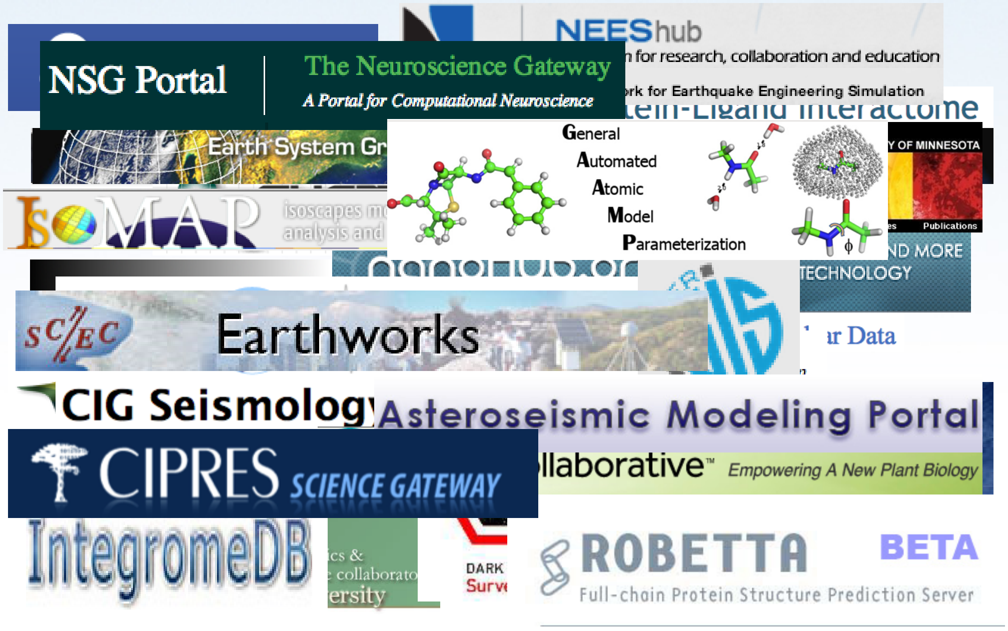
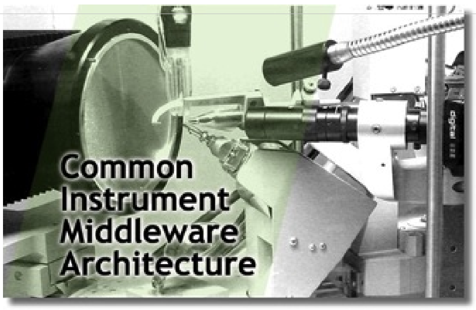
NCAR
SDSC
UC San Diego
UofChicago
NCSA
Illinois
Purdue
Indiana
OSC
Ohio State
PSC
Carnegie Mellon/Pitt
Cornell
SURA
UVA
Shodor
NICS
UofTennessee/ORNL
TACC
UofTexas
Rice
UTHSCSA
GERMANY
Jülich
XSEDE
Extreme Science and Engineering
Discovery Environment

Today, there are over 30 gateways using XSEDE

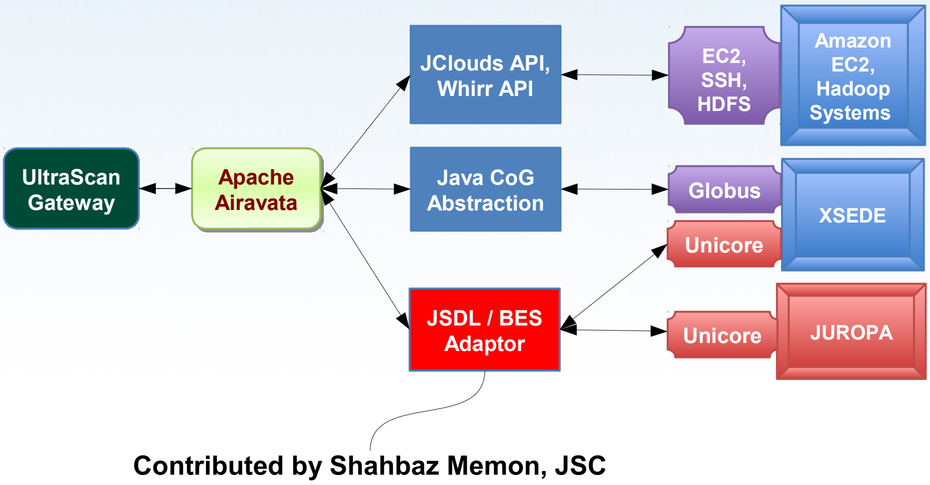




What Is Apache Airavata?

- Science Gateway software system to
  - Compose, manage, execute, and monitor distributed, computational workflows
  - Wrap legacy command line scientific applications with Web services.
  - Abstract job submission and provide uniform API for all resources
  - Run jobs on computational resources ranging from local resources to computational grids and clouds
- Airavata software is largely derived from NSF-funded academic research.

Jülich Contributions to Airavata


UltraScan Gateway

Apache Airavata

JClouds API, Whirr API

Java CoG Abstraction

JSDL / BES Adaptor

EC2, SSH, HDFS

Amazon EC2, Hadoop Systems

Globus

Unicore

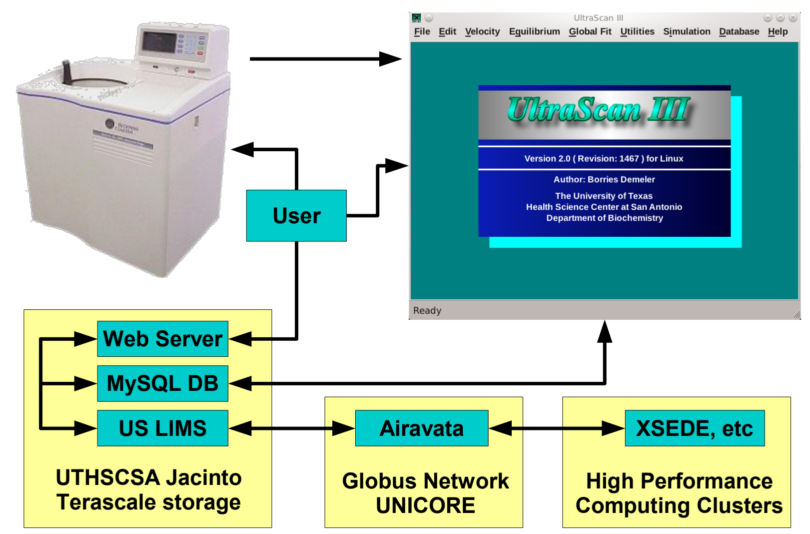
XSEDE

Unicore

JUROPA

Contributed by Shahbaz Memon, JSC

UltraScan Organization (open source, multi-platform)



Version 2.0 (Revision: 1467) for Linux

Author: Borries Demeler

The University of Texas
Health Science Center at San Antonio
Department of Biochemistry

User

Web Server

MySQL DB

US LIMS

UTHSCSA Jacinto
Terascale storage

Airavata

Globus Network
UNICORE

XSEDE, etc

High Performance
Computing Clusters

A Science Gateway for Biophysical Analysis

UltraScan (US) components and 3rd party software:

US-GUI: (Linux, Mac, Windows): used for data processing, editing, uploading, visualization, report generation (C++/Qt).

US-LIMS: web-based interface to the MySQL database. Gives the user web-based access to their data, visualizations and analysis reports (PHP).

US-HPC: includes finite element solver for multiple models and performs all optimization algorithms (2DSA, GA, Monte Carlo)

US-Gridcontrol: PHP daemon to manage job submission, communications and reporting from US-HPC,

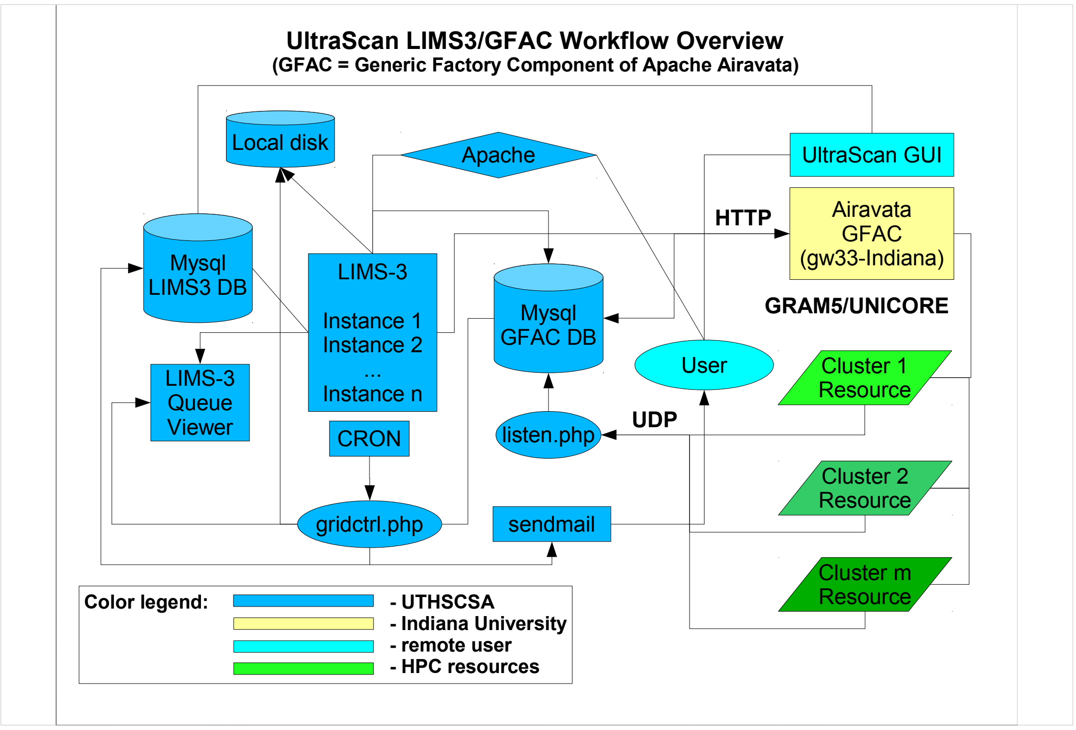
MySQL: houses all LIMS data, a separate Airavata DB holds job status info. Each institution has a separate database and separate US-LIMS instance. All interactions with MySQL are performed through stored procedure calls.

Airavata: accepts job requests and brokers them over the appropriate grid middleware to the requested supercomputer, controls job status in Airavata DB.

GRAM/UNICORE grid middleware

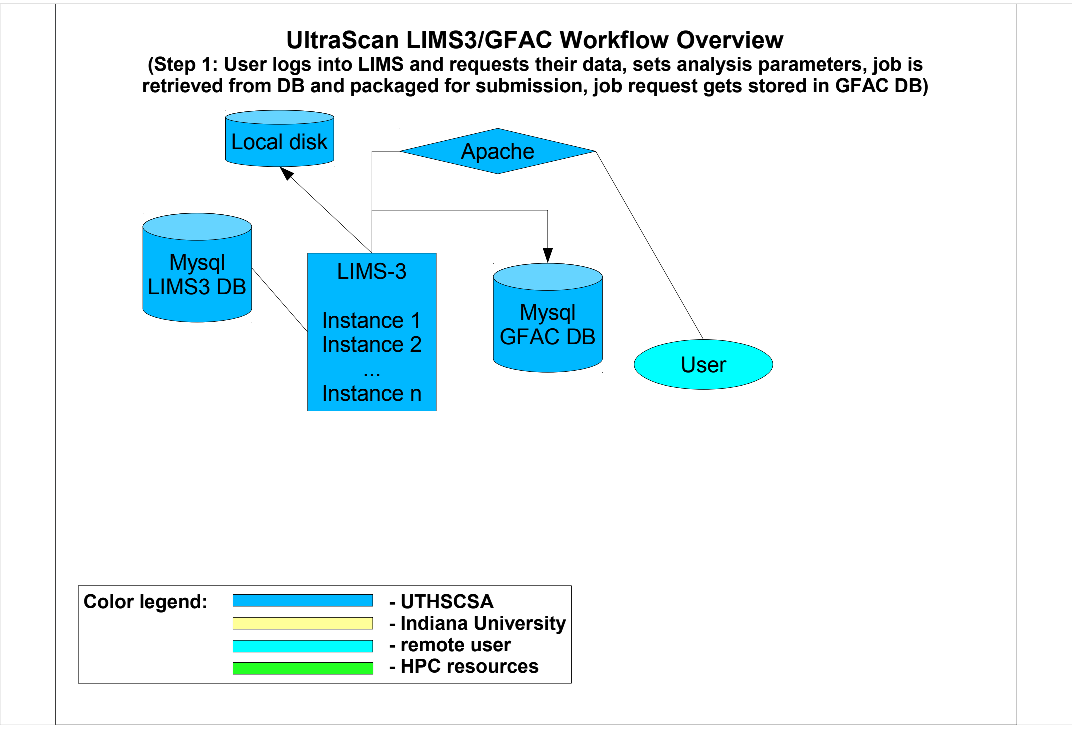
SSL communications: All communications and data transfers are SSL encrypted. All database access and LIMS access requires authentication.

Statistic scripts: queries database and reports usage and provides details for XSEDE reporting.



UltraScan LIMS3/GFAC Workflow Overview
(GFAC = Generic Factory Component of Apache Airavata)

We can represent the sedimentation problem as a 2-dimensional parameter space (s and f/f0, or s and MW, or MW and f/f0, or s and D, or D and MW, or D and f/f0, etc.). Each one of these representations is valid and provides the entire information necessary to describe completely the solution properties of individual solutes. The problem is then to identify the solutes (blue dots in the plane), and their relative concentration that when combined make up the experimental data shown as a blue concentration traces for differen time and radius values.



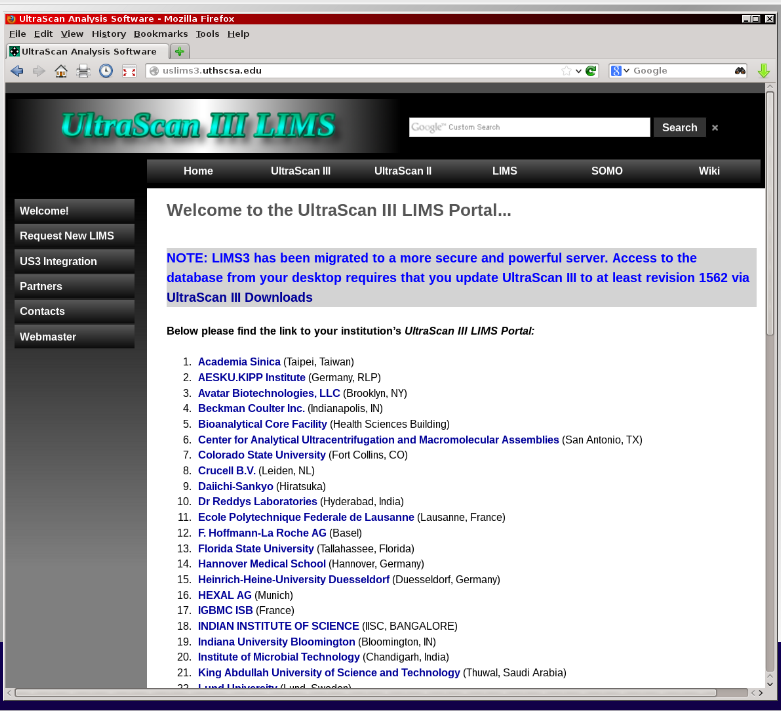
UltraScan LIMS3/GFAC Workflow Overview

(Step 1: User logs into LIMS and requests their data, sets analysis parameters, job is retrieved from DB and packaged for submission, job request gets stored in GFAC DB)

Color legend:
🟦 **- UTHSCSA**
🟨 **- Indiana University**
🟦 **- remote user**
🟩 **- HPC resources**

We can represent the sedimentation problem as a 2-dimensional parameter space (s and f/f0, or s and MW, or MW and f/f0, or s and D, or D and MW, or D and f/f0, etc.). Each one of these representations is valid and provides the entire information necessary to describe completely the solution properties of individual solutes. The problem is then to identify the solutes (blue dots in the plane), and their relative concentration that when combined make up the experimental data shown as a blue concentration traces for differen time and radius values.

3. Selecting Gateway Instance



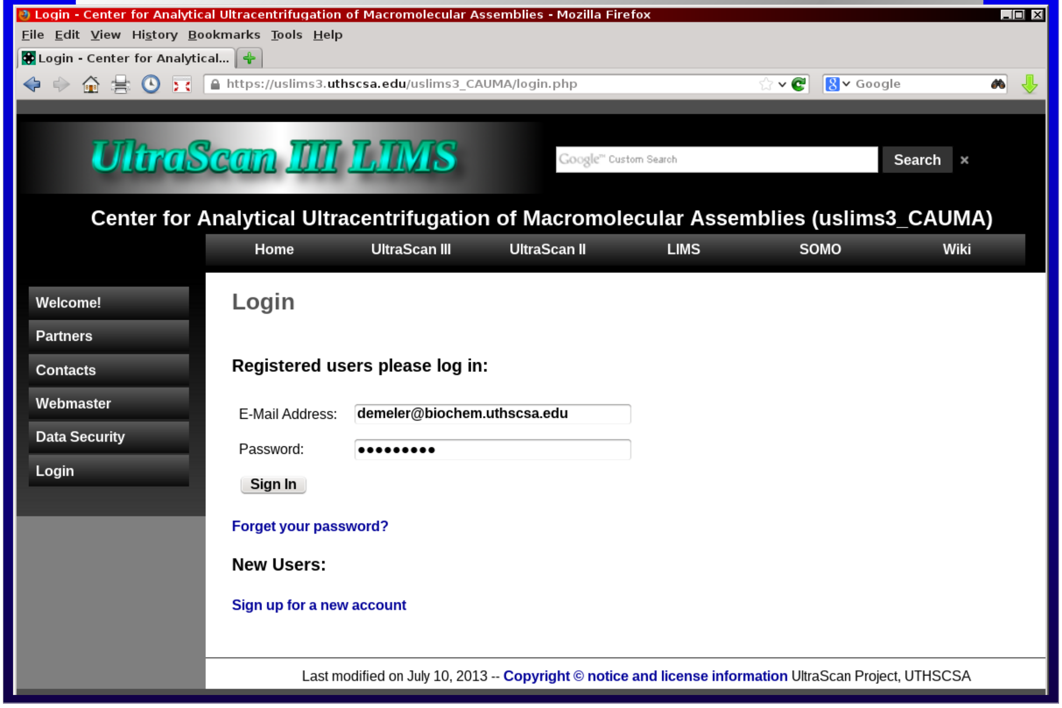
Welcome to the UltraScan III LIMS Portal...

NOTE: LIMS3 has been migrated to a more secure and powerful server. Access to the database from your desktop requires that you update UltraScan III to at least revision 1562 via UltraScan III Downloads

Below please find the link to your institution's *UltraScan III LIMS Portal:*

1. **Academia Sinica** (Taipei, Taiwan)
2. **AESKU.KIPP Institute** (Germany, RLP)
3. **Avatar Biotechnologies, LLC** (Brooklyn, NY)
4. **Beckman Coulter Inc.** (Indianapolis, IN)
5. **Bioanalytical Core Facility** (Health Sciences Building)
6. **Center for Analytical Ultracentrifugation and Macromolecular Assemblies** (San Antonio, TX)
7. **Colorado State University** (Fort Collins, CO)
8. **Crucell B.V.** (Leiden, NL)
9. **Daiichi-Sankyo** (Hiratsuka)
10. **Dr Reddys Laboratories** (Hyderabad, India)
11. **Ecole Polytechnique Federale de Lausanne** (Lausanne, France)
12. **F. Hoffmann-La Roche AG** (Basel)
13. **Florida State University** (Tallahassee, Florida)
14. **Hannover Medical School** (Hannover, Germany)
15. **Heinrich-Heine-University Duesseldorf** (Duesseldorf, Germany)
16. **HEXAL AG** (Munich)
17. **IGBMC ISB** (France)
18. **INDIAN INSTITUTE OF SCIENCE** (IISC, BANGALORE)
19. **Indiana University Bloomington** (Bloomington, IN)
20. **Institute of Microbial Technology** (Chandigarh, India)
21. **King Abdullah University of Science and Technology** (Thuwal, Saudi Arabia)
22. **Lund University** (Lund, Sweden)

4. Authentication...



Center for Analytical Ultracentrifugation of Macromolecular Assemblies (uslims3_CAUMA)

Login

Registered users please log in:

E-Mail Address: **demeler@biochem.uthscsa.edu**

Password: ●●●●●●●●●

Sign In

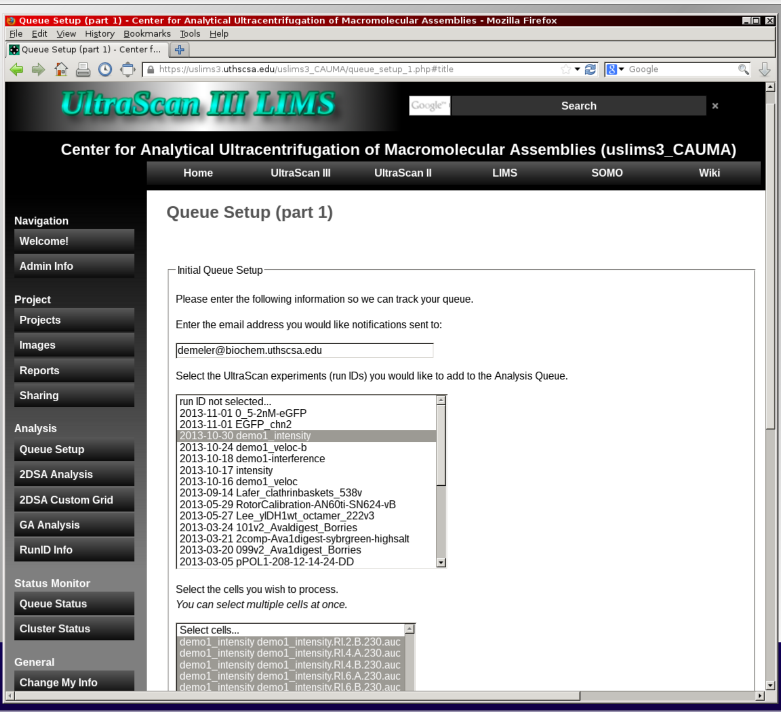
Forget your password?

New Users:

Sign up for a new account

Last modified on July 10, 2013 -- **Copyright © notice and license information** UltraScan Project, UTHSCSA

5. Data Selection



Queue Setup (part 1)

Initial Queue Setup

Please enter the following information so we can track your queue.

Enter the email address you would like notifications sent to:

demeler@biochem.uthscsa.edu

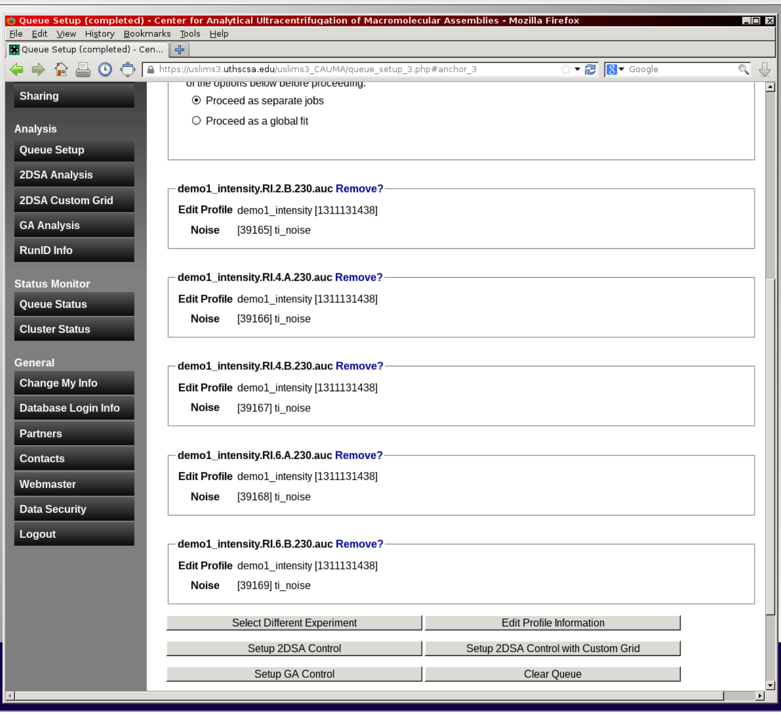
Select the UltraScan experiments (run IDs) you would like to add to the Analysis Queue.

run ID not selected...
2013-11-01 0_5-2nM-eGFP
2013-11-01 EGFP_chn2
2013-10-30 demo1_intensity
2013-10-24 demo1_veloc-b
2013-10-18 demo1-interference
2013-10-17 intensity
2013-10-16 demo1_veloc
2013-09-14 Lafer_clathrinbaskets_538v
2013-05-29 RotorCalibration-AN60ti-SN624-vB
2013-05-27 Lee_ylDH1wt_octamer_222v3
2013-03-24 101v2_Avaldigest_Borries
2013-03-21 2comp-Ava1digest-sybrgreen-highsalt
2013-03-20 099v2_Ava1digest_Borries
2013-03-05 pPOL1-208-12-14-24-DD

Select the cells you wish to process.
You can select multiple cells at once.

Select cells...
demo1_intensity demo1_intensity.RI.2.B.230.auc
demo1_intensity demo1_intensity.RI.4.A.230.auc
demo1_intensity demo1_intensity.RI.4.B.230.auc
demo1_intensity demo1_intensity.RI.6.A.230.auc
demo1_intensity demo1_intensity.RI.6.B.230.auc

6. Analysis Method Selection



of the options below before proceeding.

● Proceed as separate jobs

○ Proceed as a global fit

demo1_intensity.RI.2.B.230.auc Remove?

Edit Profile demo1_intensity [1311131438]

Noise [39165] ti_noise

demo1_intensity.RI.4.A.230.auc Remove?

Edit Profile demo1_intensity [1311131438]

Noise [39166] ti_noise

demo1_intensity.RI.4.B.230.auc Remove?

Edit Profile demo1_intensity [1311131438]

Noise [39167] ti_noise

demo1_intensity.RI.6.A.230.auc Remove?

Edit Profile demo1_intensity [1311131438]

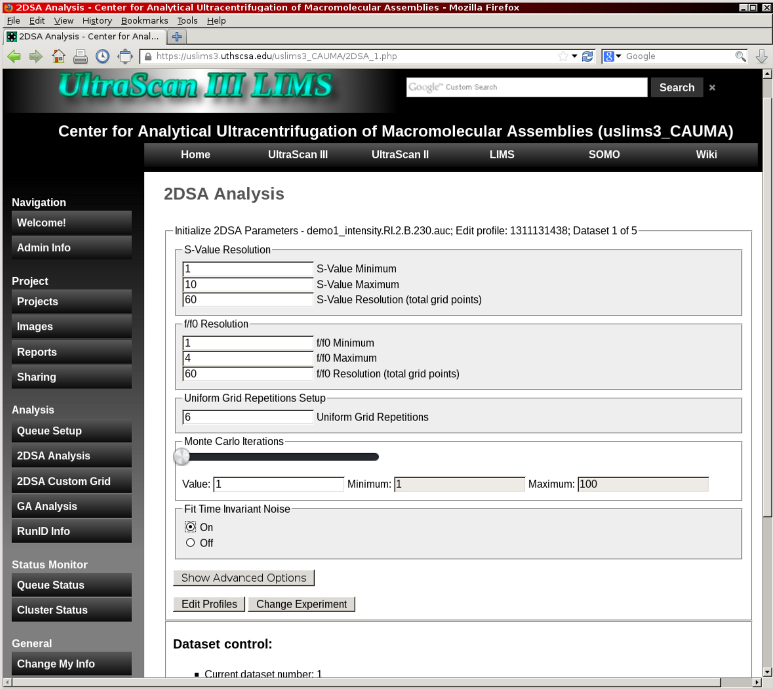
Noise [39168] ti_noise

demo1_intensity.RI.6.B.230.auc Remove?

Edit Profile demo1_intensity [1311131438]

Noise [39169] ti_noise

7. Analysis Method Parameter Selection



Center for Analytical Ultracentrifugation of Macromolecular Assemblies (uslims3_CAUMA)

2DSA Analysis

Initialize 2DSA Parameters - demo1_intensity.RI.2.B.230.auc; Edit profile: 1311131438; Dataset 1 of 5

S-Value Resolution

1 S-Value Minimum
10 S-Value Maximum
60 S-Value Resolution (total grid points)

f/f0 Resolution

1 f/f0 Minimum
4 f/f0 Maximum
60 f/f0 Resolution (total grid points)

Uniform Grid Repetitions Setup

6 Uniform Grid Repetitions

Monte Carlo Iterations

Value: 1 Minimum: 1 Maximum: 100

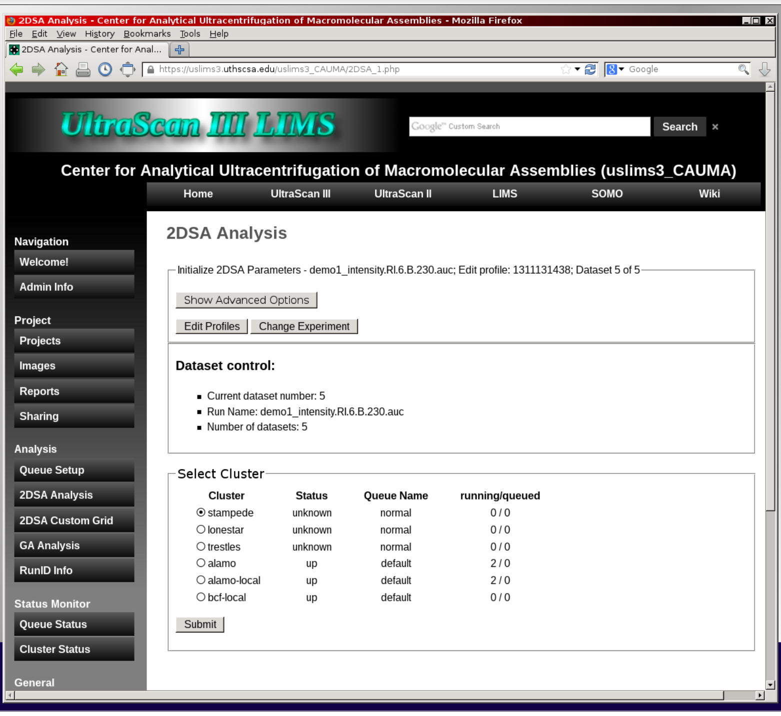
Fit Time Invariant Noise

● On
○ Off

Dataset control:

- Current dataset number: 1

9. Cluster Resource Selection



Center for Analytical Ultracentrifugation of Macromolecular Assemblies (uslims3_CAUMA)

2DSA Analysis

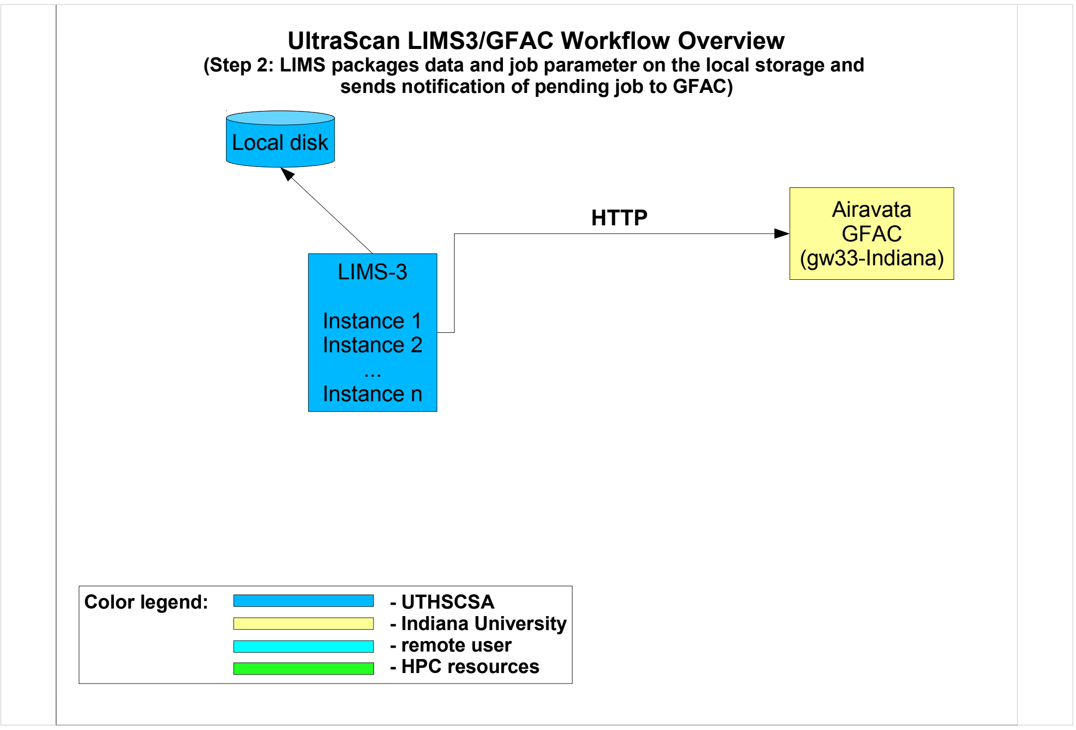
Initialize 2DSA Parameters - demo1_intensity.RI.6.B.230.auc; Edit profile: 1311131438; Dataset 5 of 5

Dataset control:

- Current dataset number: 5
- Run Name: demo1_intensity.RI.6.B.230.auc
- Number of datasets: 5

Select Cluster

Cluster	Status	Queue Name	running/queued
● stampede	unknown	normal	0 / 0
○ lonestar	unknown	normal	0 / 0
○ trestles	unknown	normal	0 / 0
○ alamo	up	default	2 / 0
○ alamo-local	up	default	2 / 0
○ bcf-local	up	default	0 / 0



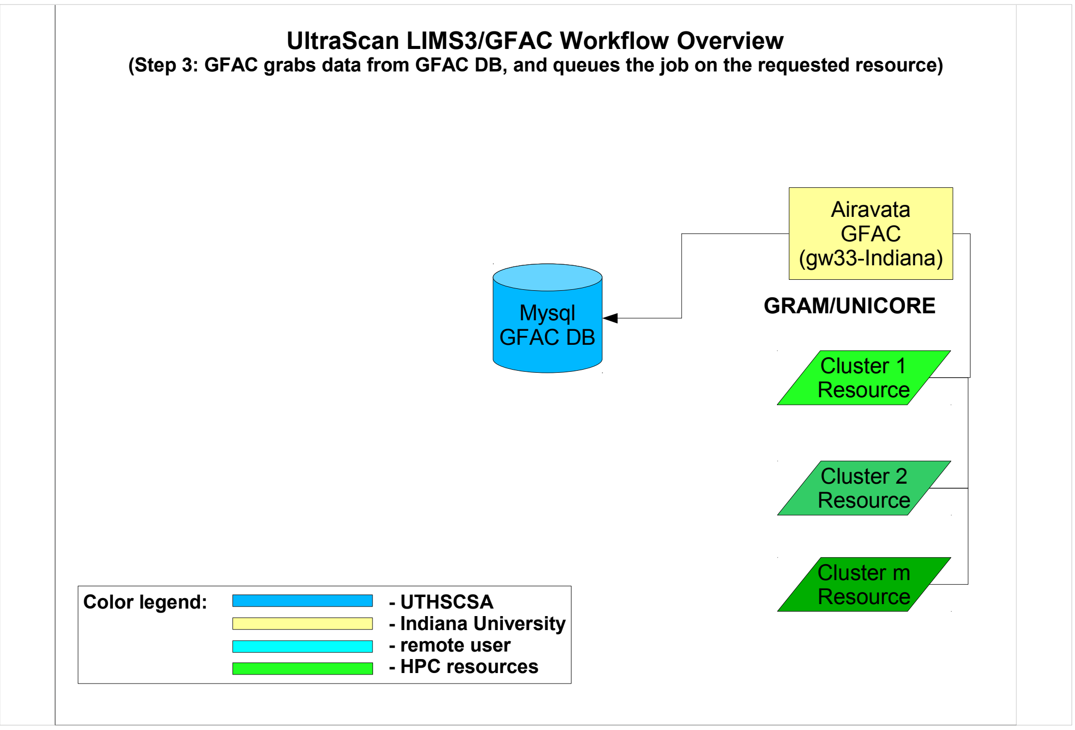
UltraScan LIMS3/GFAC Workflow Overview

(Step 2: LIMS packages data and job parameter on the local storage and sends notification of pending job to GFAC)

Color legend:

- 🟦 - **UTHSCSA**
- 🟨 - **Indiana University**
- 🟦 - **remote user**
- 🟩 - **HPC resources**

We can represent the sedimentation problem as a 2-dimensional parameter space (s and f/f0, or s and MW, or MW and f/f0, or s and D, or D and MW, or D and f/f0, etc.). Each one of these representations is valid and provides the entire information necessary to describe completely the solution properties of individual solutes. The problem is then to identify the solutes (blue dots in the plane), and their relative concentration that when combined make up the experimental data shown as a blue concentration traces for differen time and radius values.



UltraScan LIMS3/GFAC Workflow Overview

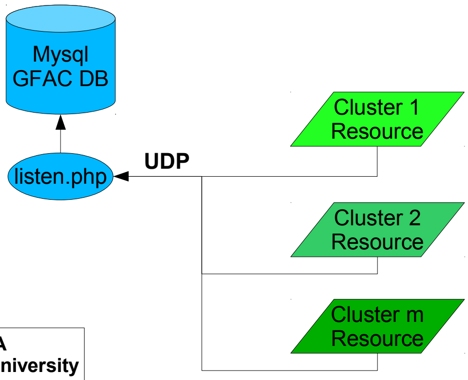
(Step 3: GFAC grabs data from GFAC DB, and queues the job on the requested resource)

Color legend:
- 🟦 - **UTHSCSA**
- 🟨 - **Indiana University**
- 🟦 - **remote user**
- 🟩 - **HPC resources**

We can represent the sedimentation problem as a 2-dimensional parameter space (s and f/f0, or s and MW, or MW and f/f0, or s and D, or D and MW, or D and f/f0, etc.). Each one of these representations is valid and provides the entire information necessary to describe completely the solution properties of individual solutes. The problem is then to identify the solutes (blue dots in the plane), and their relative concentration that when combined make up the experimental data shown as a blue concentration traces for differen time and radius values.

UltraScan LIMS3/GFAC Workflow Overview

(Step 4: US-HPC sends job status over UDP to a daemon which updates GFAC DB)



Color legend:
- 🟦 **- UTHSCSA**
- 🟨 **- Indiana University**
- 🟦 **- remote user**
- 🟩 **- HPC resources**

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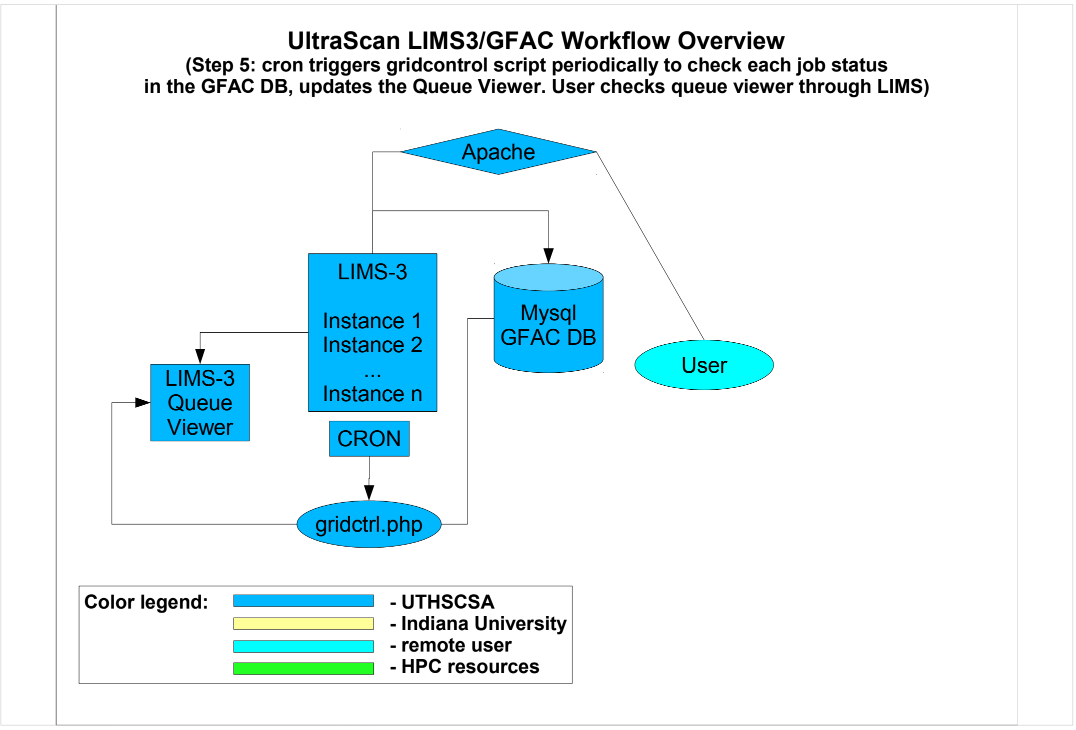
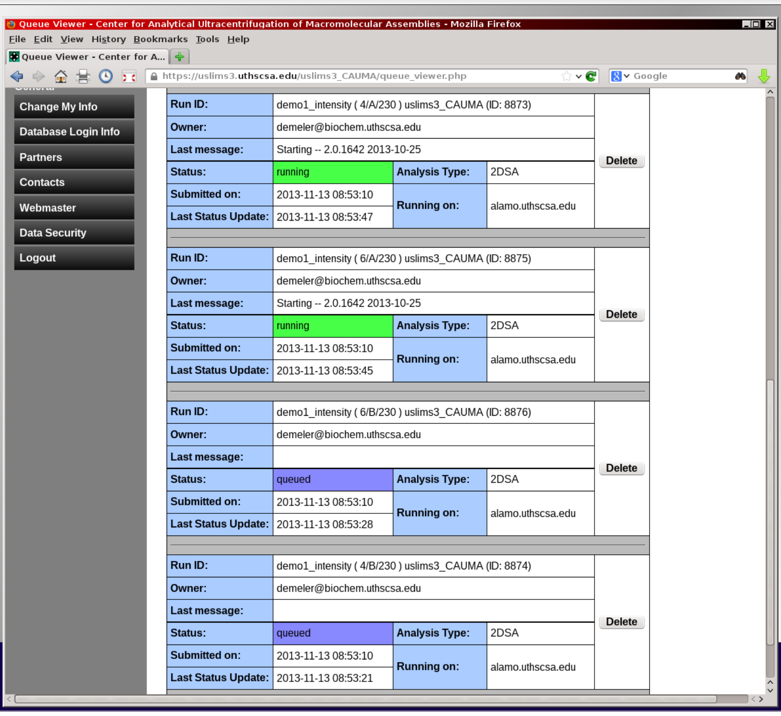

UltraScan LIMS3/GFAC Workflow Overview

(Step 5: cron triggers gridcontrol script periodically to check each job status in the GFAC DB, updates the Queue Viewer. User checks queue viewer through LIMS)

We can represent the sedimentation problem as a 2-dimensional parameter space (s and f/f0, or s and MW, or MW and f/f0, or s and D, or D and MW, or D and f/f0, etc.). Each one of these representations is valid and provides the entire information necessary to describe completely the solution properties of individual solutes. The problem is then to identify the solutes (blue dots in the plane), and their relative concentration that when combined make up the experimental data shown as a blue concentration traces for differen time and radius values.

10. Queue Monitor

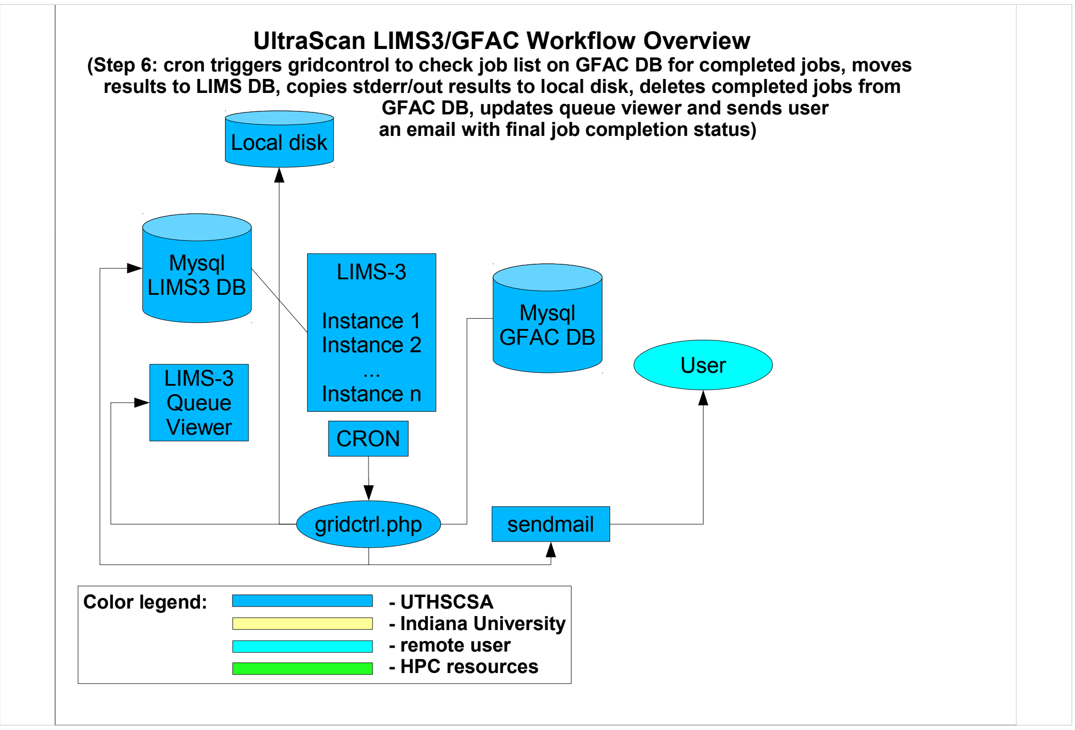


Run ID:	demo1_intensity (4/A/230) uslims3_CAUMA (ID: 8873)			
Owner:	demeler@biochem.uthscsa.edu			
Last message:	Starting -- 2.0.1642 2013-10-25			
Status:	running	**Analysis Type:**	2DSA	Delete
Submitted on:	2013-11-13 08:53:10	**Running on:**	alamo.uthscsa.edu	
Last Status Update:	2013-11-13 08:53:47			

Run ID:	demo1_intensity (6/A/230) uslims3_CAUMA (ID: 8875)			
Owner:	demeler@biochem.uthscsa.edu			
Last message:	Starting -- 2.0.1642 2013-10-25			
Status:	running	**Analysis Type:**	2DSA	Delete
Submitted on:	2013-11-13 08:53:10	**Running on:**	alamo.uthscsa.edu	
Last Status Update:	2013-11-13 08:53:45			

Run ID:	demo1_intensity (6/B/230) uslims3_CAUMA (ID: 8876)			
Owner:	demeler@biochem.uthscsa.edu			
Last message:				
Status:	queued	**Analysis Type:**	2DSA	Delete
Submitted on:	2013-11-13 08:53:10	**Running on:**	alamo.uthscsa.edu	
Last Status Update:	2013-11-13 08:53:28			

Run ID:	demo1_intensity (4/B/230) uslims3_CAUMA (ID: 8874)			
Owner:	demeler@biochem.uthscsa.edu			
Last message:				
Status:	queued	**Analysis Type:**	2DSA	Delete
Submitted on:	2013-11-13 08:53:10	**Running on:**	alamo.uthscsa.edu	
Last Status Update:	2013-11-13 08:53:21			



UltraScan LIMS3/GFAC Workflow Overview

(Step 6: cron triggers gridcontrol to check job list on GFAC DB for completed jobs, moves results to LIMS DB, copies stderr/out results to local disk, deletes completed jobs from GFAC DB, updates queue viewer and sends user an email with final job completion status)

Color legend:
- 🟦 - UTHSCSA
- 🟨 - Indiana University
- 🟦 - remote user
- 🟩 - HPC resources

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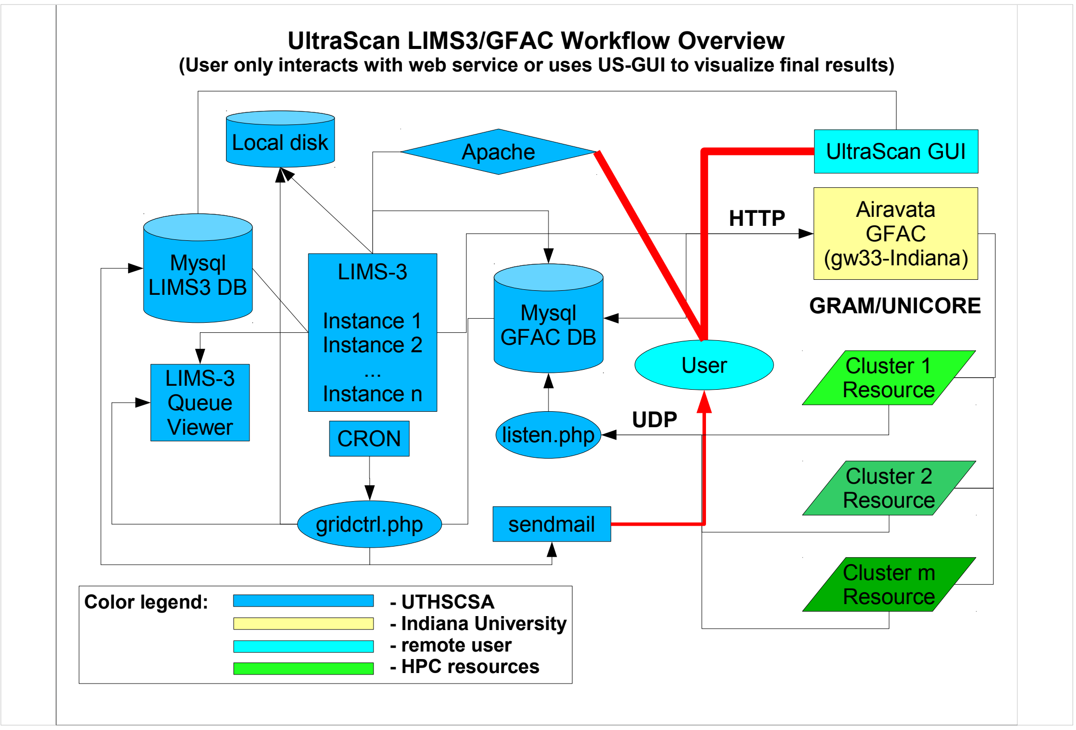


UltraScan LIMS3/GFAC Workflow Overview

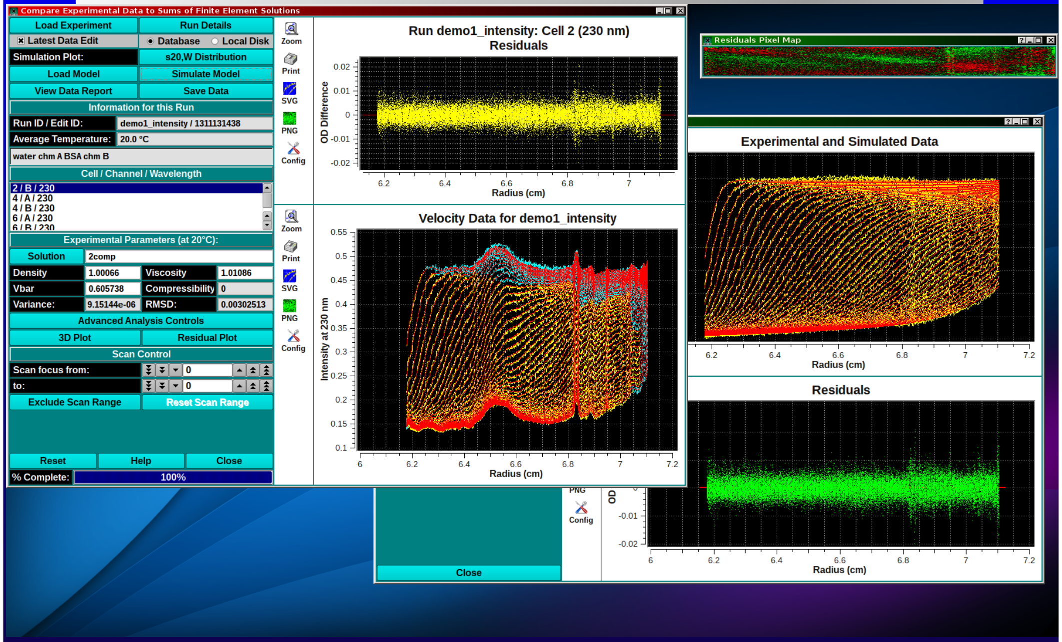
(User only interacts with web service or uses US-GUI to visualize final results)

Color legend:

- UTHSCSA
- Indiana University
- remote user
- HPC resources

We can represent the sedimentation problem as a 2-dimensional parameter space (s and f/f0, or s and MW, or MW and f/f0, or s and D, or D and MW, or D and f/f0, etc.). Each one of these representations is valid and provides the entire information necessary to describe completely the solution properties of individual solutes. The problem is then to identify the solutes (blue dots in the plane), and their relative concentration that when combined make up the experimental data shown as a blue concentration traces for differen time and radius values.

11. Result Visualization



Compare Experimental Data to Sums of Finite Element Solutions

☒ Latest Data Edit

● Database ○ Local Disk

Simulation Plot: s20,W Distribution

Run ID / Edit ID: demo1_intensity / 1311131438

Average Temperature: 20.0 °C

water chm A BSA chm B

Cell / Channel / Wavelength: 2 / B / 230

Solution: 2comp

Density: 1.00066

Viscosity: 1.01086

Vbar: 0.605738

Compressibility: 0

Variance: 9.15144e-06

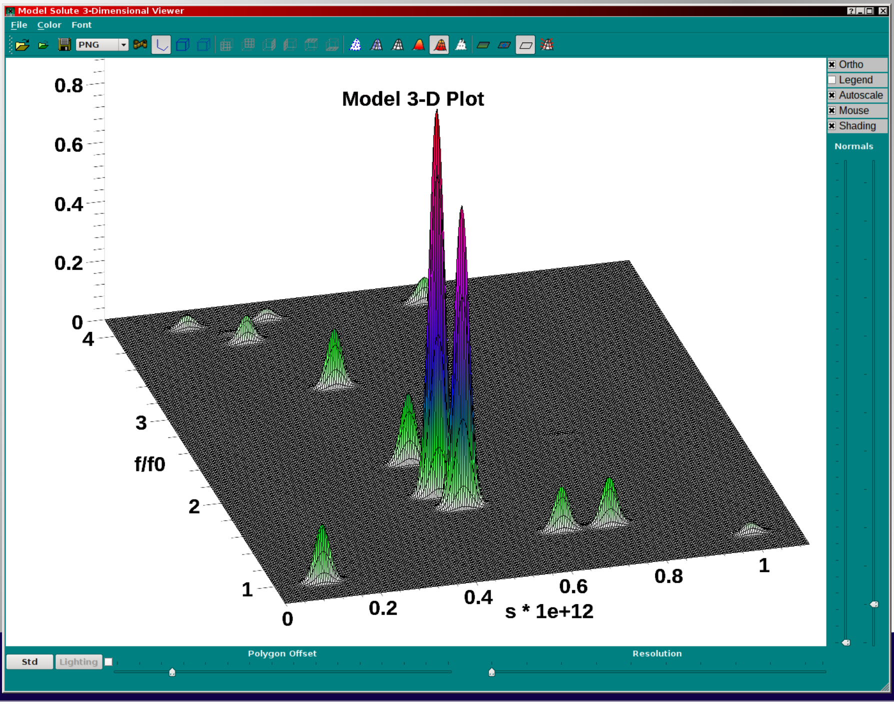
RMSD: 0.00302513

Scan focus from: 0

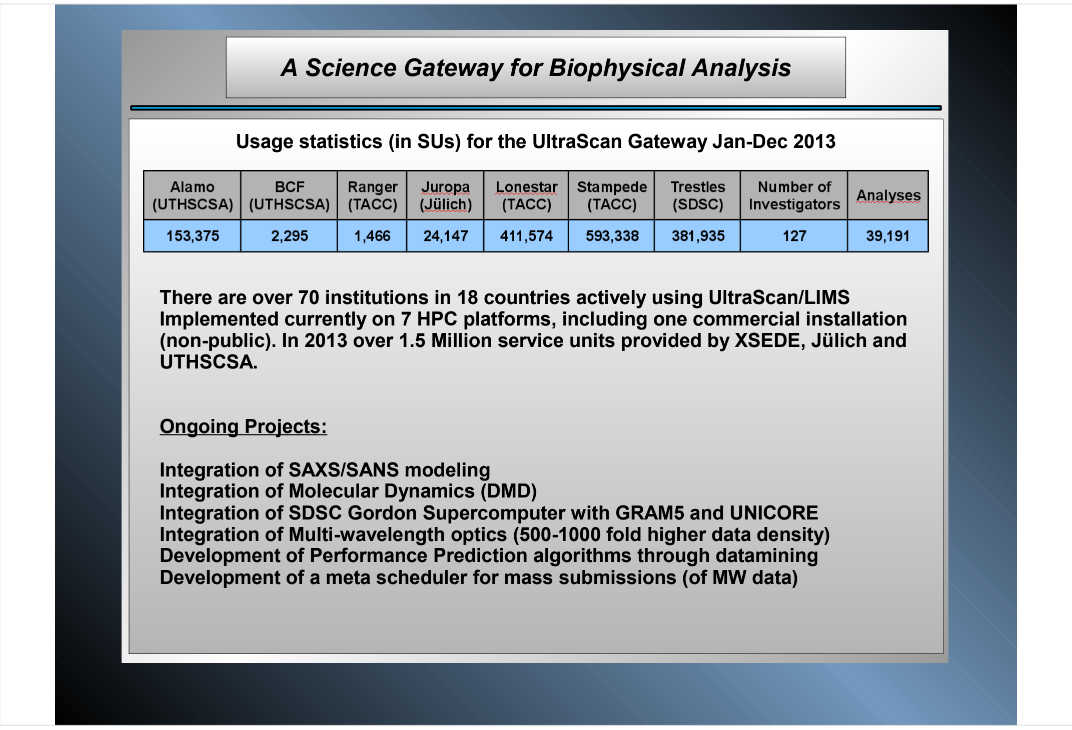
to: 0

% Complete: 100%

12. Result Metadata analysis



☒ Ortho
☐ Legend
☒ Autoscale
☒ Mouse
☒ Shading



A Science Gateway for Biophysical Analysis

Usage statistics (in SUs) for the UltraScan Gateway Jan-Dec 2013

Alamo (UTHSCSA)	BCF (UTHSCSA)	Ranger (TACC)	Juropa (Jülich)	Lonestar (TACC)	Stampede (TACC)	Trestles (SDSC)	Number of Investigators	Analyses
153,375	2,295	1,466	24,147	411,574	593,338	381,935	127	39,191

There are over 70 institutions in 18 countries actively using UltraScan/LIMS Implemented currently on 7 HPC platforms, including one commercial installation (non-public). In 2013 over 1.5 Million service units provided by XSEDE, Jülich and UTHSCSA.

Ongoing Projects:

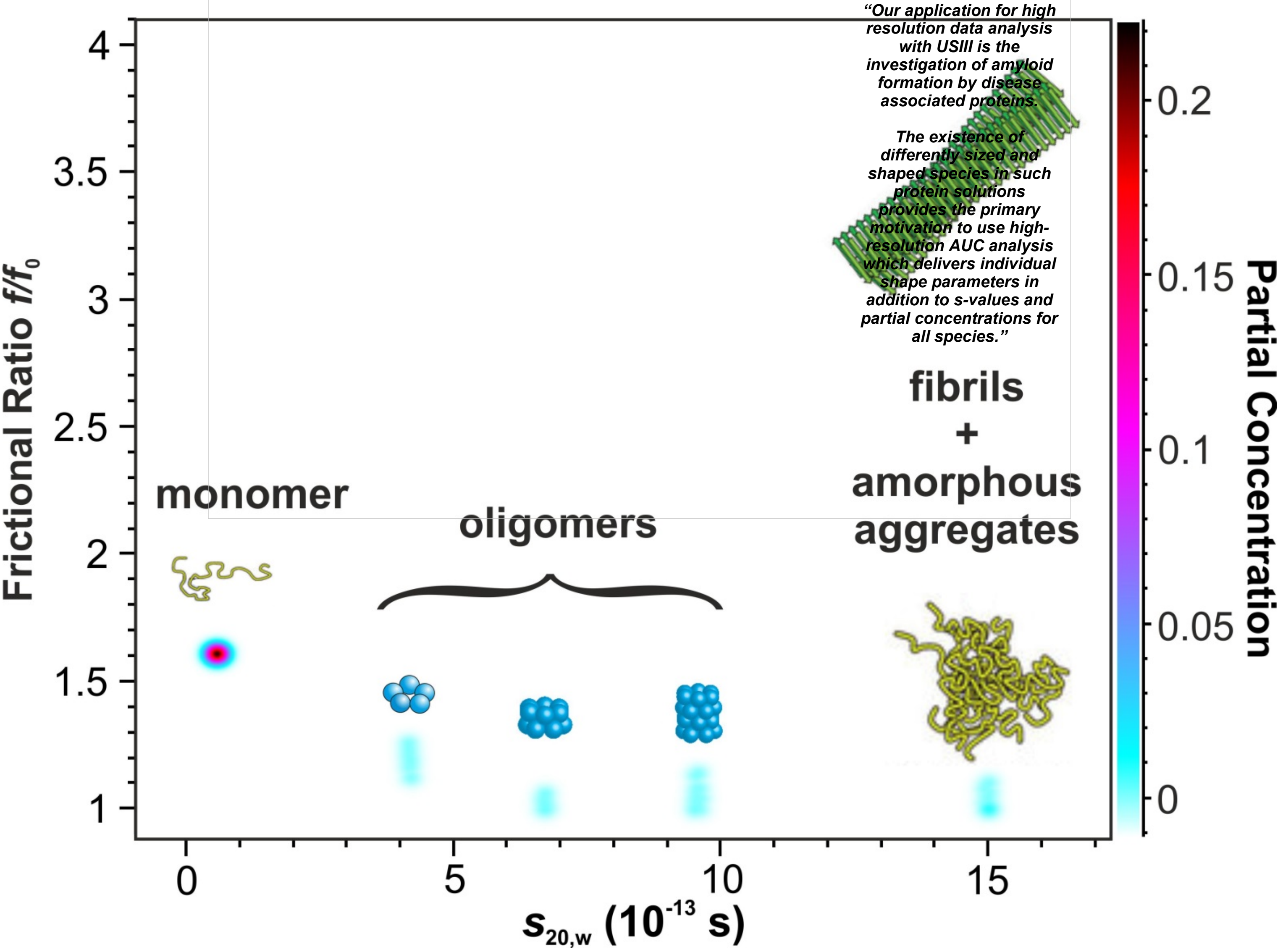
Integration of SAXS/SANS modeling
Integration of Molecular Dynamics (DMD)
Integration of SDSC Gordon Supercomputer with GRAM5 and UNICORE
Integration of Multi-wavelength optics (500-1000 fold higher data density)
Development of Performance Prediction algorithms through datamining
Development of a meta scheduler for mass submissions (of MW data)

Amyloid-β Aggregation studied by Sedimentation Velocity Analytical Ultracentrifugation

*L. Nagel-Steger at the Dept. of Physical Biology, Heinrich-Heine-University Düsseldorf
& ICS-6, RC-Jülich, Germany*

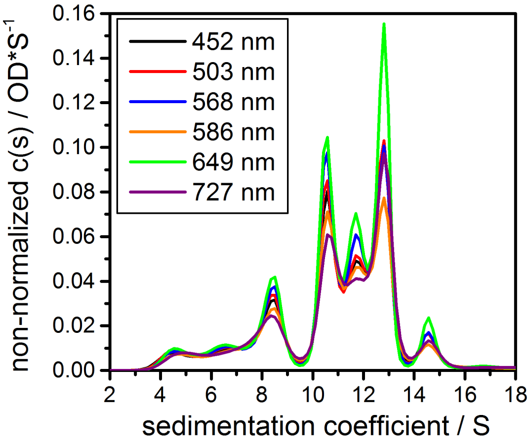
"Our application for high resolution data analysis with USIII is the investigation of amyloid formation by disease associated proteins.

The existence of differently sized and shaped species in such protein solutions provides the primary motivation to use high-resolution AUC analysis which delivers individual shape parameters in addition to s-values and partial concentrations for all species."



Sedimentation analysis of single-walled carbon nanotube composition with a multi-wavelength AUC detector.

Walter, J. and W. Peukert, Dept. of Feststoff- und Grenzflächenverfahrenstechnik, Friedrich-Alexander-Universität Erlangen-Nürnberg.



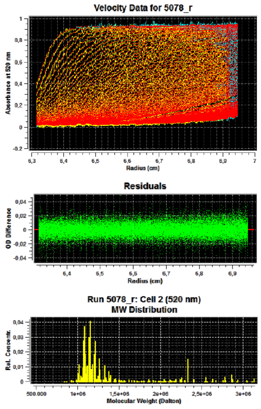
1. Analysis of quantum dots

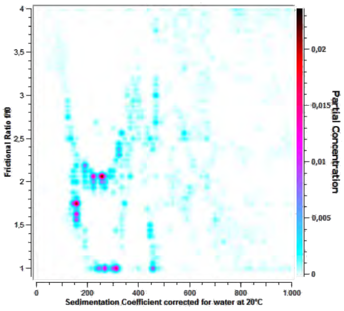
We want to study the size dependent optical properties by means of multi-wavelength AUC analysis. Hydrodynamic analysis will be complemented by simultaneous spectral analysis. We are also interested in the effect of surface modifications using different surfactants. AUC allows us to study surface properties and stabilizer interactions of particles in the lower nanoscale.

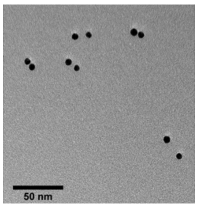
2. Analysis of carbon nanotubes
The evaluation of carbon nanotubes using AUC allows us to distinguish between different species of tubes in even complex mixtures exploiting their unique optical and hydrodynamic properties.

Synthesis and Characterization of DNA-Metal Hybrid Materials

Urban, M. and H. Cölfen, Dept. of Chemistry and biofunctional Materials
University of Konstanz







Development of new plasmonic devices.

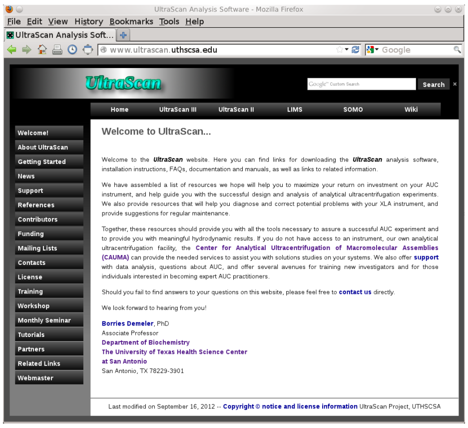
We want to develop DNA-Metal hybrid materials by linking two gold nanoparticles by DNA single- and double-stranded oligomers. The number of bases in the oligomer allows us to precisely control the distances between the metal cores to optimize plasmon resonance and fluorescence properties.

AUC provides the necessary size and shape characterization of DNA-Metal hybrid particles to allow us to bulk-characterize mixtures of nanoparticles and their assemblies with DNA.

Links:

UltraScan-III:
http://www.ultrascan.uthscsa.edu
XSEDE Science Gateway:
https://portal.xsede.org/science-gateways

SciGaP Project:
http://www.scigap.org
Airavata Project:
http://airavata.apache.org/



Welcome to UltraScan...

Welcome to the ***UltraScan*** website. Here you can find links for downloading the ***UltraScan*** analysis software, installation instructions, FAQs, documentation and manuals, as well as links to related information.

We have assembled a list of resources we hope will help you to maximize your return on investment on your AUC instrument, and help guide you with the successful design and analysis of analytical ultracentrifugation experiments. We also provide resources that will help you diagnose and correct potential problems with your XLA instrument, and provide suggestions for regular maintenance.

Together, these resources should provide you with all the tools necessary to assure a successful AUC experiment and to provide you with meaningful hydrodynamic results. If you do not have access to an instrument, our own analytical ultracentrifugation facility, the **Center for Analytical Ultracentrifugation of Macromolecular Assemblies (CAUMA)** can provide the needed services to assist you with solutions studies on your systems. We also offer **support** with data analysis, questions about AUC, and offer several avenues for training new investigators and for those individuals interested in becoming expert AUC practitioners.

Should you fail to find answers to your questions on this website, please feel free to **contact us** directly.

We look forward to hearing from you!

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The University of Texas Health Science Center
at San Antonio
San Antonio, TX 78229-3901

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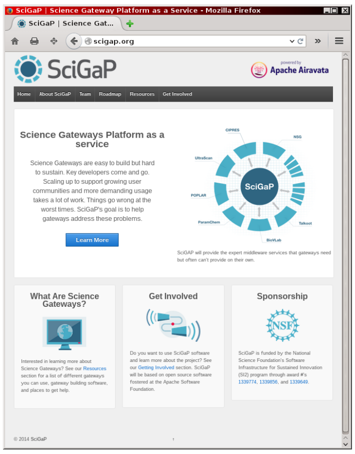

Science Gateways Platform as a service

Science Gateways are easy to build but hard to sustain. Key developers come and go. Scaling up to support growing user communities and more demanding usage takes a lot of work. Things go wrong at the worst times. SciGaP's goal is to help gateways address these problems.

SciGAP will provide the expert middleware services that gateways need but often can't provide on their own.

What Are Science Gateways?

Interested in learning more about Science Gateways? See our Resources section for a list of different gateways you can use, gateway building software, and places to get help.

Get Involved

Do you want to use SciGaP software and learn more about the project? See our Getting Involved section. SciGaP will be based on open source software fostered at the Apache Software Foundation.

Sponsorship

SciGaP is funded by the National Science Foundation's Software Infrastructure for Sustained Innovation (SI2) program through award #'s 1339774, 1339856, and 1339649.

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A copy of this presentation:
http://www.demeler.uthscsa.edu/unicore-2014.pdf

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