

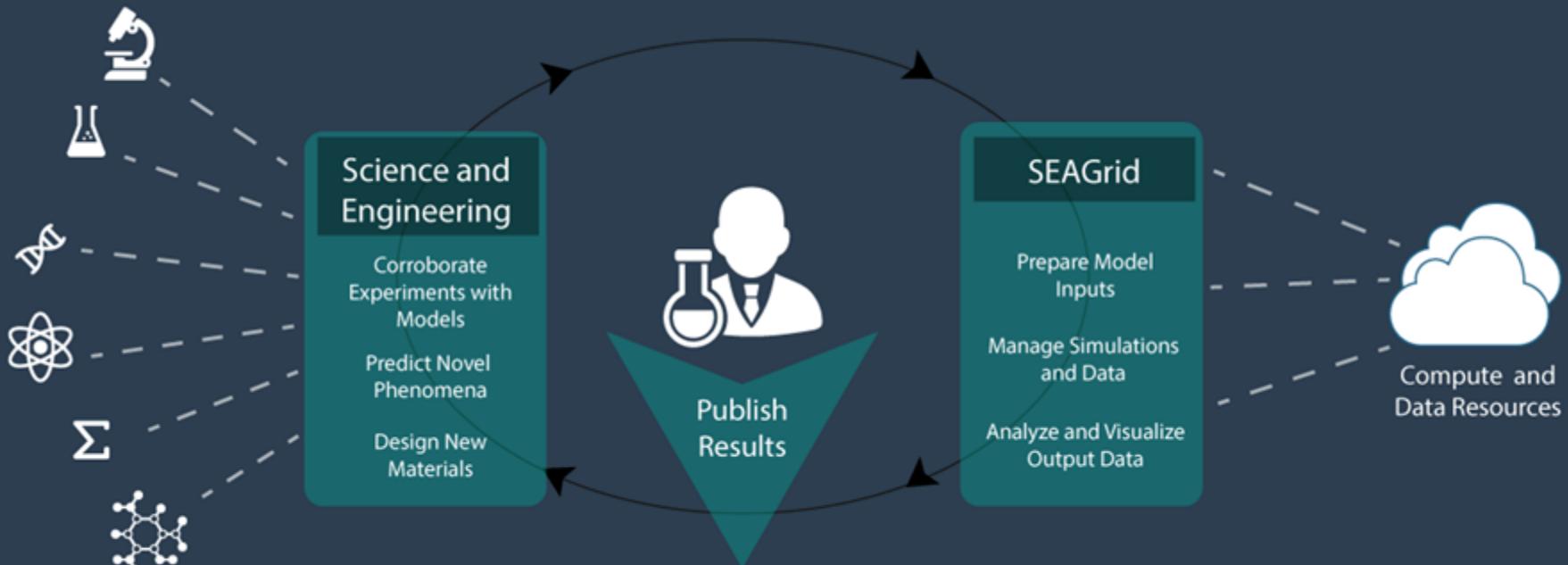


APACHE
AIRAVATA

Apache Airavata: Enabling Science with Science Gateways

Marlon Pierce, Suresh Marru

sgg@iu.edu



SEAGrid.org is an Apache Airavata-powered gateway

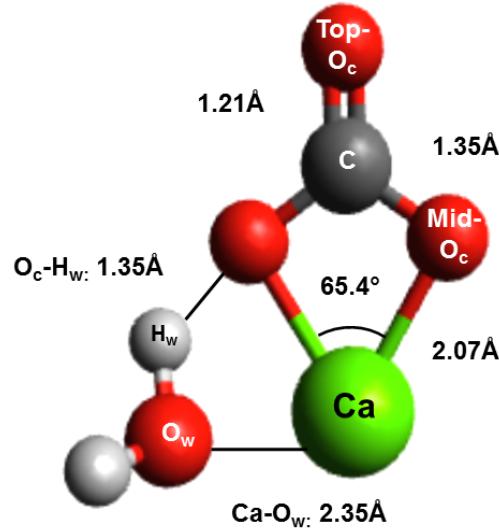
Hydrated Calcium Carbonate in Action



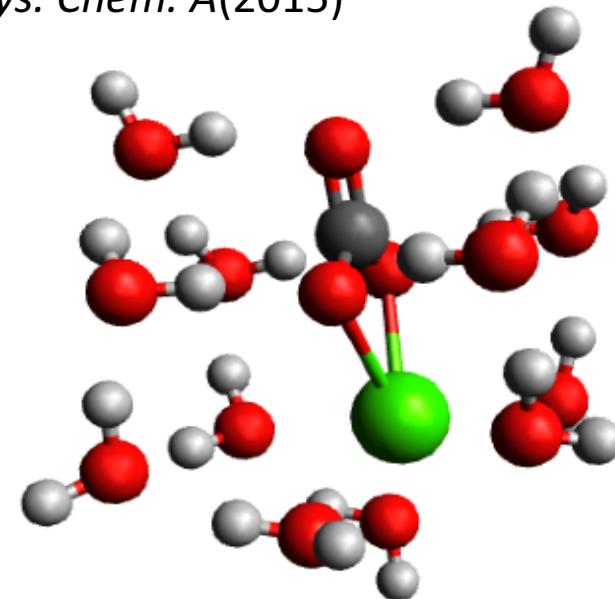
What is the chemistry of hydrated calcium carbonate?

- Bio-mineralization of skeletons and shells
- Geological CO₂ sequestration
- Cleanup of contaminated environments

Lopez-Berganza, et al. *J Phys. Chem. A*(2015)

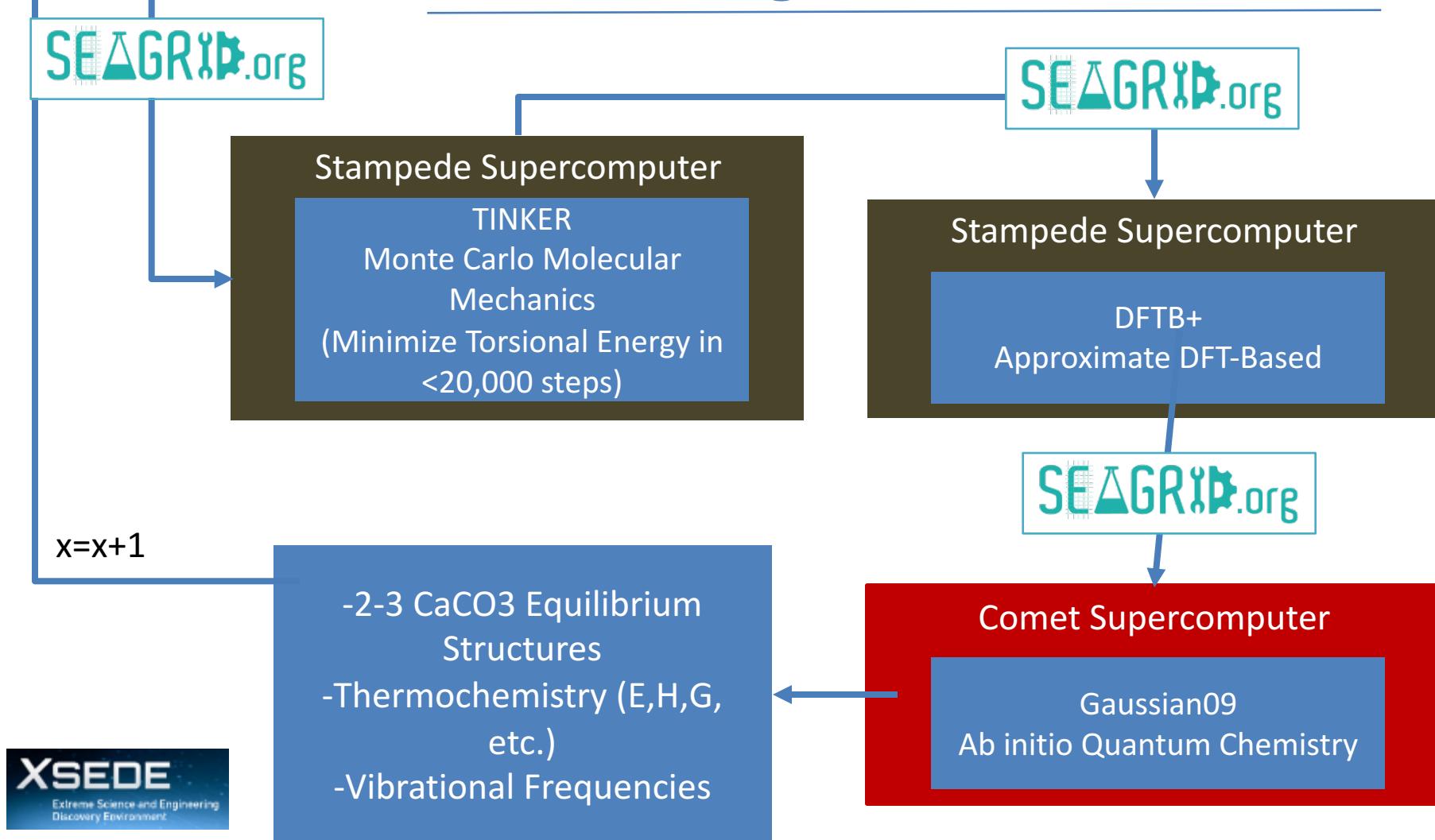


CaCO₃·1H₂O



$\text{CaCO}_3 \cdot x\text{H}_2\text{O}$ Initial
guess

SEAGrid.org enabled workflow



SEAGrid Input Preparation Tools

The image displays four windows from the SEAGrid Input Preparation Tools:

- Molecular Editor:** Shows a 3D molecular model of a complex organic molecule with red and grey spheres representing atoms. A coordinate system (x, y, z) is shown. The menu bar includes "Import Structure", "Atom", "Database", "My Files", "Function-Group", "Ion", "Molecule". A status bar at the bottom shows "Current Element: H".
- Gaussian Input Generator:** A window titled "Gaussian 03 Input GUI". It shows a tree view of "Molecular Specification", "Methods", "Basis Sets", "Job Types", and "Keywords". Under "Basis Sets", "Frequently-used basis sets" is expanded, showing options like STO-3G, 3-21G, 6-21G, etc. A "Job Name" field is set to "default_job".
- CSD Search:** A window titled "CSD Search". It has fields for "Search Text" (set to "norbornane") and "Limit" (set to 5). Below is a table with columns "Formula" and "Chemical Name". The first row is highlighted: Formula "C25 H52 P2 Rh1 1+,C32 H12 B1 F24 1-" and Chemical Name "(Norbornane)-(P,P,P',P'-tetraisobutyl-1,2-diph...".
- Import Structure:** A window showing a dropdown menu with options: "Group", "Geometry", "Forces", "Structure", "CSD", "Indiana Database", "H", "Select", and "Current Element: H". The "CSD" option is currently selected.

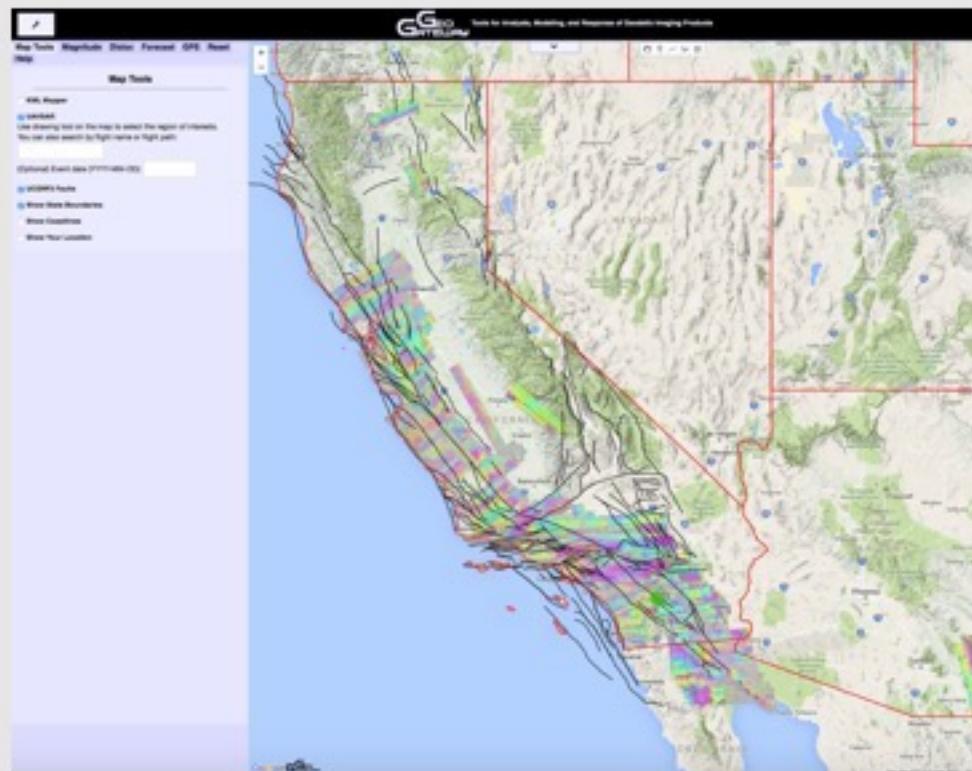


**Dr. Sudhakar Pamidighantam will
give a full lecture on SEAGrid**

Tentatively September 20th

GeoGateway

Data product search and analysis gateway for scientific discovery, field use, and disaster response

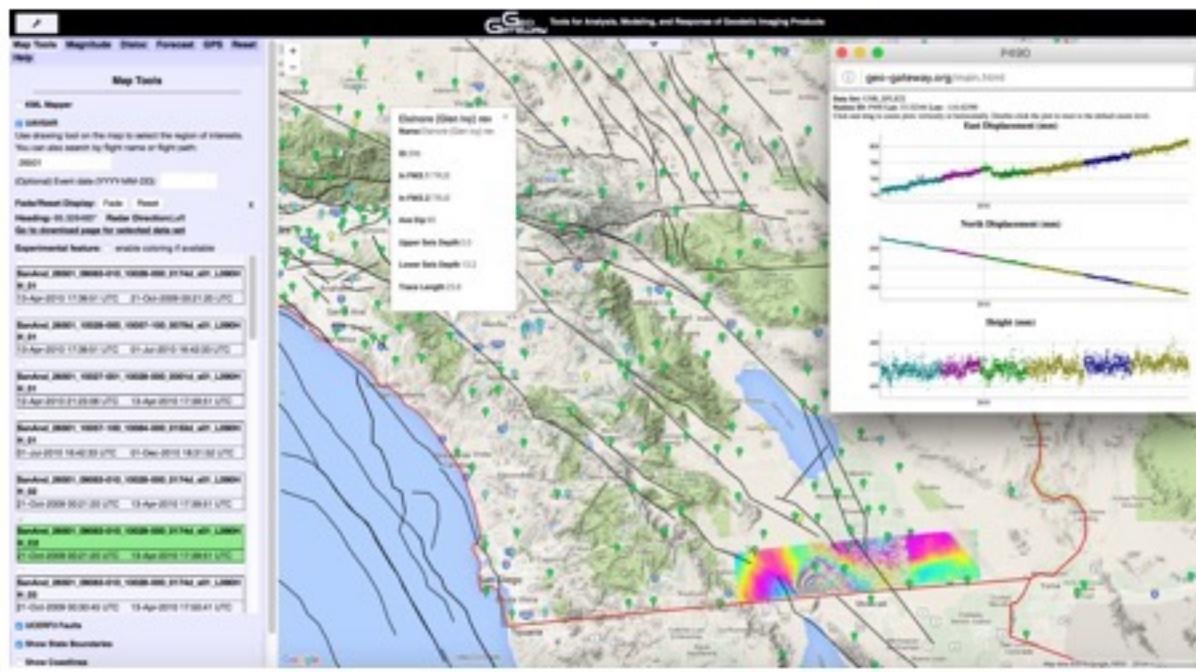


- For studying earthquakes and crustal deformation
- Analysis, modeling, and response of geodetic imaging products
- Web-enabled map-based
 - Useable on computers, tablets, and mobile devices

User Needs

Users require

- Data overlay and visualization
- Interactive analysis features
- Data product download

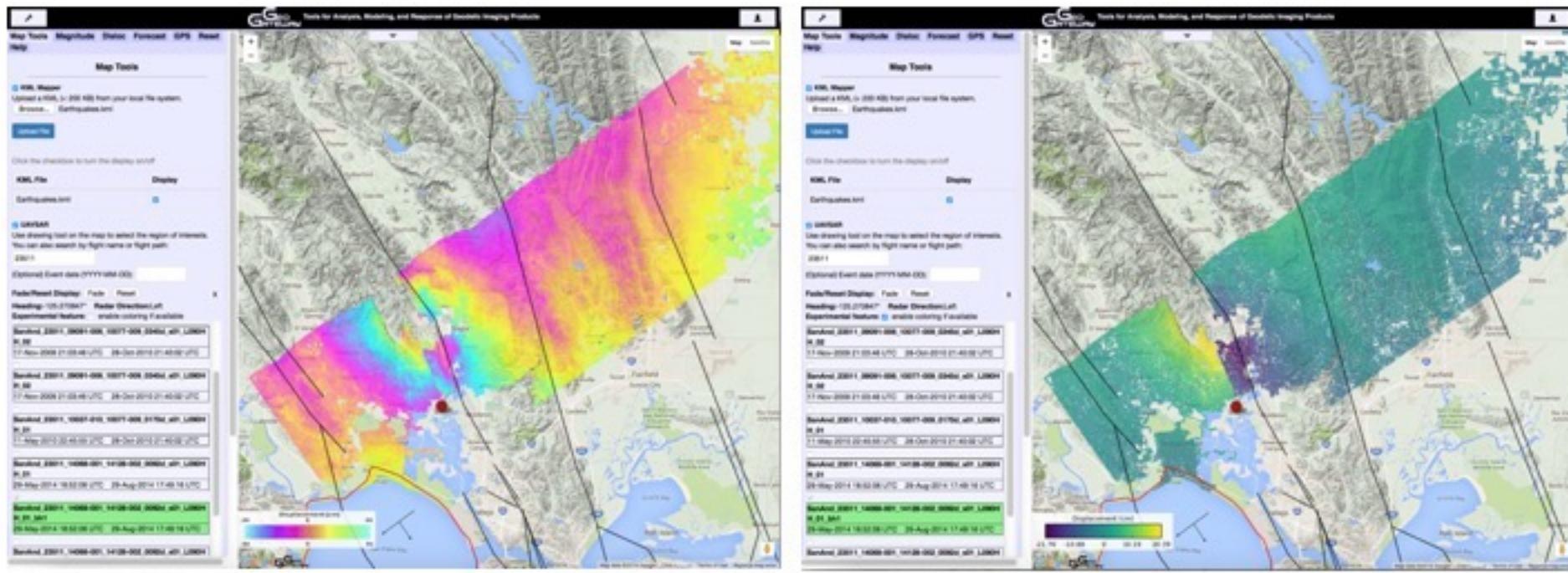


Data products

- NASA's UAVSAR
- Spaceborne interferometric radar (InSAR)
- Geologic earthquake faults
- Global Positioning System (GPS) position time series
- Seismicity
- Topographic imaging

Presentation of UAVSAR Data Products

- Users can view interferograms in their original fringes or using a single range color map
 - Allows for more intuitive interpretation of the data products



2014 M6.0 South Napa Earthquake

Dr. Andrea Donnellan will give a
guest lecture on GeoGateway

September 29th



Analytical Ultracentrifugation Data Analysis

Borries Demeler

University of Texas Health Science
Center, San Antonio

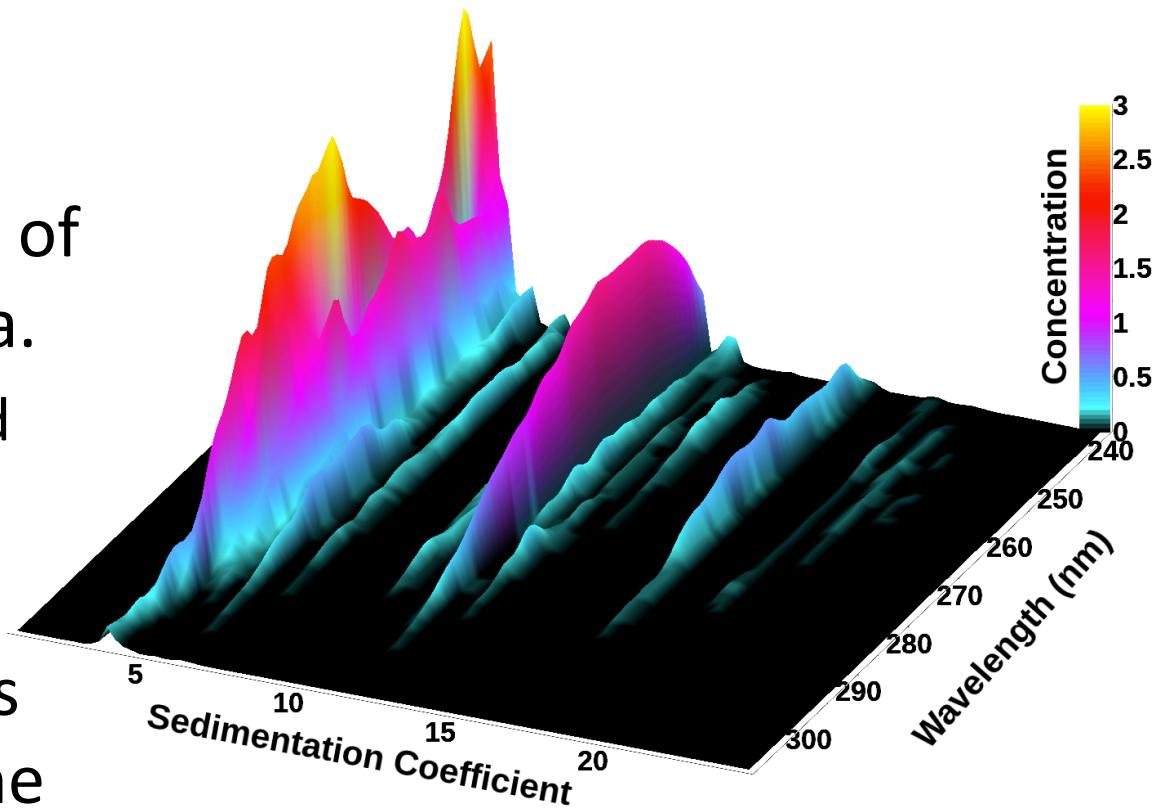
sgg@iu.edu



sgg@iu.edu

Revolution in Ultracentrifugation

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



Cauma3d Test Database (uslims3_cauma3d)

[Home](#) [UltraScan III](#) [UltraScan II](#) [LIMS](#) [SOMO](#) [Wiki](#)

Welcome to the TeraGrid Science Gateway for UltraScan!

This website offers access to the UltraScan Laboratory Information Management System (USLIMS), a [TeraGrid Science Gateway](#) supported by an allocation through a TeraGrid community account. This system provides web and database support for users of the [UltraScan software](#). You can use this portal to access data associated with your sedimentation experiments, and share your data with collaborators. Authorized users can also use this site to model analytical ultracentrifugation experiments with UltraScan's high-performance analysis modules by submitting analysis jobs to computing clusters available at the [University of Texas Health Science Center](#) and [TeraGrid sites at the Texas Advanced Computing Center](#) and at a community account (see below for director).

DISCLAIMER:

We do not take any responsibility for your responsibility to always make provided via the [UltraScan mailing list](#) assume all risks involved with placing information placed on this server will a make arrangements for such a service.

Funding for this facility is provided thru

- [Department of Biochemistry, U](#)
- User fees collected from collabora
- San Antonio Life Science Institu
- [The National Science Foundation](#)
- Demeler)
- [The National Institutes of Health](#)

When publishing, please credit our fac

Calculations were performed on the Bioinformatics Core Facility at the University of Texas Health Science Center at San Antonio and the Texas Advanced Computing Center site #MCB070038 (to Borries Demeler)."

Please enter the link to each manusc

Before logging in, if you have not done so will make it easier to use the secure port

Borries Demeler, Ph.D.
Associate Professor
UltraScan Project Director

Navigation

[Welcome!](#)[Admin Info](#)

Project

[Projects](#)[Images](#)[Reports](#)[Sharing](#)

Analysis

[Queue Setup](#)[2DSA Analysis](#)[2DSA Custom Grid](#)[GA Analysis](#)[RunID Info](#)[Status Monitor](#)[Queue Status](#)[Cluster Status](#)

General

[Change My Info](#)[Database Login Info](#)[Partners](#)[Contacts](#)[Webmaster](#)[Data Security](#)[Logout](#)

Launch analysis and monitor through a browser

2DSA Analysis

Initialize 2DSA Parameters - demo1_veloc_rs.RA.2.A.260.auc; Edit profile: 1308301540; Dataset 1 of 1

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

[Show Advanced Options](#)[Edit Profiles](#) [Change Experiment](#)

Dataset control:

- Current dataset number: 1
- Run Name: demo1_veloc_rs.RA.2.A.260.auc
- Number of datasets: 1

Select Cluster

Cluster	Status	Queue Name	running/queued
<input checked="" type="radio"/> stampede	*	normal	* / *
<input type="radio"/> lonestar	unknown	normal	0 / 0
<input type="radio"/> trestles	*	normal	* / *
<input type="radio"/> juropa	*	default	* / *
<input type="radio"/> alamo	unknown	default	0 / 0
<input type="radio"/> bcf	up	default	0 / 0

[Submit](#)

Desktop analysis tools are integrated with the Web portal.

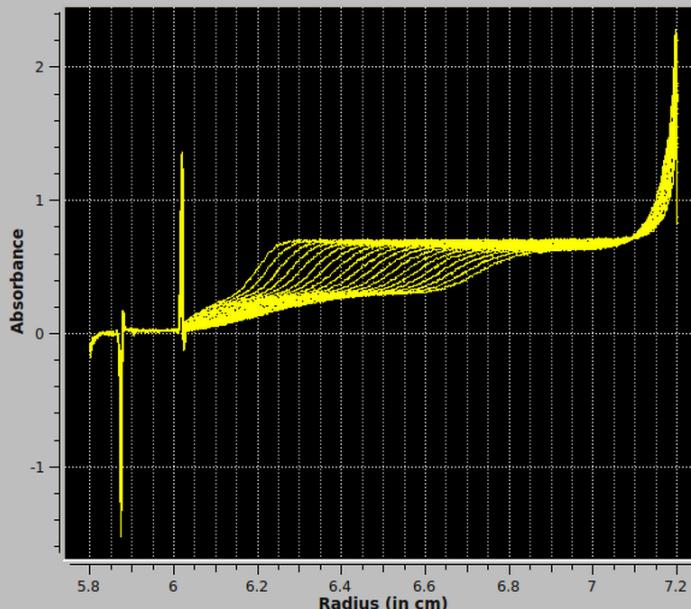
The UltraScan science gateway enables experimental scientists to their analyze data on supercomputers.

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

Run ID: demo1_veloc_rs
Cell 2, Channel A, Wavelength 260
Edited Dataset:

Raw Scan Data (PNG Plot)
Filename:cvt.2A260.raw.png

Radial Absorbance Data
Run ID: demo1_veloc_rs
Cell: 2 Channel: A Wavelength: 260





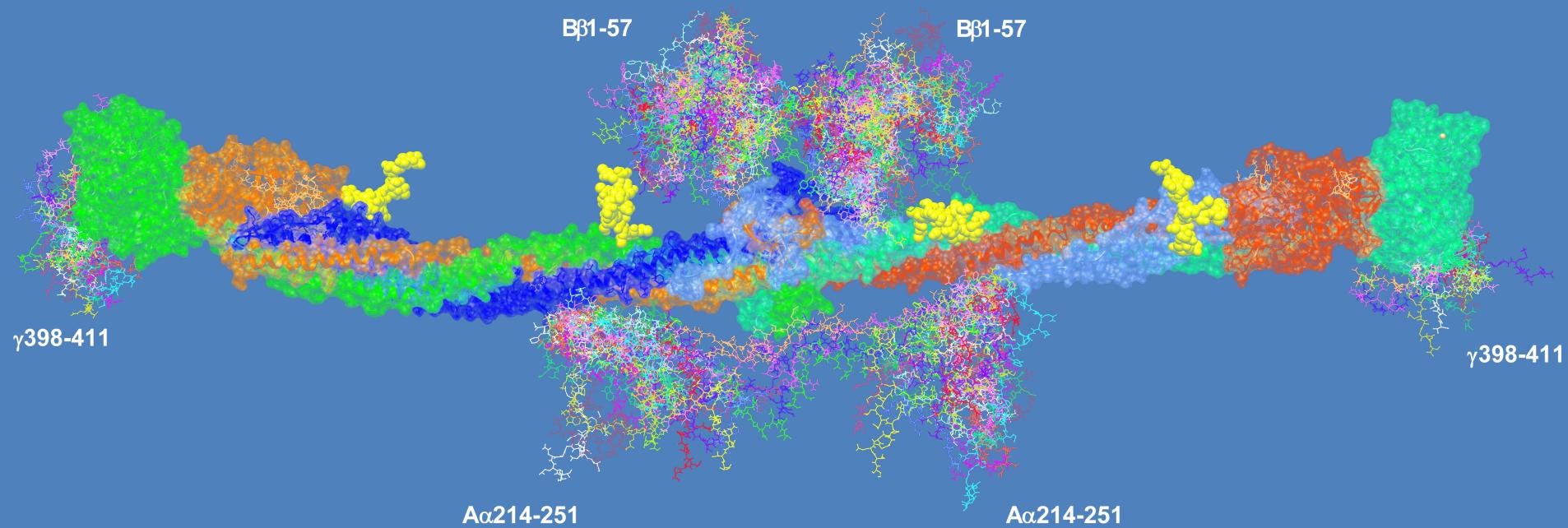
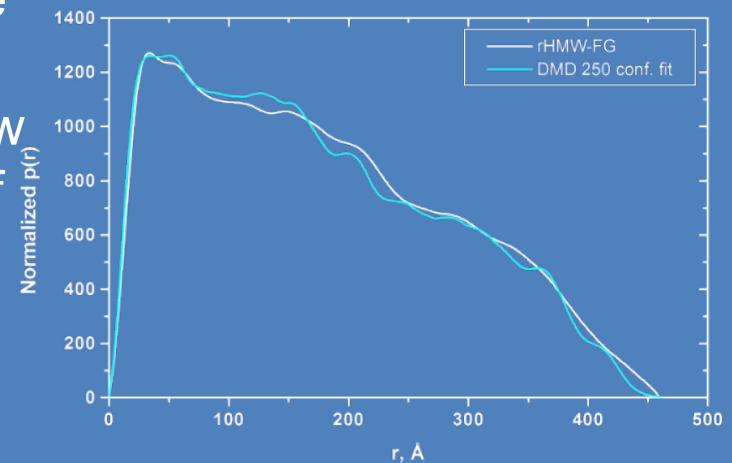
Science Gateways for Small Angle Scattering

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

sgg@iu.edu

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



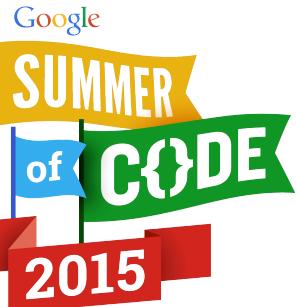
Images credit: Mattia Rocco

Why a US-SOMO Gateway?

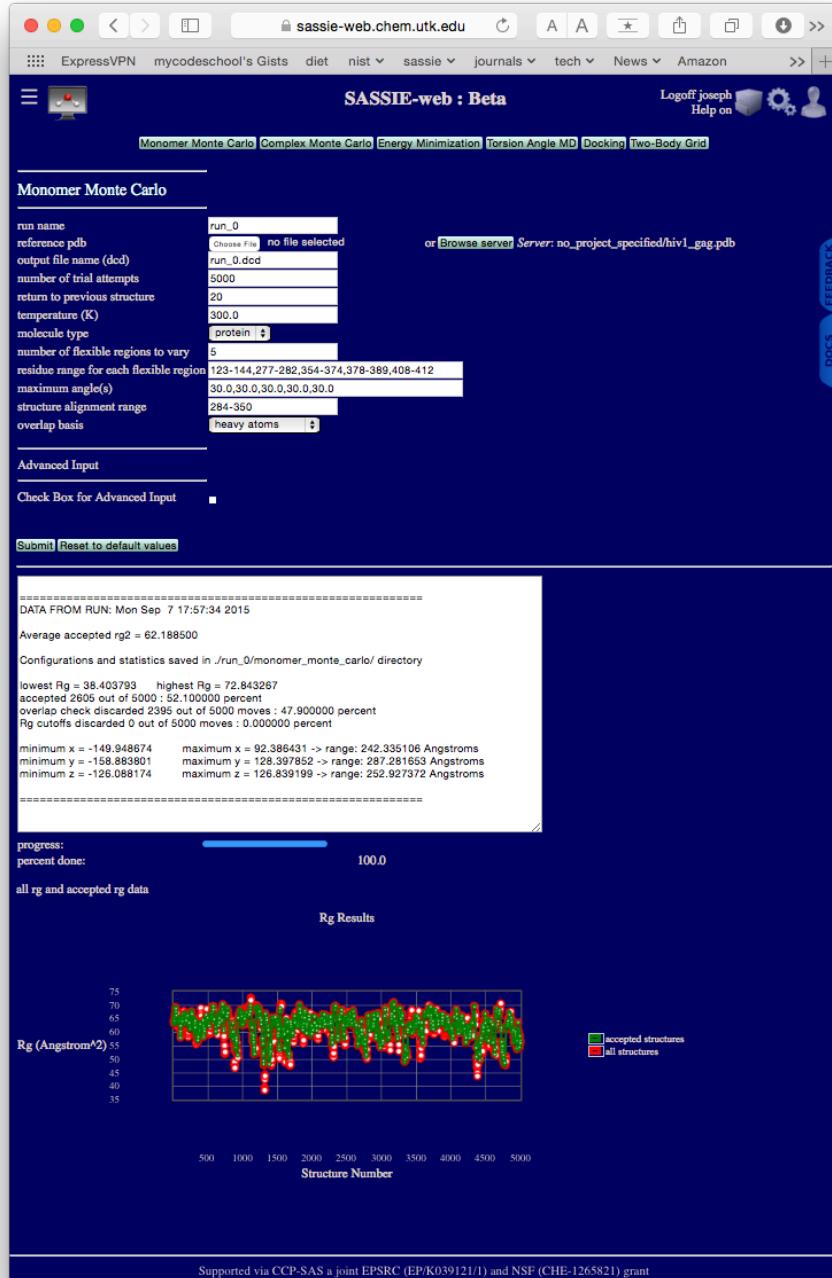
- Data analysis requires both computational and experimental expertise.
 - Lower the barrier to HPC usage.
 - Help support staff be more efficient
- Codes are very idiosyncratic
 - Can be hard to distribute, install, and use
 - So make them available as a service.

- 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.

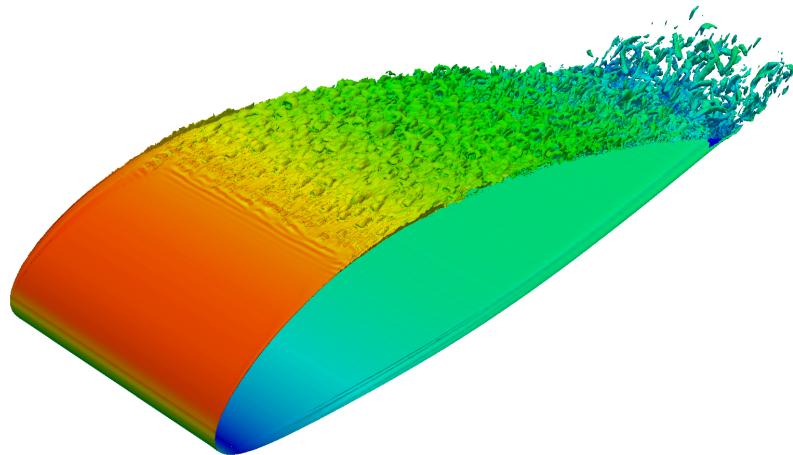
- Code: <http://genapp.rocks>
- Example:



sgg@iu.edu



Supported via CCP-SAS a joint EPSRC (EP/K039121/1) and NSF (CHE-1265821) grant



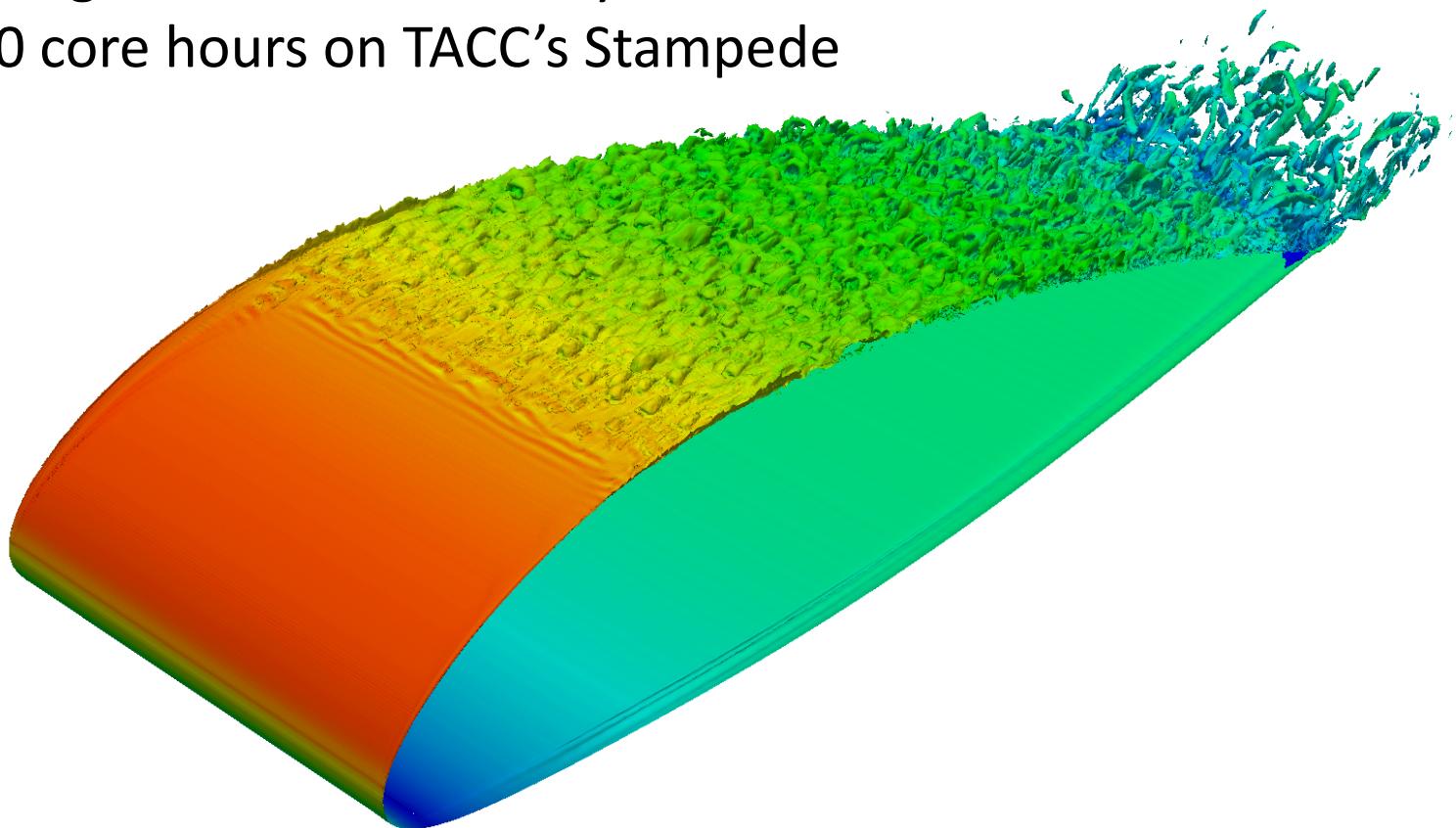
Large Eddy Simulations of Turbulent Flow

Cameron Smith, Steve Tran, and
Onkar Sahni

Rensselaer Polytechnic Institute

sgg@iu.edu

- 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



PHP Gateway with Airavata

PGA is a science gateway built with the Airavata API. You can reference PGA as you integrate Airavata into your own gateway, or you can create your gateway on top of PGA by cloning it at the link below. PGA is known to work well in the Chrome, Firefox, and Internet Explorer browsers.

[See the code ↗](#)

[XSEDE 2015 tutorial documentation ↗](#)



SciGaP is a hosted service with a public API that science gateways can use to manage applications and workflows running on remote supercomputers, as well as other services. Gateway developers can thus concentrate their efforts on building their scientific communities and not worry about operations.

Science Gateway Platform as a Service (SciGaP) provides application programmer interfaces (APIs) to hosted generic infrastructure services that can be used by domain science communities to create Science Gateways.

[Learn more ↗](#)



powered by

Apache Airavata

Apache Airavata is a software framework which is dominantly used to build Web-based science gateways and assist to compose, manage, execute and monitor large scale applications and workflows on distributed computing resources such as local clusters, supercomputers, national grids, academic and commercial clouds. Airavata mainly supports long running applications and workflows on distributed computational resources.

[Learn more ↗](#)

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

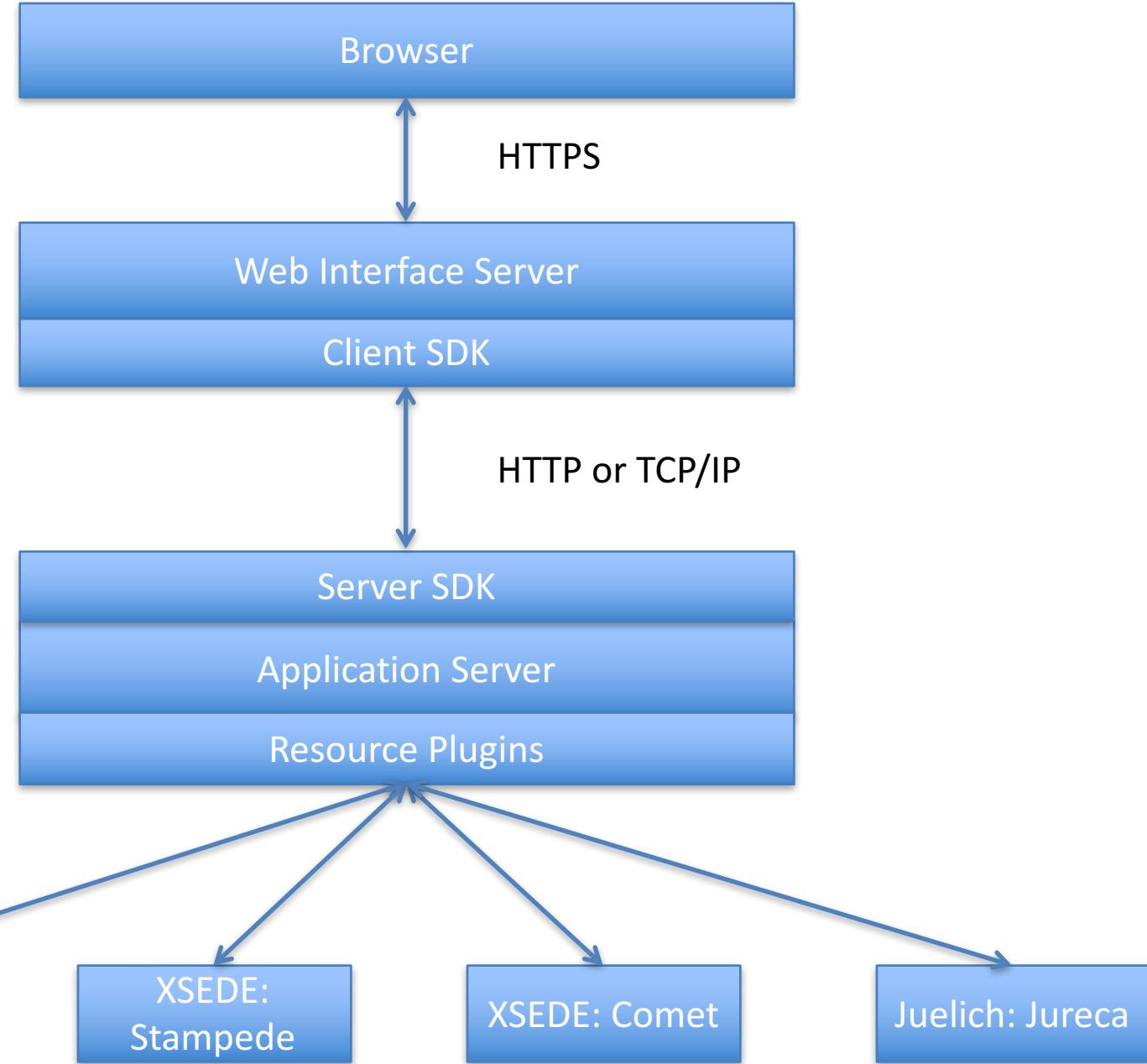
PHASTA team uses
Apache Airavata and the
PGA to run simulations
on TACC's Stampede.

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 ↗ geom.smd ↗ geom.sms ↗ solver.inp ↗
Outputs	Phasta-Output-TAR : Phasta_Output.tar.gz ↗ Phasta-Standard-Error : Phasta_P.stderr ↗ Phasta-Standard-Out : Phasta_P.stdout ↗

[Clone](#)

Classic Web
architectures
can be used
to build
science
gateways.



Time to Rethink This Architecture?

This is what the class is about.

Science Gateway Platform as a Service

Mark Miller, Amit Majumdar

San Diego Supercomputer Center

sgg@iu.edu

Missing results?

Send us the [job handle](#),
and we may be able to
help.

More Information

About Us

Requirements

Known Issues

Usage Statistics

User Locations

Enabled Publications

The CIPRES Science Gateway now offers PhyloBayes MPI and DPPDIV, along with fast RAxML and MrBayes codes.

First Time Users: Please review the [XSEDE Primer](#) and our [Fair Use Policy](#).

CIPRES Login:

*Username:

*Password:

[Forgot Password?](#)

iPlant users login here:



[What is this?](#)

Status: Routine Maintenance will occur on Mar 14, 2014; because this will kill running jobs, submissions that could enter that time period will be held in the queue until maintenance is complete.

CIPRES Gateway News

PhyloBayes MPI and MrBayes 3.2.2 now available
10/7/2013

Command Change Issues for MB 3.2.1
8/23/2013

Simplified access to phylogenetics codes on powerful XSEDE resources

Folders

-  [sarahm](#)
-  [amy](#)
-  [pamela](#)
-  [andy](#)
-  [James MrBayes](#)
-  [peggy](#)
-  [phylobayes](#)
-  [Jana](#)
-  [John Philips](#)
-  [paul mrbayes 3.2.2](#)
 -  [Data \(1\)](#)
 -  [Tasks \(3\)](#)
-  [phylobayes](#)
-  [oldmrbayes](#)
-  [joe](#)
-  [susana](#)
-  [aelys](#)
-  [vanessa](#)
-  [readseq](#)
-  [truncated_tree](#)
-  [selma](#)
-  [diogo](#)
-  [torsten](#)
-  [mike_hawaii](#)
-  [raxml_test](#)

MrBayes 3.2.2 on XSEDE: Tree Inference Using Bayesian Analysis - run on XSEDE ([John P. Huelsenbeck and Fred Ronquist](#))

Simple Parameters



OPEN / CLOSE

My Data Contains a MrBayes Data Block (CHECK THIS OR MrBayes BLOCK ENTRIES WILL BE OVERWRITTEN!!!) *

I confirm that there is not an "autoclose = no" statement in my MrBayes block *

My MrBayes Block species nrnns=

My MrBayes Block species ncchains=

Maximum Hours to Run (click here for help setting this correctly) *

My Data Type Is (only one data type can be used through the web form, see help below) * nucleic acid

Set the Seed Number Set seed=

Set the Swapseed=

Use scientific notation

How many decimals should we print?



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

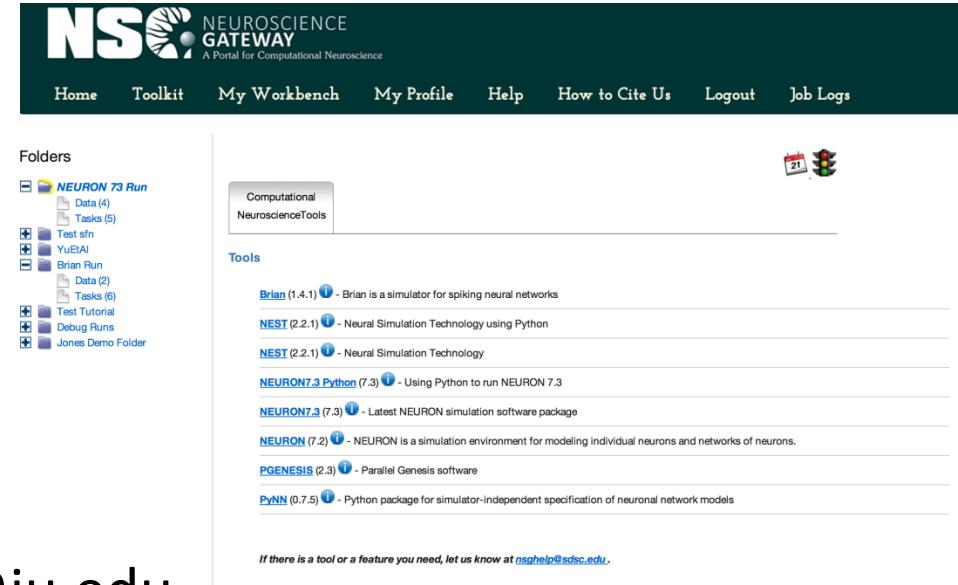
<http://www.nsgportal.org>

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



The screenshot shows the NSG portal homepage. At the top, there's a navigation bar with links for Home, Toolkit, My Workbench, My Profile, Help, How to Cite Us, Logout, and Job Logs. A small calendar icon and a traffic light icon are also present. On the left, there's a sidebar titled 'Folders' containing a tree view of project structures: 'NEURON 7.3 Run' (Data 4, Tasks 5), 'Test.sif', 'YuBAI', 'Brian Run' (Data 2, Tasks 6), 'Test Tutorial', 'Debug Runs', and 'Jones Demo Folder'. The main content area has a header 'Computational NeuroscienceTools'. Below it, a list of tools is shown with their descriptions:

- Brian** (1.4.1) - Brian is a simulator for spiking neural networks
- NEST** (2.2.1) - Neural Simulation Technology using Python
- NEST** (2.2.1) - Neural Simulation Technology
- NEURON7.3 Python** (7.3) - Using Python to run NEURON 7.3
- NEURON7.3** (7.3) - Latest NEURON simulation software package
- NEURON** (7.2) - NEURON is a simulation environment for modeling individual neurons and networks of neurons.
- GENESIS** (2.3) - Parallel Genesis software
- PyNN** (0.7.5) - Python package for simulator-independent specification of neuronal network models

At the bottom, a footer note reads: 'If there is a tool or a feature you need, let us know at nsghelp@sdsc.edu'.

sgg@iu.edu