Cyber Infrastructure for Molecular Science Communities

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Outline

- What is cyberinfrastructure and Science gateway
- Apache Airavata Collaboration Platform
- SEAGrid Science Gateway
- CIRC Collaborations

Acknowledgements

CYBERINFRASTRUCTURE
INTEGRATION RESEARCH CENTER
PERVASIVE TECHNOLOGY INSTITUTE

POWERED BY

APACHE
AIRAVATA

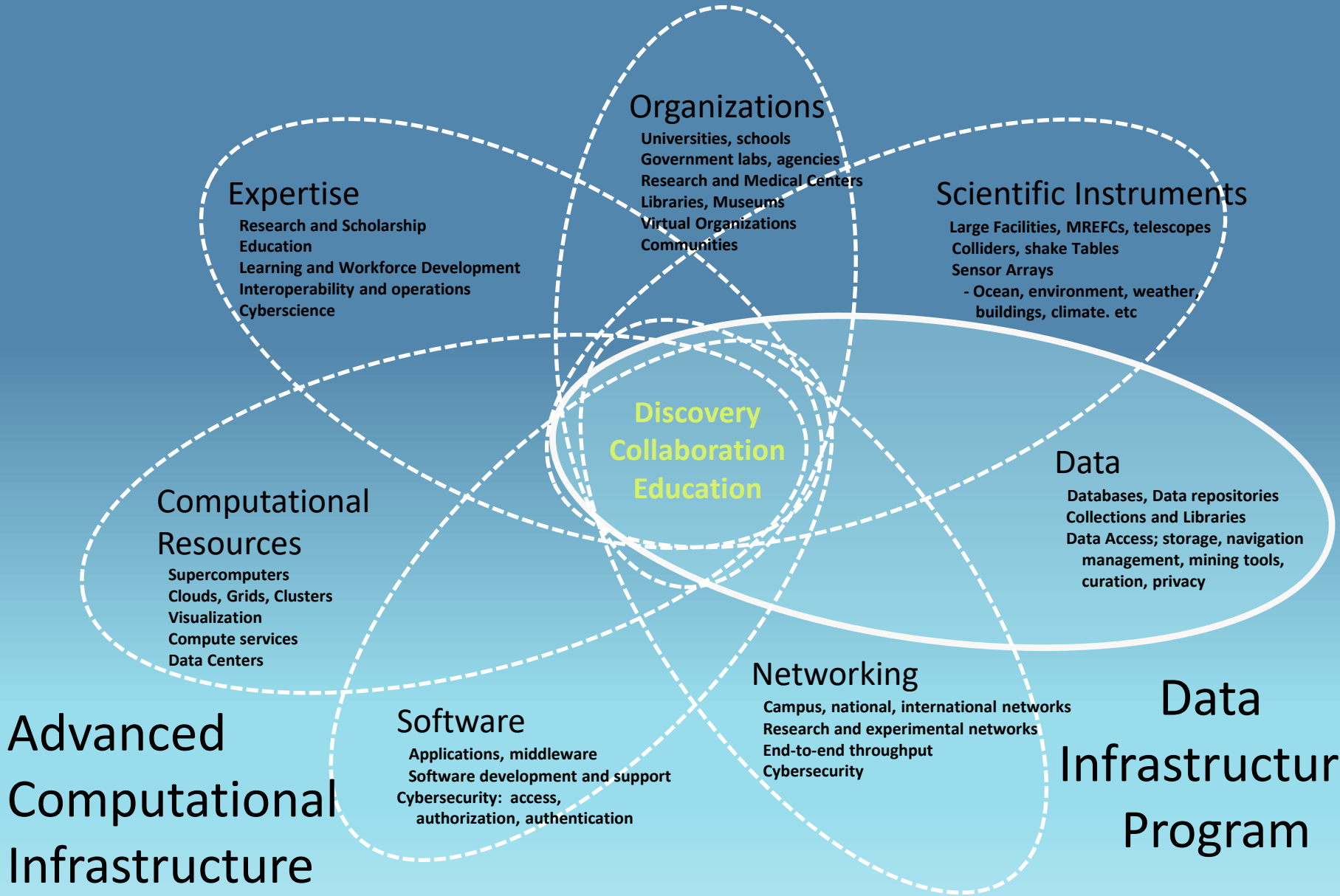
SciGaP

Cyberinfrastructure

- Laboratory, Local to Campus, State, National and International Resources of Data, Computing, Networks and Software frameworks integrated together to provide seamless access to the scientist for research and teaching.

NSF Supercomputer Centers XSEDE, Frontera, Regional and Local systems

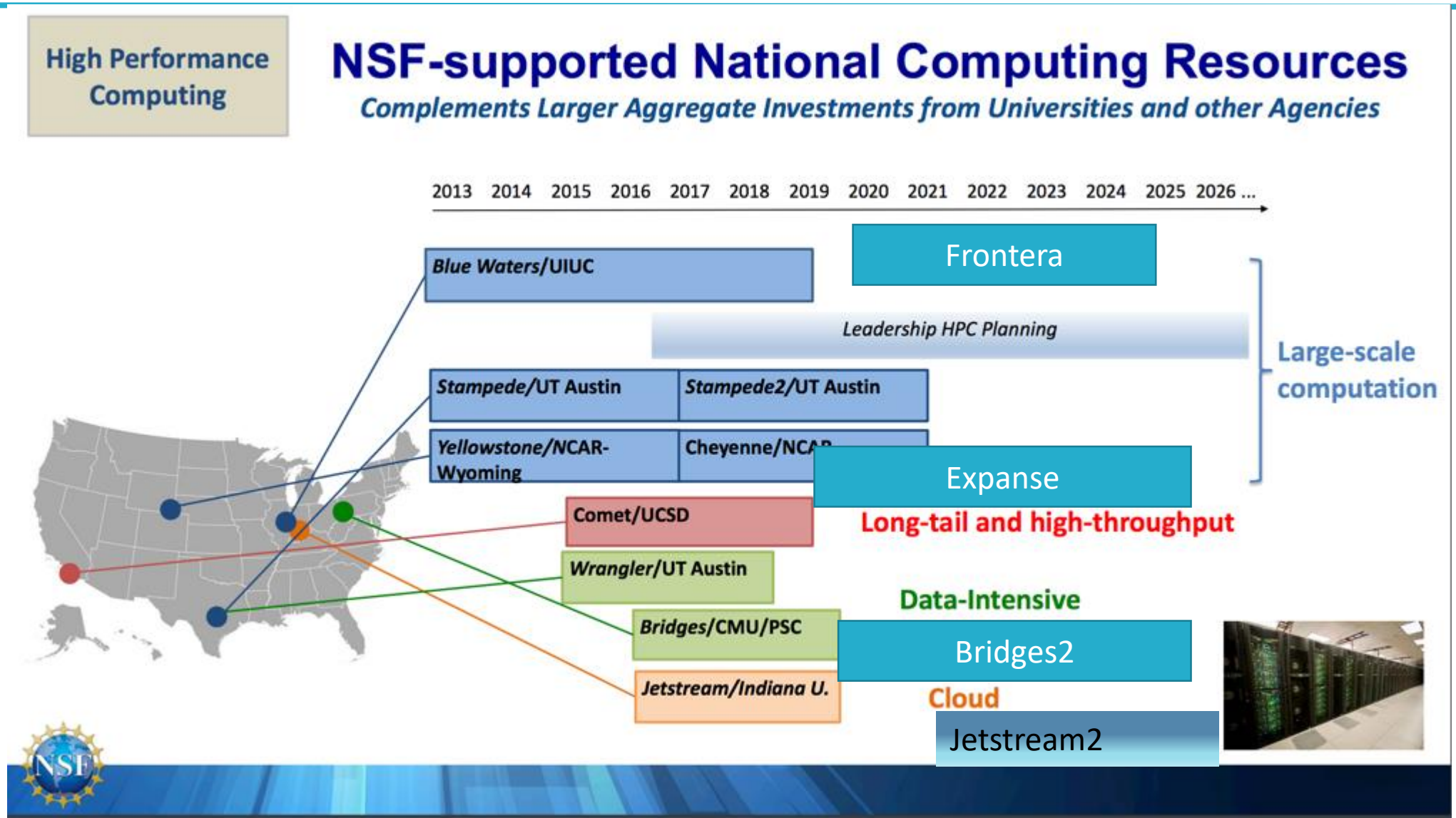
NSF CIF21 Major Areas



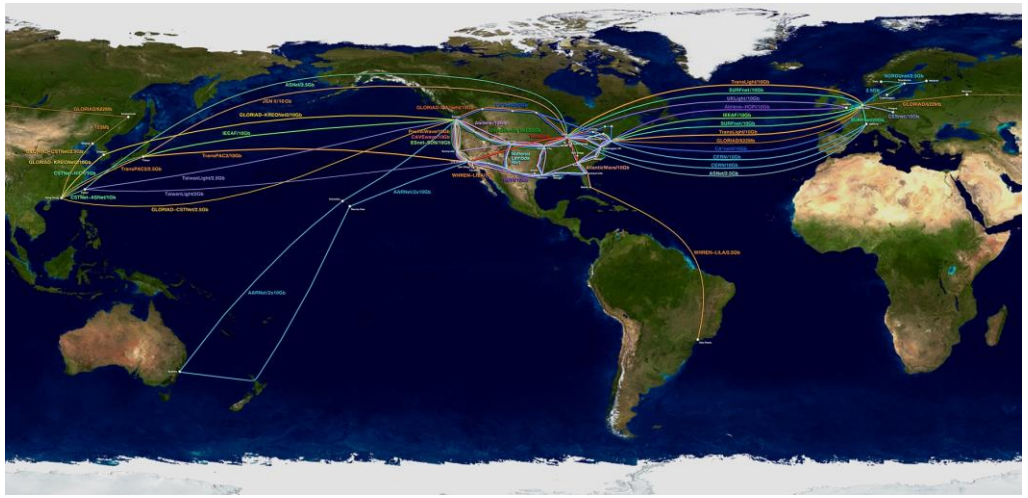
Current XSEDE Resources

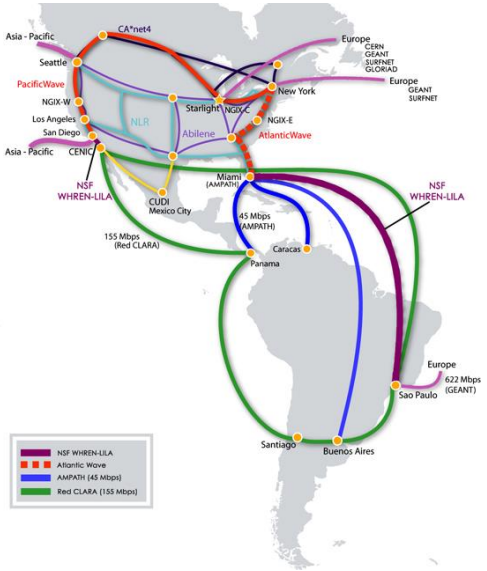
Resource	Organization	Type
HP/NVIDIA Interactive Visualization and Data Analytics System (Maverick)	TACC	vis
IU/TACC (Jetstream)	Indiana U	compute
IU/TACC Storage (Jetstream Storage)	UT Austin	storage
LSU Cluster (superMIC)	LSU CCT	compute
Open Science Grid (OSG)	OSG	compute
PSC Bridges GPU (Bridges2 GPU)	PSC	compute
PSC Large Memory Nodes (Bridges2 Large)	PSC	compute
PSC Regular Memory (Bridges2)	PSC	compute
PSC Storage (Bridges Pylon)	PSC	storage
SDSC Comet GPU Nodes (Expanse GPU)	SDSC	compute
SDSC Dell Cluster with Intel Haswell Processors (Expanse)	SDSC	compute
SDSC Medium-term disk storage (Data Oasis)	SDSC	storage
Stanford University GPU Cluster (XStream)	Stanford U	compute
TACC Data Analytics System (Jetstream)	TACC	compute
TACC Dell/Intel Knights Landing, Skylake System (Stampede2)	UT Austin	compute
TACC Long-term Storage (Jetstream Storage)	TACC	storage
TACC Long-term tape Archival Storage (Corral)	TACC	storage

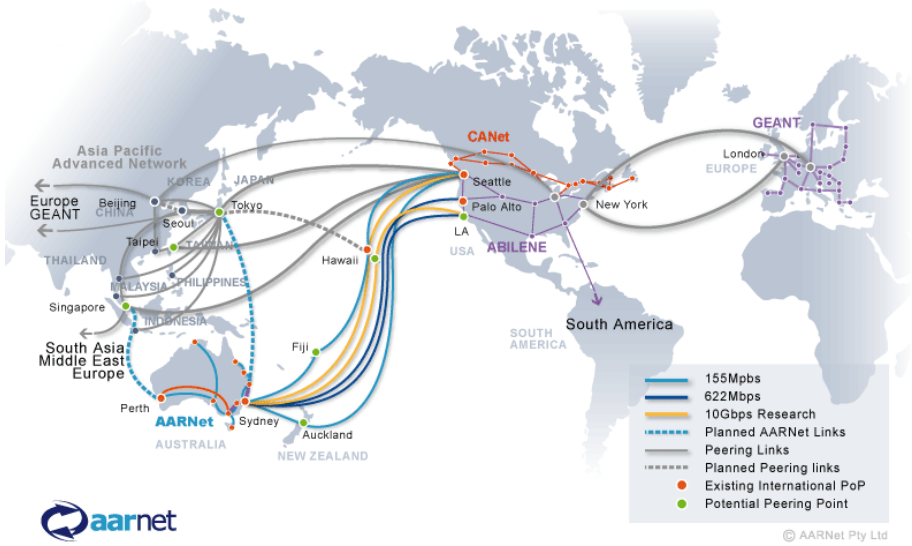
NSF HPC Resources



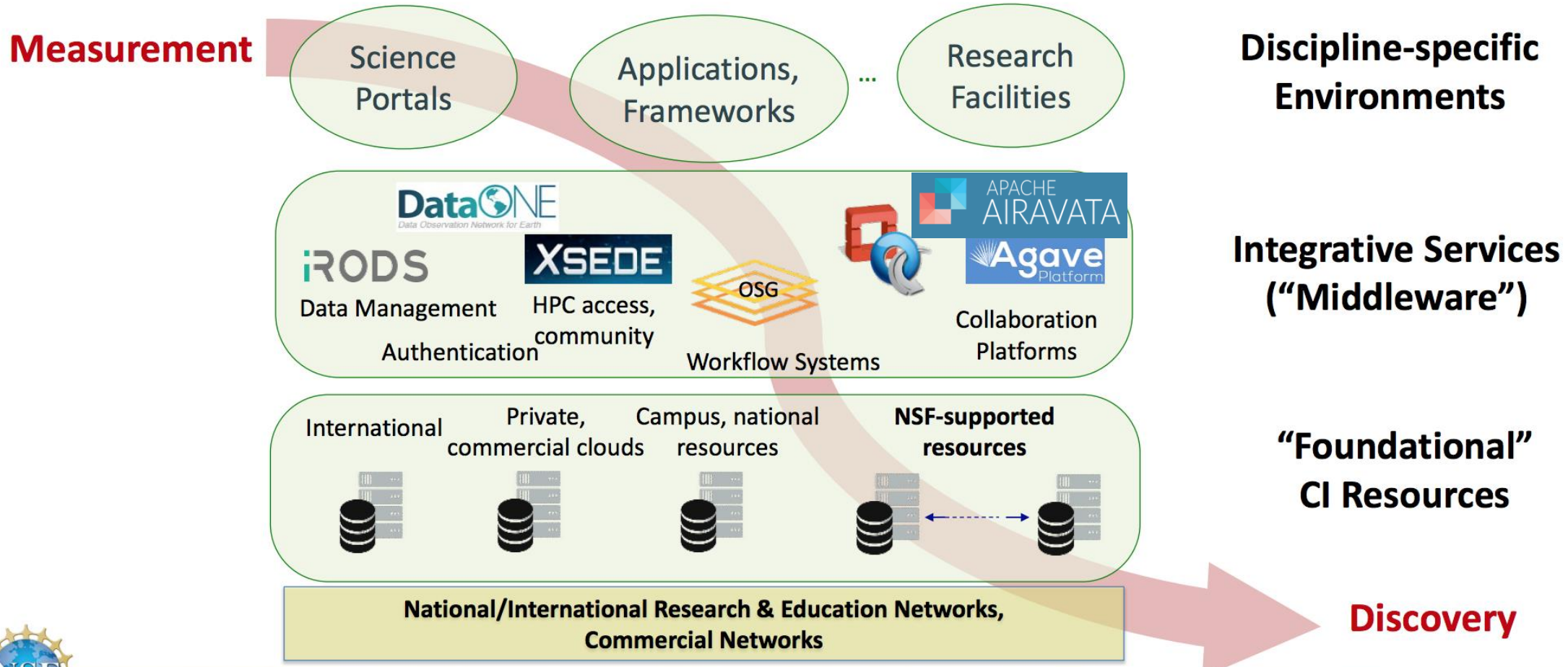
VO-Global: International R&E Networking







Emerging discovery pathways at scale: Architecture view



Science Gateways

Web interfaces and middleware for integrating distributed computing, automating expertise, controlling access, managing results, and speeding up your critical computational workflows

Science gateways are Web and desktop interfaces to high performance computing clusters, computing clouds.

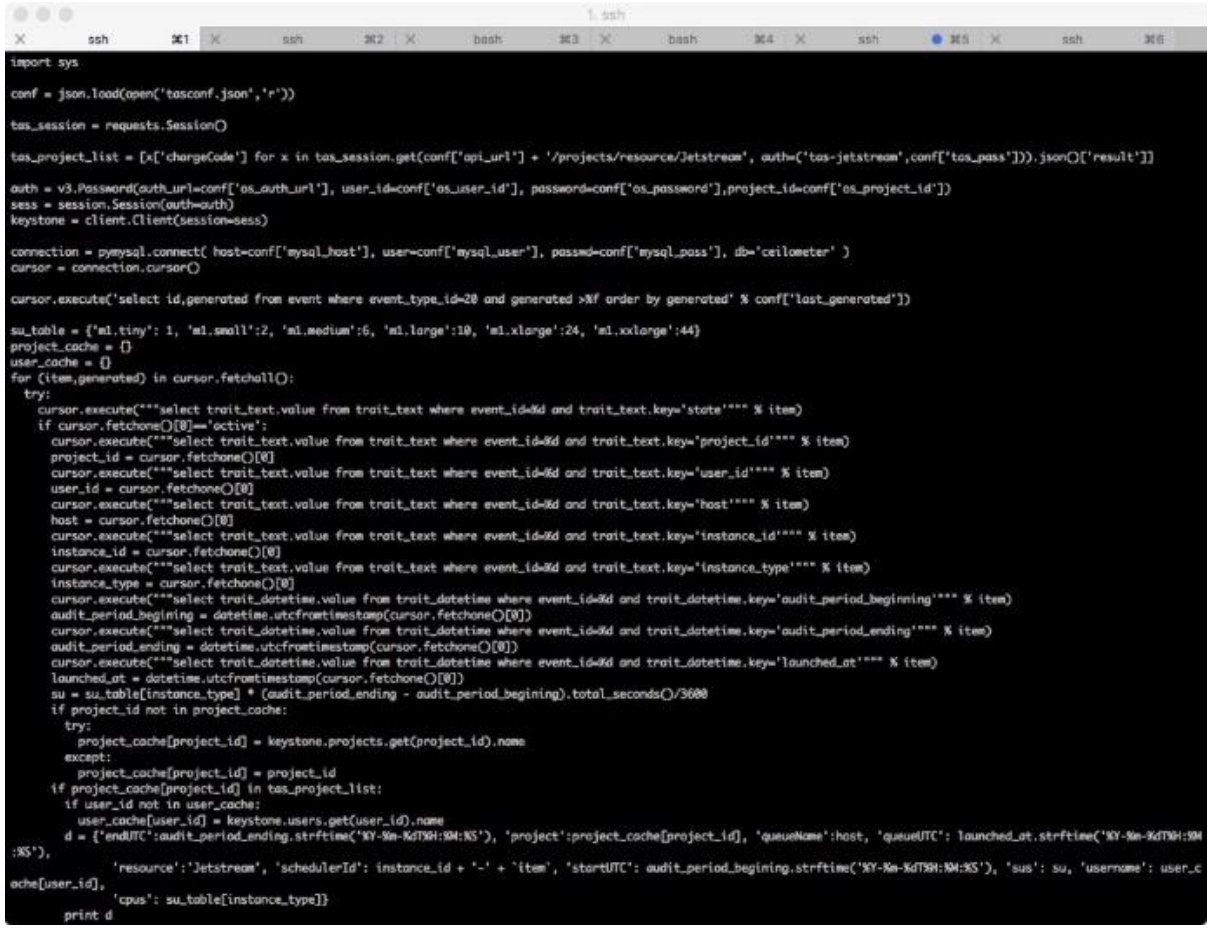
Science gateways encode expertise

- Running specific scientific application
- Running jobs on diverse, nonlocal machines
- Moving data to and from world-wide resources

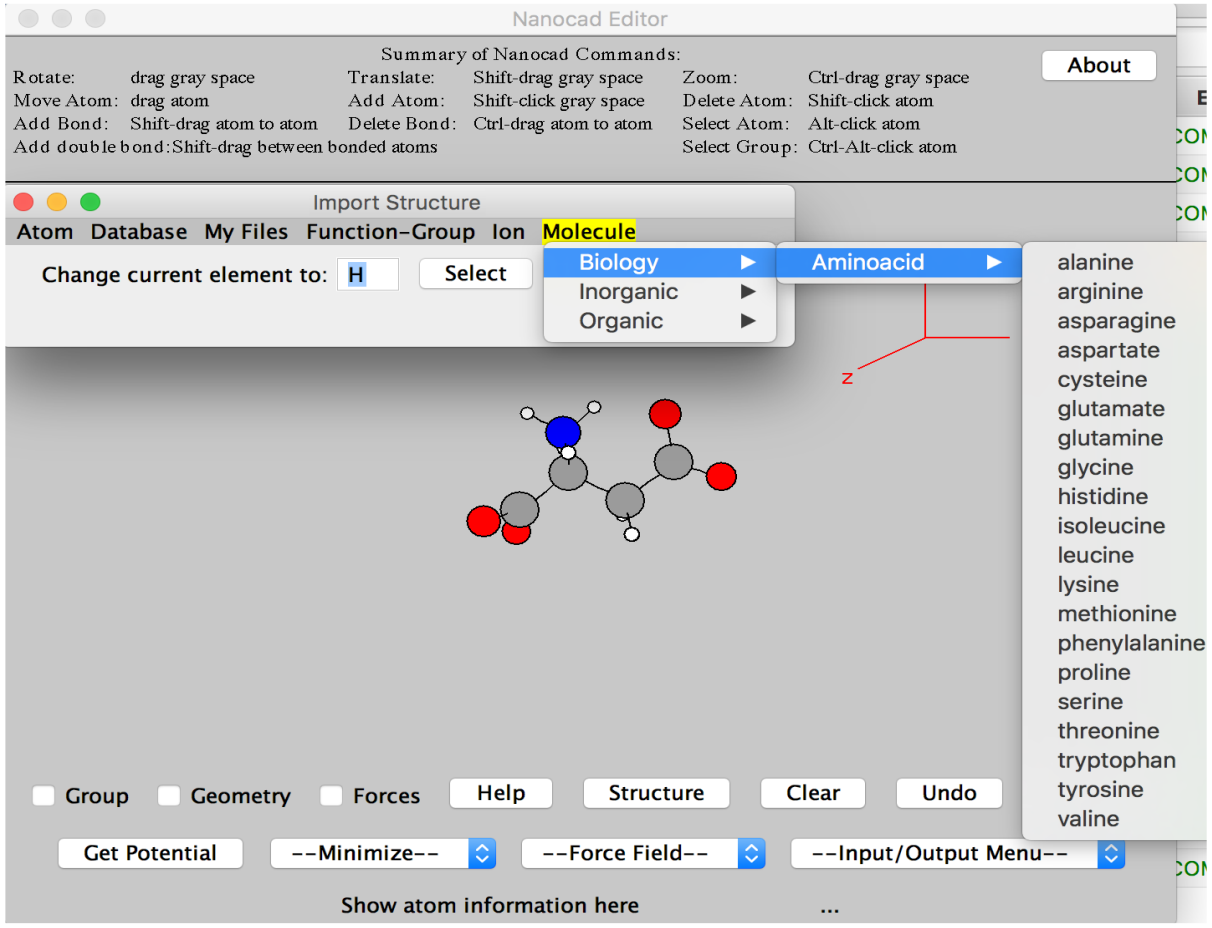
Science gateways enable sharing of results

Science gateways make results recoverable and reproducible

Technology Adoption Choices

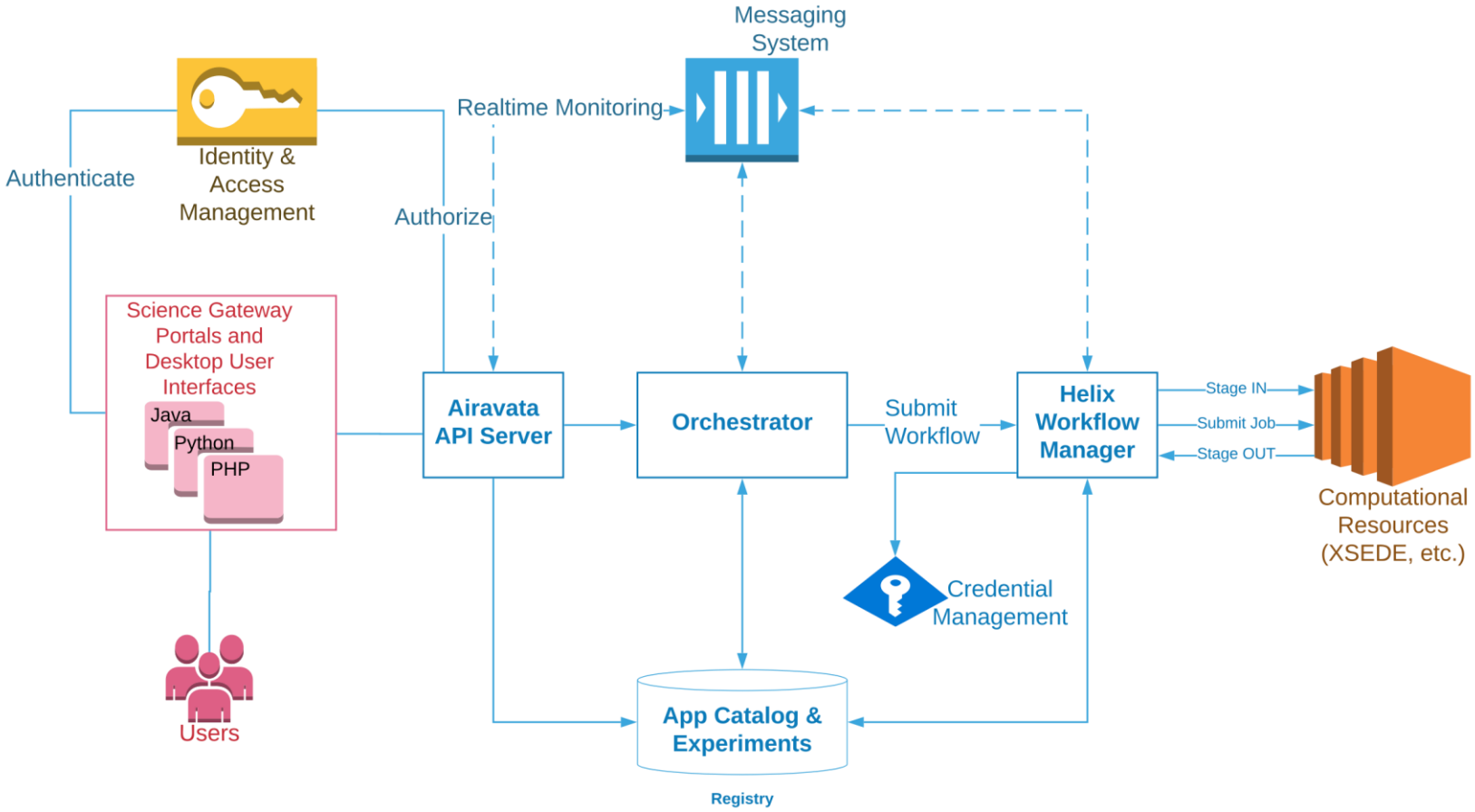


```
import sys

conf = json.load(open('tasconf.json','r'))

tas_session = requests.Session()

tas_project_list = [x['chargeCode'] for x in tas_session.get(conf['api_url'] + '/projects/resource/Jetstream', auth=('tas-jetstream',conf['tas_pass'])).json()['result']]

auth = v3.Password(auth_url=conf['os_auth_url'], user_id=conf['os_user_id'], password=conf['os_password'],project_id=conf['os_project_id'])
sess = session.Session(auth=auth)
keystone = client.Client(session=sess)

connection = pymysql.connect( host=conf['mysql_host'], user=conf['mysql_user'], passwd=conf['mysql_pass'], db='ceilometer' )
cursor = connection.cursor()

cursor.execute('select id,generated from event where event_type_id=20 and generated >%f order by generated' % conf['last_generated'])

su_table = {'m1.tiny': 1, 'm1.small':2, 'm1.medium':6, 'm1.large':10, 'm1.xlarge':24, 'm1.xxlarge':44}
project_cache = {}
user_cache = {}
for (item,generated) in cursor.fetchall():
  try:
    cursor.execute("""select trait_text.value from trait_text where event_id=%d and trait_text.key='state'""" % item)
    if cursor.fetchone()[0]=='active':
      cursor.execute("""select trait_text.value from trait_text where event_id=%d and trait_text.key='project_id'""" % item)
      project_id = cursor.fetchone()[0]
      cursor.execute("""select trait_text.value from trait_text where event_id=%d and trait_text.key='user_id'""" % item)
      user_id = cursor.fetchone()[0]
      cursor.execute("""select trait_text.value from trait_text where event_id=%d and trait_text.key='host'""" % item)
      host = cursor.fetchone()[0]
      cursor.execute("""select trait_text.value from trait_text where event_id=%d and trait_text.key='instance_id'""" % item)
      instance_id = cursor.fetchone()[0]
      cursor.execute("""select trait_text.value from trait_text where event_id=%d and trait_text.key='instance_type'""" % item)
      instance_type = cursor.fetchone()[0]
      cursor.execute("""select trait_datetime.value from trait_datetime where event_id=%d and trait_datetime.key='audit_period_beginning'""" % item)
      audit_period_begining = datetime.utcfromtimestamp(cursor.fetchone()[0])
      cursor.execute("""select trait_datetime.value from trait_datetime where event_id=%d and trait_datetime.key='audit_period_ending'""" % item)
      audit_period_ending = datetime.utcfromtimestamp(cursor.fetchone()[0])
      cursor.execute("""select trait_datetime.value from trait_datetime where event_id=%d and trait_datetime.key='launched_at'""" % item)
      launched_at = datetime.utcfromtimestamp(cursor.fetchone()[0])
      su = su_table[instance_type] * (audit_period_ending - audit_period_begining).total_seconds()/3600
      if project_id not in project_cache:
        try:
          project_cache[project_id] = keystone.projects.get(project_id).name
        except:
          project_cache[project_id] = project_id
      if project_cache[project_id] in tas_project_list:
        if user_id not in user_cache:
          user_cache[user_id] = keystone.users.get(user_id).name
        d = {'endUTC':audit_period_ending.strftime('%Y-%m-%dT%H:%M:%S'), 'project':project_cache[project_id], 'queueName':host, 'queueUTC': launched_at.strftime('%Y-%m-%dT%H:%M
:%S'),
             'resource':'Jetstream', 'schedulerId': instance_id + '-' + `item`, 'startUTC': audit_period_begining.strftime('%Y-%m-%dT%H:%M:%S'), 'sus': su, 'username': user_c
ache[user_id],
             'cpus': su_table[instance_type]}
        print d
```



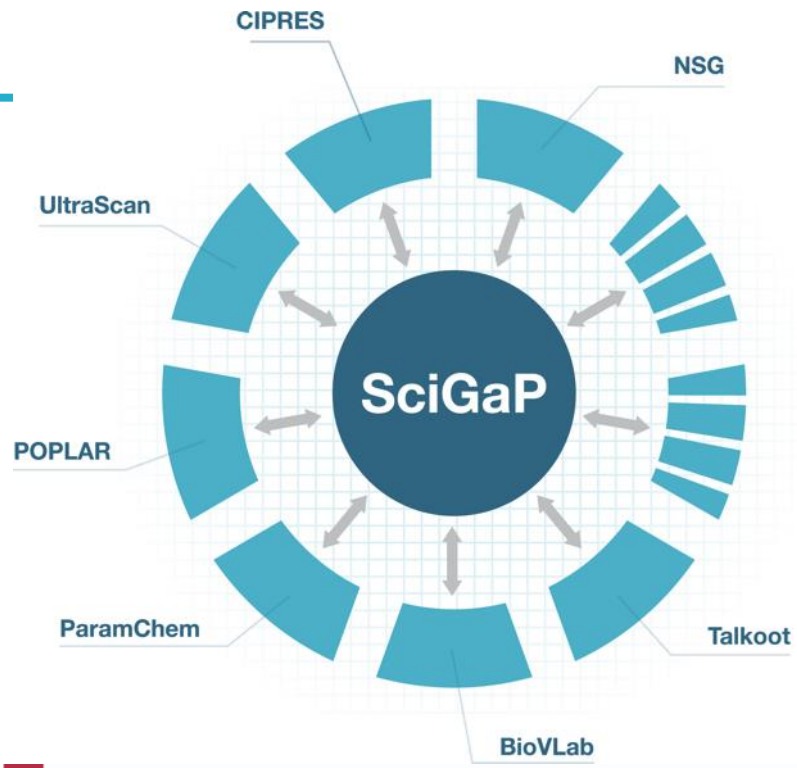
Apache Airavata

- Open source science gateway framework (airavata.apache.org)
- Enable sharing of
  - Applications
  - Compute/storage resources
  - Simulation results
- API and full-featured UI clients



SciGaP Hosting Services

- Airavata is multi-tenanted
- The SciGaP project runs a hosted instance of Airavata, supports 30+ science gateways
- Web Portal hosting
- Common use case: Software-as-a-service science gateway
- Consulting help also available
- Request a gateway at https://scigap.org
- Sustainably operated by SGRC after NSF funding through NSF SI2 program

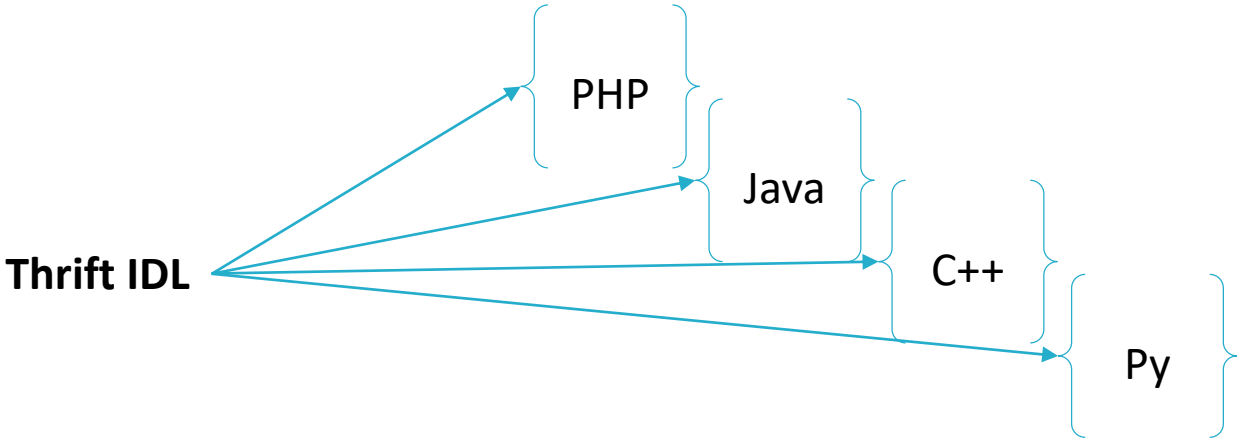


SCIENCE GATEWAYS RESEARCH CENTER
INDIANA UNIVERSITY
Pervasive Technology Institute

Building an Airavata client

Option 1: Build your own

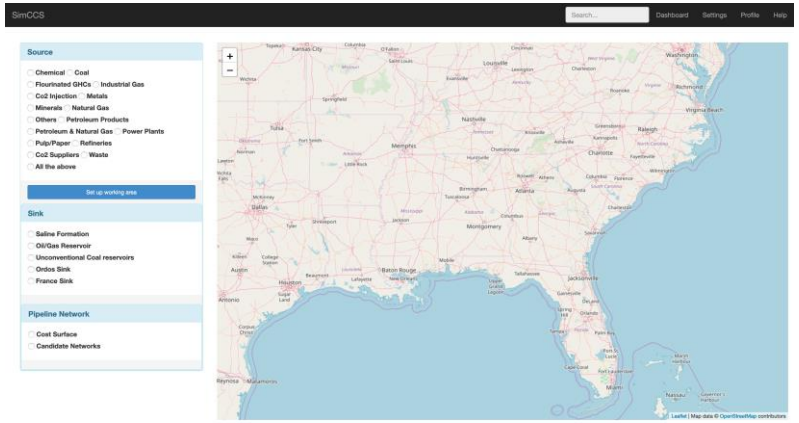
- Thrift based API
- Clients exist in Java, Python, PHP, but many more target languages possible
- Example code is available



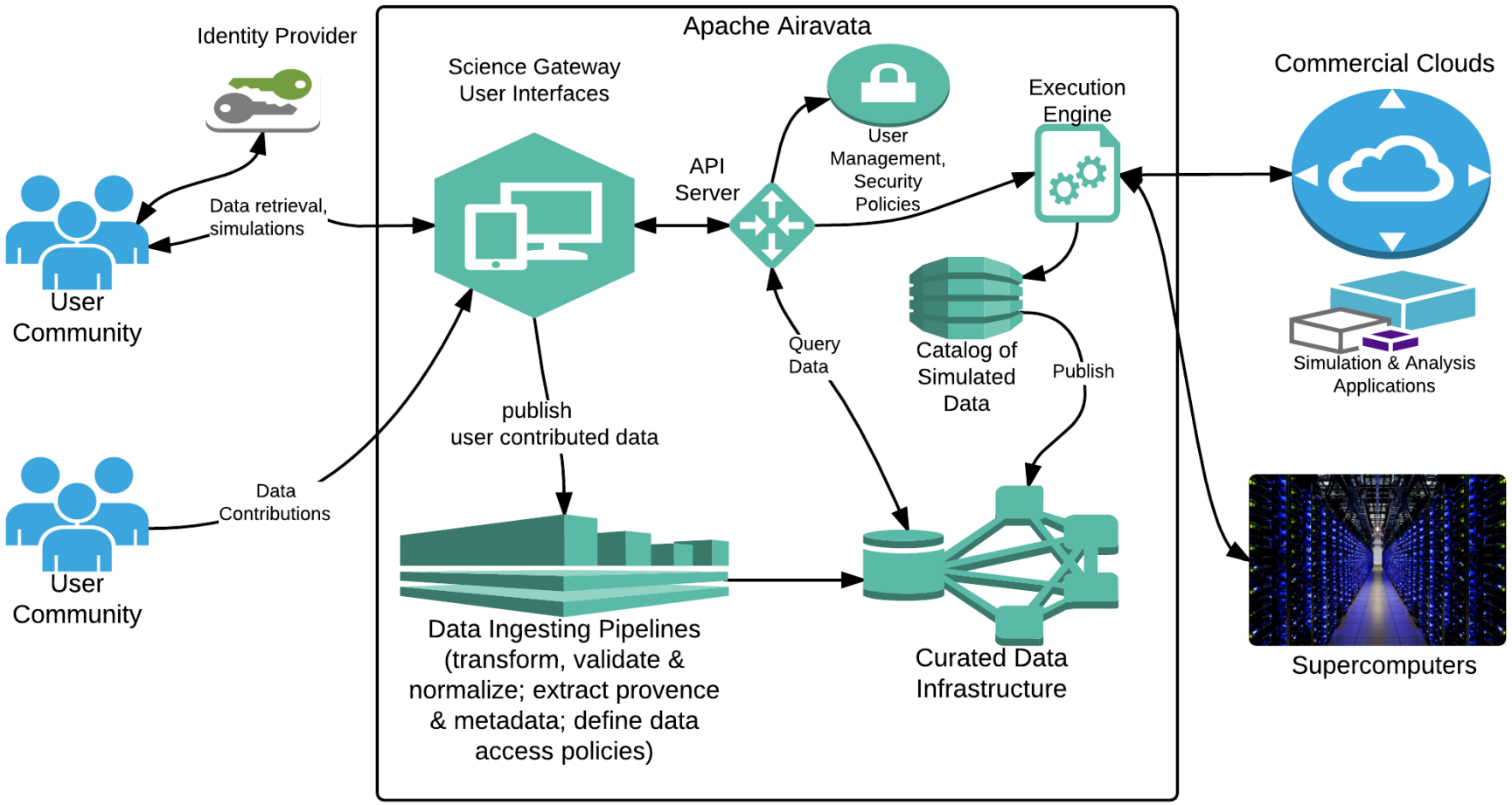
Option 2: Build extensions to Django Portal

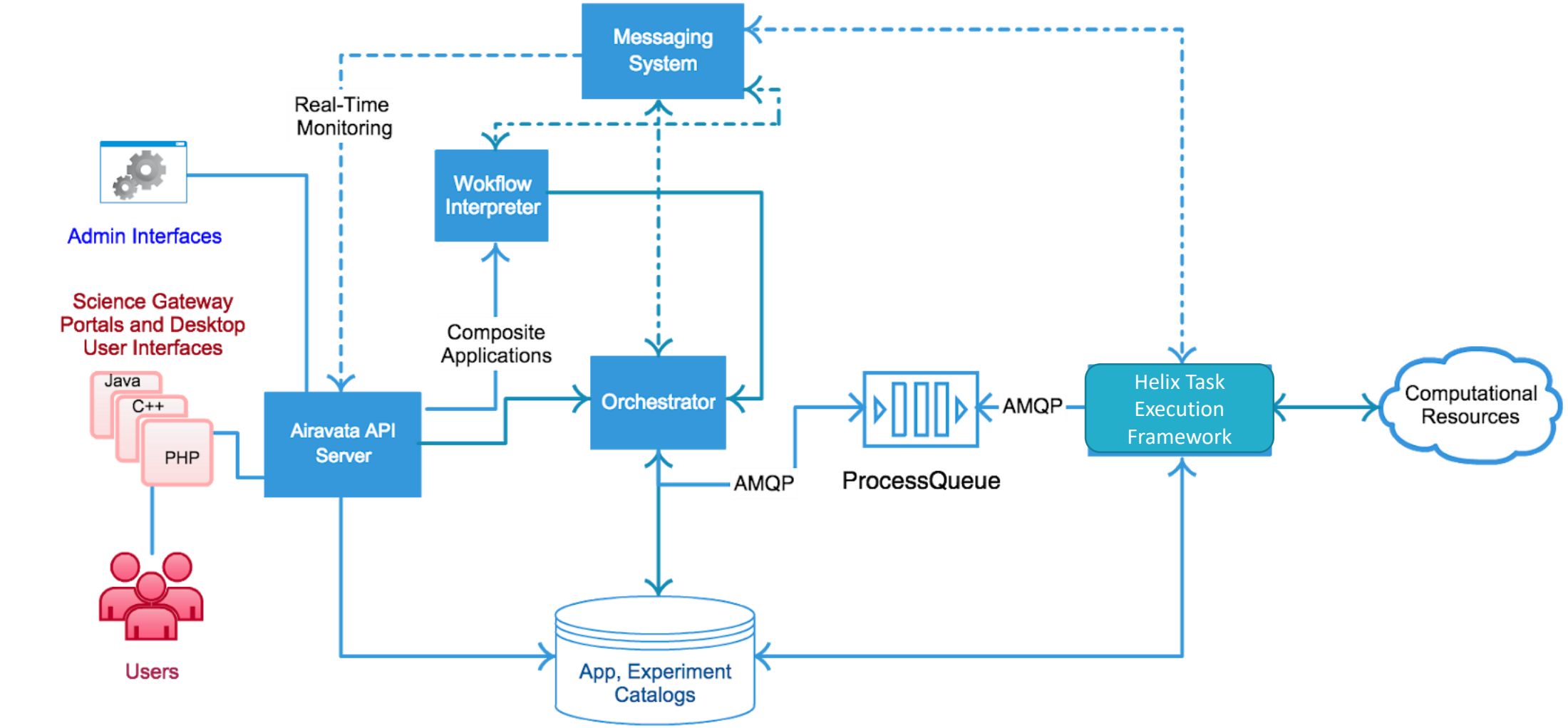
- New Django Portal (beta)
  - production availability this summer
- Extensibility
  - Add additional Django apps
  - Custom experiment input editors
  - Custom experiment output viewers
  - Leverage REST API and JS libraries

Example custom Django app: SimCCS Maptool



Science Gateway Architecture




Messaging System
Real-Time Monitoring
Wokflow Interpreter
Admin Interfaces
Science Gateway Portals and Desktop User Interfaces
Java
C++
PHP
Airavata API Server
Composite Applications
Orchestrator
AMQP
ProcessQueue
AMQP
Helix Task Execution Framework
Computational Resources
Users
App, Experiment Catalogs

What Is Apache Airavata?

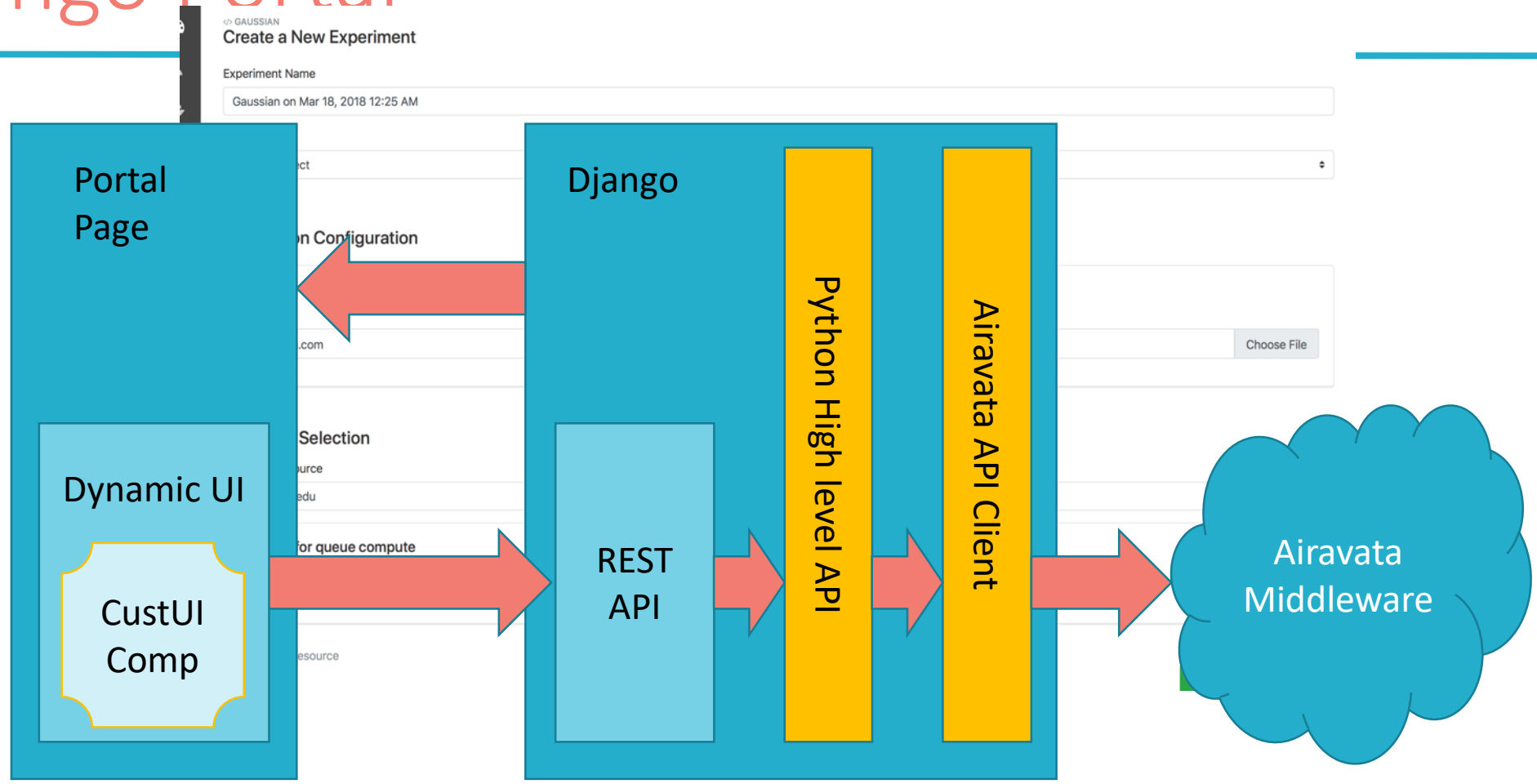
- Apache Airavata is software for building science gateways.
  - Don’t start from scratch
- Airavata-based gateways integrate clusters and supercomputers from all over the world.
  - We can make your resources available to your team.
  - We can help you access supercomputers, clusters, and computing clouds from outside your institution or enterprise.

Some Gateways Built with Apache Airavata

Gateway	Description
UltraScan	Support for data analysis of analytical ultracentrifugation experiments
GeoGateway	Earthquake modeling and data access to support NASA and other researchers
IU Cybergateway	Campus gateway for accessing campus resources (in revision)
University of South Dakota Gateway	Campus gateway specializing in chemistry and bio applications. Other campus gateways: Oklahoma University , University of Utah, Georgia State University
dREG Science Gateway	Gateway for locating and understanding Transcriptional Regulatory Elements (TREs) that encode the temporal and spatial patterns of gene expression.
Oklahoma Innovation Institute Gateway	Gateway for computational chemistry and engineering applications
PHASTA Gateway	Gateway for computational engineering, finite element simulation

For a complete list, please see https://circ.iu.edu/collaborations.html

Django Portal



Custom UI Components

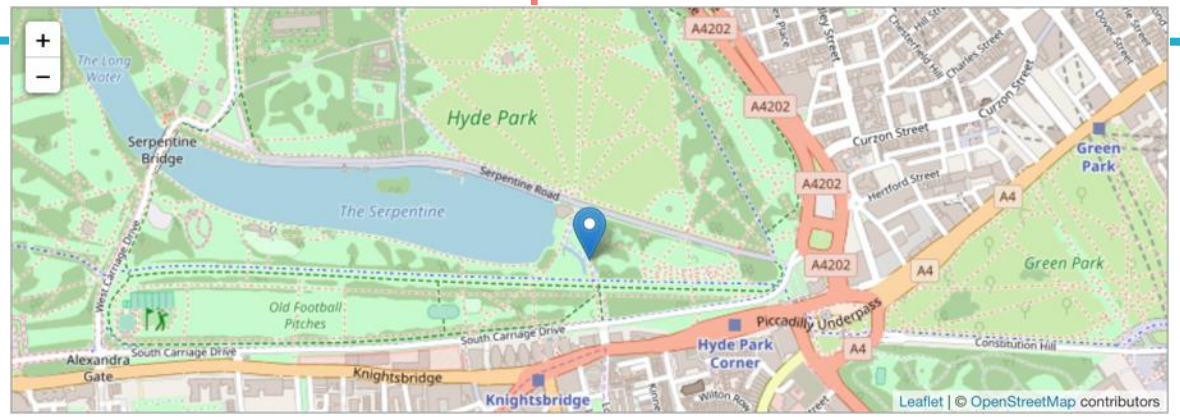


Image credit: leafletjs.com website

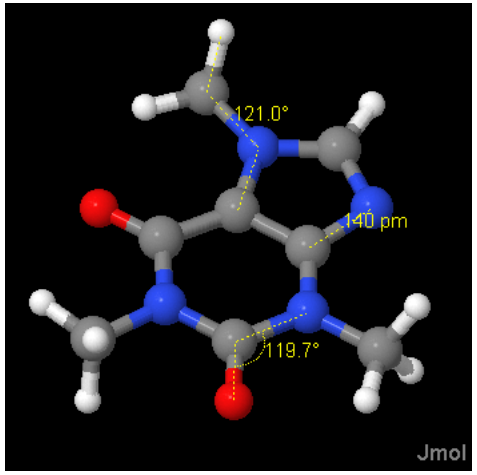
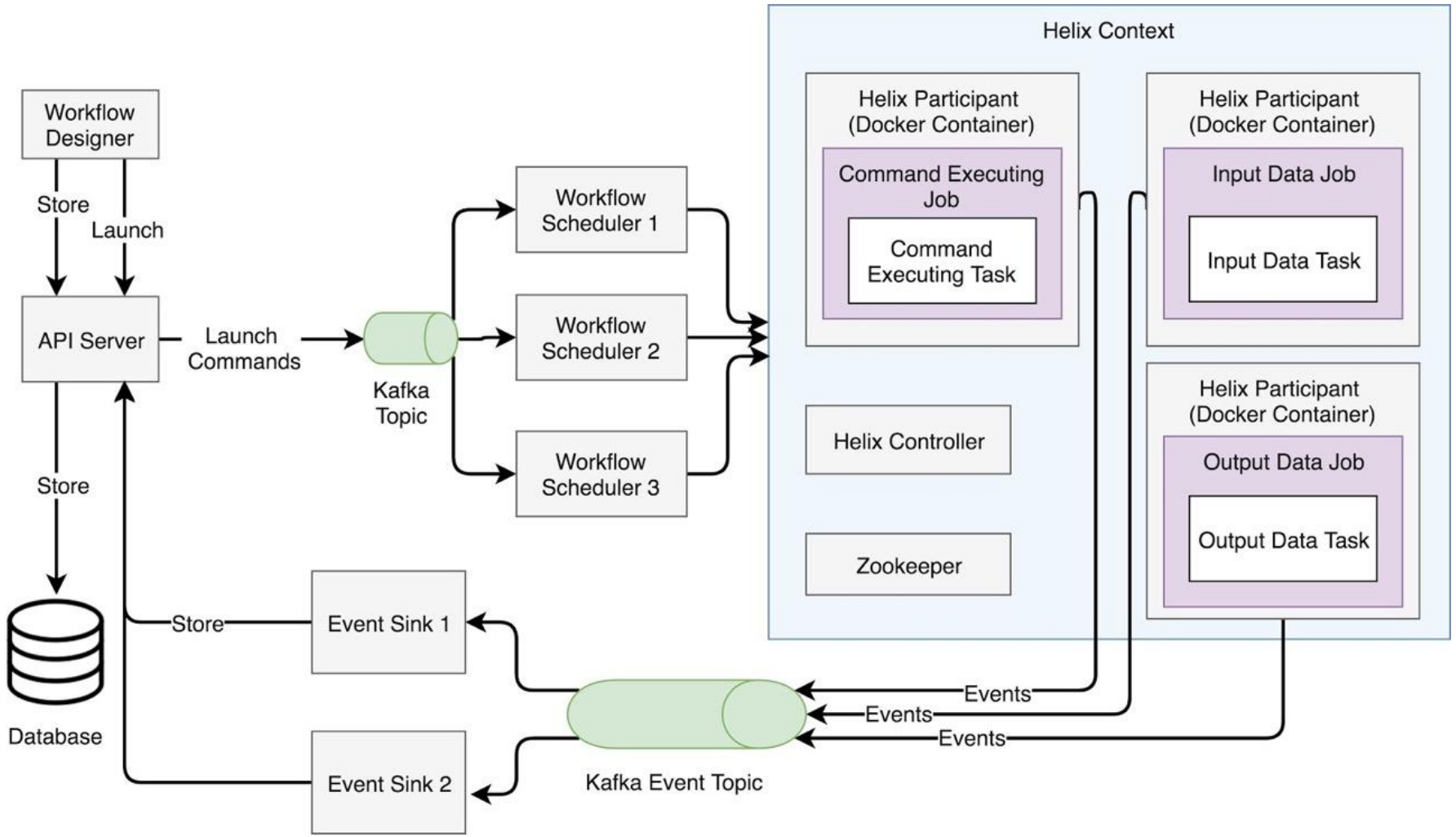


Image credit: jmol.sourceforge.net website

Helix-based Task Execution



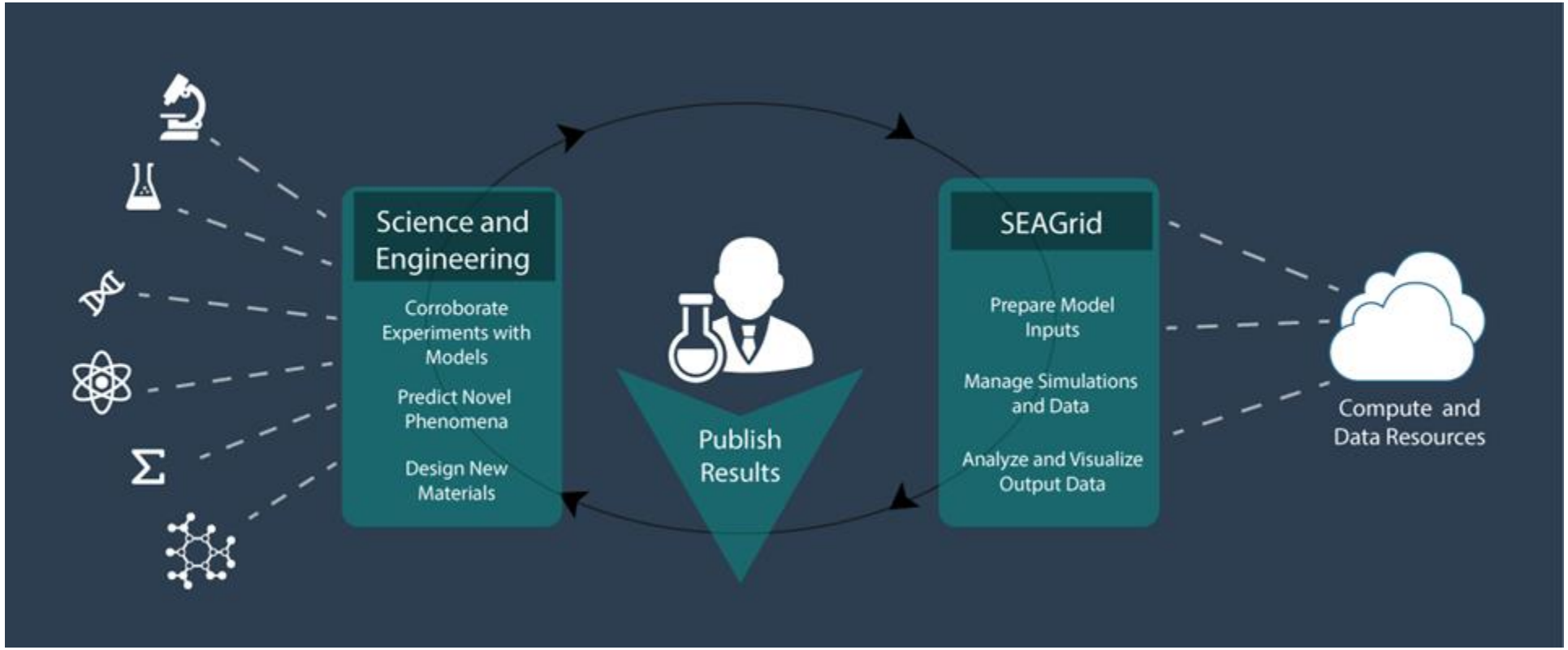
Group-based Authorization

- Currently, authorization based on statically defined roles
- Group-based authorization gives gateway admins more fine-grained control
- But also opens the door to allowing users to share resources and applications with other users

Apache Airavata Summary

- Apache Airavata has been used as the basis for several kinds of gateways, Single Application, Campus, Domain Specific, Multi-disciplinary etc..
- We can integrate Workflows, Data and Metadata, Data reuse mechanisms, sharing and Group wise access control
- Apache Airavata is Open Source Open Community software framework and can accommodate contributors from many disciplines
- Education, Training, Work-force development opportunities to get involved are available

SEAGrid.org



SEAGrid.org is an Apache Airavata-powered gateway

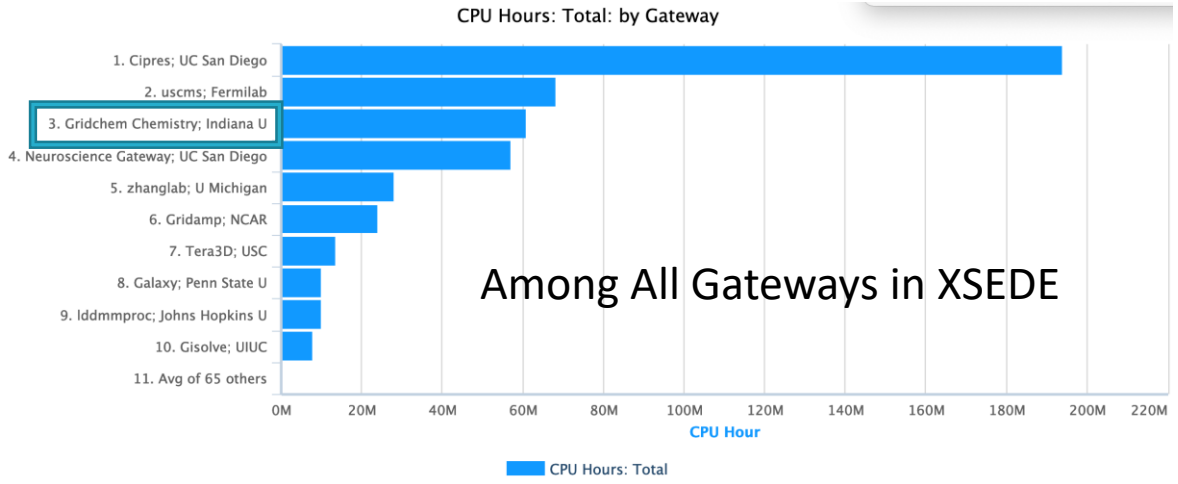
SEAGrid 16 Years in Service

- NSF XSEDE Gateway 2021 Allocation valued at $2,974,326.00
- NSF XSEDE Resources NCSA, SDSC, TACC, PSC, IU, LSU
- Bigred3 and Carbonate (IU), CCR U. Buffalo
- 1662 Registered Users, ~ 400 Active
- 222M XD SUs for 222K Jobs Since 2005
- More than 80 Publications since 2015
- Mainly Chemistry Applications

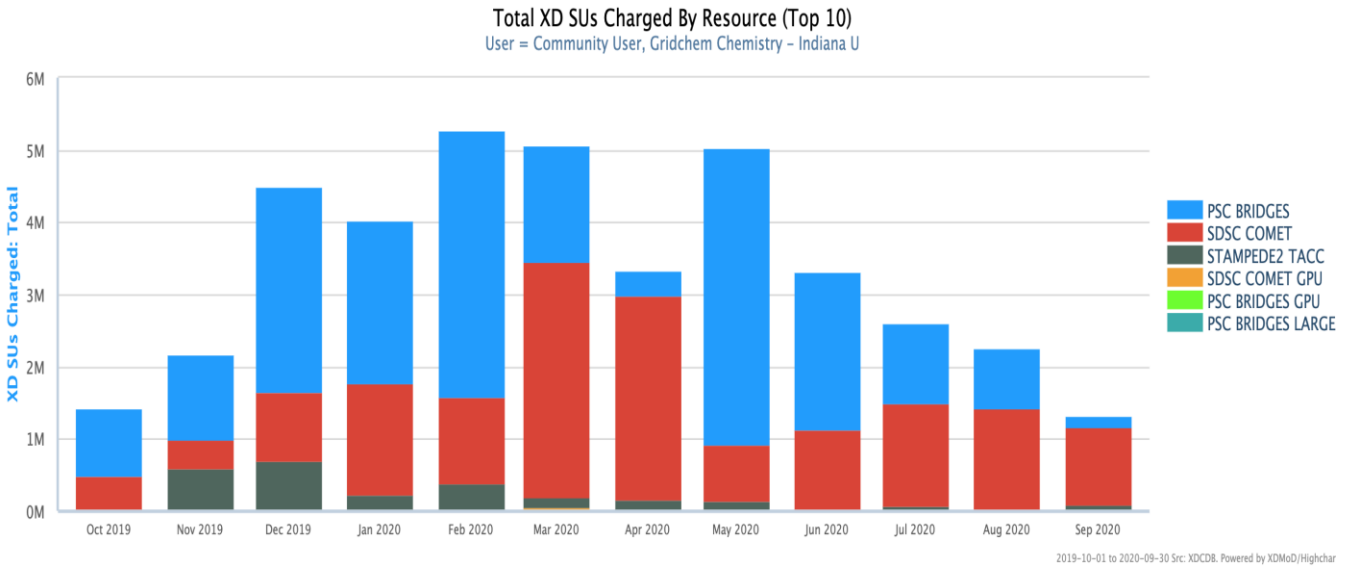
- Desktop Client for Pre and Post processing
- Dynamic Information Services (RSS, HPC Load data, Queue Prediction) Inherent workflow capability – Checkpoint Reuse, High throughput and Coupled Applications
- Allocations, PI specific user and resource management and Job level usage monitoring
- Consulting – Adaptive Services
- Data Archive

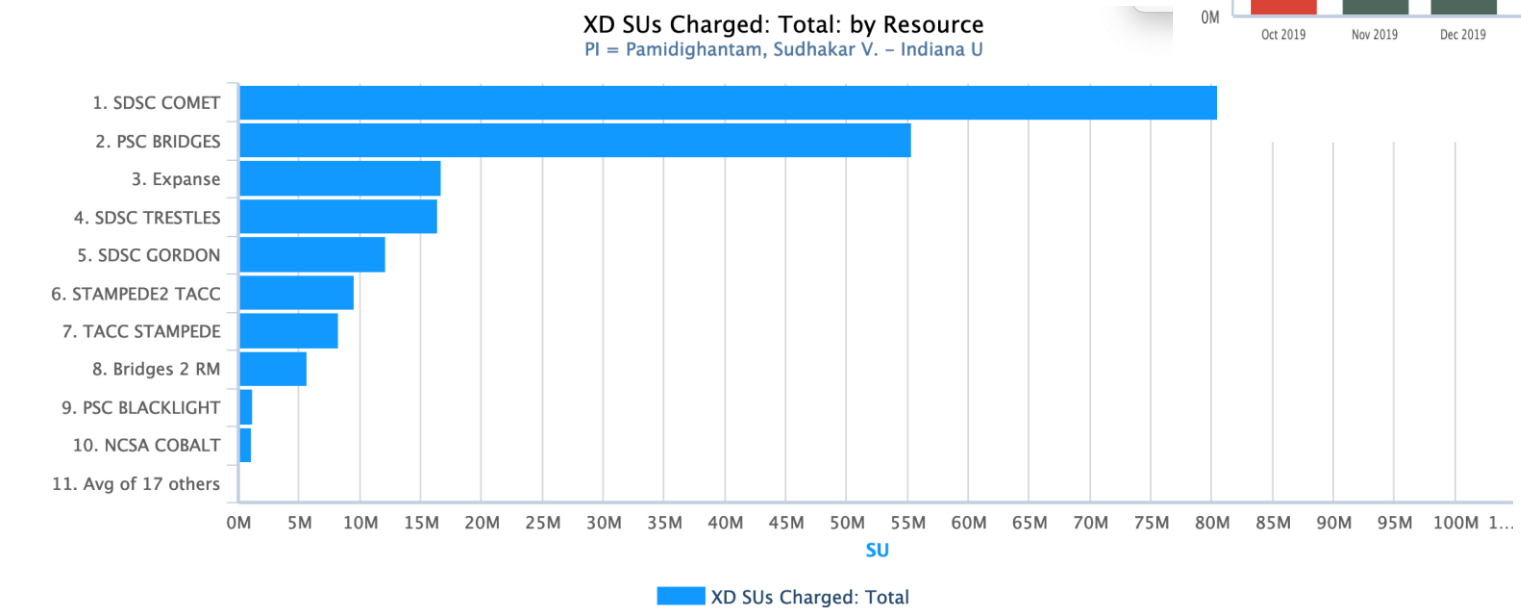
Application	Site	Host
Abaqus 6.14-1/6.13-3	SDSC	Comet
Abinit	Multiple	TACC/SDSC
AceMD	SDSC	Comet-GPU
Amber	Multiple	Systems in XSEDE
AutoDock-Vina	TACC,SDSC	Stampede2,Comet
BoltzTrap	SDSC	Comet
Charmm	SDSC	Comet
CP2K	SDSC	Comet
CPMD	SDSC	Comet
Dalton	PSC	Bridges
DDScat	SDSC	Comet
DFTB+	TACC	Stampede2
Gamd-Namd	SDSC	Comet
Gamess	SDSC	Comet, Bigred3, Karst
Gaussian 09/16	SDSC	Comet, Bridges, Bigred3, CO3
GNAT	TACC	Stampede2
Graph-MBT-ONIOM`	PSC	Bridges
Gromacs	Multiple	Systems in XSEDE
Lammps	Multiple	Systems in XSEDE
Molcas	TACC	Stampede
Nek5000	SDSC	Comet, Bigred3
NWChem	Multiple	Systems in XSEDE
Octopus	TACC	Stampede2
OpenMM	SDSC	Comet
Orca	TACC,PSC	Stampede2, Bridges
PolyUMod	SDSC	Comet
PSI4	SDSC	Comet, Stampede2
Quantum Espresso/6.1	Multiple	Systems in XSEDE

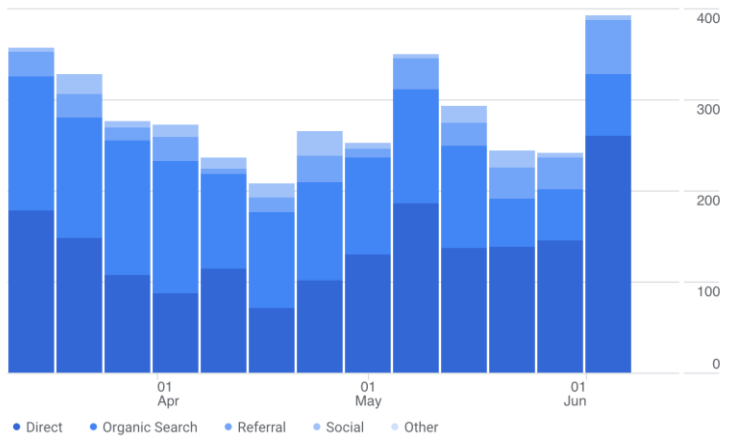
SEAGrid Usage



Among All Gateways in XSEDE

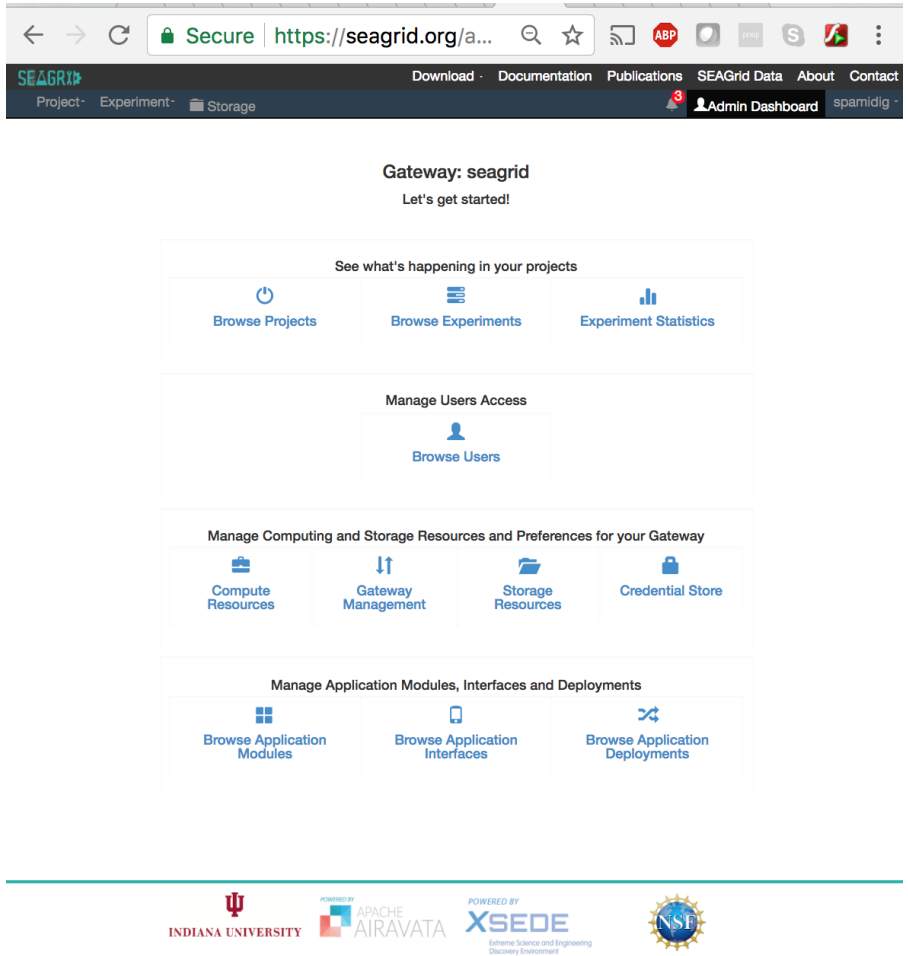


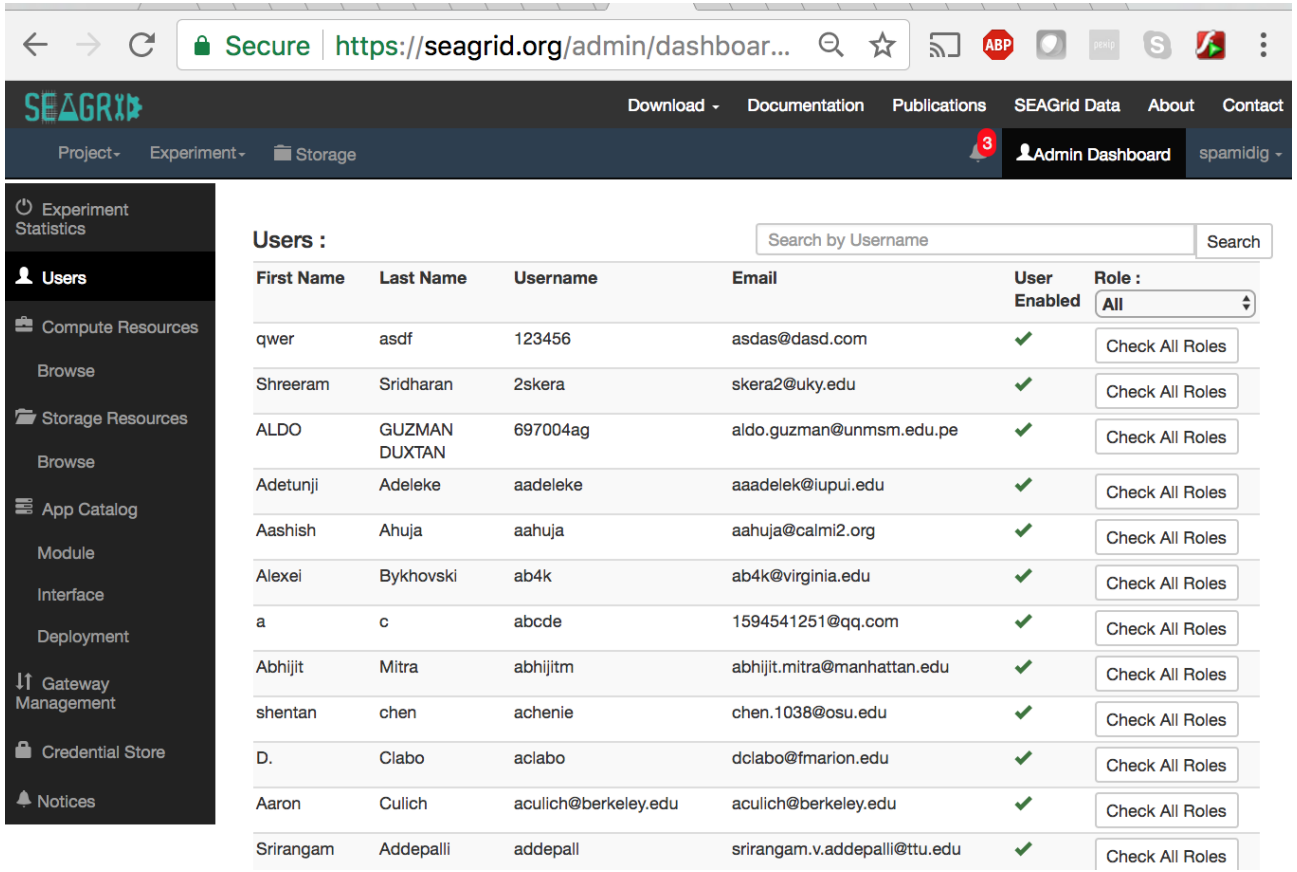




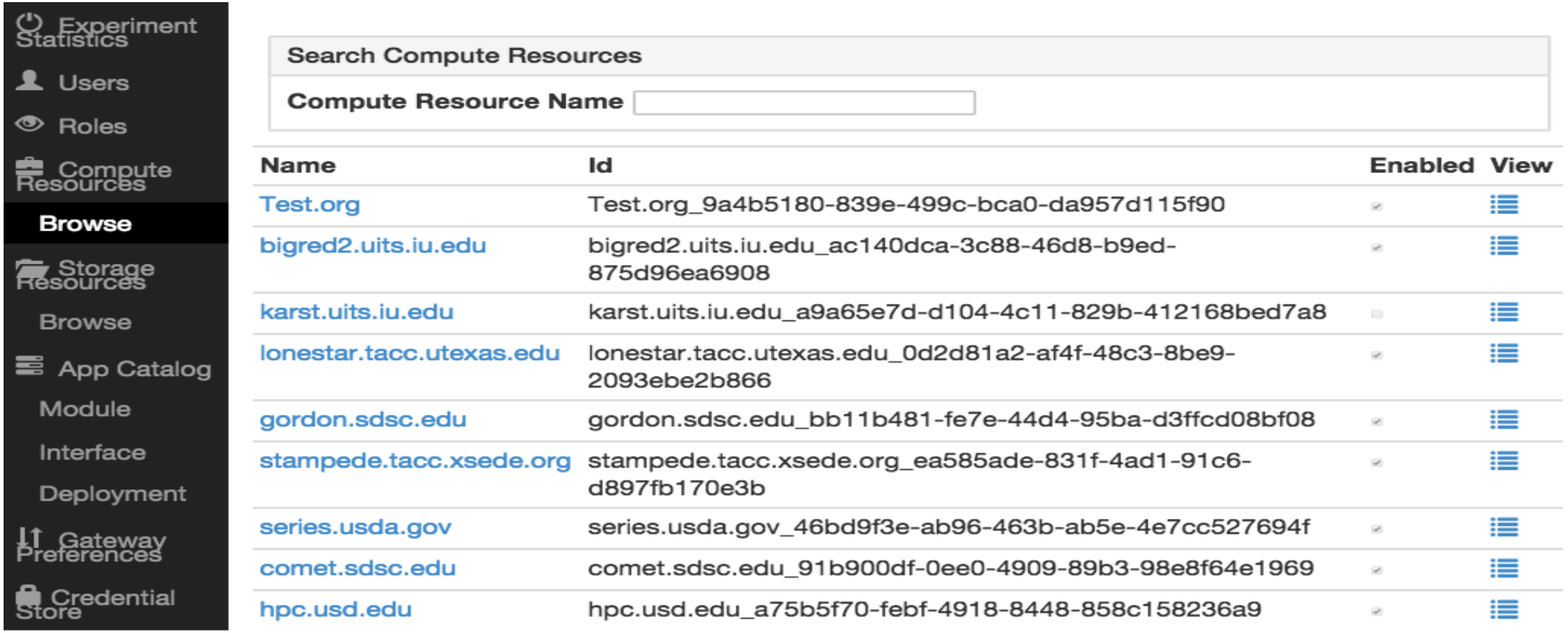
Google Analytics User Counts

SEAGrid Gateway Admin View



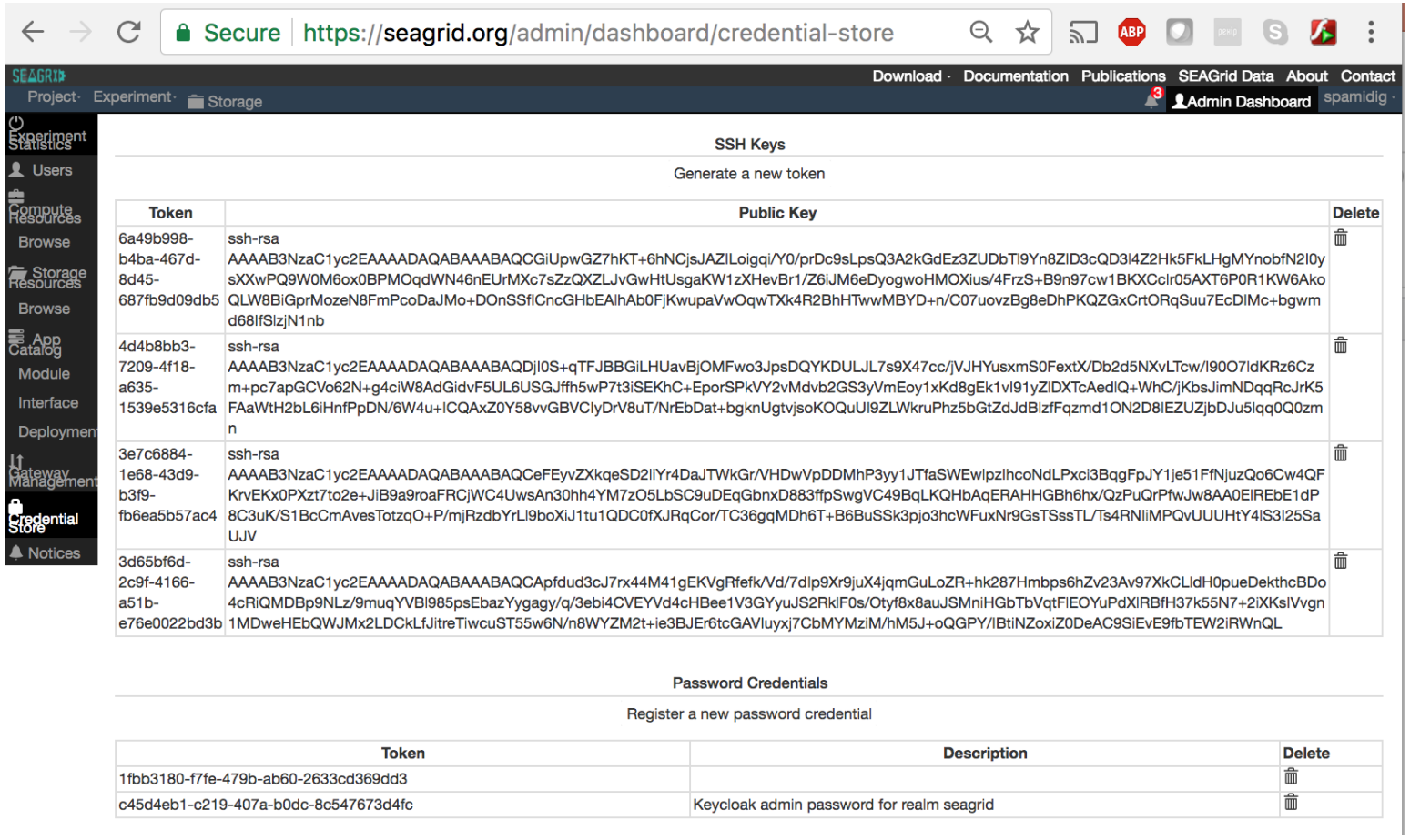


SEAGrid Admin Dashboard Compute Resource Browser

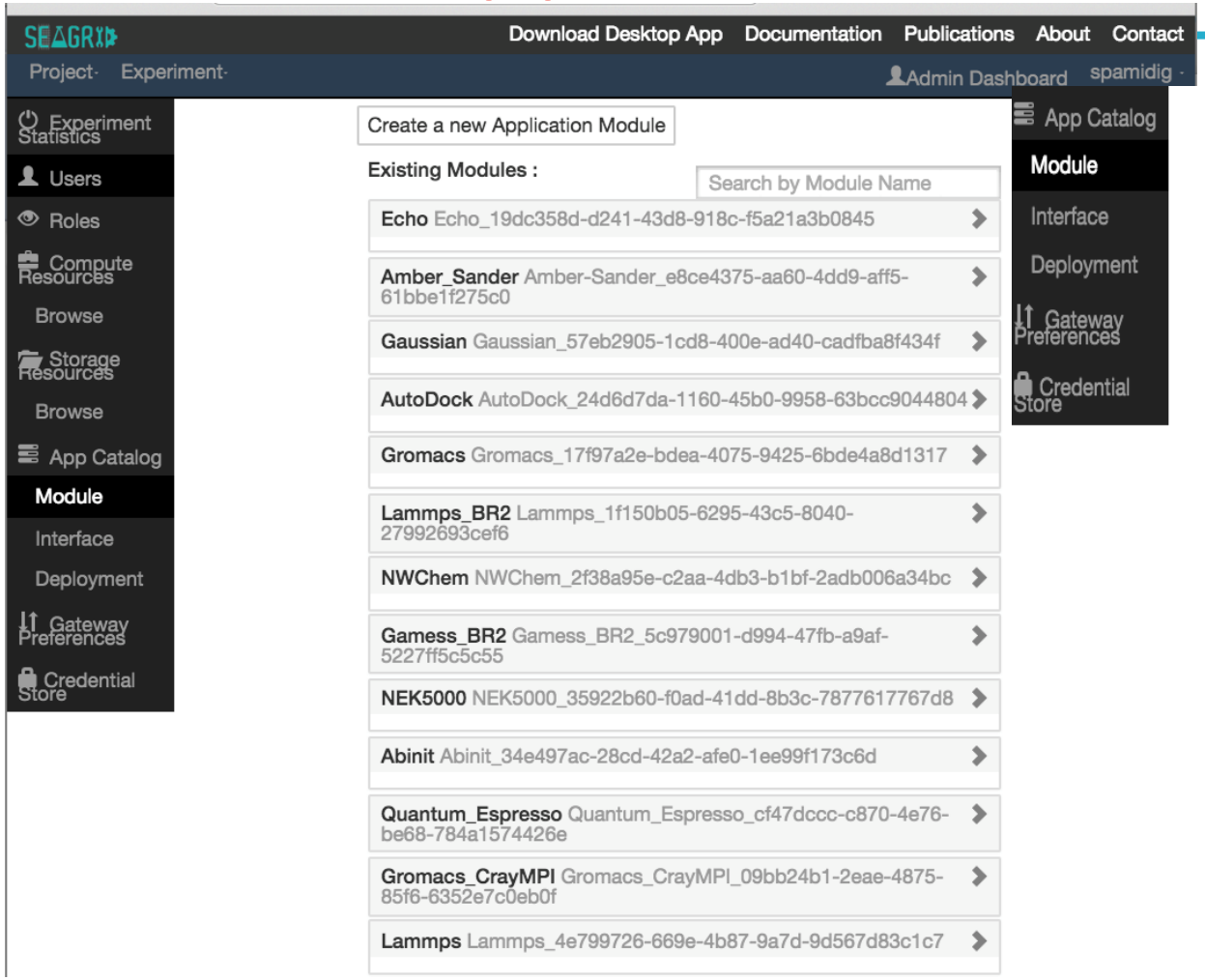


Name	Id	Enabled	View
Test.org	Test.org_9a4b5180-839e-499c-bca0-da957d115f90	☑	☰
bigred2.uits.iu.edu	bigred2.uits.iu.edu_ac140dca-3c88-46d8-b9ed-875d96ea6908	☑	☰
karst.uits.iu.edu	karst.uits.iu.edu_a9a65e7d-d104-4c11-829b-412168bed7a8	☐	☰
lonestar.tacc.utexas.edu	lonestar.tacc.utexas.edu_0d2d81a2-af4f-48c3-8be9-2093ebe2b866	☑	☰
gordon.sdsc.edu	gordon.sdsc.edu_bb11b481-fe7e-44d4-95ba-d3ffcd08bf08	☑	☰
stampede.tacc.xsede.org	stampede.tacc.xsede.org_ea585ade-831f-4ad1-91c6-d897fb170e3b	☑	☰
series.usda.gov	series.usda.gov_46bd9f3e-ab96-463b-ab5e-4e7cc527694f	☑	☰
comet.sdsc.edu	comet.sdsc.edu_91b900df-0ee0-4909-89b3-98e8f64e1969	☑	☰
hpc.usd.edu	hpc.usd.edu_a75b5f70-febf-4918-8448-858c158236a9	☑	☰

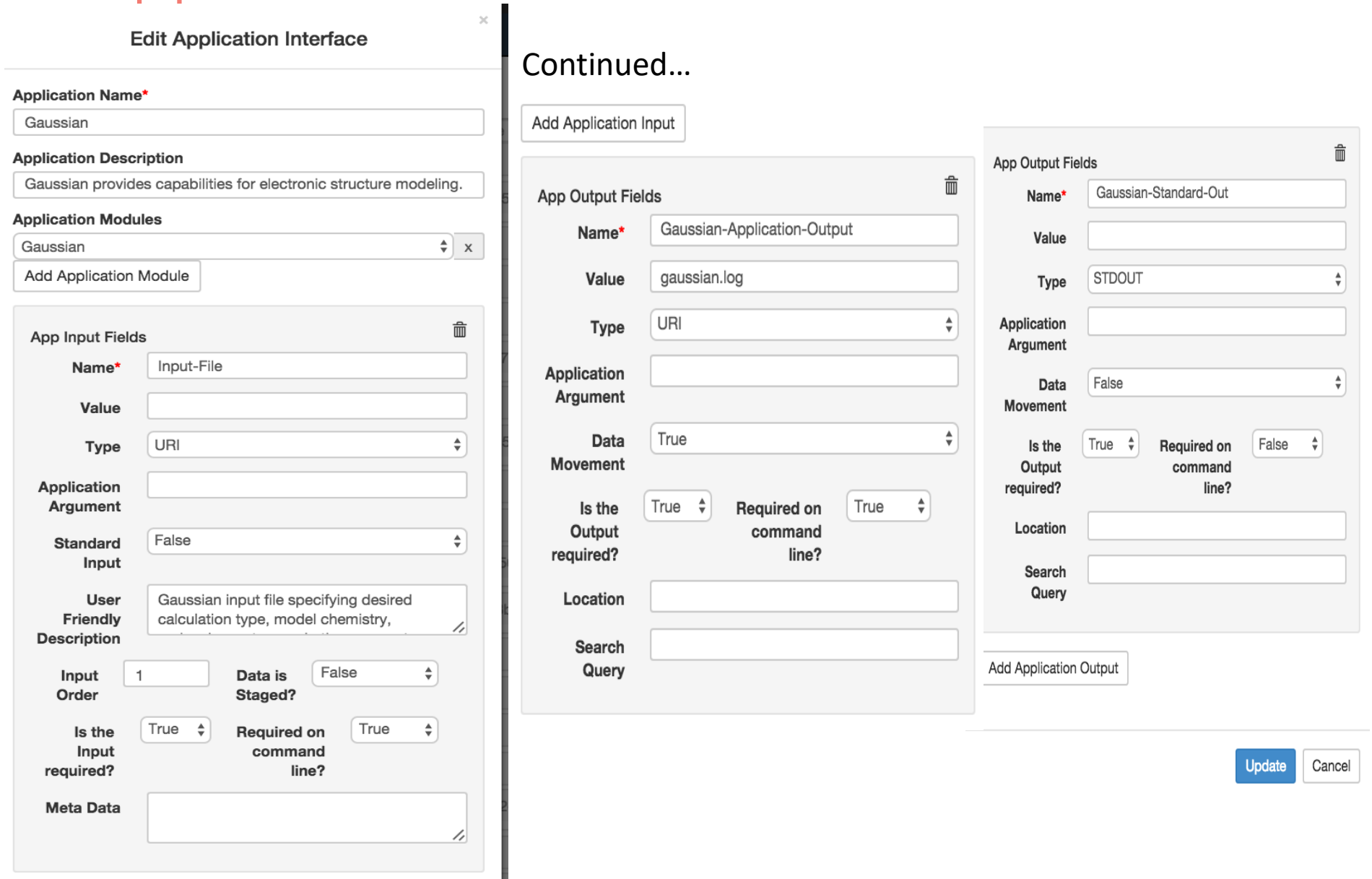
SEAGrid Gateway Credential Store



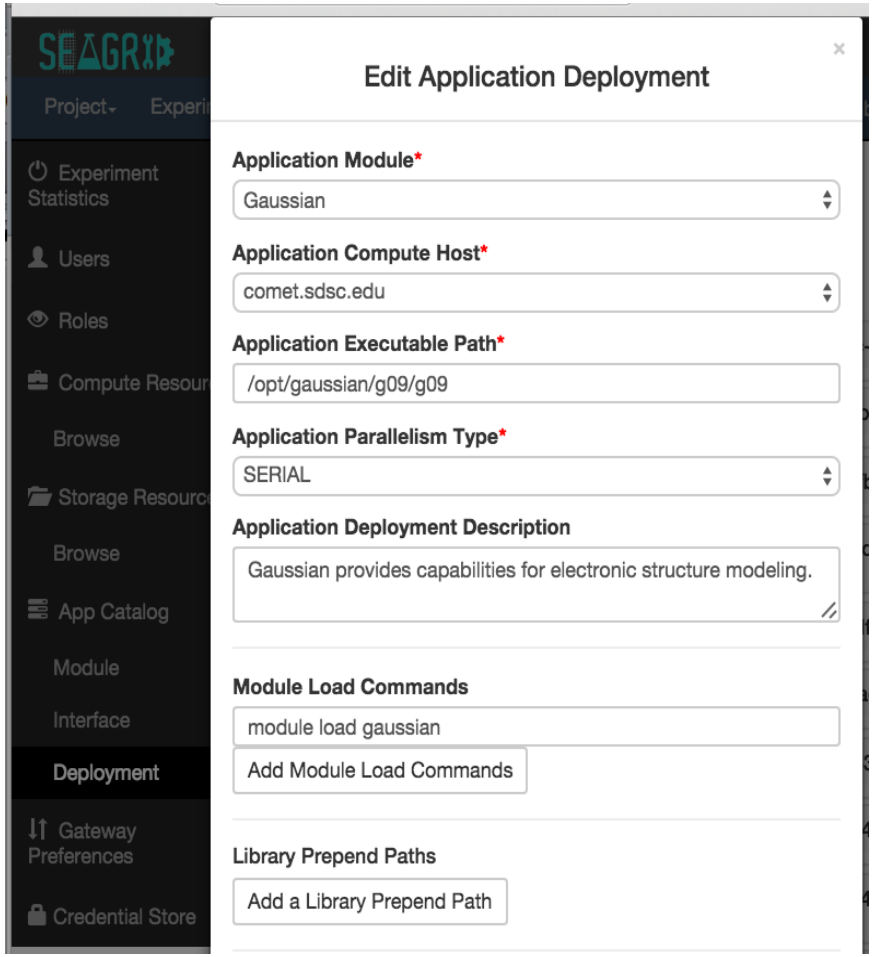
SEAGrid Application Catalog



Application Interface Editor



Application Deployment Editor



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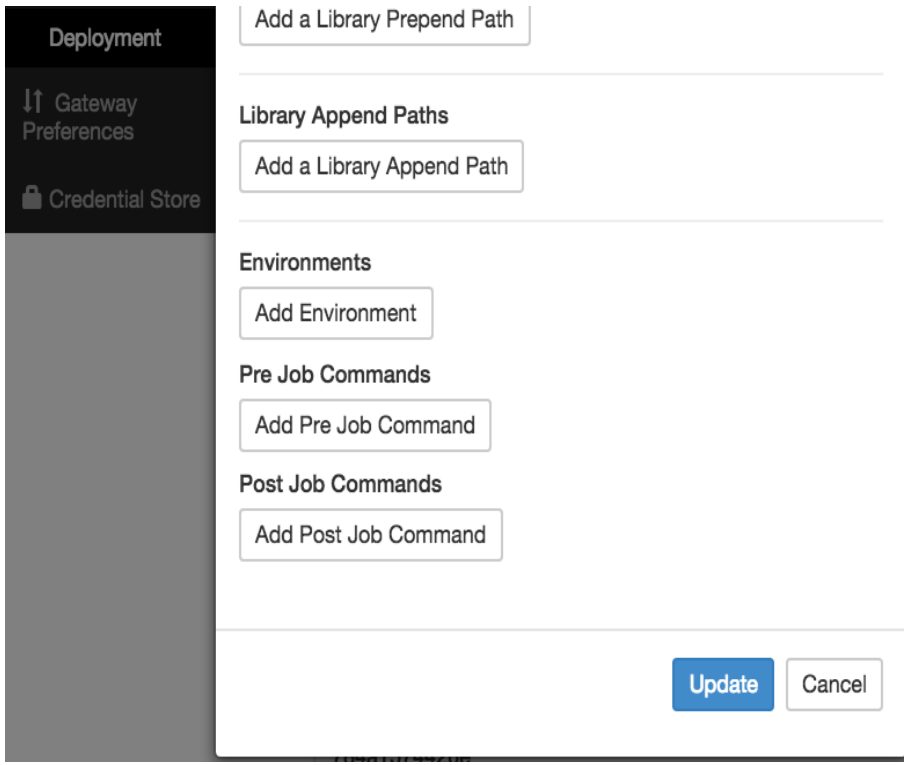
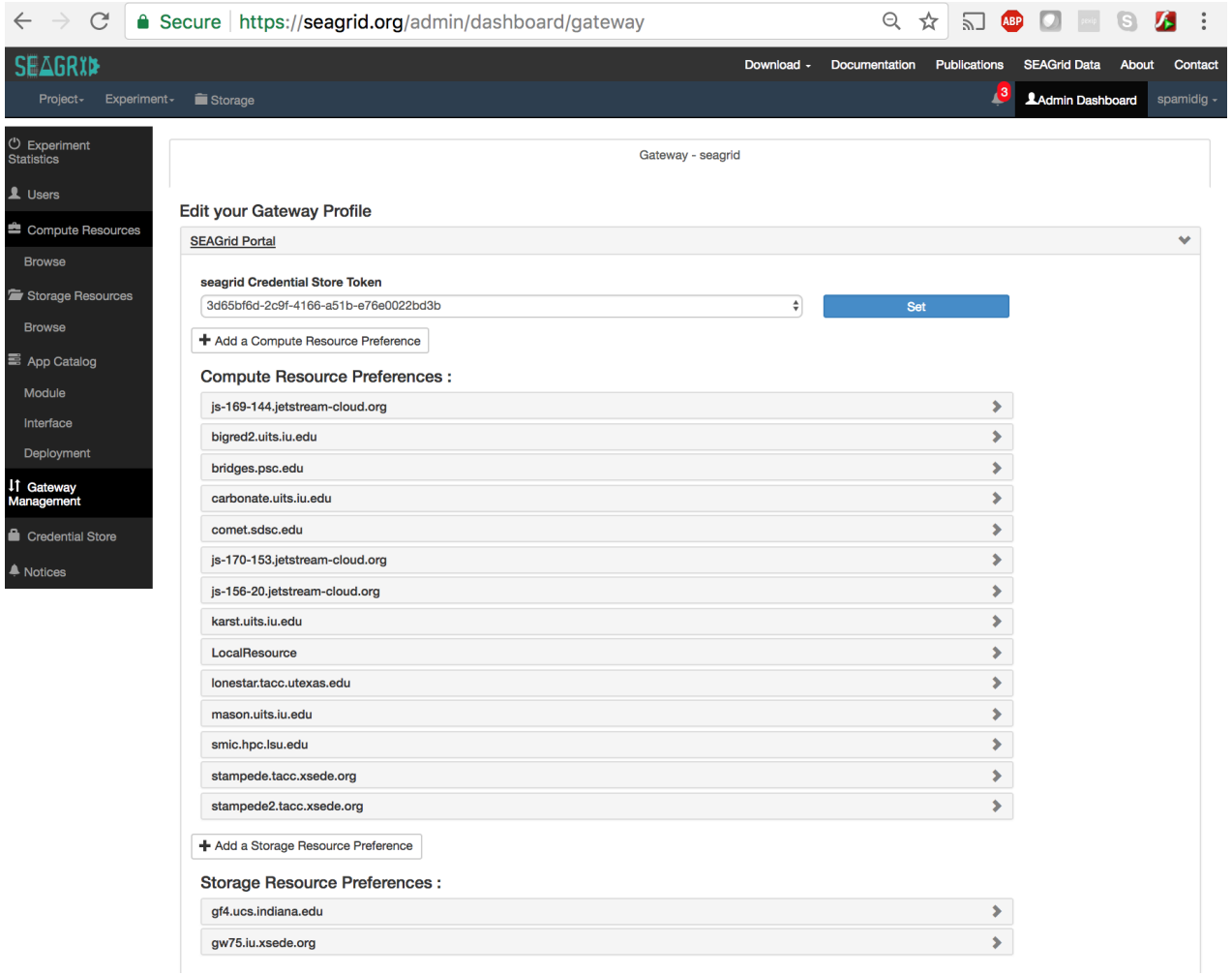
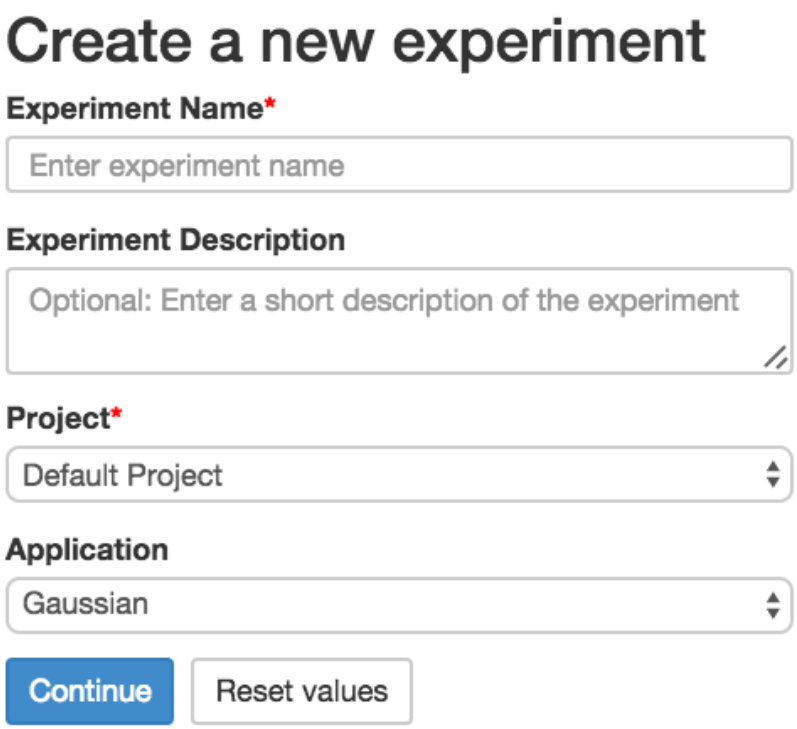
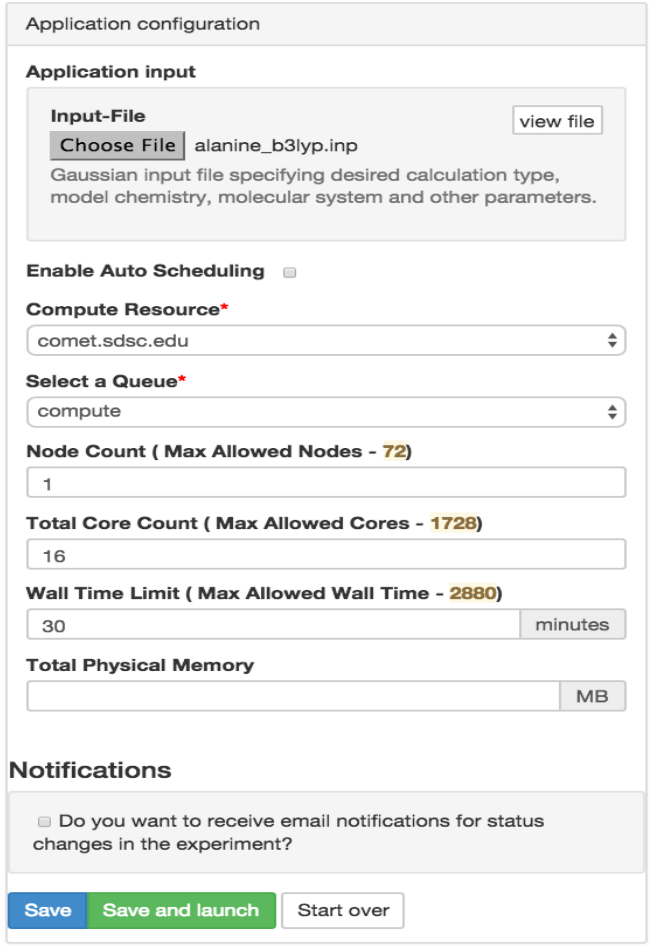


Gateway Profile



SEAGrid Experiment Creation





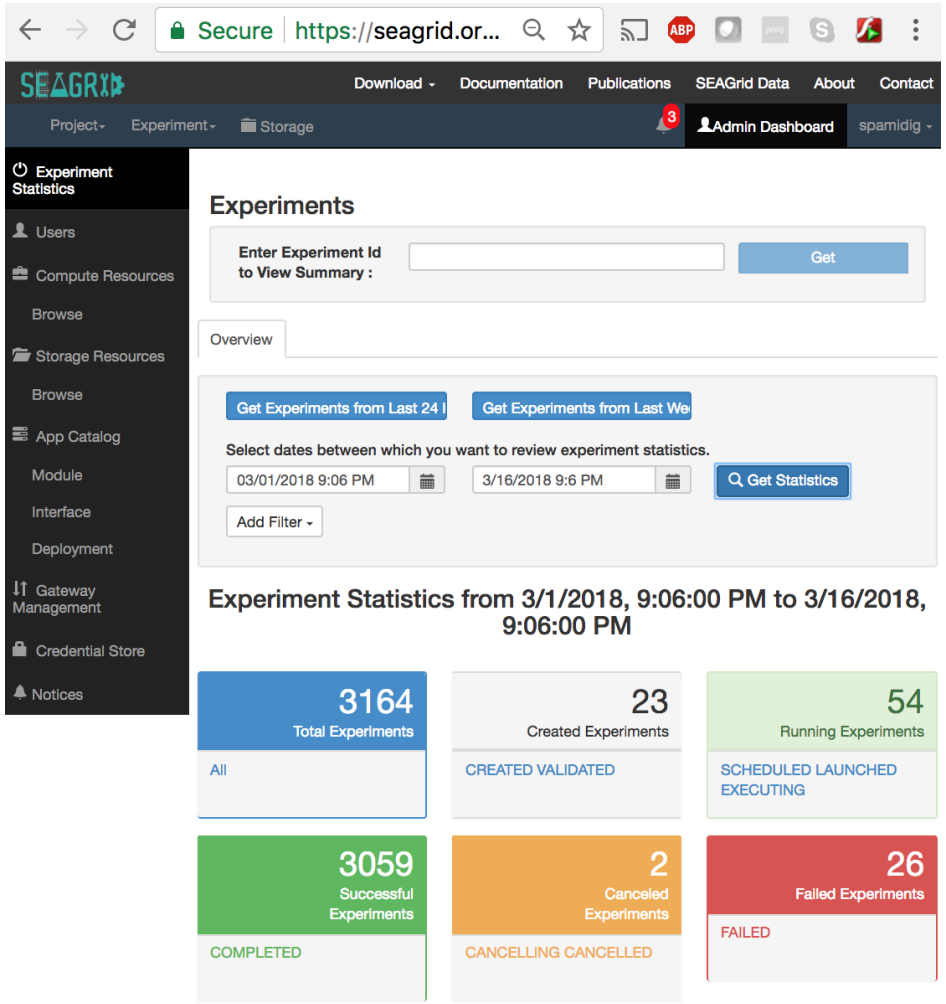
SEAGrid Experiment Status

Experiment Summary

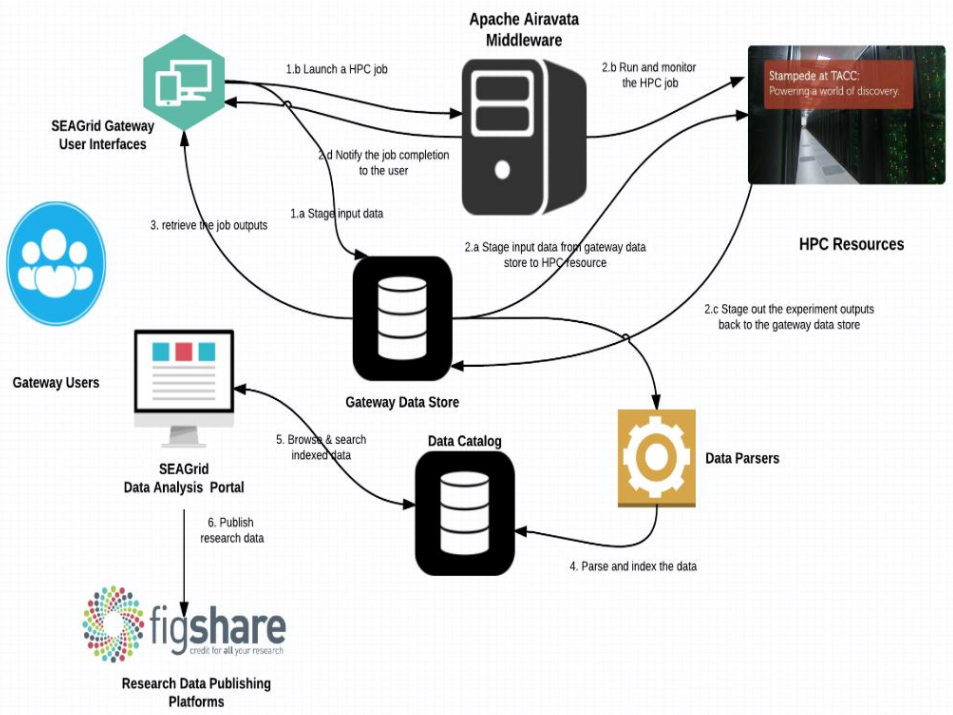
Enable Auto Refresh ON OFF

Experiment Id	Tests_3299e7ce-e87c-433c-96f7-f8514123ef07
Name	Tests
Description	Tests
Project	Default Project
Application	Gaussian
Compute resource	comet.sdsc.edu
Experiment Status	EXECUTING
Job	Name: A920254545 | ID: 1739851 | Status: QUEUED | Creation Time: 2016-03-11, 9:45 AM - GMT-0600 (CST)
Creation time	2016-03-11, 9:45 AM - GMT-0600 (CST)
Last Modified Time	2016-03-11, 9:45 AM - GMT-0600 (CST)
Enable Auto Schedule	false
Wall time	30
CPU count	16
Node count	1
Queue	compute
Inputs	alanine_b3lyp.inp
Outputs	Experiment hasn't completed. Experiment Status is : EXECUTING
Storage Directory	Open
Errors	

SEAGrid Admin Experiment Viewer



SEAGrid Data Catalog



SEAGrid Data Catalog | Search | Directory Browser | spamidig

AND OR | + Add rule | Add group

Formula | contains | C5H12O2 | Delete

Reset | Search | Page Size 10

Experiment Name	Owner Name	Package	Formula	Finished Time	Basis Set	Number of Basis Functions	Energy
Clone_of_neopentanediol_G16_B5	spamidig	Gaussian 16, Revision B.01	C5H12O2	07-Mar-2019	CC-pVDZ	158	-348.2027935
synpentane24diol.153	spamidig	Gaussian 16, Revision B.01	C5H12O2	24-Jul-2018	CC-pVDZ	158	-348.2198212
npenatne12diol	spamidig	Gaussian 16, Revision B.01	C5H12O2	24-Jul-2018	CC-pVDZ	158	-348.2027935
NPENTANEDIOL.153	spamidig	Gaussian 16, Revision B.01	C5H12O2	24-Jul-2018	CC-pVDZ	158	-348.2174693
npentane24diol.153	spamidig	Gaussian 16, Revision A.03	C5H12O2	23-Jul-2018	CC-pVDZ	158	-348.2174692
isopentane13diol	spamidig	Gaussian 16, Revision A.03	C5H12O2	20-Jul-2018	CC-pVDZ	158	-348.2018422
Clone_of_Neopentane	spamidig	Gaussian 16, Revision B.01	C5H12O2	20-Jul-2018	CC-pVDZ	158	-348.2027935
Clone_of_Clone_of_Neopentane	spamidig	Gaussian 16, Revision B.01	C5H12O2	20-Jul-2018	CC-pVDZ	158	-348.2027935
neopentanediol	spamidig	Gaussian 16, Revision B.01	C5H12O2	17-Jul-2018	CC-pVDZ	158	-348.2027935
npentane24diol.153	spamidig	Gaussian 16, Revision B.01	C5H12O2	17-Jul-2018	CC-pVDZ	158	-348.2174692

Export to CSV | next

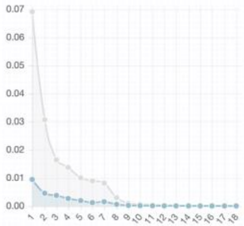
Output Metadata

SEAGrid Data Catalog Search Directory Browser spamidig

N.B: This data is automatically extracted using set of configured parser and may contain errors. Please report any issues in the issue tracker

Organization	
Experiment	LongCC_HC1.1521059306868
Project	sharingtest
Owner	spamidig
Indexed Time	2019-05-10 22:10:31
Molecule	
Formula	C42H26
Number of Atoms	68
Electron Symmetry	1-A
Multiplicity	1
Charge	0
Orbital Symmetry	Occupied A
Identifiers	
InChI	InChI=1S/C42H26/c1-5-13-33-27(9-1)17-18-28-10-2-6-14-34(28)41(33)37-25-23-31-21-22-32-24-26-38(40(37)39(31)32)42(41)35-15-7-3-11-29(35)19-20-30-12-4-8-16-36(30)42/h1-26H
InChI Key	QQYNKBIOZSXWGD-UHFFFAOYSA-N
SMILES	c12ccccc1C=Cc1c(cccc1)[C@@]12[C@]2(c3ccccc3C=Cc3c2cccc3)c2ccc3c4c2c1ccc4C=C3

Final Molecular Structure



Gradient vs Iteration

Canonical SMILES	c1ccc2c(c1)C=Cc1c([C@@]32c2ccc4c5c2c([C@@]23c3ccccc3C=Cc3c2cccc3)ccc5C=C4)cccc1
Calculation	
Package	Gaussian 09, Revision E.01
Calculation Type	FOpt; Freq
Methods	RB3LYP; RB3LYP
Basis Set	6-31G(d,p)
Number of Basis Functions	760
Number of Molecular Orbitals in the Calculation	760
Keywords	# RB3LYP/6-31G(d,p) GFInput GFPrint Iop(6/7=3) Opt Freq; #NGeom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d,p) Freq
Job Status	CalcDone
Calculated Properties	
Energy (au)	-1616.0971637
Dipole (debye)	-0.0328227,-0.1402467,0.0158595
HF (au)	-1616.0971637
Homos	138
Homo Eigenvalue (ev)	-5.340506429913
Homo Eigenvalues (ev)	Homo - 1 : -5.3832283044415, Homo - 2 : -5.78514046163, Homo - 3 : -5.8621486813215, Homo - 4 : -6.3320893011349995, Homo - 5 : -6.3739948341120005, Homo - 6 : -6.556311113946999, Homo - 7 : -6.667333564951, Homo - 8 : -6.744613898493, Homo - 9 : -6.965570345099,

Lumo Eigenvalue (ev)	-1.9453419172245
Lumo Eigenvalues (ev)	Lumo + 1 : -1.3630182771545, Lumo + 2 : -0.9167515623345, Lumo + 3 : -0.5586497350765, Lumo + 4 : -0.3235433682445, Lumo + 5 : -0.0383680529205, Lumo + 6 : 0.1820441659845, Lumo + 7 : 0.4051775233945, Lumo + 8 : 0.519737454455, Lumo + 9 : 0.573615996854,
Zero Point Energy (Hartree/Particle)	0.5430401
NImag	0
Thermal (Hartree/Particle)	0.5721956
Enthalpy (Hartree/Particle)	0.573140;
Gibbs (Hartree/Particle)	0.485218;
Execution Environment	
Calculated By	GCOMMUNI
Calculated Machine	GINC-R677
Finished Time	14-Mar-2018
Job CPU Run Time	130491.1 seconds
Memory	3000 MB
Number of Shared Processors	28
Input File Configuration	
Link 0 Commands	%nproc=28;%mem=3000MB;%Chk=longccHC_CeN.chk
Route Commands	# RB3LYP/6-31G(d,p) GFInput GFPrint Iop(6/7=3) Opt Freq

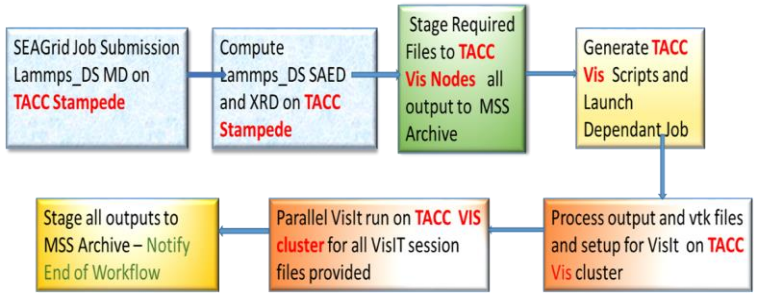
File Set	
Gaussian Input File	gaussian.in
Gaussian Output File	gaussian.log
Gaussian Checkpoint File	longccHC_CeN.chk
SDF Structure File	structure.sdf
PDB Structure File	structure.pdb
InChI File	inchi.txt
SMILES File	smiles.txt

Make Public

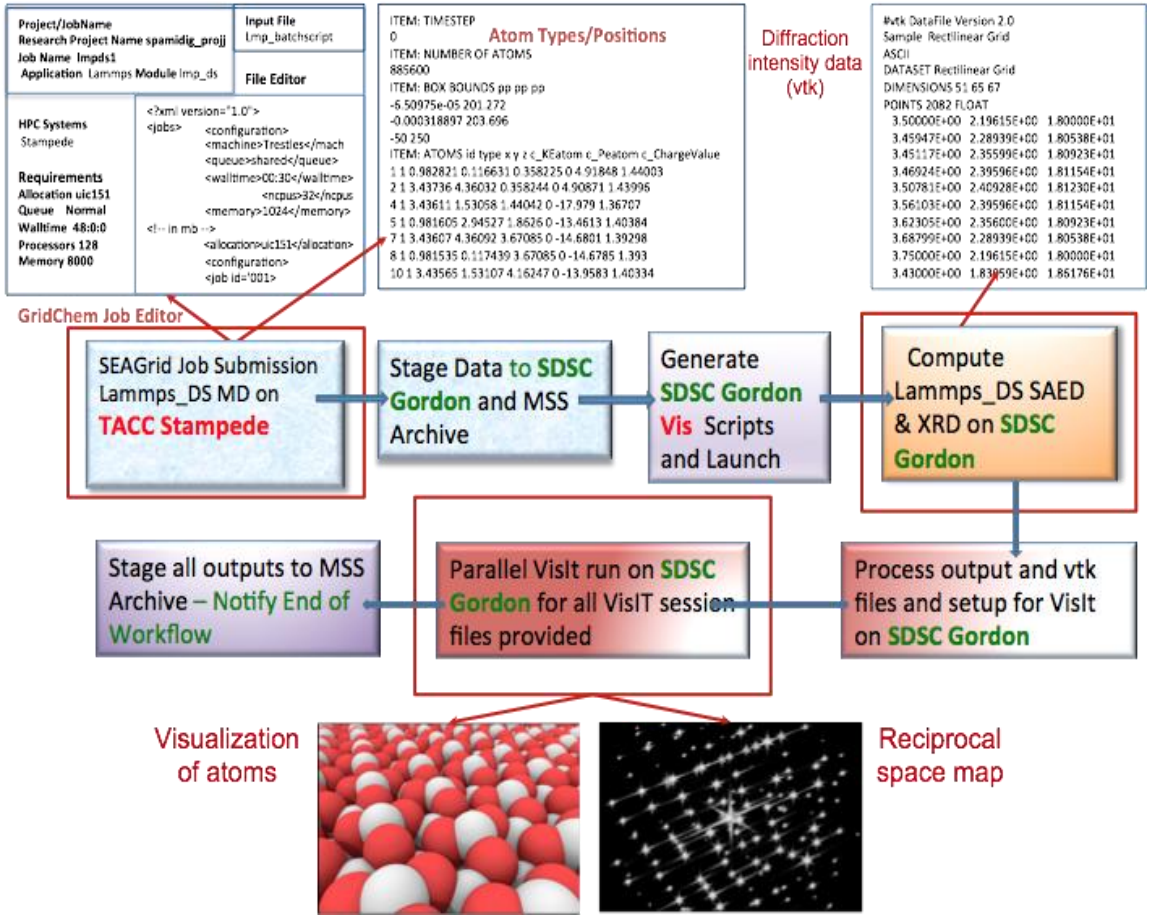
Workflow and Visualization

An XSEDE ECSS Project

- For large memory calculations a workflow is required to use the appropriate XSEDE resource
  - TACC Stampede: Atomistic simulation of alumina
  - SDSC Gordon: Calculation of diffraction intensities + Visualization
- Workflow implemented through SEAGrid Science gateway
  - Supports a private “DS” LAMMPS build
  - Supports single job ID handle for multi-resource job submission
  - Supports the development of a XML script for high throughput job submission
  - Compatible with parallel VisIt executions so that diffraction pattern generation is automated

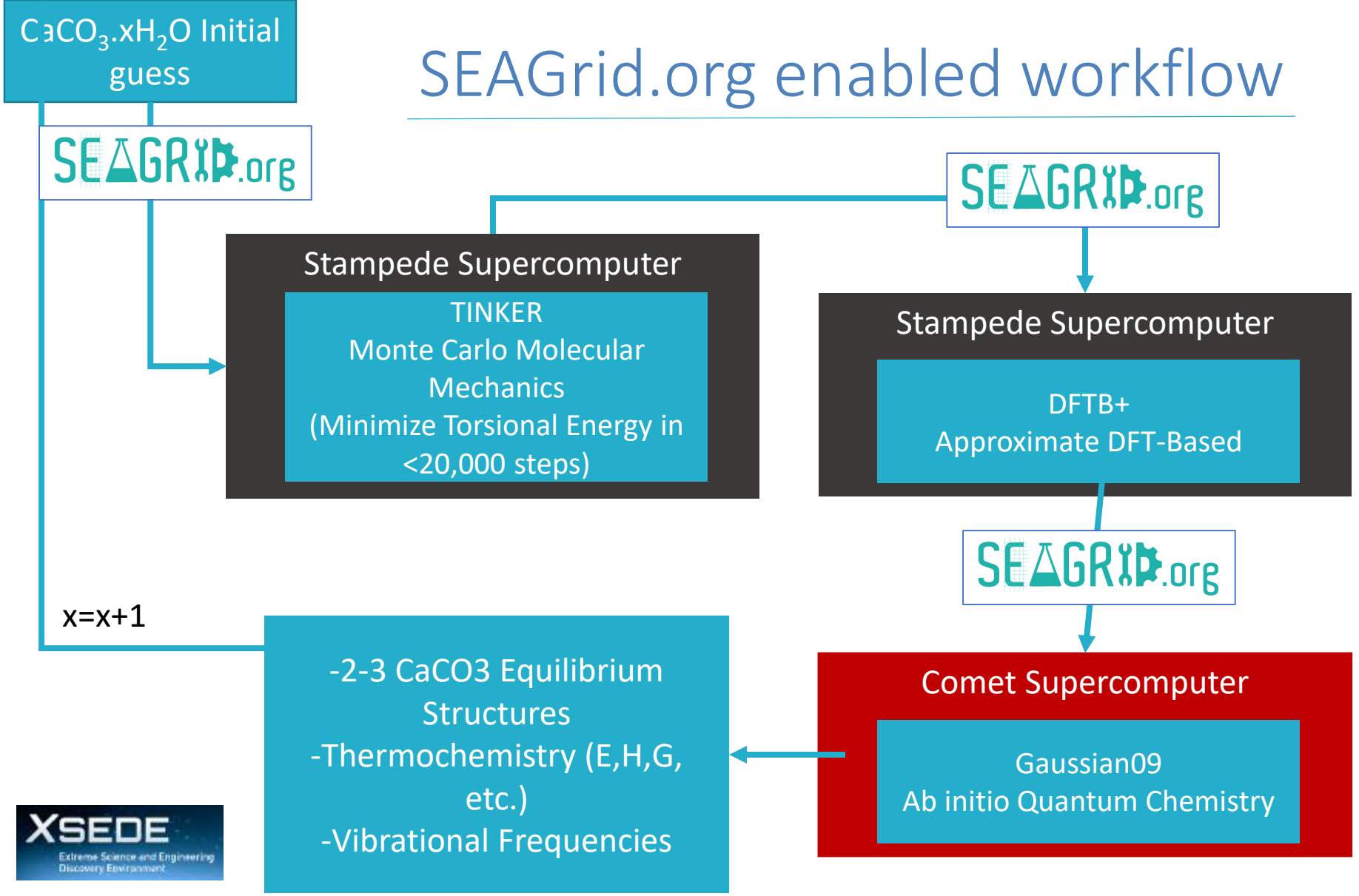


Workflow to run on TACC resources only



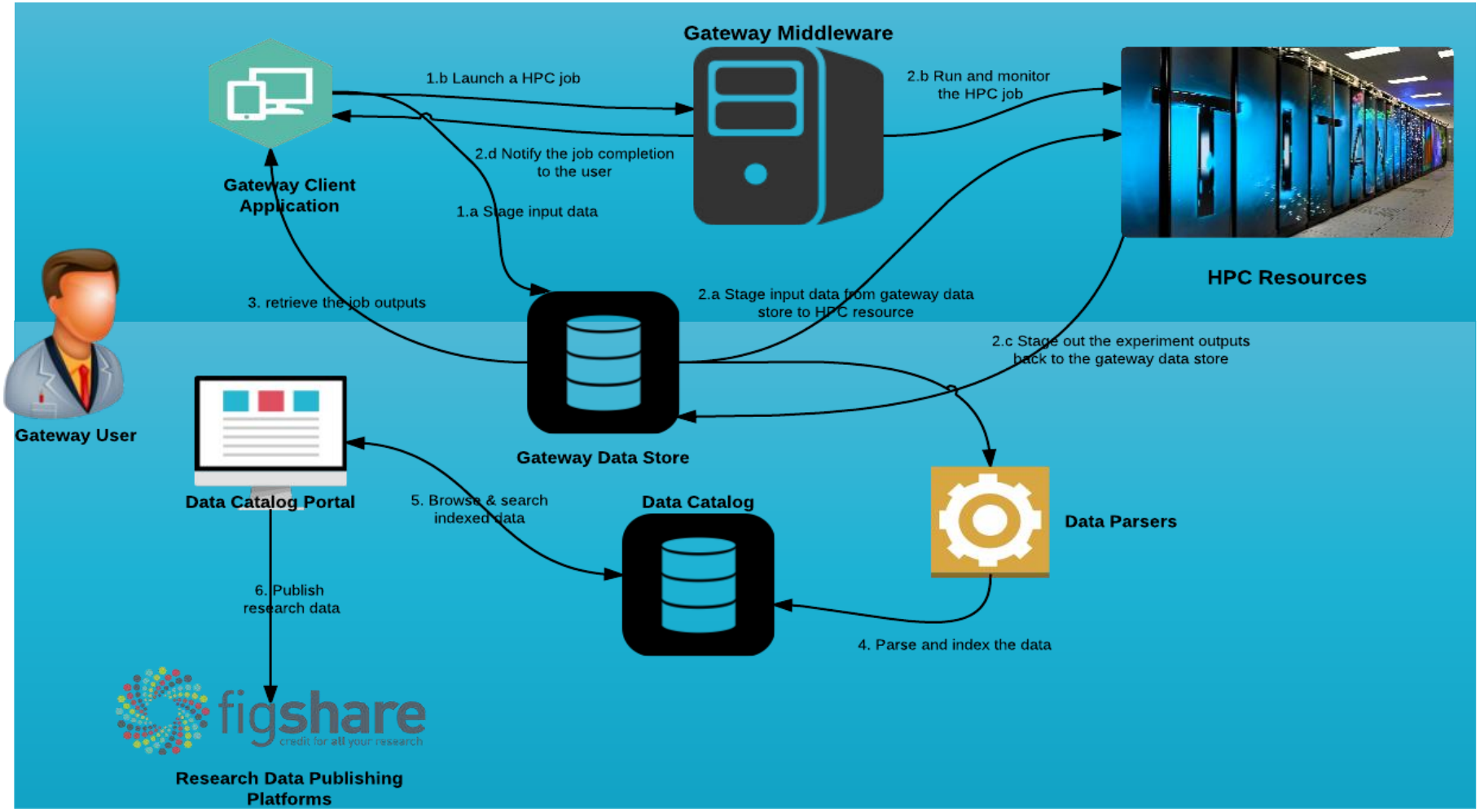
Workflow running on TACC and SDSC Resources

SEAGrid.org enabled workflow

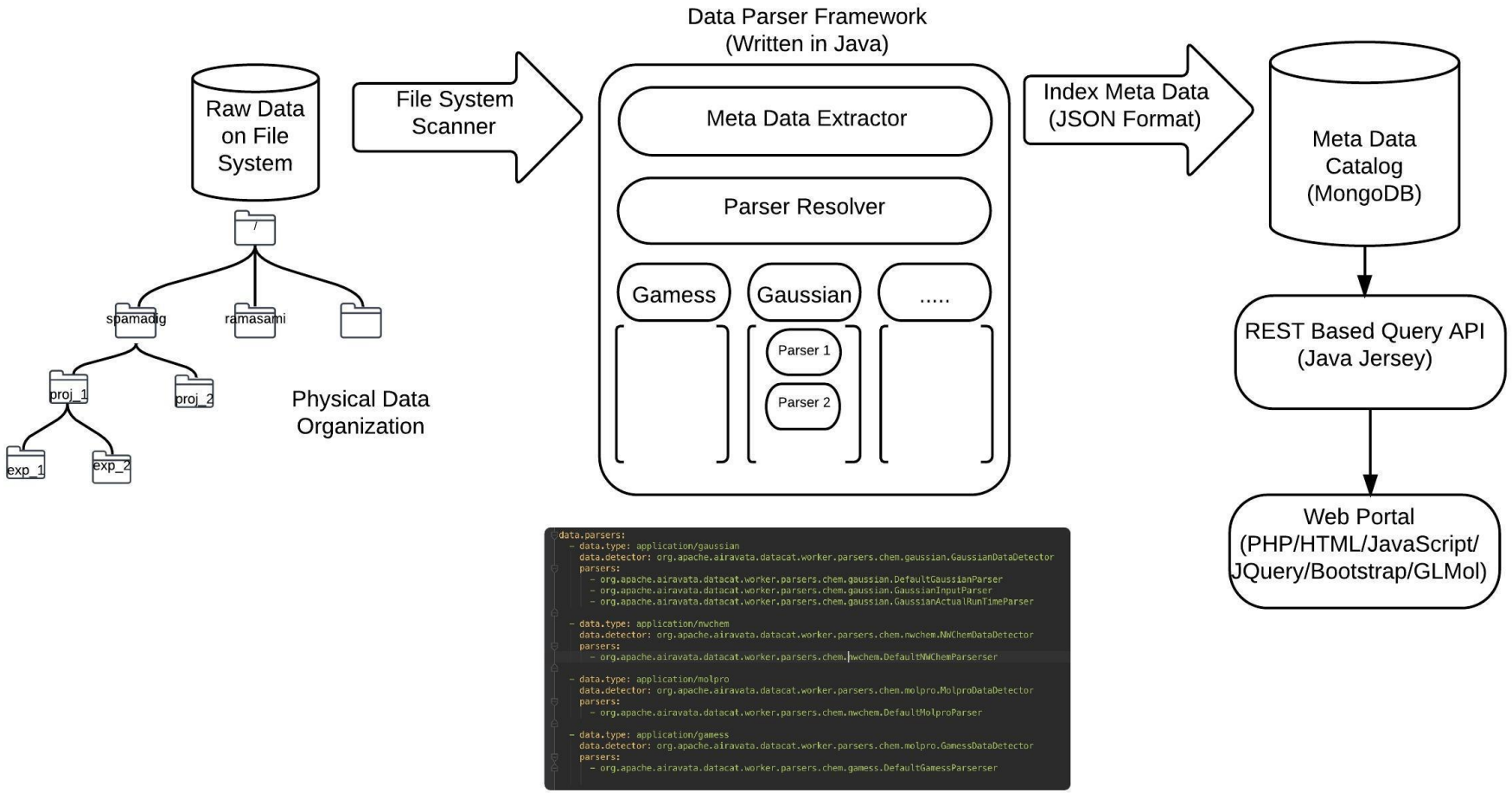


Lopez-Berganza, et al. *J Phys. Chem. A*(2015)

SEAGrid Data Catalog

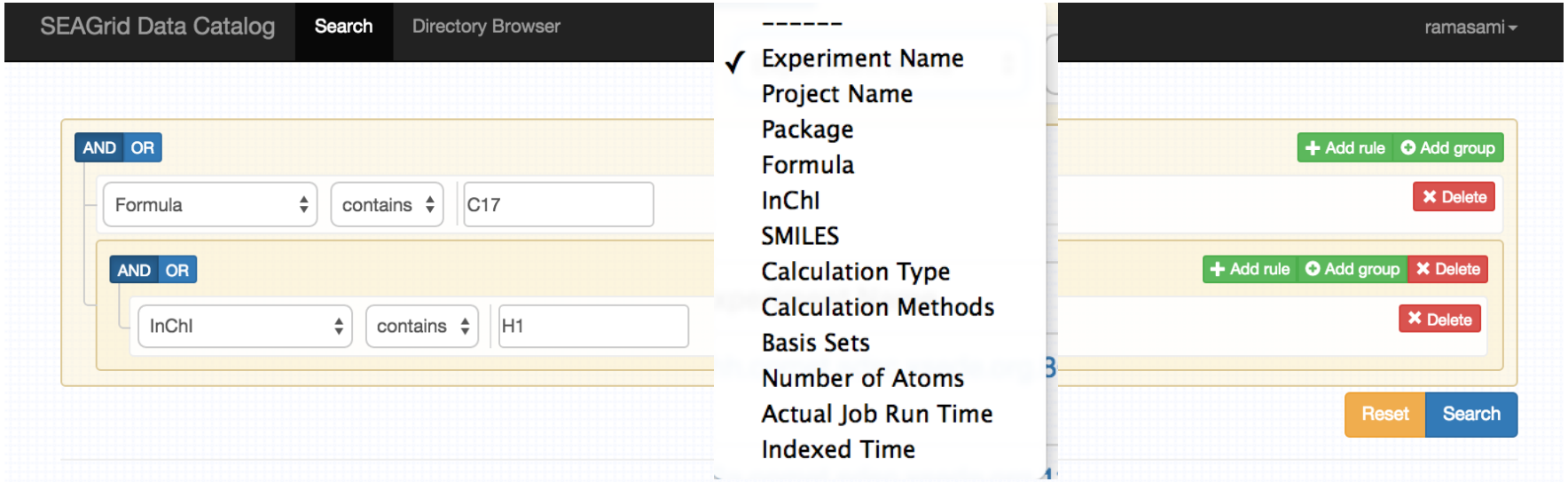


SEAGrid Data System Architecture



Parser Configuration

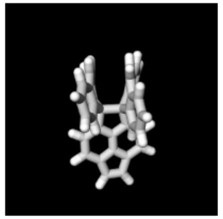
Searching for Cataloged Data



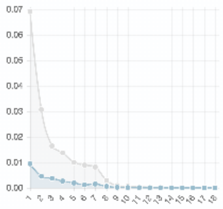
Experiment Name	Project Name	Package	Formula	Indexed Time
bm28.comet.sdsc.xsede.org.738999.150801	ramasami_proj	Gaussian 09, Revision D.01	C17H11NO2S	2016-03-03 23:53:15
h_dv1.trestles.sdsc.teragrid.org.2532797.150303	ramasami_proj	Gaussian 09, Revision D.01	C17H15NO	2016-03-03 23:28:46
ms95.gordon.sdsc.edu.2048727.150513	ramasami_proj	Gaussian 09, Revision D.01	C17H11NO2S	2016-03-03 23:21:40
mb20.trestles.sdsc.teragrid.org.2583124.150422	ramasami_proj	Gaussian 09, Revision D.01	C17H11NO2S	2016-03-03 23:16:17
bm23.comet.sdsc.xsede.org.738994.150801	ramasami_proj	Gaussian 09, Revision D.01	C17H11NO2S	2016-03-03 23:12:08
mre3.comet.sdsc.xsede.org.678254.150709	ramasami_proj	Gaussian 09, Revision D.01	C17H13Br2ClFeN3O2S(2)	2016-03-03 23:09:35

Output Metadata

Organization	
Experiment	LongCC_HC1.1521059306868
Project	sharingtest
Owner	spamidig
Indexed Time	2018-03-14 17:50:40
Molecule	
Formula	C42H26
Number of Atoms	68
Electron Symmetry	1-A
Multiplicity	1
Charge	0
Orbital Symmetry	Occupied A
Identifiers	
InChI	InChI=1S/C42H26/c1-5-13-33-27(9-1)17-18-28-10-2-6-14-34(28)41(33)37-25-23-31-21-22-32-24-26-38(40(37)39(31)32)42(41)35-15-7-3-11-29(35)19-20-30-12-4-8-16-36(30)42/h1-26H
InChI Key	QQYNKBIOZSXWGD-UHFFFAOYSA-N
SMILES	c12ccccc1C=Cc1c(cccc1)[C@@]12[C@]2(c3ccccc3C=Cc3c2cccc3)c2ccc3c4c2c1ccc4C=C3



Final Molecular Structure



Gradient vs Iteration

Canonical SMILES	c1ccc2c(c1)C=Cc1c([C@@]32c2ccc4c5c2c([C@@]23c3ccccc3C=Cc3c2cccc3)ccc5C=C4)cccc1
Calculation	
Package	Gaussian 09, Revision E.01
Calculation Type	FOpt; Freq
Methods	RB3LYP; RB3LYP
Basis Set	6-31G(d,p)
Number of Basis Functions	760
Number of Molecular Orbitals in the Calculation	760
Keywords	# RB3LYP/6-31G(d,p) GFInput GFPrint Iop(6/7=3) Opt Freq; #NGeom=AllCheck Guess=TCheck SCRF=Check Test GenChk RB3LYP/6-31G(d,p) Freq
Job Status	CalcDone
Calculated Properties	
Energy	-1616.0971637
Dipole	-0.0328227,-0.1402467,0.0158595
HF	-1616.0971637
Homos	[138]

Execution Environment	
Calculated By	GCOMMUNI
Calculated Machine	GINC-R677
Finished Time	14-Mar-2018
Job CPU Run Time	130491.1 seconds
Memory	3000 MB
Number of Shared Processors	28
Input File Configuration	
Link 0 Commands	%nproc=28;%mem=3000MB;%Chk=longccHC_CeN.chk
Route Commands	# RB3LYP/6-31G(d,p) GFInput GFPrint Iop(6/7=3) Opt Freq
File Set	
Gaussian Input File	gaussian.in
Gaussian Output File	gaussian.log
Gaussian Checkpoint File	longccHC_CeN.chk
SDF Structure File	structure.sdf
PDB Structure File	structure.pdb
InChI File	inchi.txt
SMILES File	smiles.txt

Make Public

Cyberinfrastructure Integration Research Center

- Science Gateways Communities Institute EDS Activities
- XSEDE ECSS-Gateways Collaborations
- XSEDE ECSS ESRT/NIP Consulting
- NSF Grants –OGCE, SciGaP, XSEDE, JetStream, Cyberwater, DELTA_Topology, Graph-theory-based molecular fragmentation methods

- NASA Grants – GeoGateway
- Private Sector Partnerships

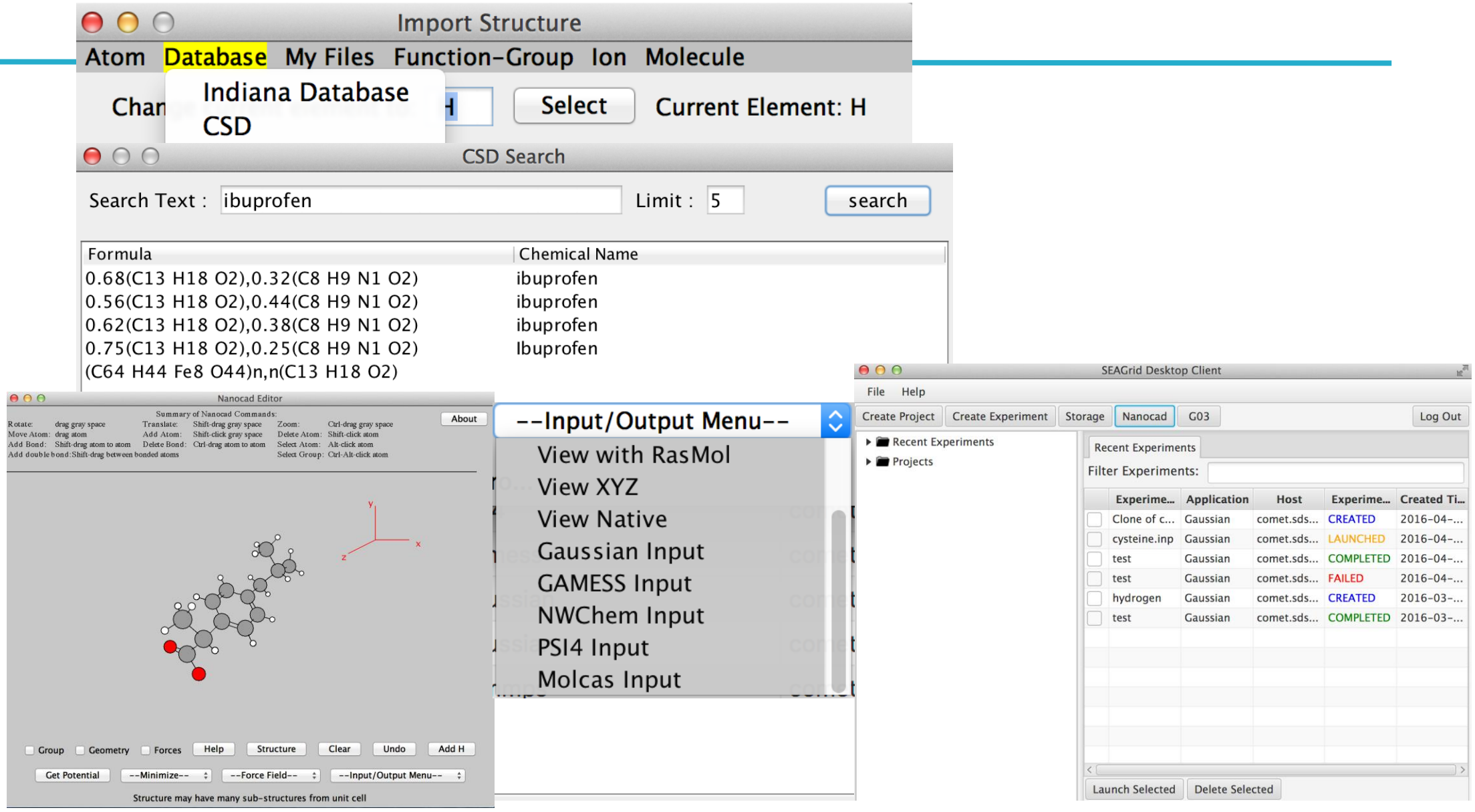
https://circ.iu.edu/

Acknowledgements and Contacts

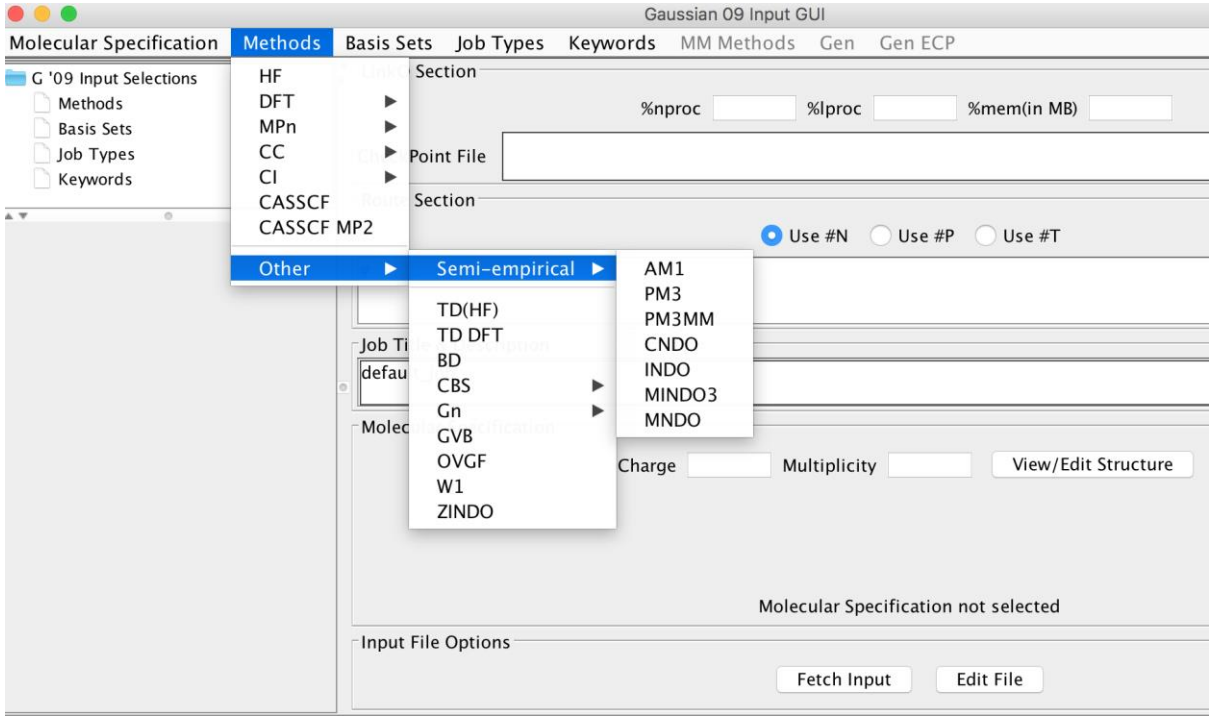
- NSF Grants ACI-1547611, ACI-1339774
- Apache Software Foundation
- Indiana University
- GSOC Programs
- Science Gateways Research Center https://circ.iu.edu/

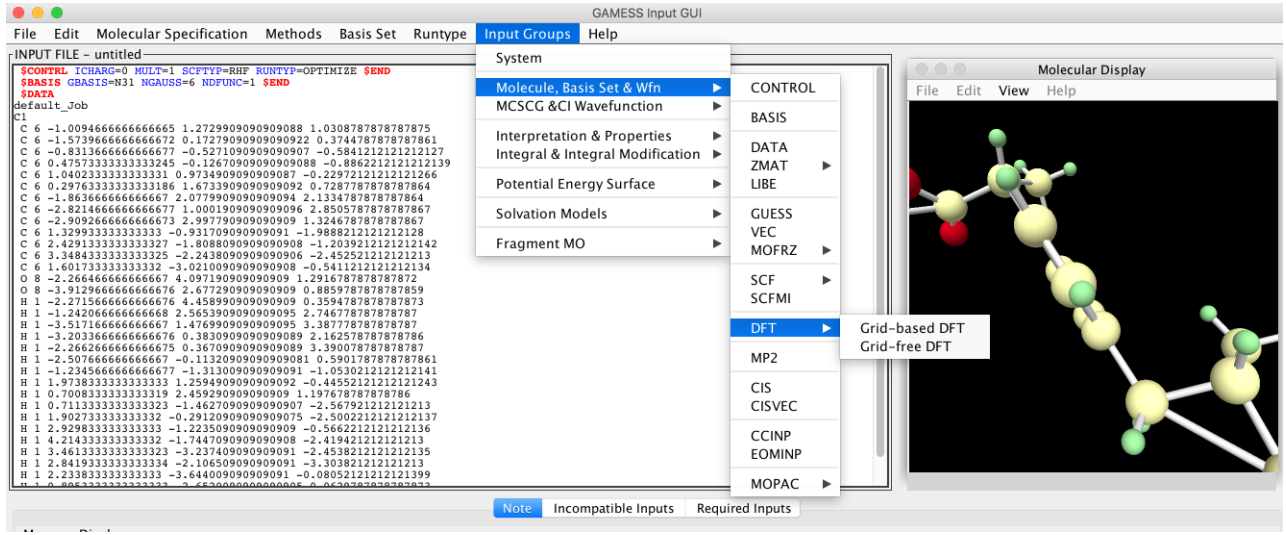
- Center email: sgrc-iu-group@iu.edu
- Marlon Pierce: marpierc@iu.edu, Director
- Apache Airavata Open Source Science Gateway Softwar http://airavata.apache.org/
- Sudhakar Pamidighantam pamidigs@iu.edu SEAGrid
- Suresh Marru: smarru@iu.edu Apache Airavata

SEAGrid Desktop Client CSD Database



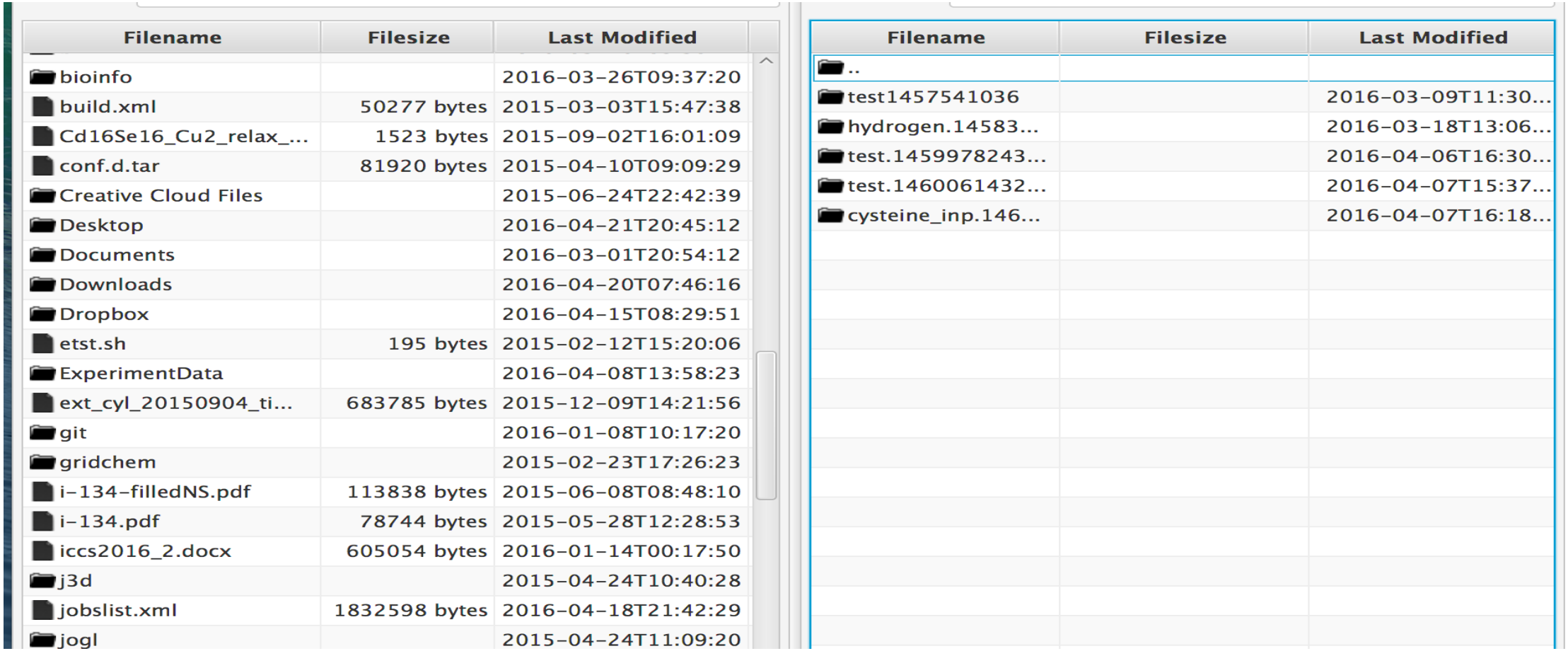
Graphical Interfaces to Application Software





SEAGrid Desktop Client

Storage Browser



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Cd16Se16_Cu2_relax_...	1523 bytes	2015-09-02T16:01:09
conf.d.tar	81920 bytes	2015-04-10T09:09:29
Creative Cloud Files		2015-06-24T22:42:39
Desktop		2016-04-21T20:45:12
Documents		2016-03-01T20:54:12
Downloads		2016-04-20T07:46:16
Dropbox		2016-04-15T08:29:51
etst.sh	195 bytes	2015-02-12T15:20:06
ExperimentData		2016-04-08T13:58:23
ext_cyl_20150904_ti...	683785 bytes	2015-12-09T14:21:56
git		2016-01-08T10:17:20
gridchem		2015-02-23T17:26:23
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i-134.pdf	78744 bytes	2015-05-28T12:28:53
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jogl		2015-04-24T11:09:20

Filename	Filesize	Last Modified
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test1457541036		2016-03-09T11:30...
hydrogen.14583...		2016-03-18T13:06...
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test.1460061432...		2016-04-07T15:37...
cysteine_inp.146...		2016-04-07T16:18...