
# Apache Airavata: Enabling Science with Science Gateways

Marlon Pierce, Suresh Marru and Collaborators

SC15, Austin TX

sgg@iu.edu

SciGaP

# Science Gateways: User Interfaces to Supercomputers

## Apache Airavata: Services that Enable Science Gateways to Work

sgg@iu.edu

SciGaP

UltraScan

# Analytical Ultracentrifugation Data Analysis

Borries Demeler

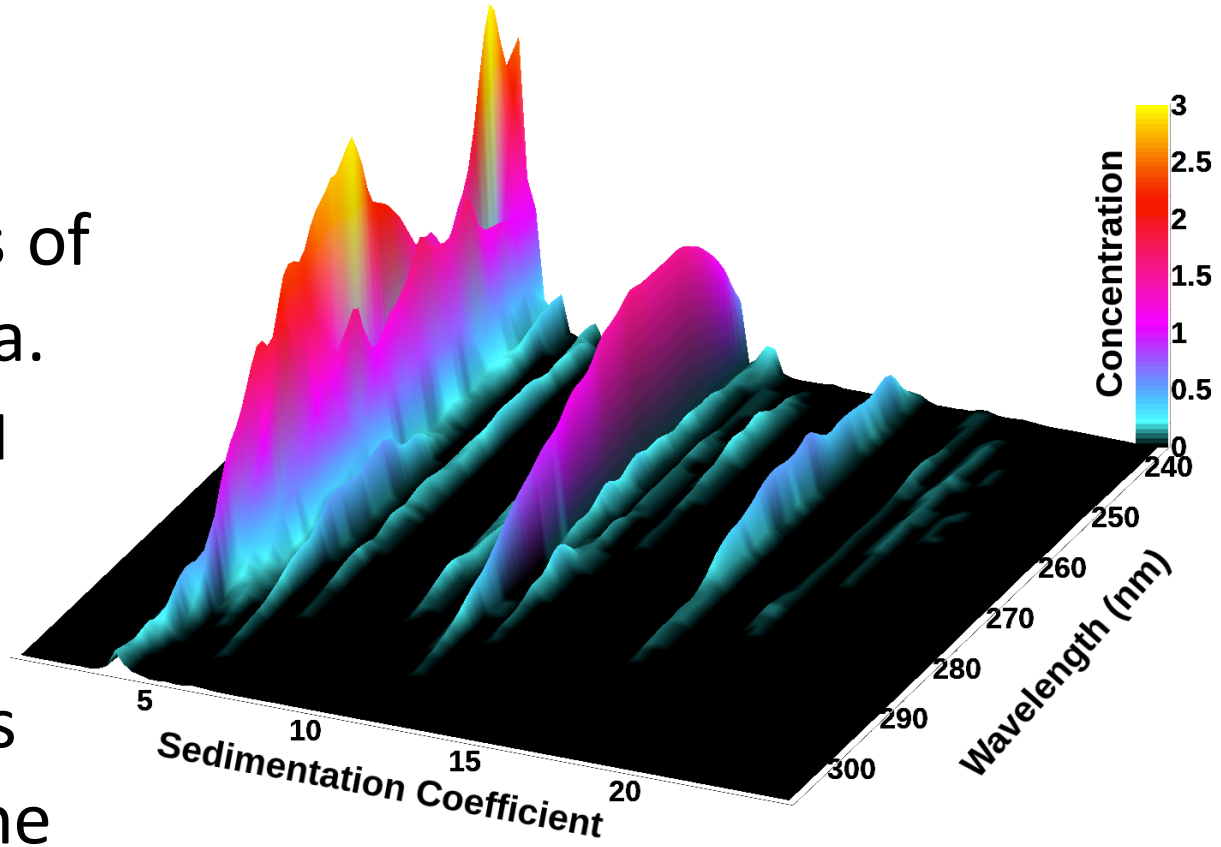
University of Texas Health Science Center, San Antonio

sgg@iu.edu

SciGaP

# Revolution in Ultracentrifugation

- New multi-wavelength instruments producing 100's of times more data.
  - Unprecedented accuracy
  - New science
- Supercomputers needed to do the analysis.

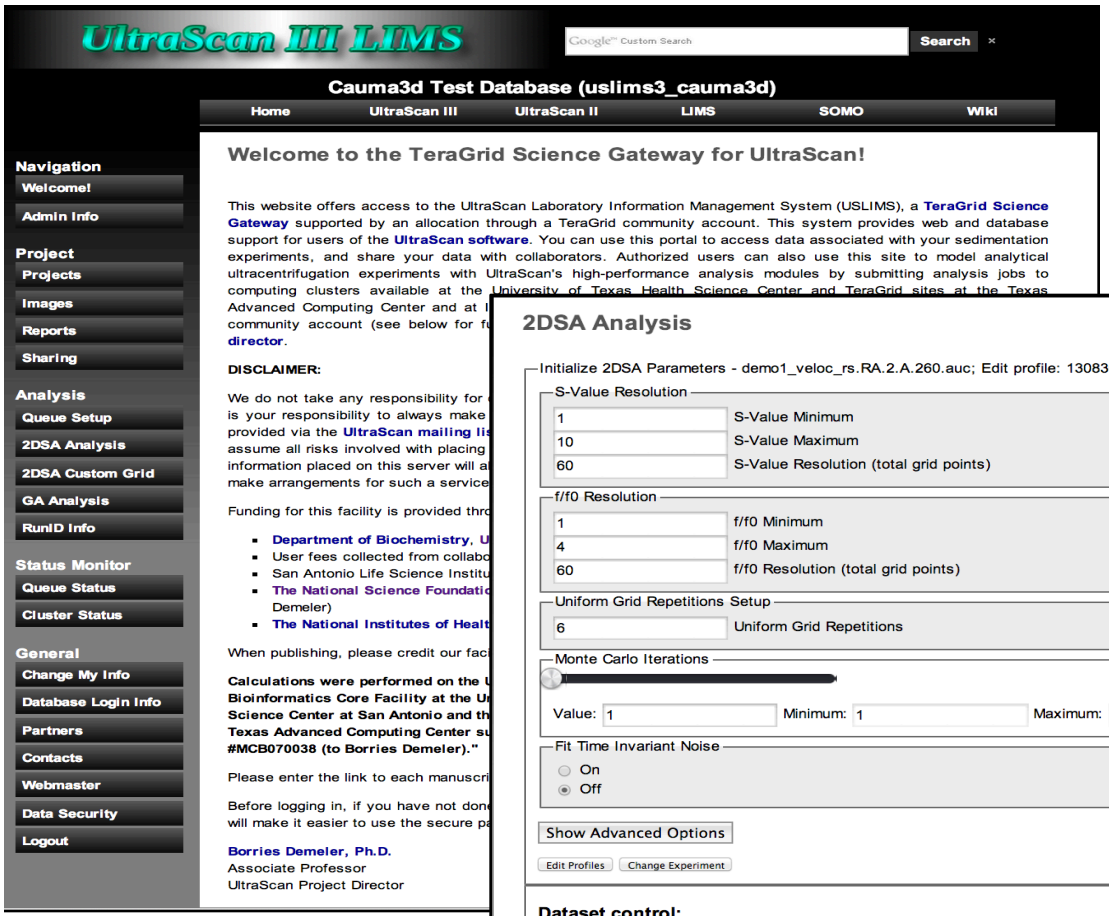


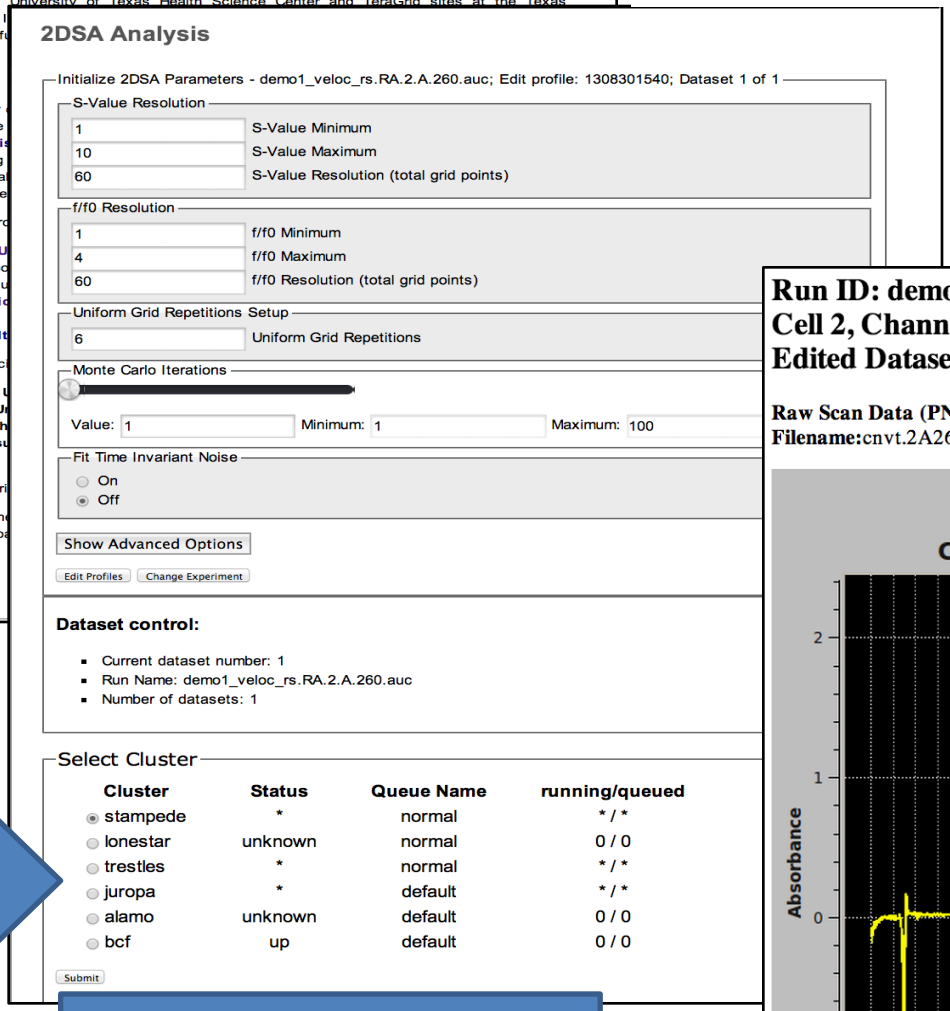

sgg@iu.edu

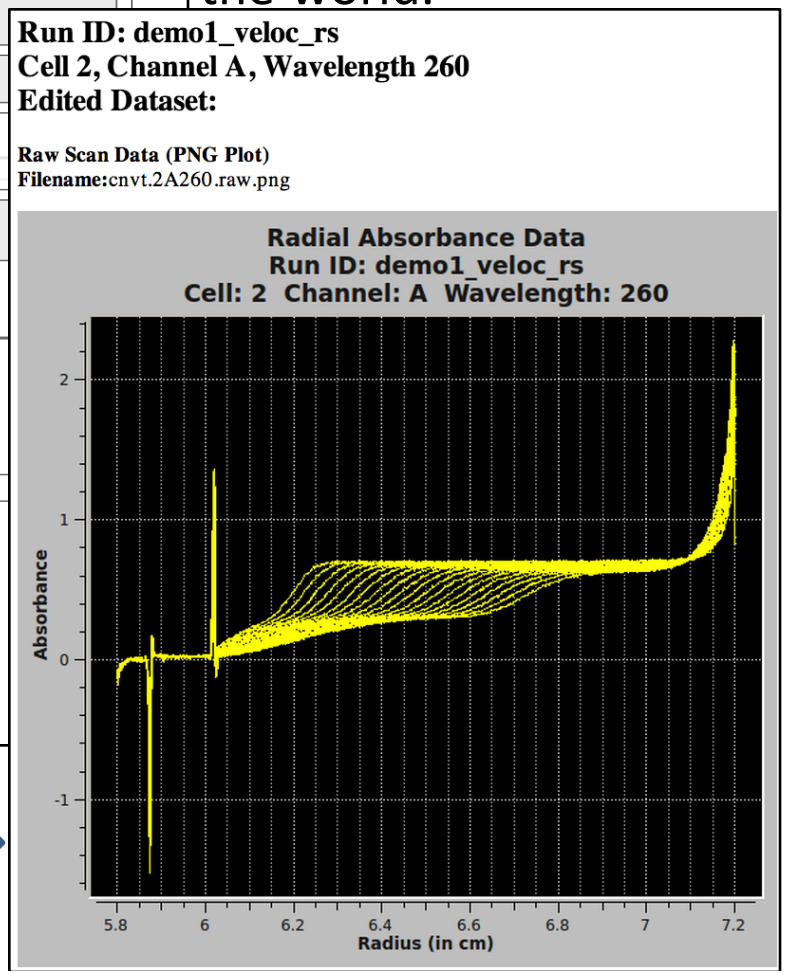
SciGaP

The UltraScan science gateway enables experimental scientists to their analyze data on supercomputers.

UltraScan uses Apache Airavata for managing analyses on HPCs across the world.

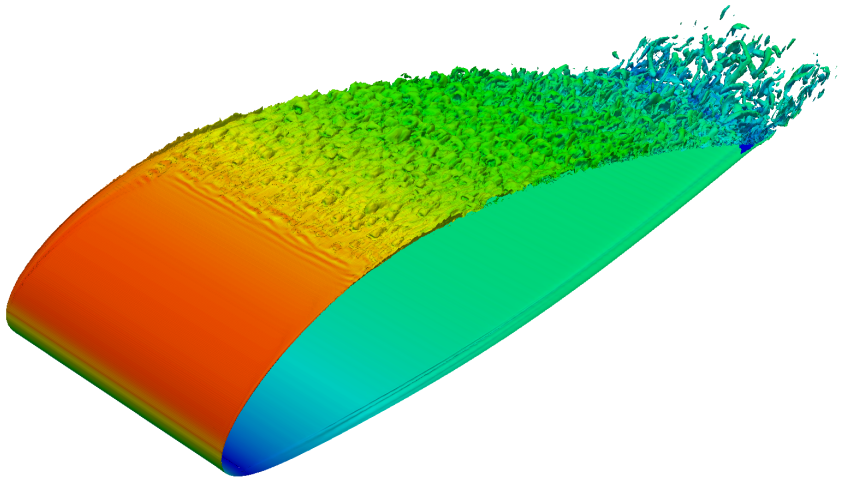



Launch analysis and monitor through a browser

Desktop analysis tools are integrated with the Web portal.



# Large Eddy Simulations of Turbulent Flow

Cameron Smith, Steve Tran, and Onkar Sahni

Rensselaer Polytechnic Institute

sgg@iu.edu

SciGaP

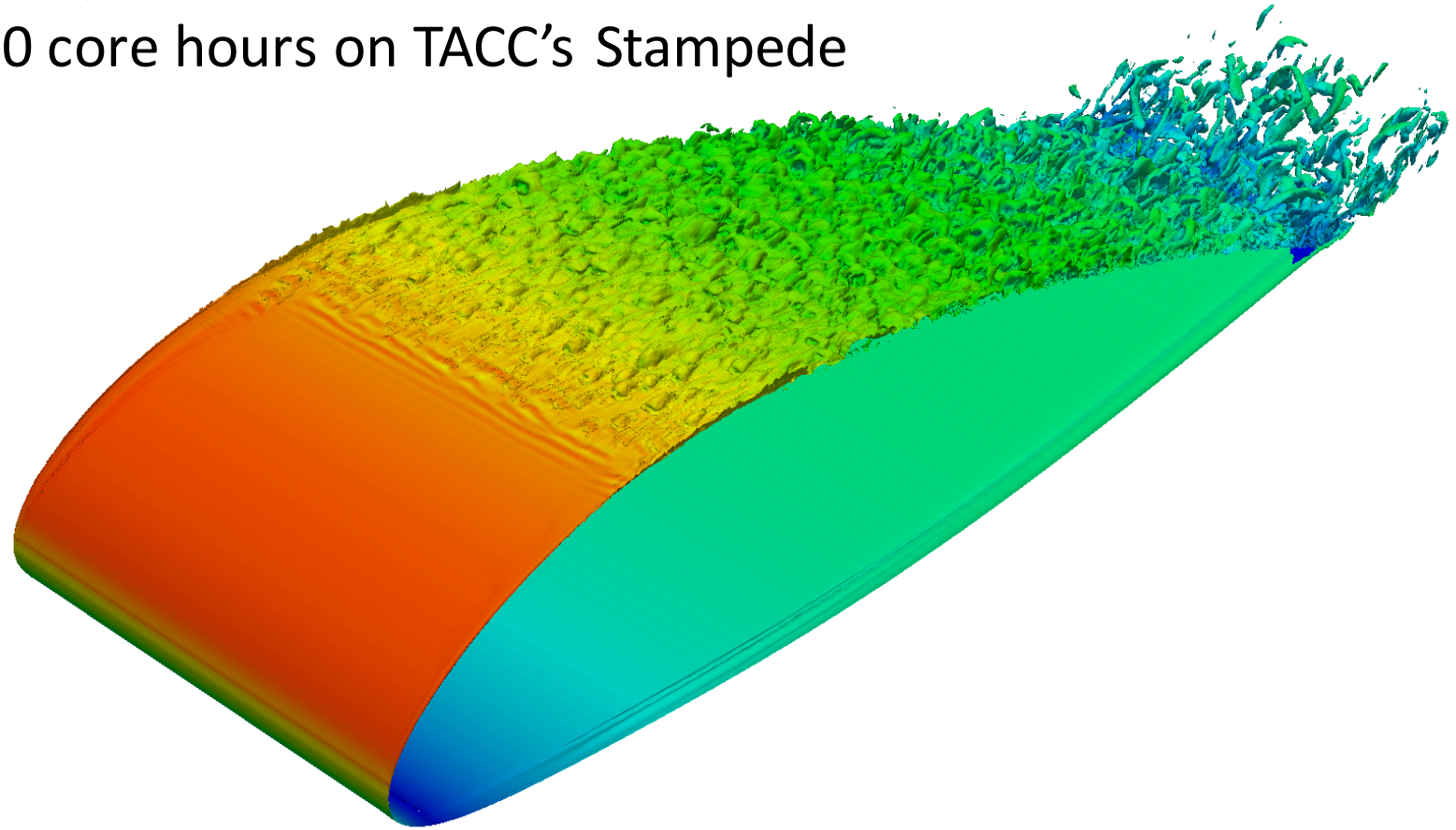
# Science Use Case: PHASTA

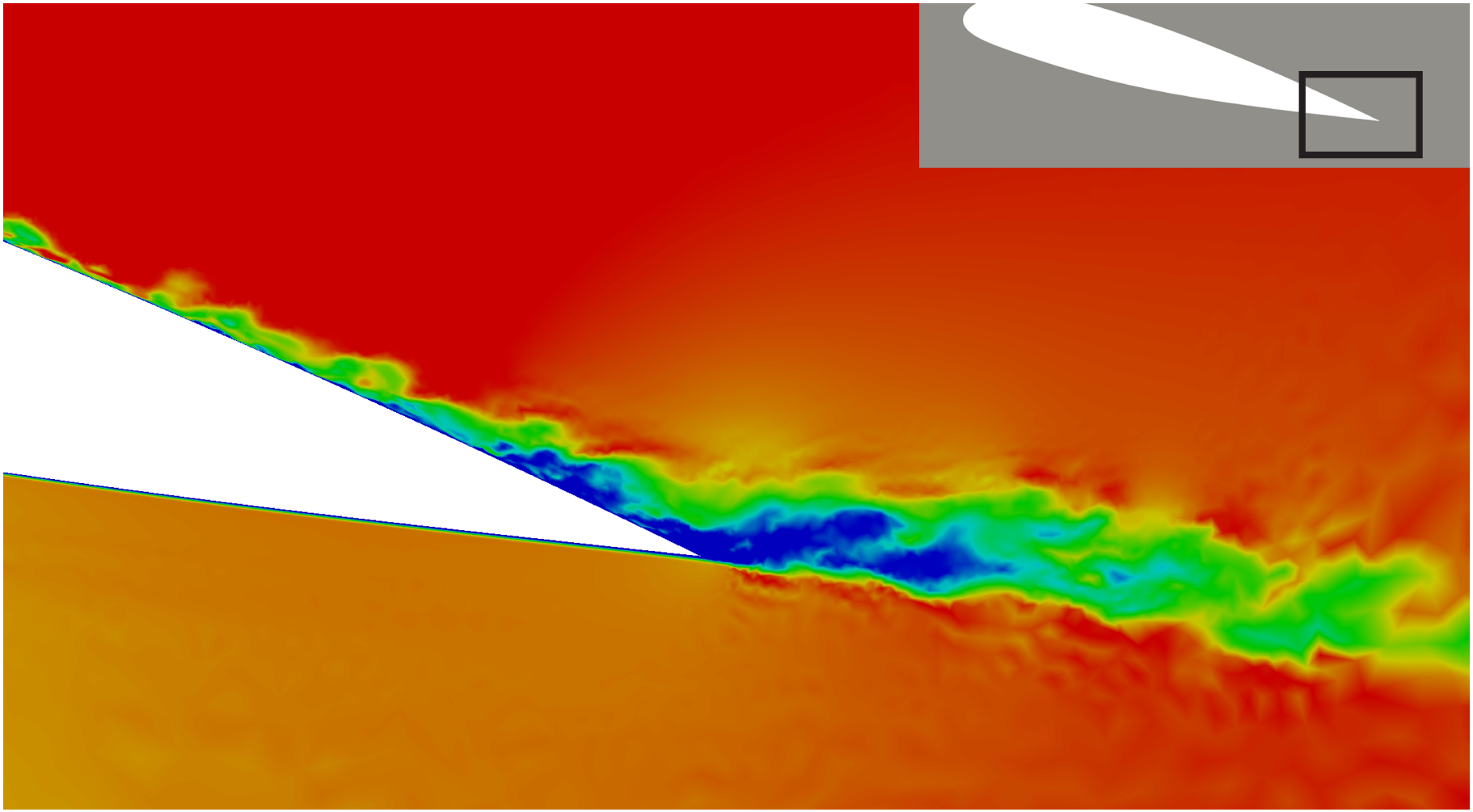
- One of the challenges in studying turbulent flows is the multiscale nature of turbulence.
  - Direct Numerical Simulation (DNS) resolves turbulent flow structures up to dissipation scale, but is not practical with current HPC resources on engineering problems of interest.
- Large Eddy Simulation (LES) is a powerful tool which is capable of accurately resolving and modeling turbulence at a reasonable cost.
  - LES resolves those flow features that can be captured by the numerical discretization/grid while modeling their interactions with the unresolved (subgrid scale) flow features.
  - To account for inhomogeneous flows, Lagrangian-averaged dynamic Smagorinsky model is employed in stabilized finite element simulation.
- Example case: Flow over Aerospatiale-A airfoil
  - Static angle of attack 13°, Reynolds number 2,000,000
  - Flow transitions to a turbulent flow and exhibits marginal flow separation near the trailing edge

sgg@iu.edu

SciGaP

- Direct Numerical Simulation (DNS) not practical for many engineering problems.
- Large Eddy Simulation (LES) models turbulence at a reasonable cost.
  - Lagrangian-averaged dynamic Smagorinsky model
- Example: flow over Aerospatiale-A airfoil
  - Static angle of attack: 13°; Reynolds number: 2,000,000
  - 75,000 core hours on TACC's Stampede





sgg@iu.edu

SciGaP


PHASTA team uses Apache Airavata and the PGA to run simulations on TACC's Stampede.

## Experiment Summary

| | |
|---|---|
| **Experiment Id** | Phast-Exp-Stampede_4e07a9e1-31a2-4210-b3b6-d32bd48cf498 |
| **Name** | Phast-Exp-Stampede |
| **Description** | Phasta exp running on Stampede |
| **Project** | November/12/2015 |
| **Application** | Phasta_P |
| **Compute resource** | stampede.tacc.xsede.org |
| **Experiment Status** | COMPLETED |
| **Job Status** | COMPLETE |
| **Creation time** | 2015-11-12, 12:43 PM - GMT-0500 (EST) |
| **Last Modified Time** | 2015-11-12, 12:44 PM - GMT-0500 (EST) |
| **Enable Auto Schedule** | false |
| **Wall time** | 30 |
| **CPU count** | 16 |
| **Node count** | 1 |
| **Queue** | normal |
| **Inputs** | geom.xmt_txt<br>geom.smd<br>geom.sms<br>solver.inp |
| **Outputs** | Phasta-Output-TAR : PHASTA_Output.tar.gz<br>Phasta-Standard-Error : Phasta_P.stderr<br>Phasta-Standard-Out : Phasta_P.stdout |

Clone

Apache Airavata manages multi-stepped workflow, multiple code versions.

# Science Gateways for Small Angle Scattering

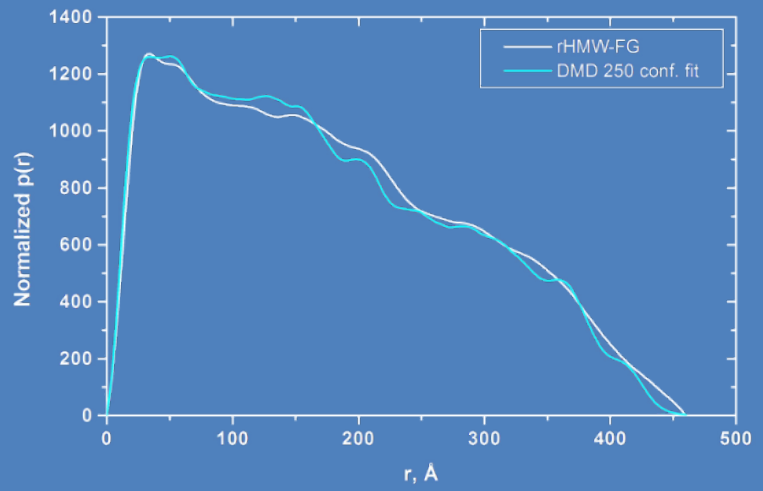
Prof. Emre Brookes, University of Texas Health Science Center, San Antonio

sgg@iu.edu

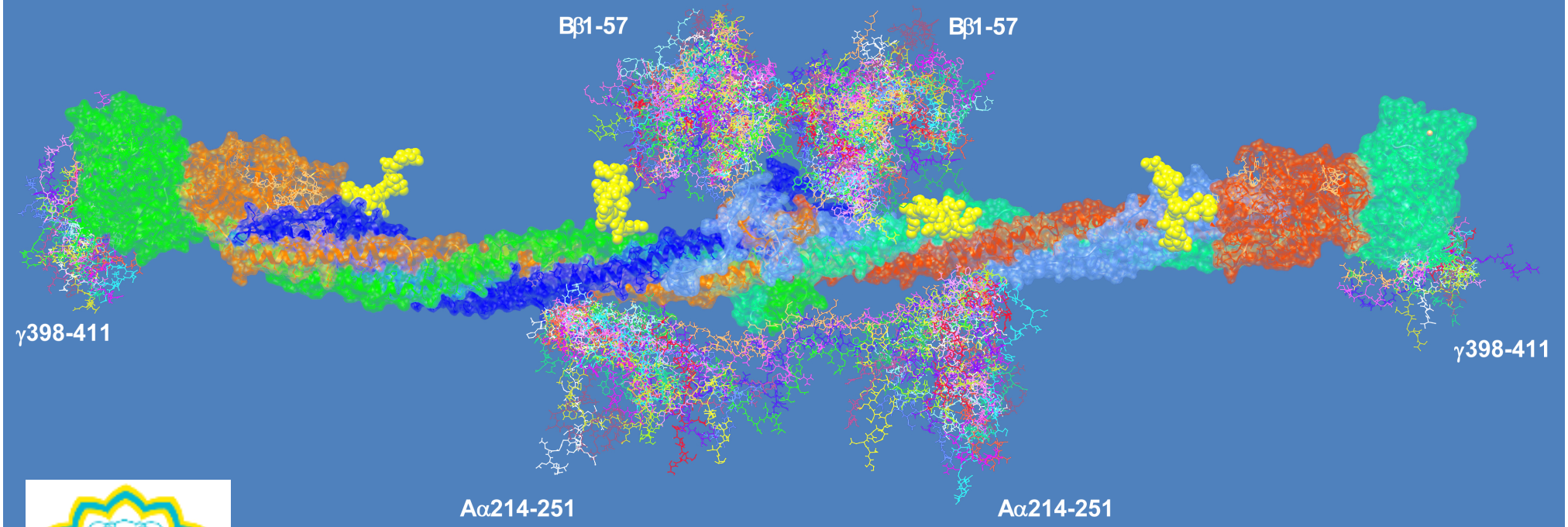
SciGaP

# Conformational variability / Fibrinogen

- Fibrinogen is an important component of the coagulation cascade, as well as a major determinant of blood viscosity and blood flow
- A centrosymmetric dimer made by 3 pairs of chains
- US-SOMO/DMD simulations of the conformational variability for comparison to experimental data

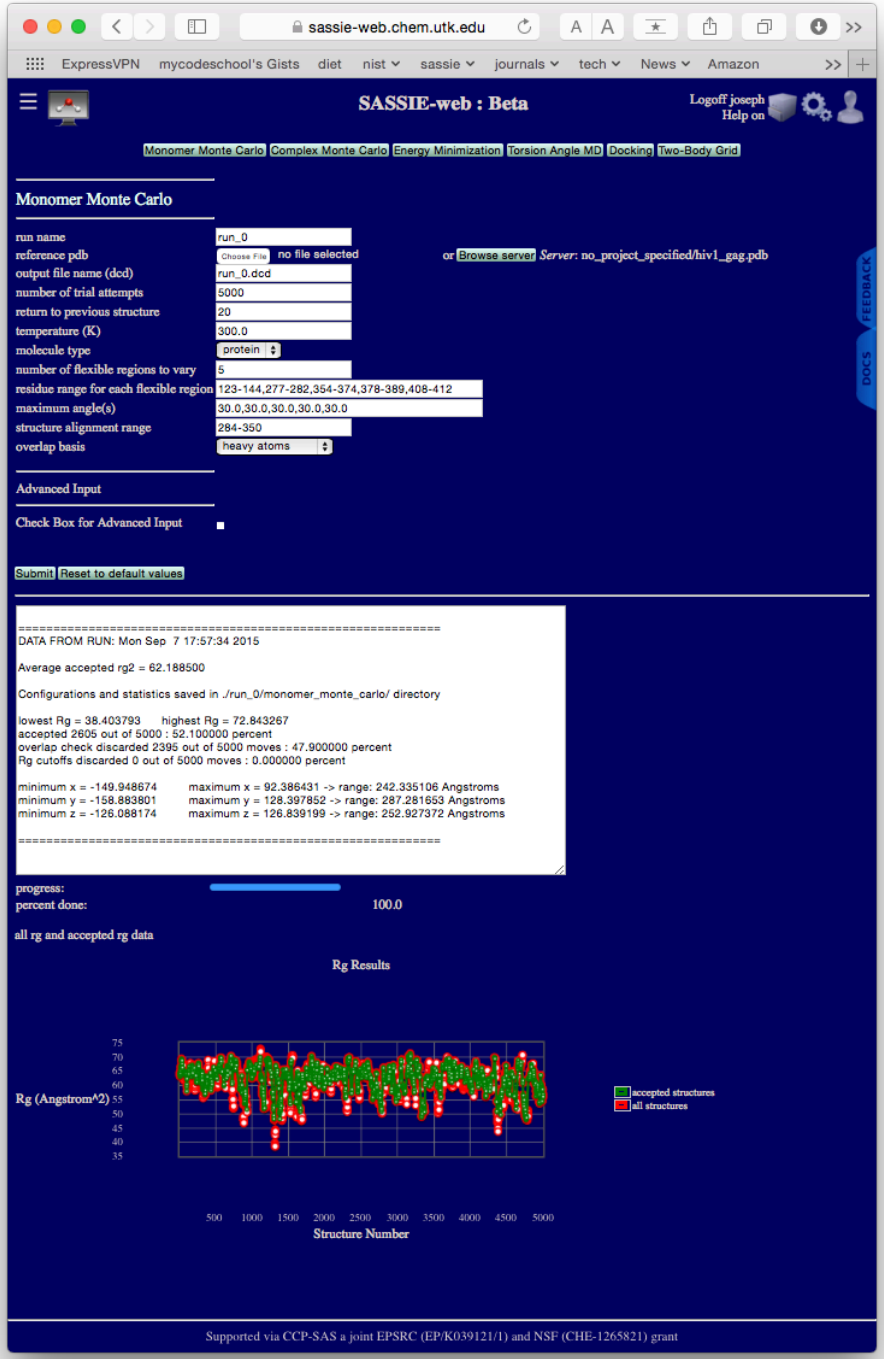


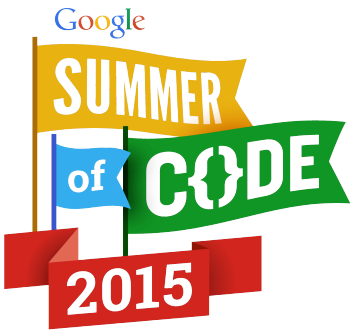

Images credit: Mattia Rocco

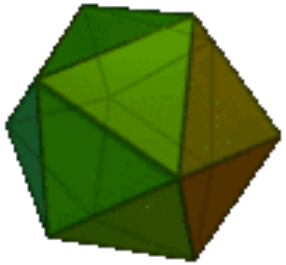



sgg@iu.edu

- GenApp generates user interfaces for the wide range of small angle scattering codes.
  - Python, Tcl/Tk, HTML5, Java
  - QT, Web Apps, iOS, Android
- GenApp uses Apache Airavata's Thrift APIs to manage workflows on HPC resources.
- Code: http://genapp.rocks
- Example:
  - https://sassie-web.chem.utk.edu/sassie2/



sgg@iu.edu

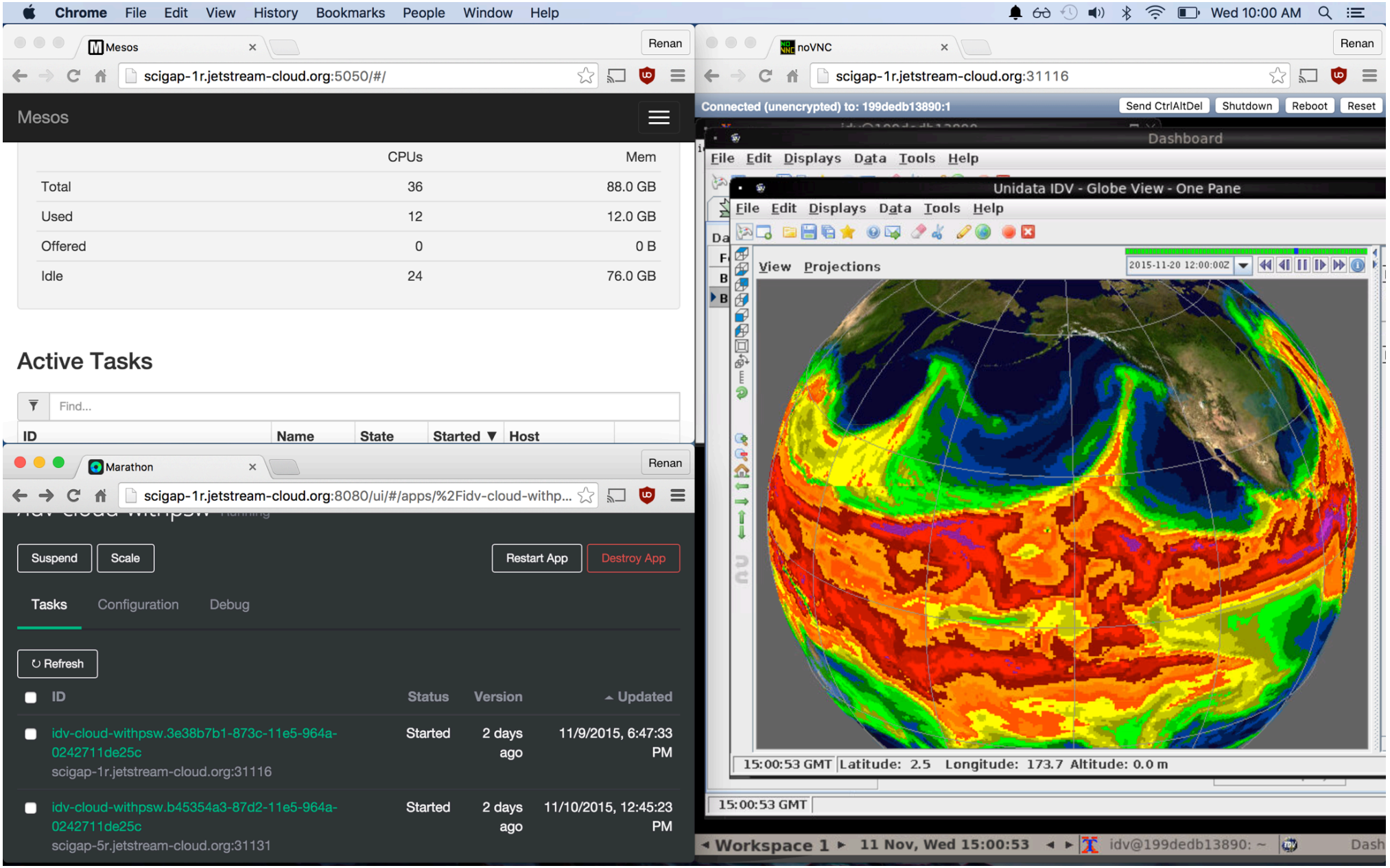
# Science Gateways and Cloud Research on Jetstream

Prof. Madhusudhan Govindaraju

State University of New York
Binghamton

sgg@iu.edu

SciGaP




sgg@iu.edu

SciGaP

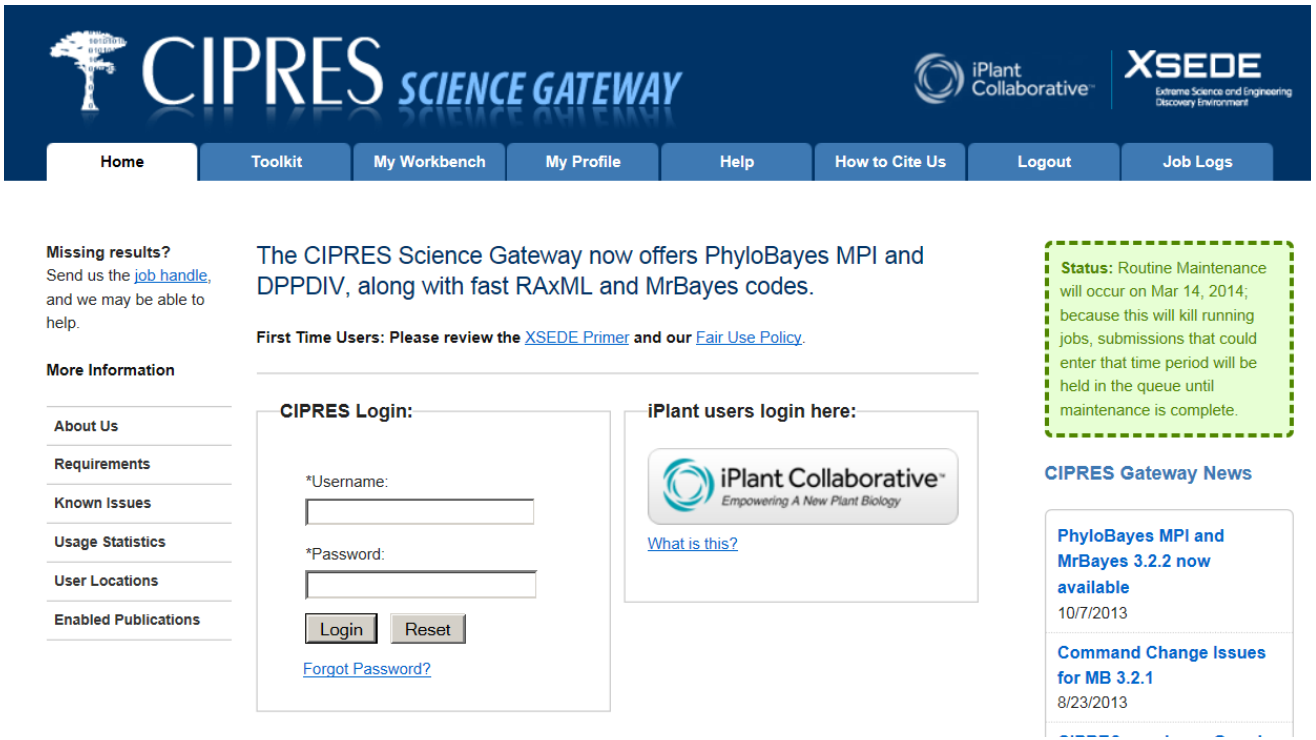
# Science Gateway Platform as a Service

Mark Miller, Amit Majumdar

San Diego Supercomputer Center

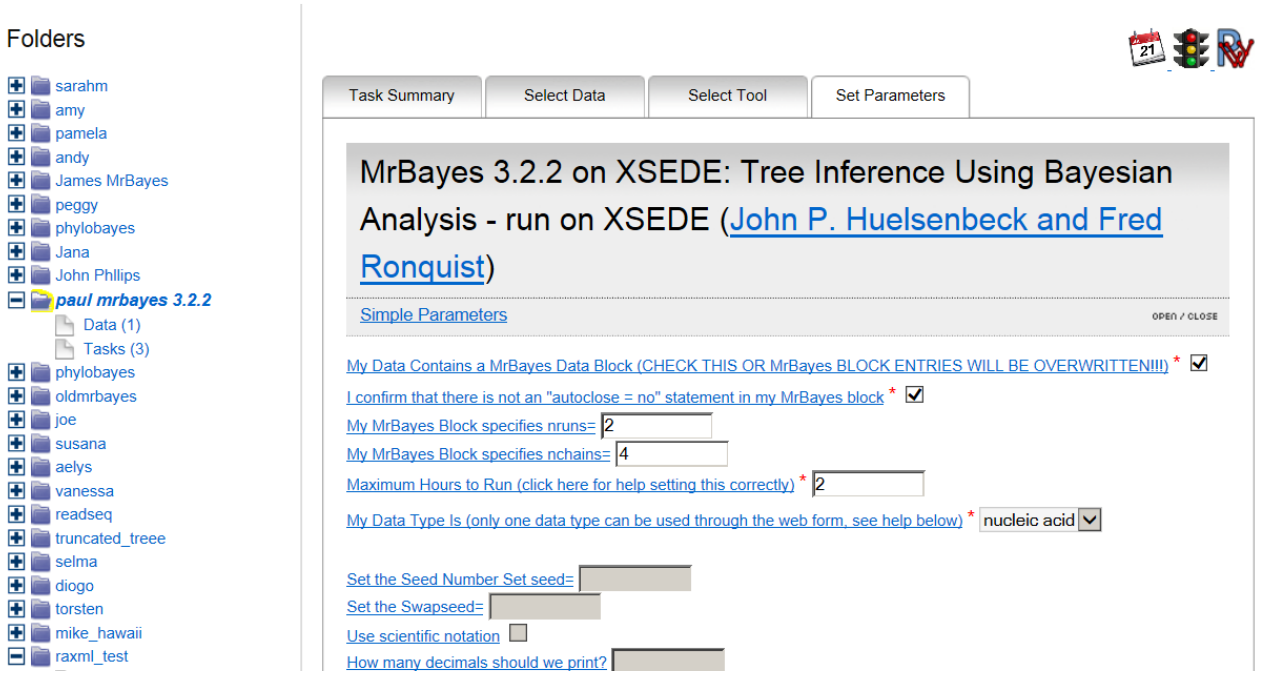
sgg@iu.edu

SciGaP




**The CIPRES Gateway has allowed 14500+ users to Access 101 million core hours of XSEDE time for 550,000 jobs, resulting in 1800+ publications.**

**Simplified access to phylogenetics codes on powerful XSEDE resources**



# NSG NEUROSCIENCE GATEWAY
A Portal for Computational Neuroscience

Amit Majumdar (PI), Maryann Martone (Co-PI), Subha Sivagnanm (Sr. Personnel)
Kenneth Yoshimoto (Sr. Personnel), Anita Bandrowski (Sr. Personnel), Vadim Astakhov UCSD
Ted Carnevale (PI), Yale School of Medicine
NSF Awards: ABI #1146949; ABI #1146830

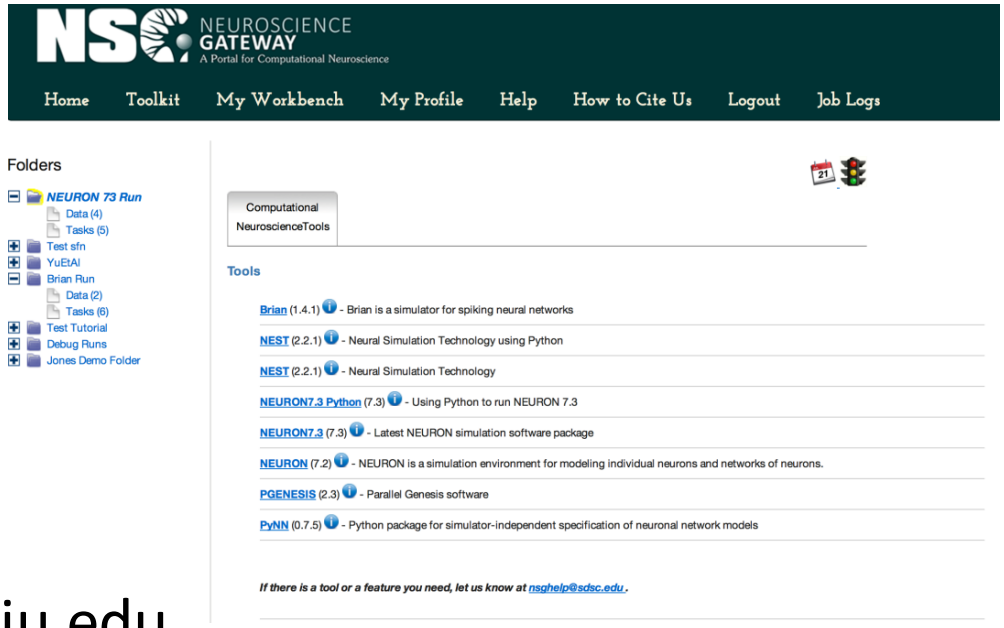
The NSG is a simple and secure online science portal that provides access to computational neuroscience codes on XSEDE HPC resources
http://www.nsgportal.org

Easy user interface – providing easy model upload, running of codes

Complete set of neuronal simulation tools – NEURON, GENESIS, Brian, NEST, PyNN – widely used by computational neuroscientists

Ability to easily get to the results, download results

*Democratize computational neuroscience*




sgg@iu.edu