



Graduate School of Biomedical Sciences, Dept. of Biochemistry

UT HEALTH SCIENCE CENTER™

San Antonio

Borries Demeler, Ph.D.

**Biophysics and HPC:
The UltraScan XSEDE Science Gateway**



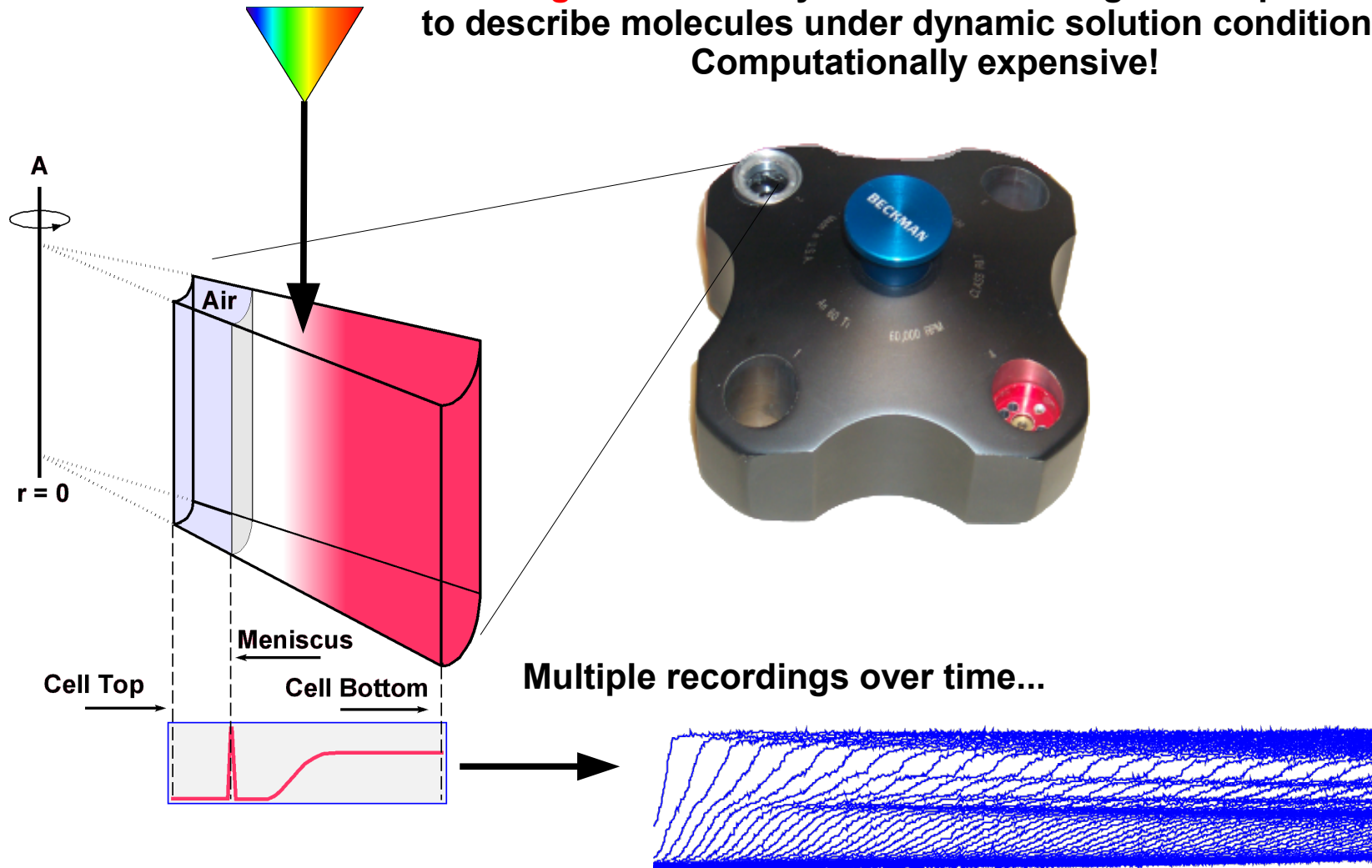
A Science Gateway for Biophysical Analysis

Goals:

- *Support analysis of experiments on molecules in solution environments*
 - *Analytical ultracentrifugation (AUC)*
 - *Laser Light Scattering (LS)*
 - *Small angle X-ray/neutron scattering (SAXS/SANS)*
- *Provide highest possible resolution in the analysis – requires HPC*
- *Offer a flexible model for multiple optimization methods*
- *Integrate a variety of HPC environments into a uniform user experience*
- *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 (GRAM4, GRAM5, Unicore...)*
- *Fast turnaround to support serial workflows (model refinement)*

A Science Gateway for Biophysical Analysis

Challenge: Model analytical ultracentrifugation experiments to describe molecules under dynamic solution conditions: Computationally expensive!



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$$L(s, D): \left(\frac{\partial C}{\partial t} \right)_r = \frac{-1}{r} \frac{\partial}{\partial r} \left[s \omega^2 r^2 C - D r \frac{\partial C}{\partial r} \right]_t$$
$$MIN: \sum_{i=1, j=1}^{r, t} \left[Y_{i, j} - \sum_{k=1}^n \left(L_k(s_k, D_k)_{i, j} \right) \right]^2$$

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

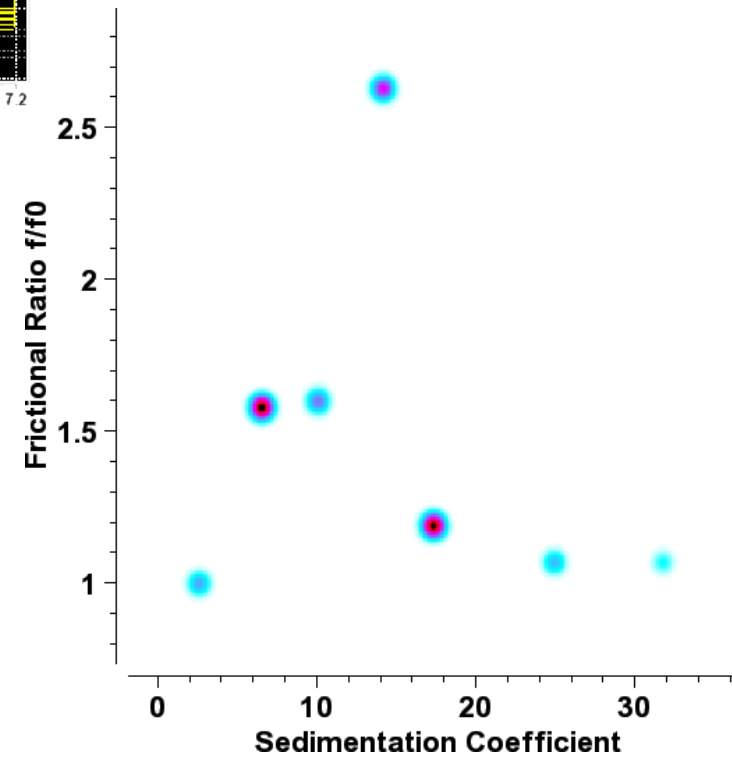
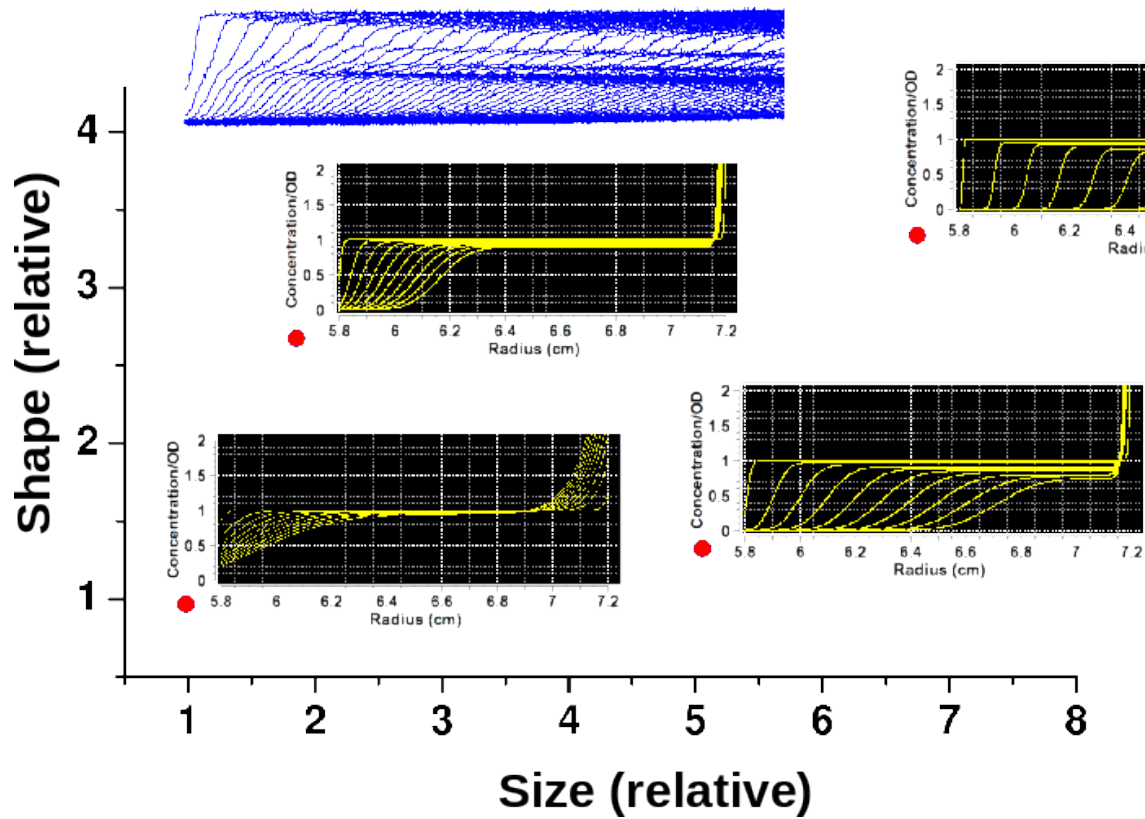
The optimization problem is solved with parallelized 2DSA, GA, MC

Brookes E, Cao W, Demeler B A two-dimensional spectrum analysis for sedimentation velocity experiments of mixtures with heterogeneity in molecular weight and shape. *Eur Biophys J.* (2010) 39(3):405-14.

Brookes E, Demeler B. Parsimonious Regularization using Genetic Algorithms Applied to the Analysis of Analytical Ultracentrifugation Experiments. *GECCO Proceedings ACM 978159593-697-4/07/0007* (2007)

Demeler B and E. Brookes. Monte Carlo analysis of sedimentation experiments. *Colloid Polym Sci* (2008) 286(2) 129-137

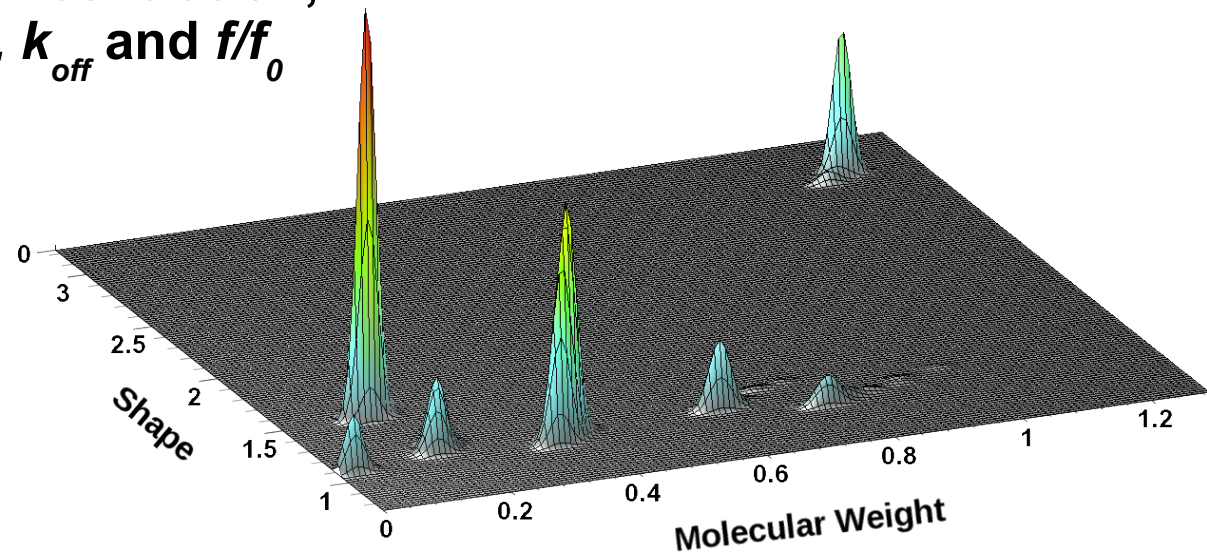
The analysis provides information about the number of components in solution, their relative concentrations, their sedimentation and diffusion properties, molar mass, anisotropy (rel. shape), interaction coefficients, and reaction rate constants



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

Optimization:

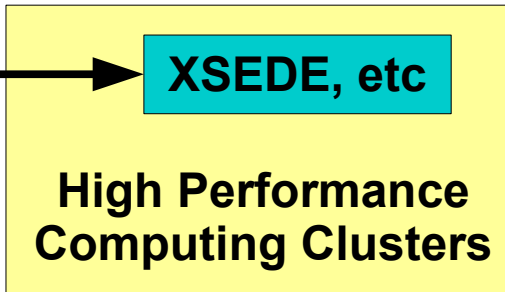
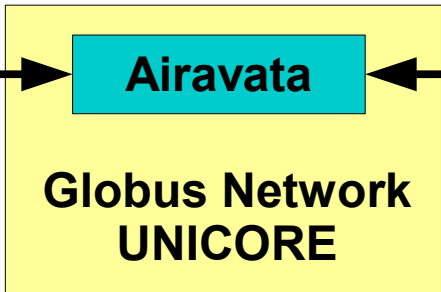
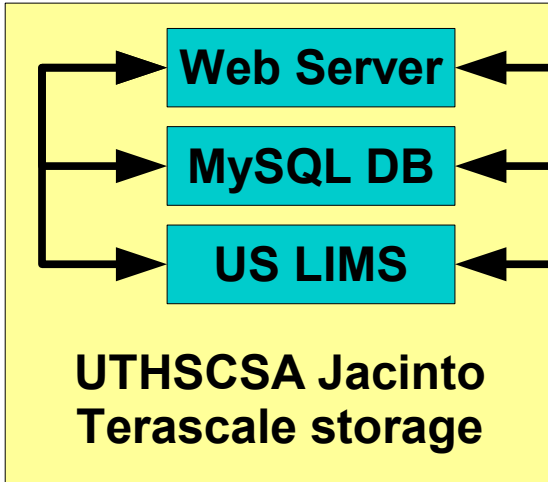
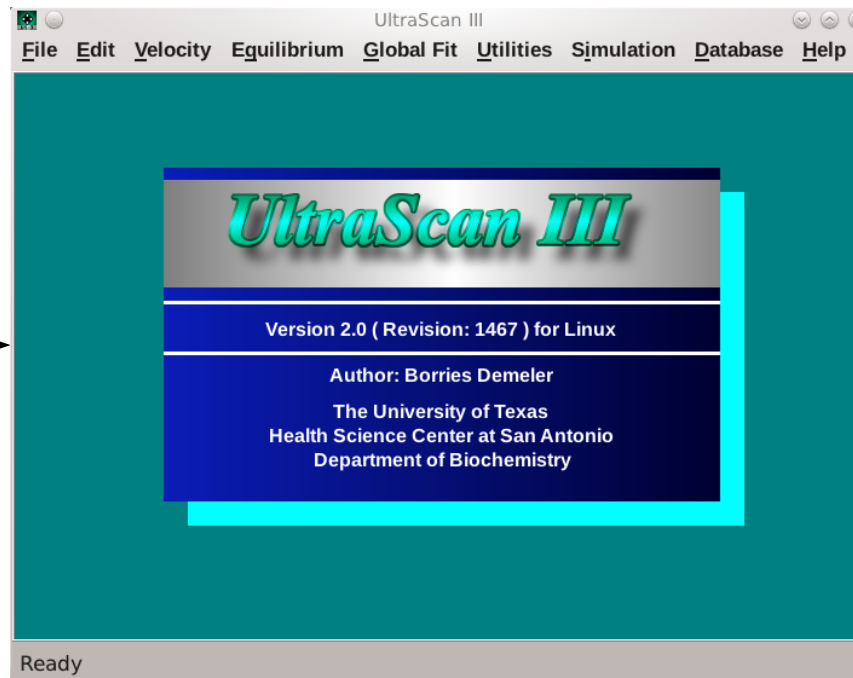
2D-Spectrum Analysis
 Genetic Algorithms
 Monte Carlo Analysis



UltraScan Organization (open source, multi-platform)



User



UltraScan (US) components and 3rd party software:

- 1. US-GUI: (Linux, Mac, Windows): used for data processing, editing, uploading, visualization, report generation (C++/Qt).**
- 2. US-LIMS: web-based interface to the MySQL database. Gives the user web-based access to their data, visualizations and analysis reports (PHP).**
- 3. US-HPC: includes finite element solver for multiple models and performs all optimization algorithms (2DSA, GA, Monte Carlo)**
- 4. US-Gridcontrol: PHP daemon to manage job submission, communications and reporting from US-HPC,**
- 5. MySQL: houses all LIMS data, a separate GFAC DB holds job status info. Each institution has a separate database and separate US-LIMS instance. All communications with MySQL are performed through stored procedure calls.**
- 6. GFAC/Airavata: accepts job requests and brokers them over the appropriate grid middleware to the requested supercomputer, controls job status in GFAC DB.**
- 7. GRAM/UNICORE grid middleware**
- 8. SSL communications: All communications and data transfers are SSL encrypted. All database access and LIMS access requires authentication.**
- 9. Statistic scripts: queries database and reports usage and provides details for XSEDE reporting.**

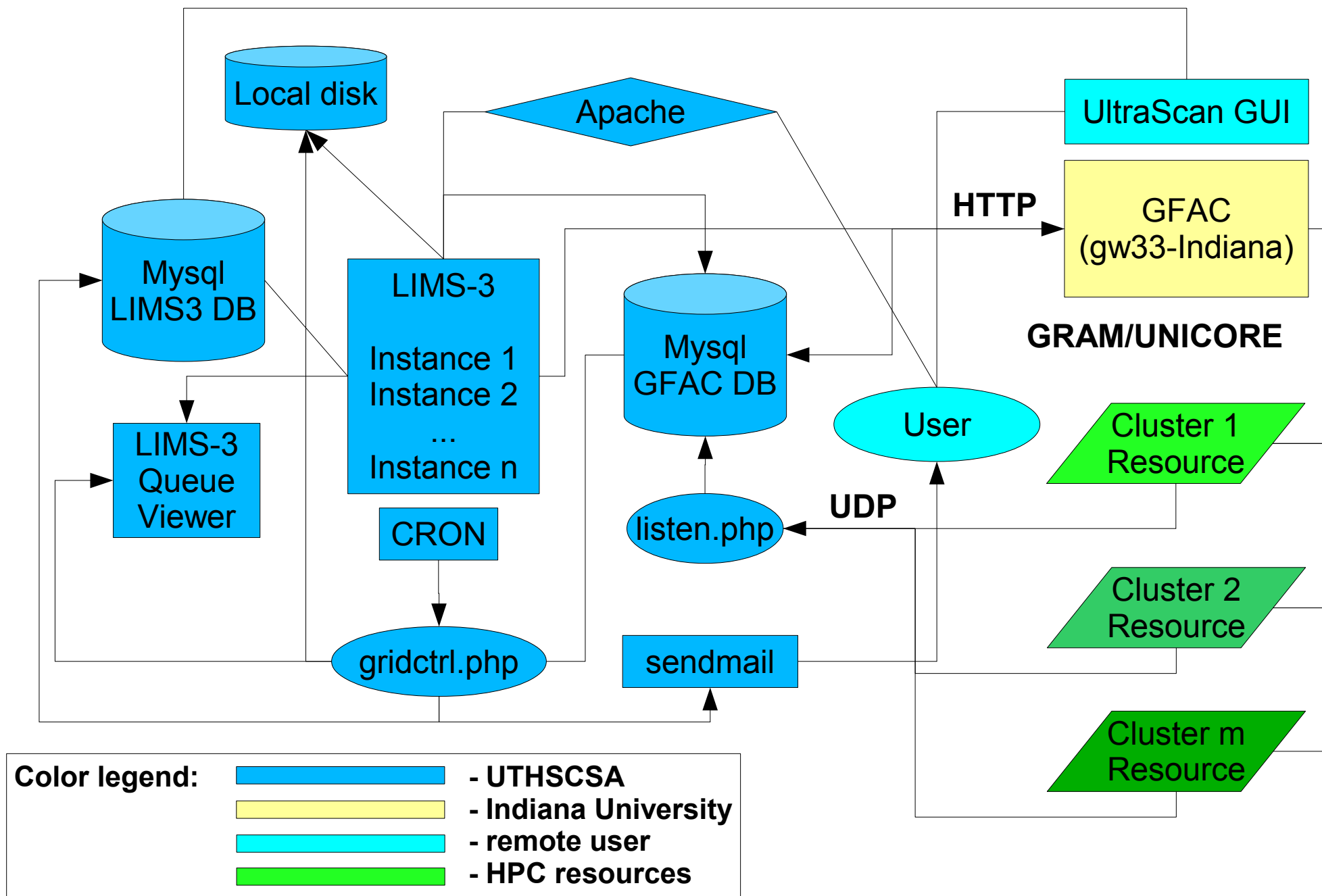
A Science Gateway for Biophysical Analysis

Data Flow:

- 1. User acquires data and stores it on a local computer.**
- 2. After authentication in US-GUI, user uploads data (converted to efficient binary format) together with all meta data (XML) information to the LIMS SQL database.**
- 3. Data editing: edited data is used by all analyses in US for further processing.**
- 4. User logs into US-LIMS website, selects data, analysis method, analysis parameters, and HPC resource, then submits the analysis request. LIMS places the data and request into a special GFAC database, and notifies GFAC.**
- 5. GFAC component brokers request for desired HPC resource, grabs data from GFAC database, and places the job into the job queue.**
- 6. US-HPC processes analysis, sending UDP status updates which are processed by US-Gridcontrol**
- 7. User monitors job queue which is periodically updated by US-Gridcontrol. When job is finished, user is also sent an e-mail, and the result (a universal model in XML) is deposited in the MySQL DB associated with the user's US-LIMS instance.**
- 8. User visualizes the results with the US-GUI and prepares items to be stored in the report. Results and reports are placed into MySQL DB.**
- 9. User can proceed with several iterations of result refinement (GA, MC)**
- 10. User can share the data with a collaborator who has an account on the same LIMS. User or collaborator can log into US-LIMS and review the results.**

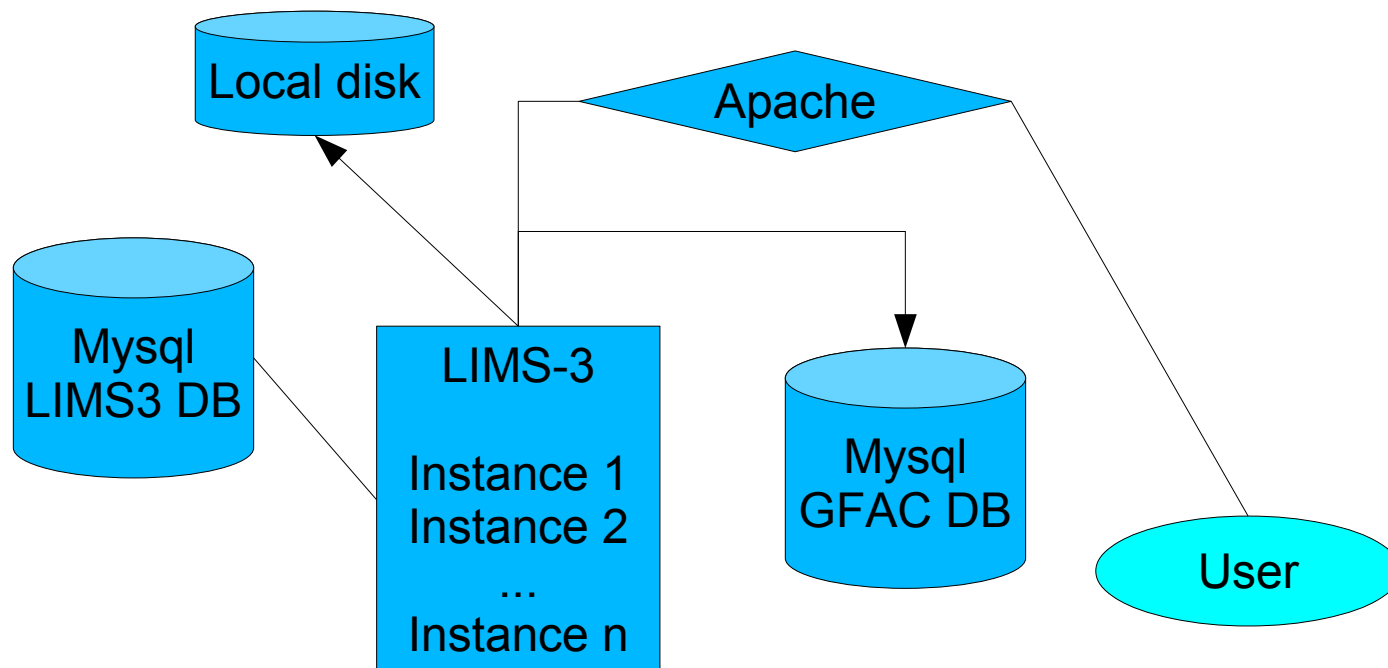
UltraScan LIMS3/GFAC Workflow Overview

(GFAC = Generic Factory Component of Apache Airavata)


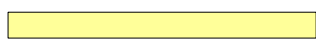




UltraScan LIMS3/GFAC Workflow Overview

(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)

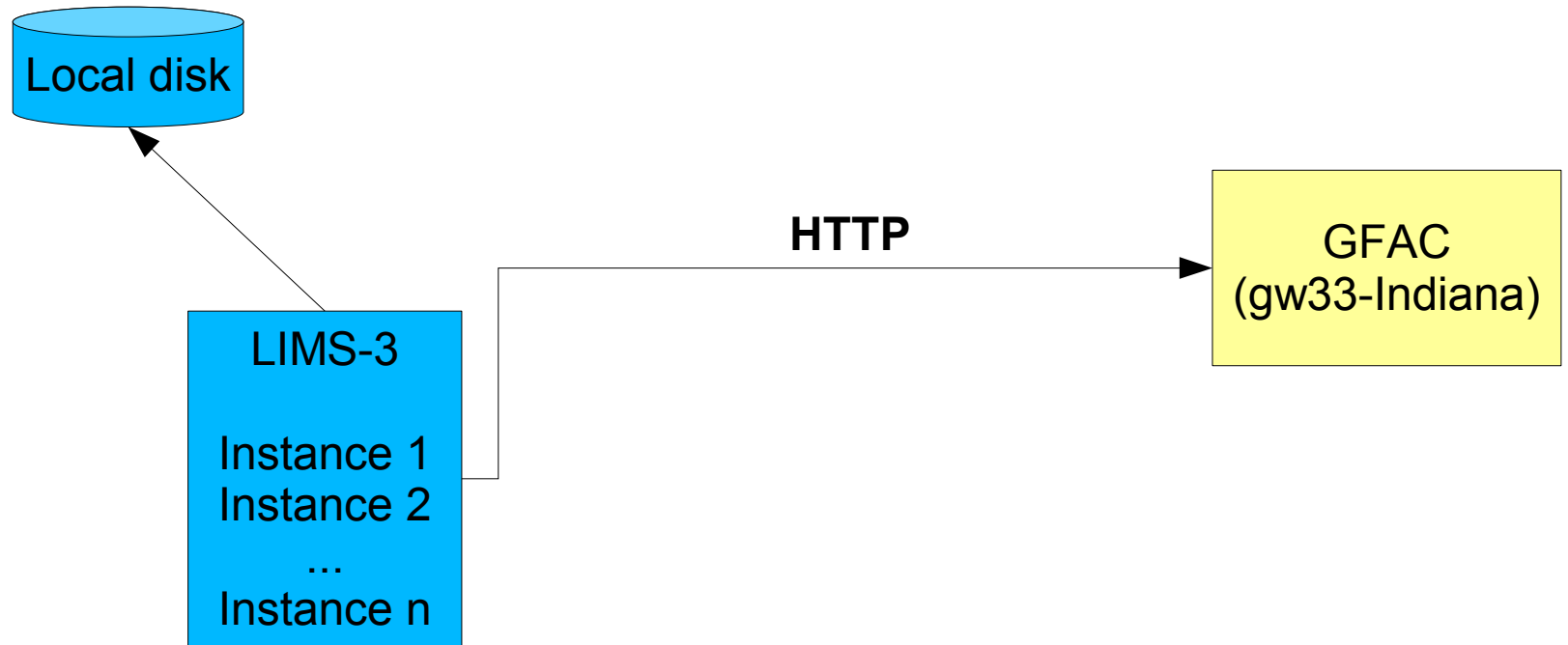


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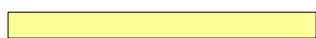


-  - UTHSCSA
-  - Indiana University
-  - remote user
-  - HPC resources

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)

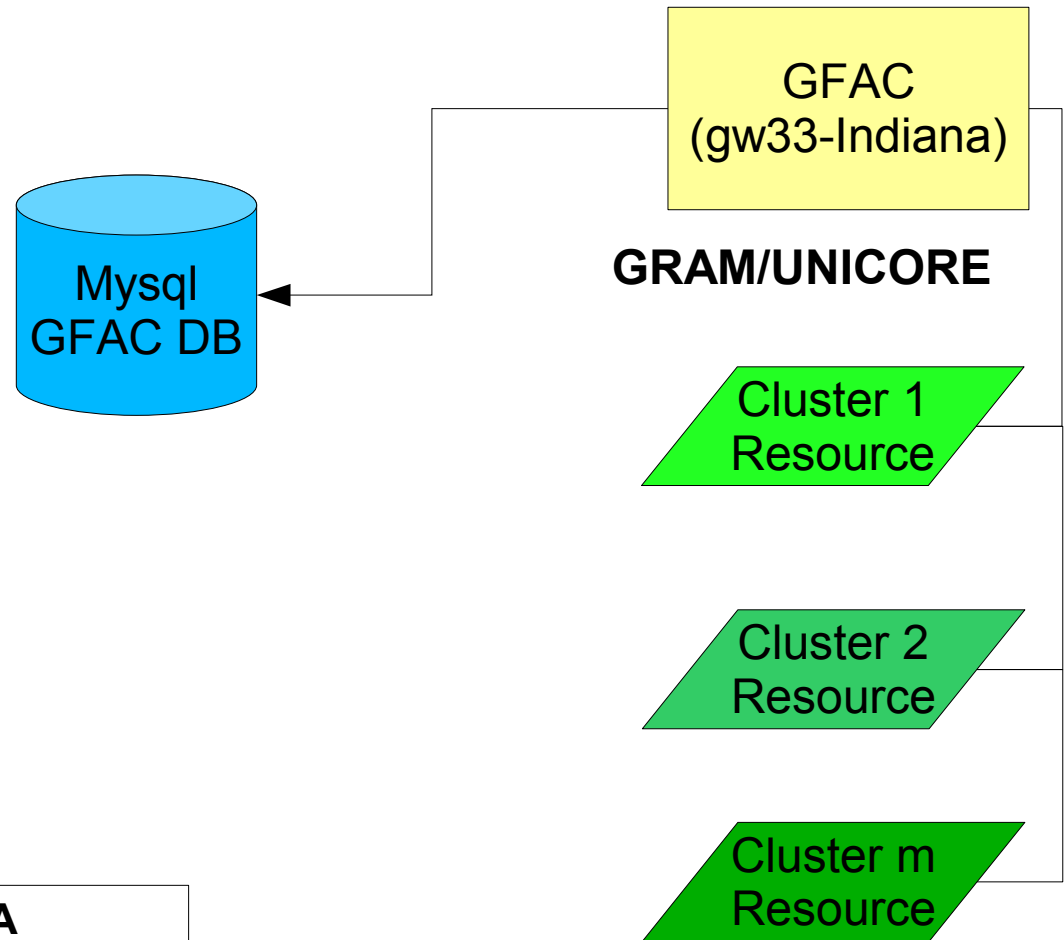


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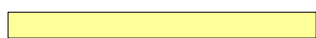


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-  - remote user
-  - HPC resources

UltraScan LIMS3/GFAC Workflow Overview

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

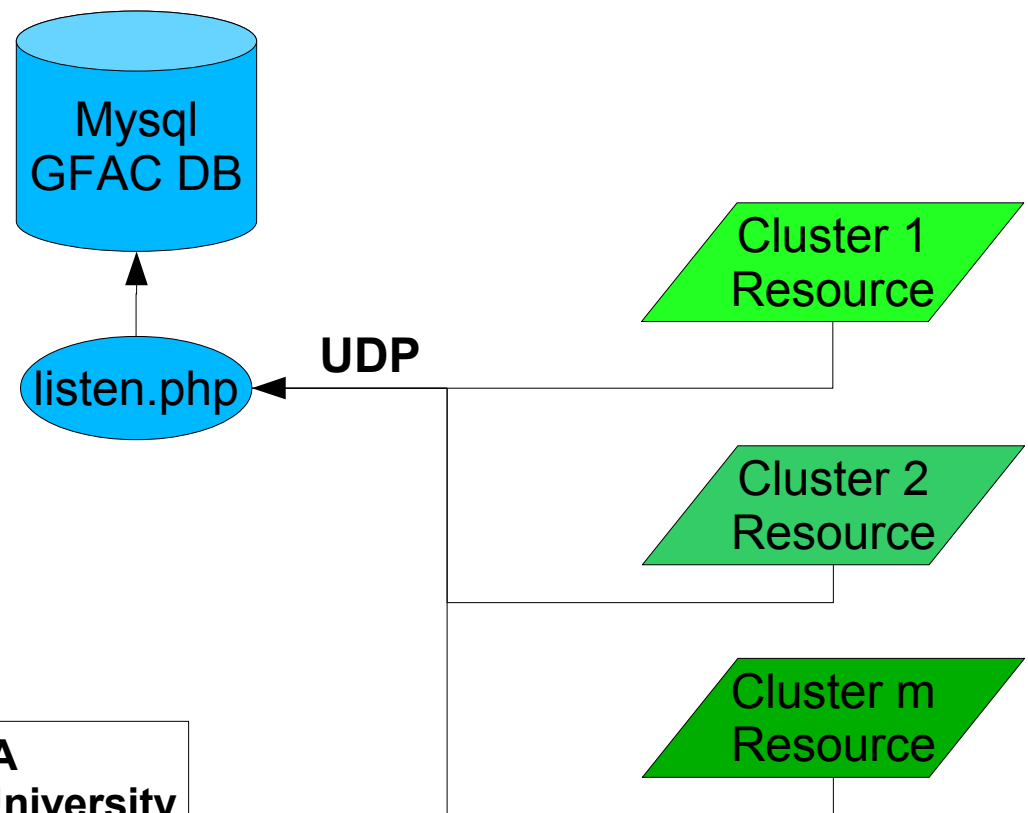


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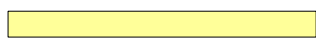


-  - UTHSCSA
-  - Indiana University
-  - remote user
-  - HPC resources

UltraScan LIMS3/GFAC Workflow Overview

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

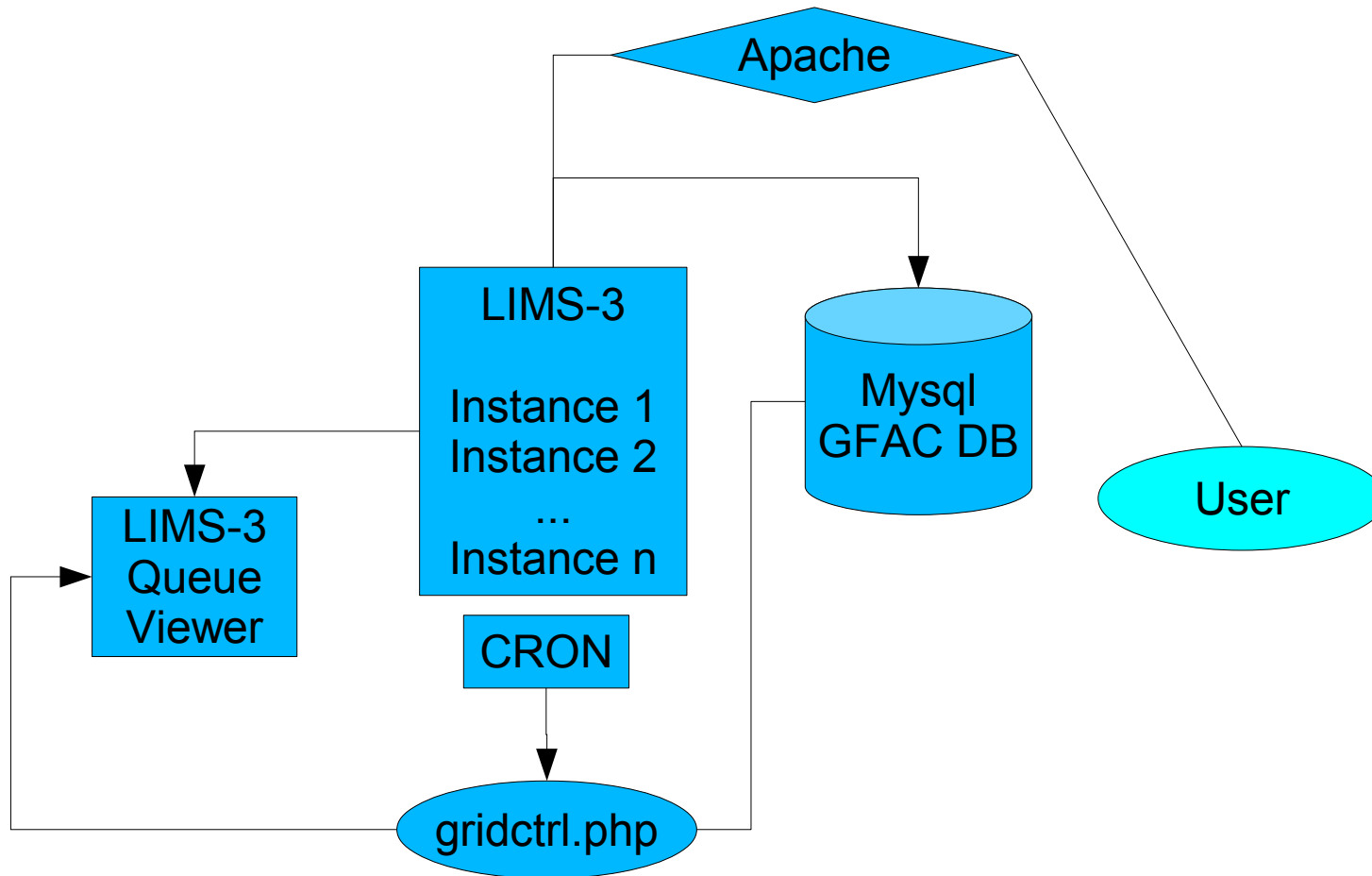


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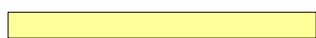


-  - UTHSCSA
-  - Indiana University
-  - remote user
-  - HPC resources

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)

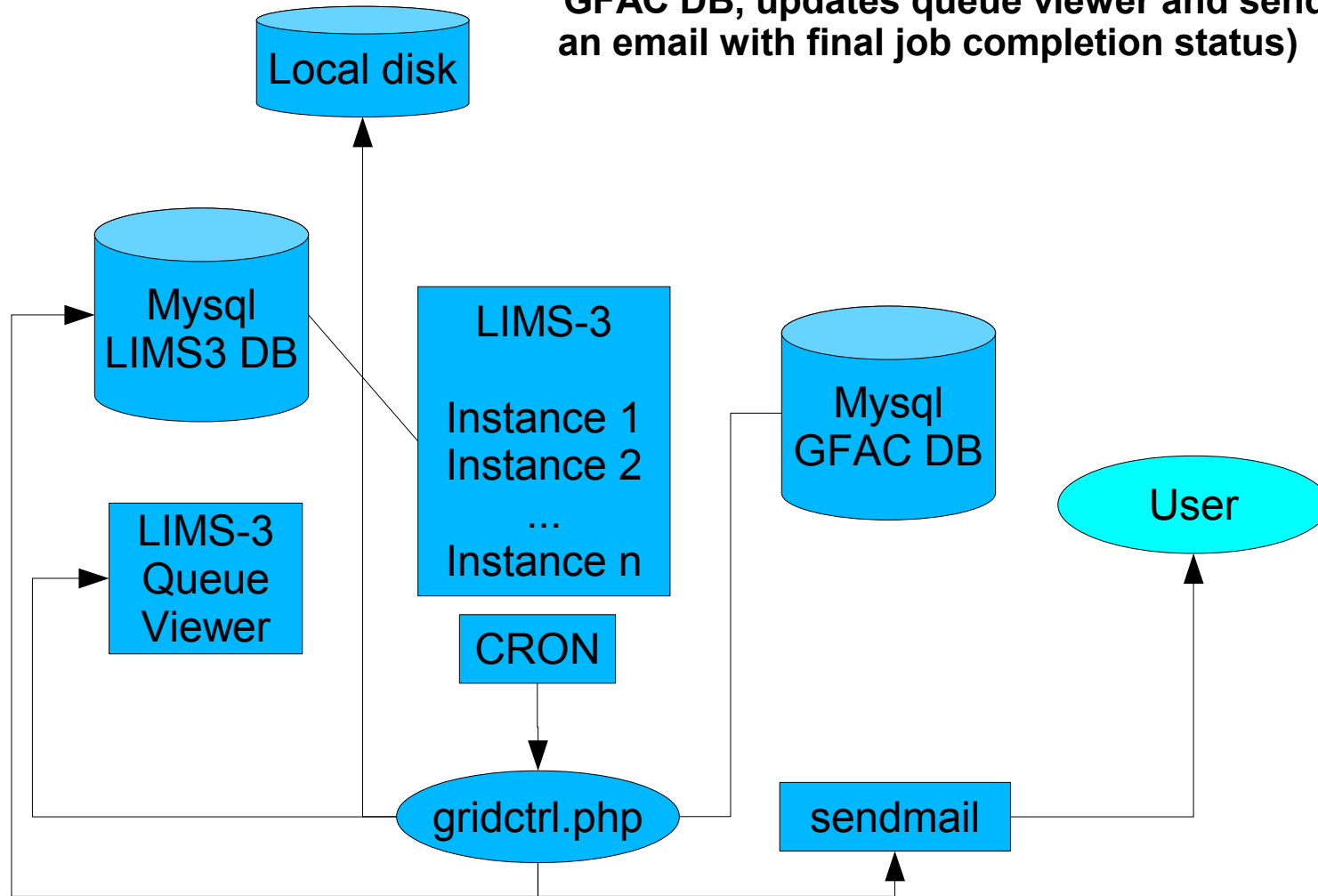


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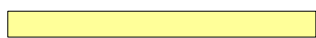


	- UTHSCSA
	- Indiana University
	- remote user
	- HPC resources

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)

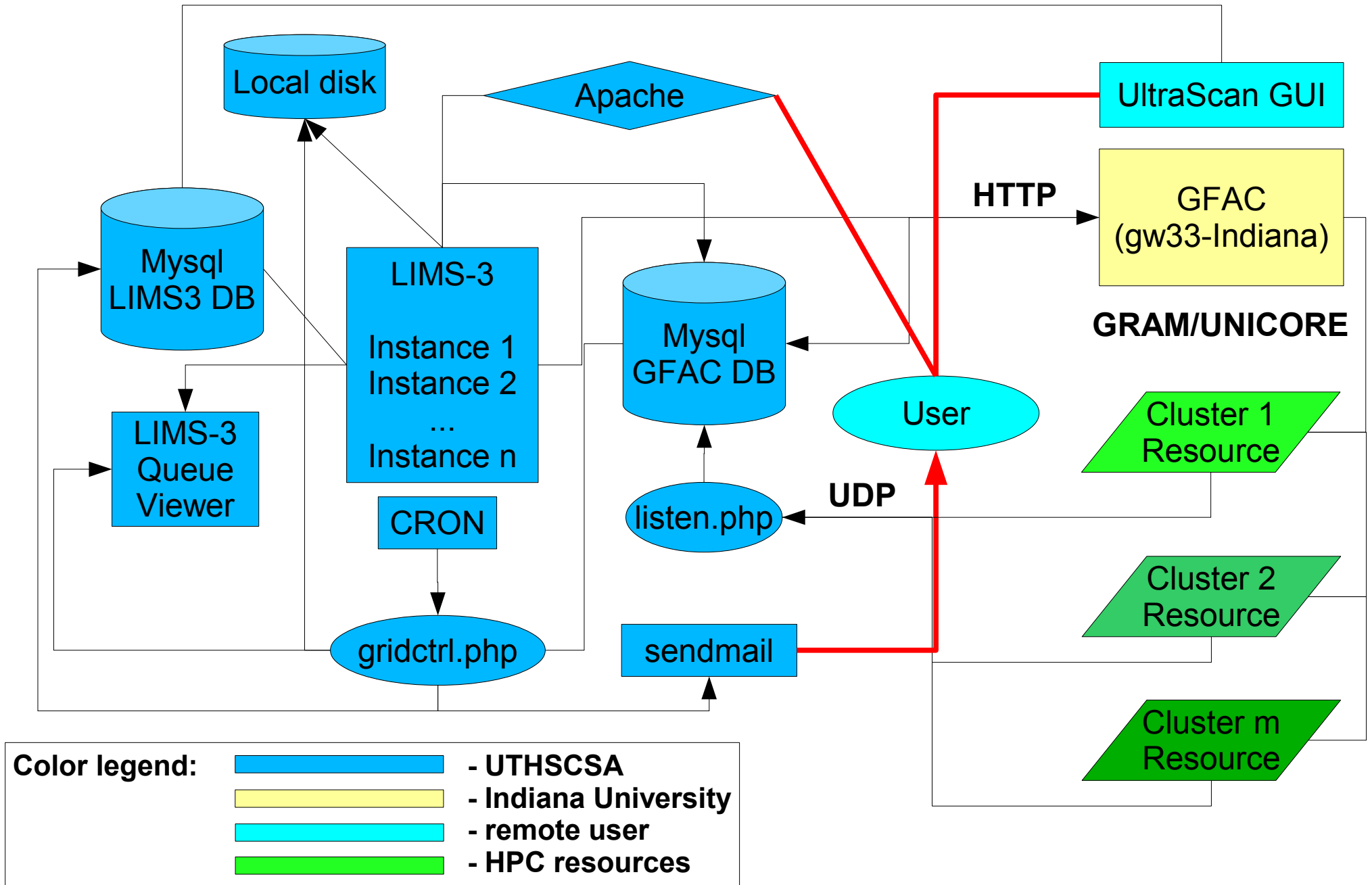


Color legend:

-  - UTHSCSA
-  - Indiana University
-  - remote user
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UltraScan LIMS3/GFAC Workflow Overview

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



A Science Gateway for Biophysical Analysis

Current usage statistics (in SUs) for the period of January-November 2012:

Alamo (UTHSCSA)	BCF (UTHSCSA)	Ranger (TACC)	Lonestar (TACC)	Trestles (SDSC)	Total SUs	Number of Investigators
438,471	14,951	696,807	337,902	4,487	1,492,618	98

- There are over 40 institutions in 10 countries actively using UltraScan/LIMS
- Implemented currently on 5 HPC platforms, including one commercial installation (non-public)

Ongoing Projects:

- Integration of SAXS/SANS modeling
- Integration of Light Scattering modules
- Integration of Molecular Dynamics (DMD)
- Integration of Jülich Supercomputing Center (Germany)
- Integration of Multi-wavelength optics (500-1000 fold higher data density)

In the planning stage:

- Integration of CFA data acquisition

Links:

UltraScan:

<http://www.ultrascan.uthscsa.edu>

XSEDE Science Gateway:

<https://portal.xsede.org/science-gateways>

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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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Below is a complete list of current science gateways, to see a detailed project description please click on the name of the science gateway.

To update the information contained in this table, please contact help@xsede.org. To register your gateway, please complete the [Gateway Registration Form](#).

Search:

TITLE	FIELD OF SCIENCE	PORTAL HOMEPAGE
Massive Pulsar Surveys using the Arecibo L-band Feed Array (ALFA)	Astronomical Sciences	Visit Portal
Center for Multiscale Modeling of Atmospheric Processes	Atmospheric Sciences	Visit Portal
Community Climate System Model (CCSM) TeraGrid Gateway	Atmospheric Sciences	Visit Portal
Biodrugscore: A portal for customized scoring and ranking of molecules docked to the human proteome	Biochemistry and Molecular Structure and Function	Visit Portal
Chemical Informatics and Cyberinfrastructure Collaboratory	Biochemistry and Molecular Structure and Function	Visit Portal
High-Resolution Modeling of Hydrodynamic Experiments with UltraScan	Biophysics	Visit Portal
Computational Chemistry Grid (GridChem)	Chemistry	Visit Portal
Science Gateway for Diffraction Facilities, Data and Methods	Chemistry	Visit Portal
User-Friendly Security Solutions for Grid Environments	Communications and Computational Systems	Visit Portal
Cyberinfrastructure for End-to-End Environmental Exploration Portal	Earth Sciences	Visit Portal

A copy of this presentation:

<http://www.demeler.uthscsa.edu/SciSoft2012/Presentation-121712.pdf>

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