

SGCI MOLSSI Workshop on Science Gateways

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Hiltonmeetings

Chemchartday4

Science Gateways

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

Welcome

- Introductions
- Agenda
- Logistics
- Workshop Survey
- Thanks

Introductions

- Registration
 - Please register – Any body not registered
s.apache.org/acs2018
- NSF Software Institutes – SGCI and MolSSI Vision and Community Engagement
- Diversity of Gateways
 - Protein Structure Prediction, Educational, Materials Research, Generic Chemistry Applications
 - Speakers: Yang Zhang, Joseph Montoya, Sudhakar Pamidighantam, Mark Perri
 - Research Exemplar for SEAGrid – Daniel Dumett
- Gateway Software and Platform as a Service
 - Apache Airavata and SciGap
- Hands On Sessions
 - SEAGrid User Oriented
 - Gateway Building

Our Goals

- This is intended to be open in multiple dimensions
- The gateways demonstrated during the workshop are only examples for Application, Discipline, Research Theme and Education specific to be broadly representative –

Gateway Technologies should be considered reasonably mature and agile to address pressing problems in Computational, Data and Integrated services for communities

Particularly software elements to be integrated into infrastructures and frameworks with Dev-Ops amenities for rapid dissemination are specific goals for gateways

Workshop Survey

We have an online Survey

Please take notes and help the community maximize the benefit by responding to the survey

We can follow up with more specific actions based on the survey

Help us improve the dissemination and impact for the workshop itself

DREAM BIG and Solve Grand Challenge Problems with Broad Societal Impacts

2-year Postdoc Position Data Curation in Chemistry

Overview

- Embedded in Chemistry and Libraries
- Co-advising by Prof Flood and librarian J. Laherty
- Papers expected
- Job prospects available

Job Description

- Develop data curation and analysis services
- Bring chemistry into the age of data (big data, cloud storage, data mining)
- Communicate science information needs between chemists, librarians,

- PhD Chemists with experience in handling data
- Excellent communication skills



Council on Library and
Information Resources



Alfred P. Sloan
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FULFILLING *the* PROMISE

Please fill the Survey

- <https://sciencegateways.org/acseval>