

Simplifying and Securing Model-Based Simulation Using Science Gateways

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Pervasive Technology Institute

What is a Science Gateway?

- Web and desktop interfaces to remote science and engineering resources
 - Supercomputers, clusters, clouds
 - Mass storage systems, data services
- Provide Software as a Service
- Support replicability
 - Capture metadata about what you did to get a result
- Support collaboration
 - Share metadata



Experiment Summary Enable Auto Refresh ON OFF

Experiment ID	Test2_ec34aed9-25e3-4861-9464-c755cc517ba1											
Name	Test2											
Description												
Project	Mar-15-Jobs											
Owner	sraeroma2017											
Application	search-SRA											
Experiment Status	COMPLETED											
Job	<table border="1"><thead><tr><th>Name</th><th>ID</th><th>Status</th><th>Creation Time</th></tr></thead><tbody><tr><td>A1185529494</td><td>128</td><td>COMPLETE</td><td>04/26/2018, 12:14 PM - GMT-0400 (EDT)</td></tr></tbody></table>				Name	ID	Status	Creation Time	A1185529494	128	COMPLETE	04/26/2018, 12:14 PM - GMT-0400 (EDT)
Name	ID	Status	Creation Time									
A1185529494	128	COMPLETE	04/26/2018, 12:14 PM - GMT-0400 (EDT)									
Notifications To:												
Creation Time	04/26/2018, 12:14 PM - GMT-0400 (EDT)											
Last Modified Time	04/26/2018, 12:21 PM - GMT-0400 (EDT)											
Inputs	Fasta-Reference-File: reference Select existing Search IDs File OR Upload your own below: Uploading my own as an optional file Optional File Inputs: sra_ids.txt											
Outputs	Downloading-Details: report.txt Search-SRA-Standard-Error: search-SRA.stderr Search-SRA-Standard-Out: search-SRA.stdout											
Storage Directory	Open											
Errors												

Sharing Details

Order By

This has not been shared

[Clone](#) [Update Sharing](#)



SimCCS Gateway

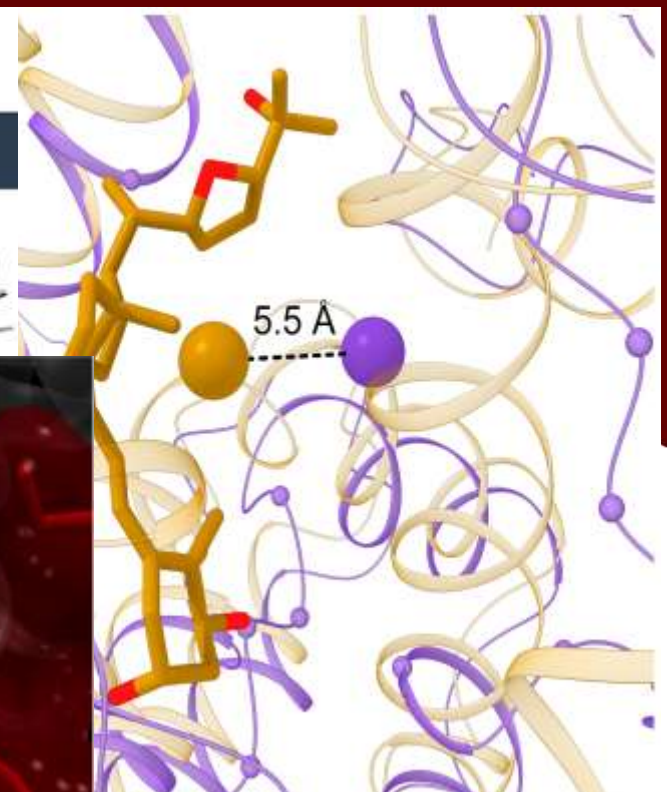
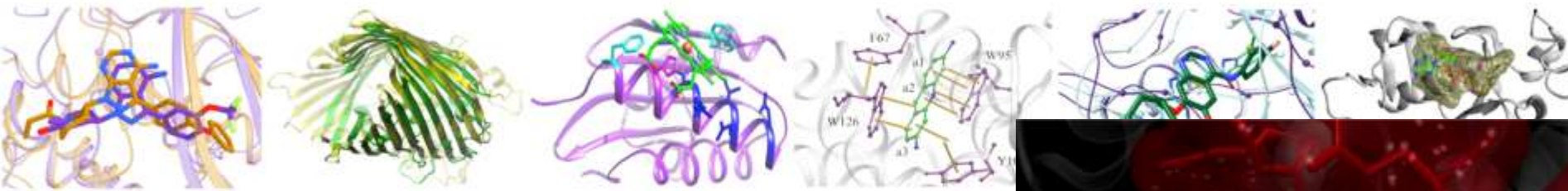
SimCCS Gateway is a cloud computing service that provides novel decision-support. Developed by members of the U.S.-China Clean Energy Research Center, Advanced energy technologies to thrive in a carbon constrained world.

SimCCS supports decision making by integrating applications in operations research design and reservoir performance prediction. Users are able to produce integrated involving multiple CO2 sources and geologic sinks. By harnessing the power of high investment solutions for implementing CCUS technologies.



The screenshot shows the SimCCS software interface. On the left, there are tabs for 'Data', 'Model', and 'Results'. Below these are sections for 'Dataset' (set to '_Ordosv2'), 'Scenario' (set to 'S1R42'), and 'Network Generation' (with buttons for 'Shortest Paths Network', 'Candidate Network', 'Reprocess All', and 'Enable All'). A 'Legend' section includes options for 'Sources' and 'Sinks' (Visible/Label) and network types (Cost Surface, Shortest Paths Network, Raw Delaunay Edges, Candidate Network). At the bottom left, coordinates are displayed: 'Lat: 41.795057317' and 'Lon: 105.62636678300001'. The main area shows a map of the Ordos Basin in China with a network of purple lines representing CO2 transport paths. An inset image shows two large industrial storage tanks. Another inset shows a map of China with the Ordos Basin highlighted. A third inset shows a histogram of 'Total CO2 (Mtpa)' with a probability curve overlaid.



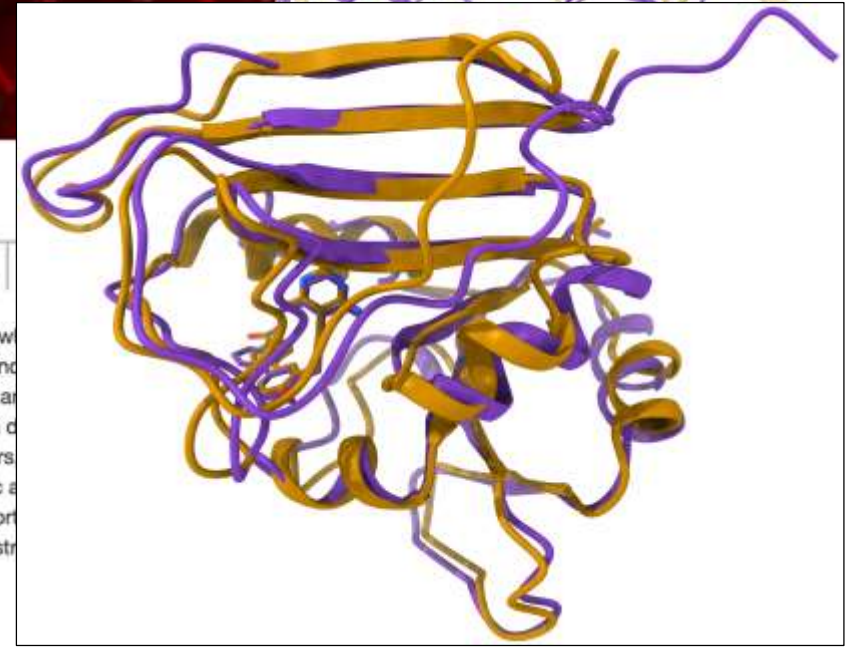
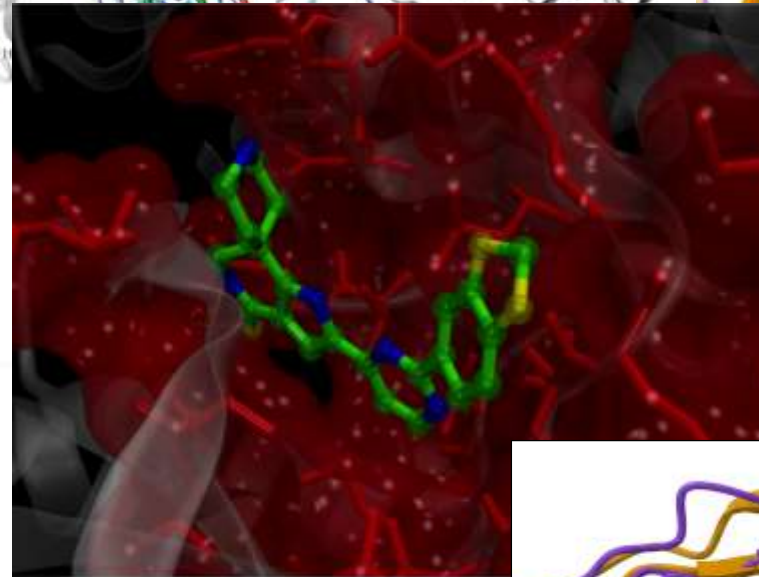


LSU Gateway Welcome!

Welcome to Louisiana State University Science Gateway

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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.

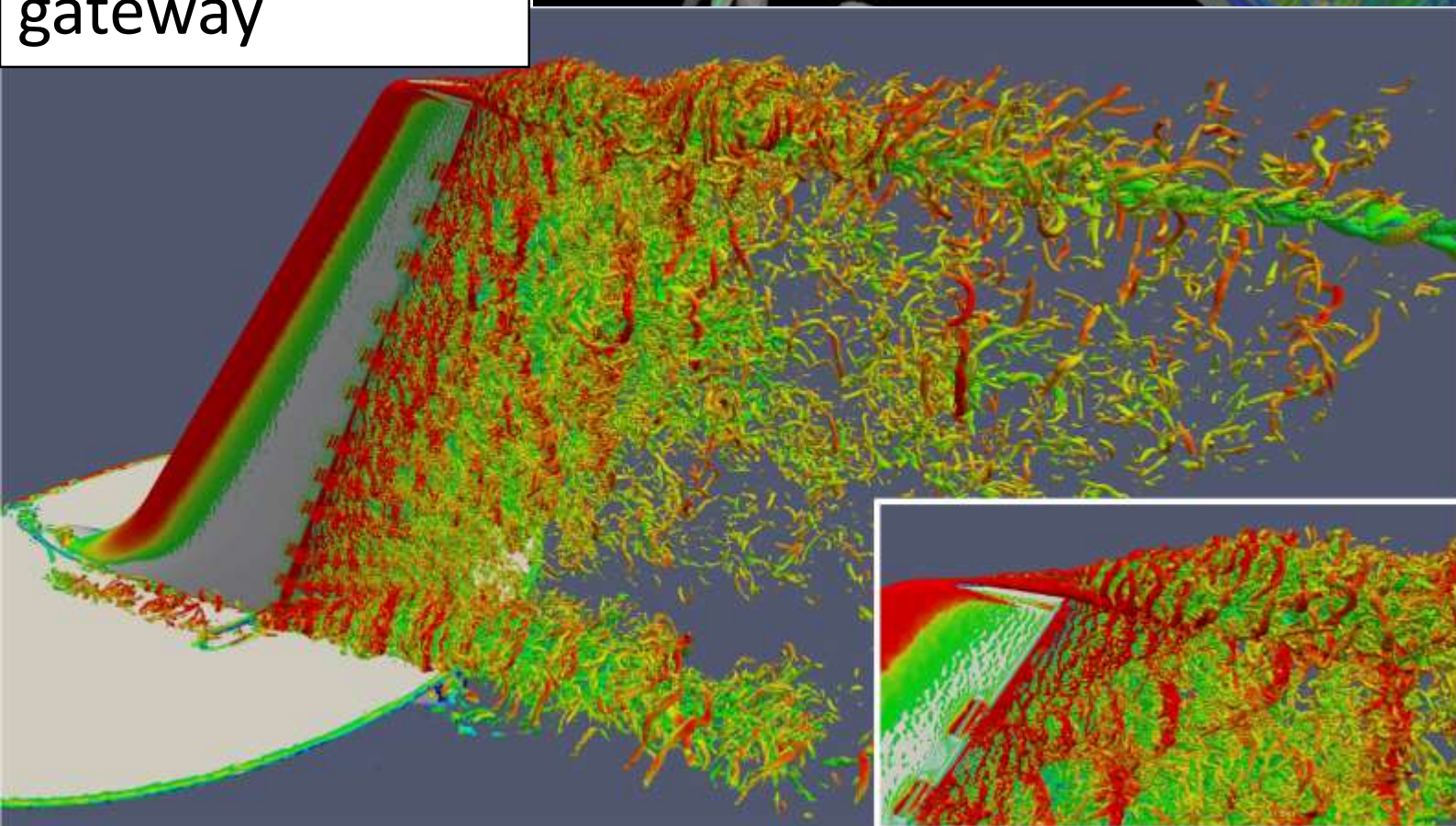
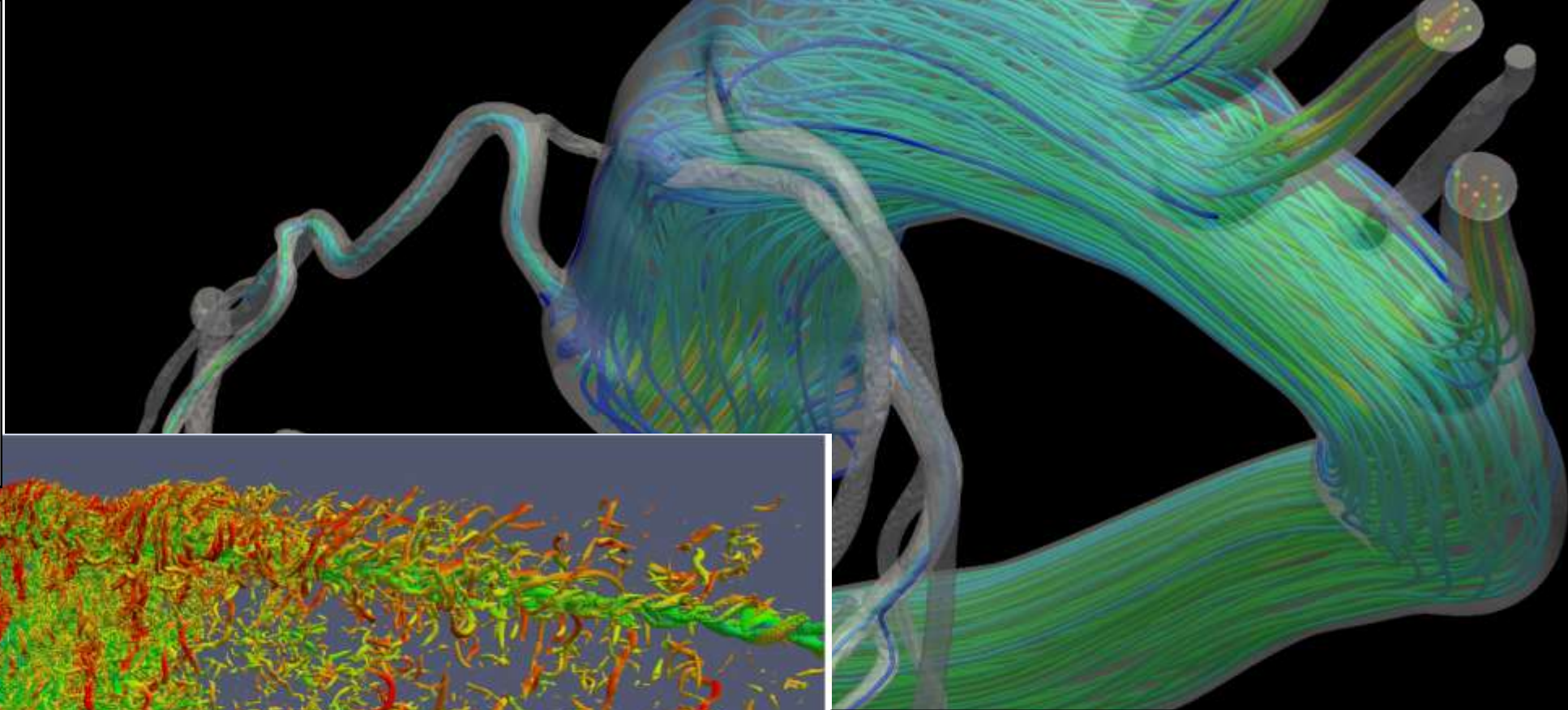
Science Gateway Platform as a Service (SciGaP) provides application programmer interfaces (APIs) to hosted generic infrastructure services that can be used by domain science communities to create Science



Apache Airavata is a software framework widely 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 running applications and workflows on distributed computational resources.

[Learn more](#)

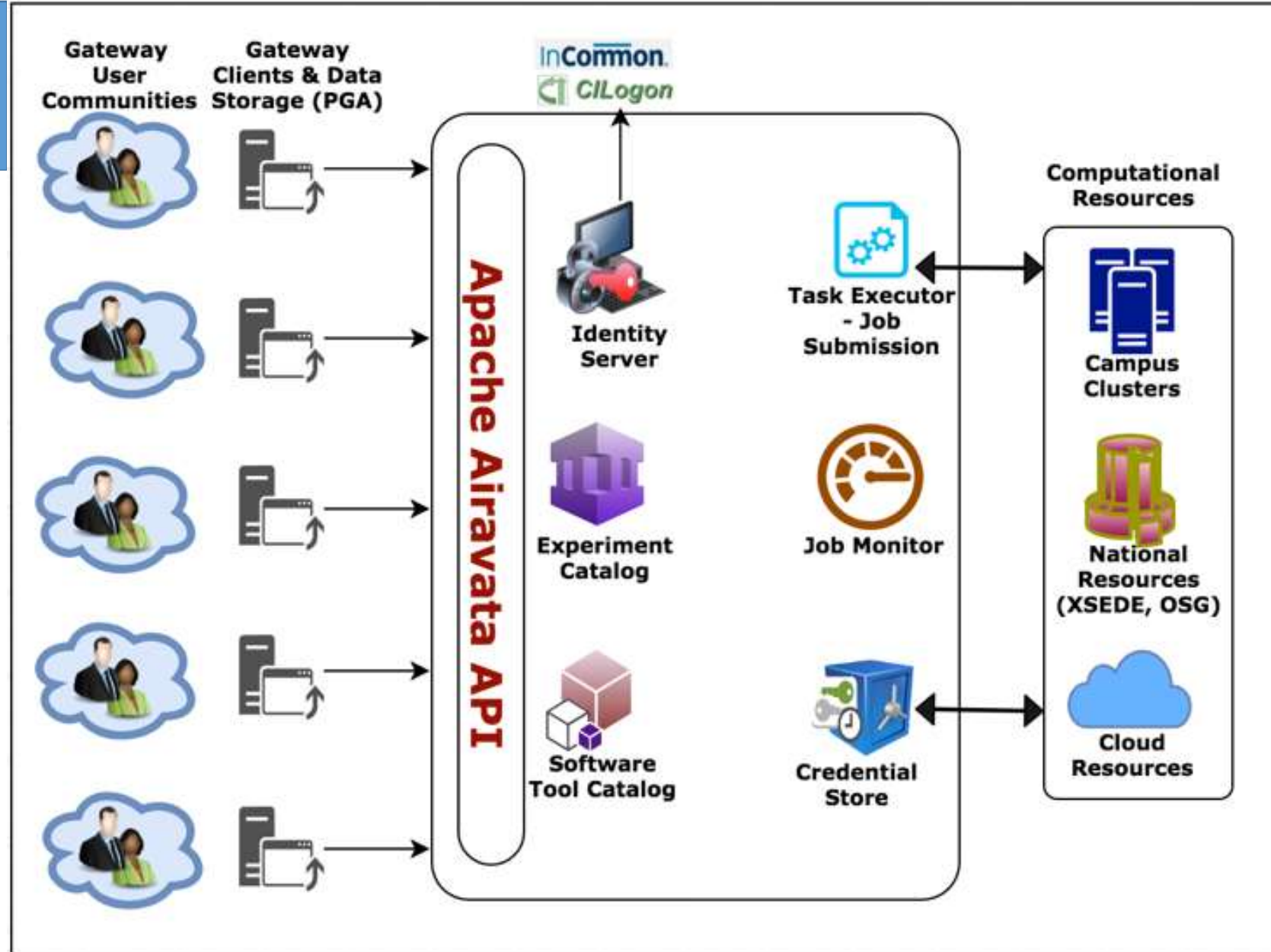
We support
ABAQUS
through
SEAGrid.org, an
Airavata client
gateway



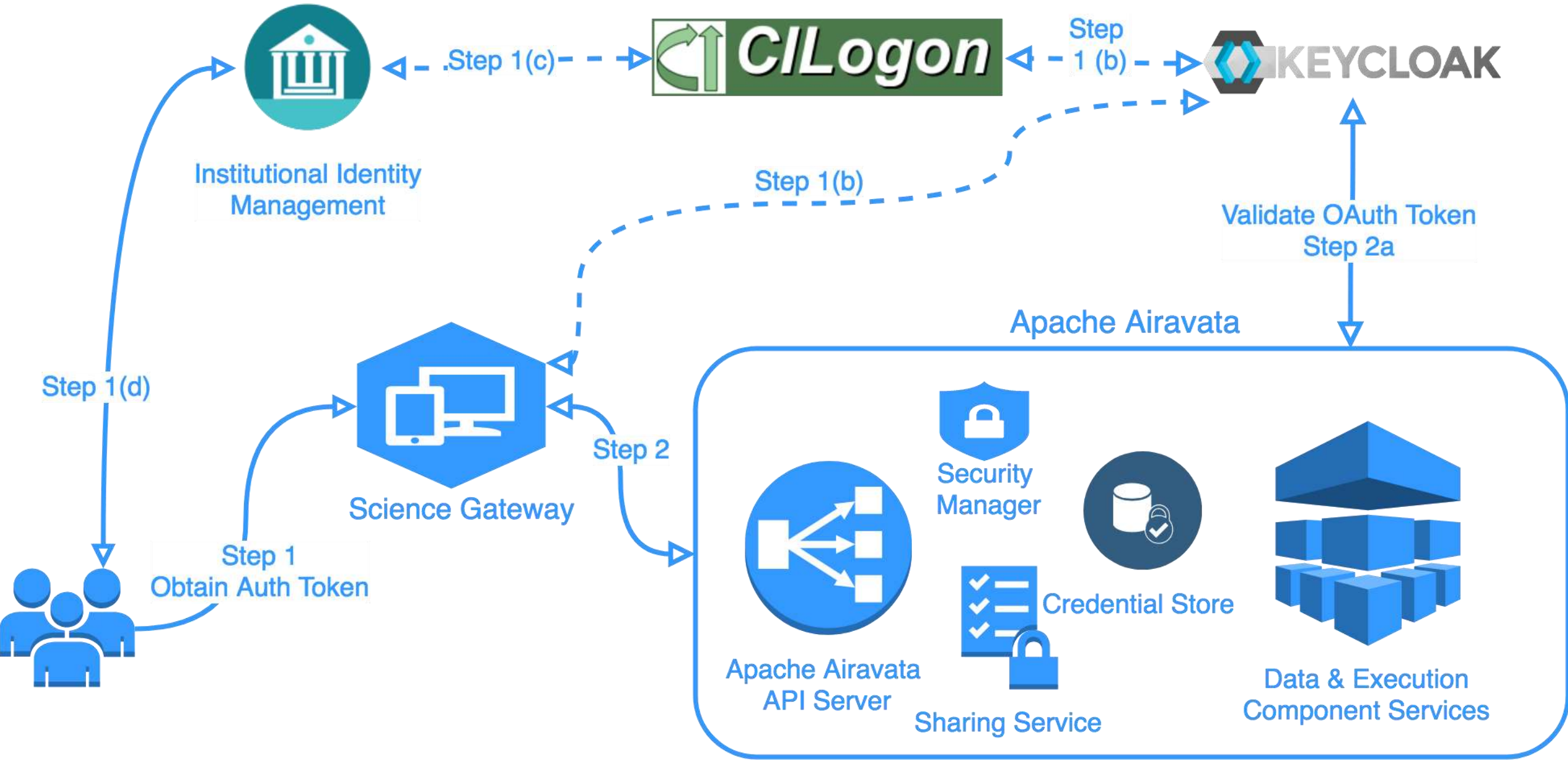
SimVascular (above) and
PHASTA (left) CFD solver
executions on diverse HPC
systems enabled using
Apache Airavata based
science gateways.

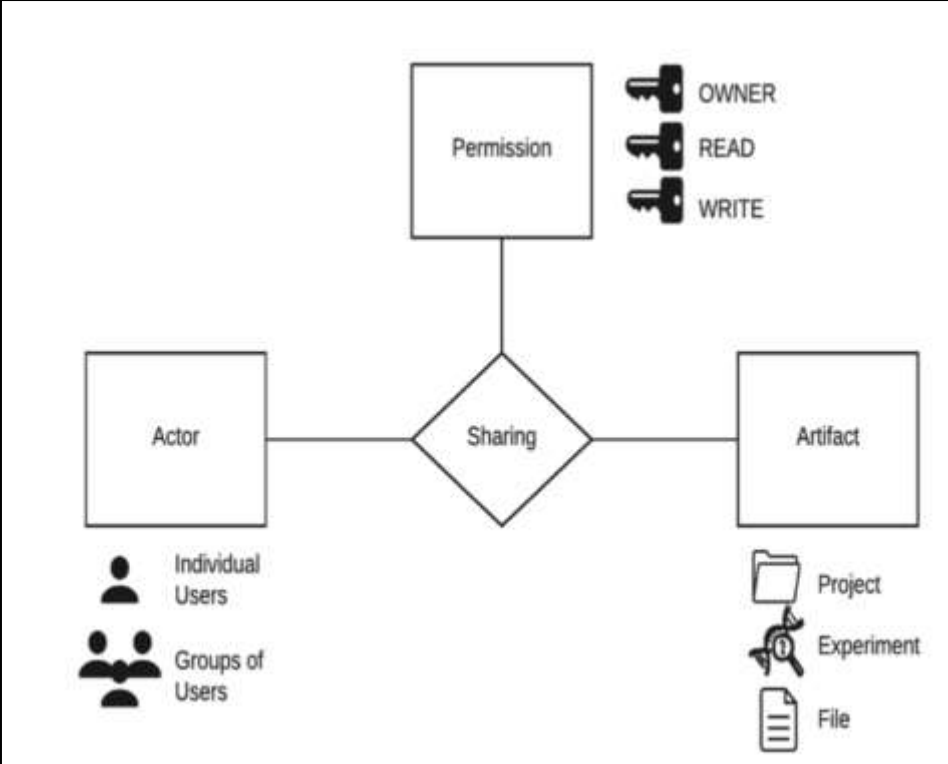
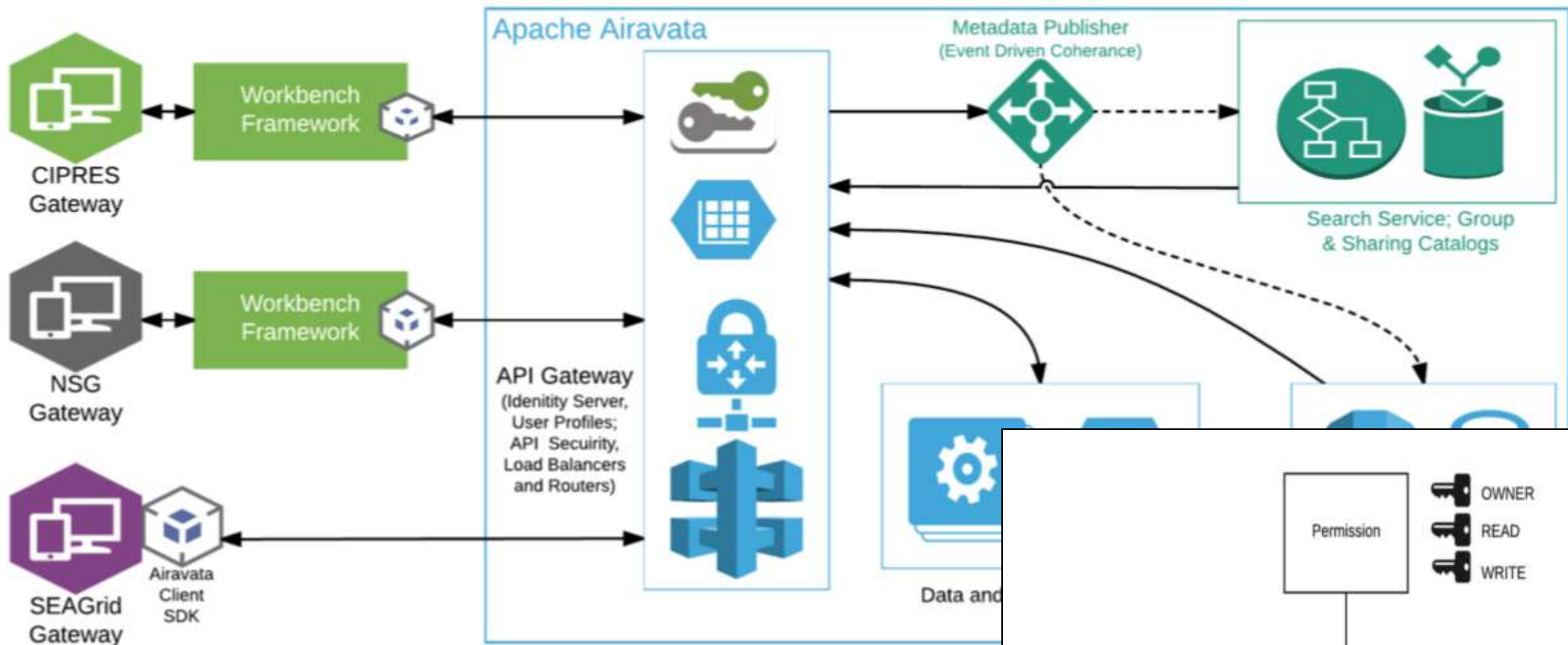
Our Approach

- Provide a “platform as a service” for gateways.
- Treat each gateway as a tenant
- Allow tenants to manage their own resources, users, applications
- Make it open source
 - Including “infrastructure as code” for production deployments

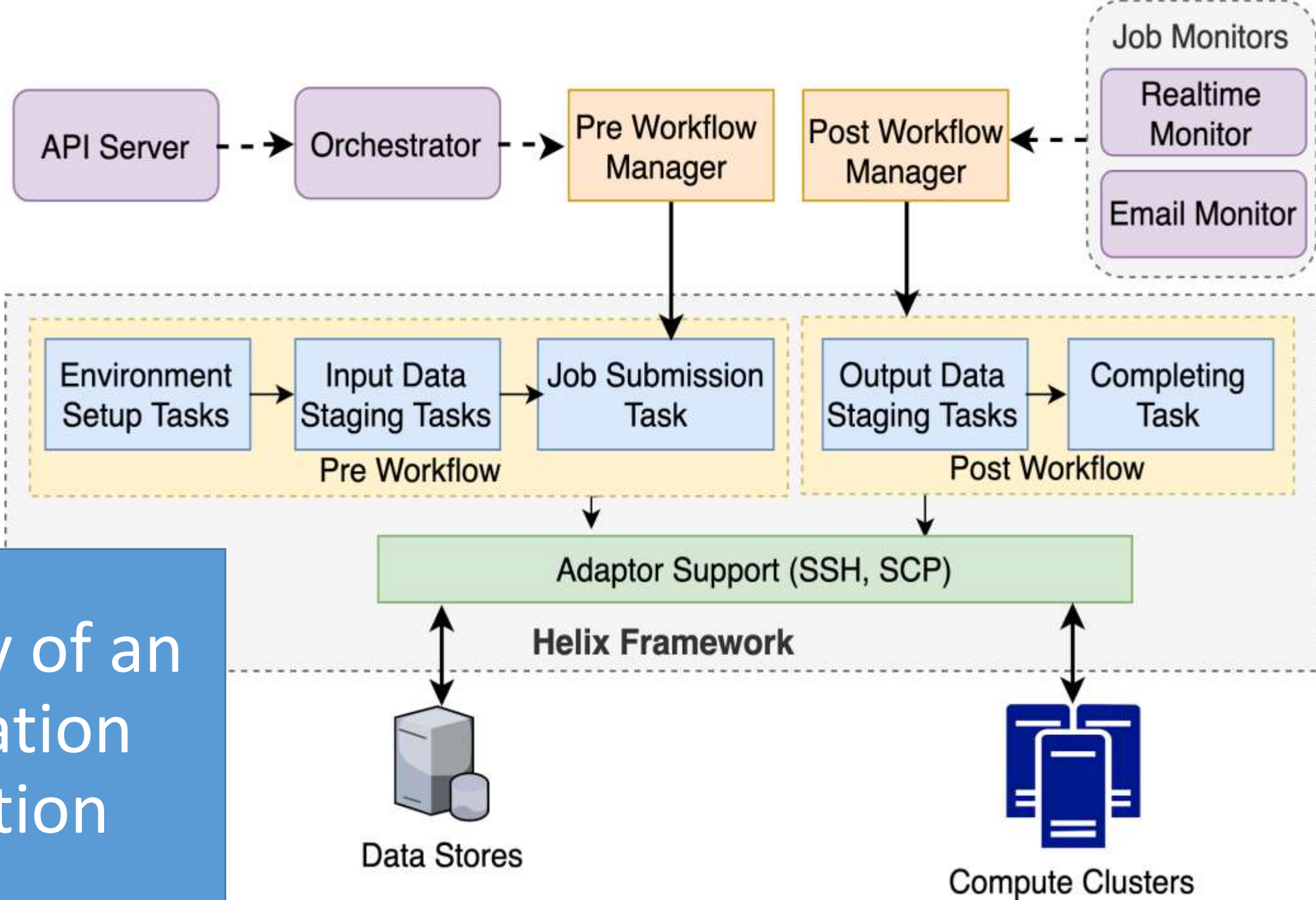
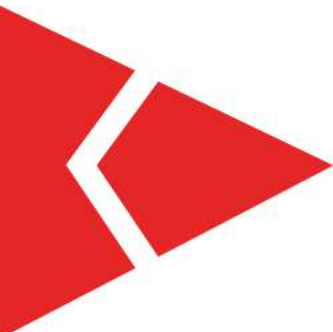


Authentication and Identity Management



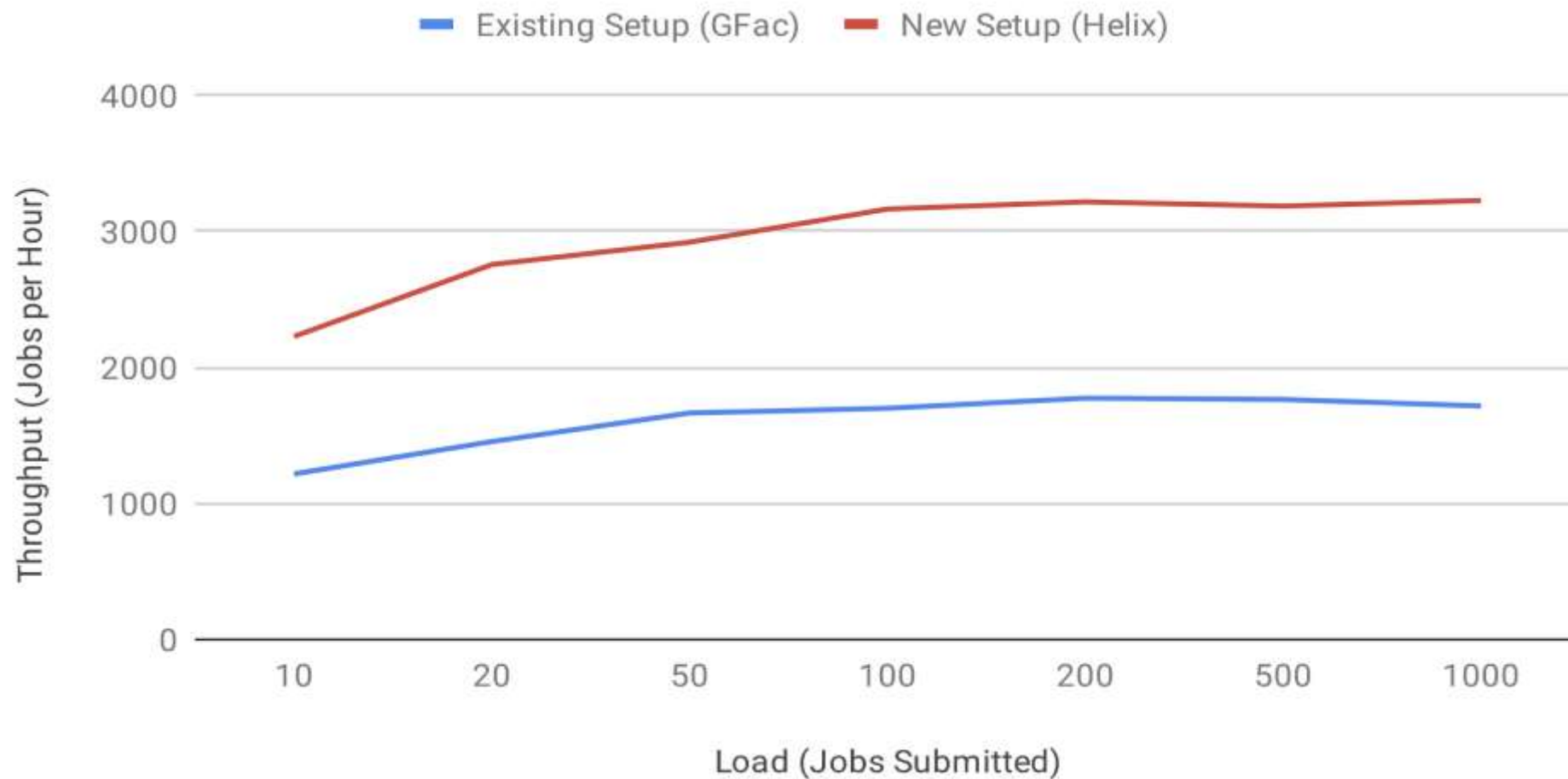


We use an actor-artifact approach for metadata sharing that is optimized for each actor to be associated with many artifacts

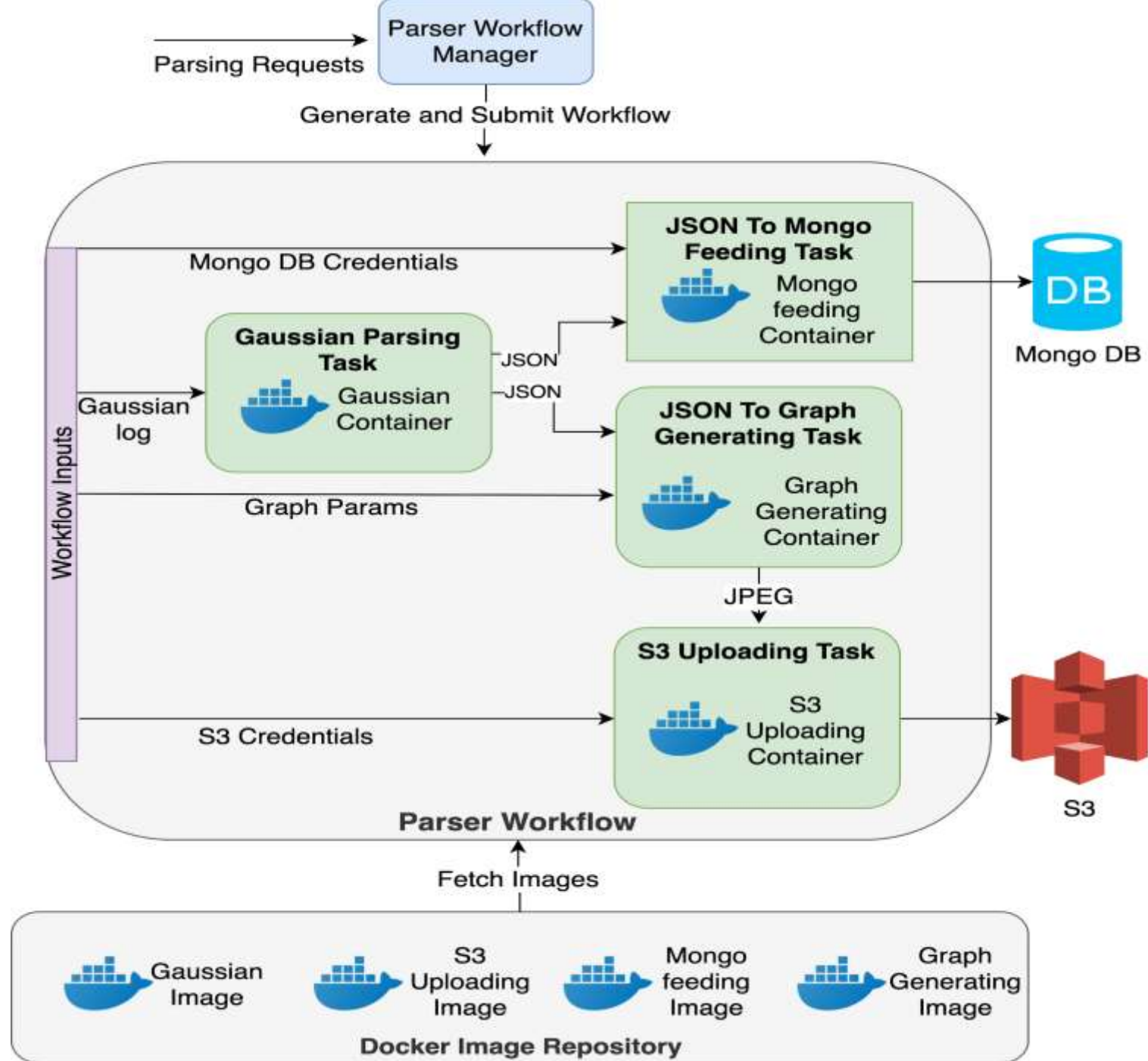


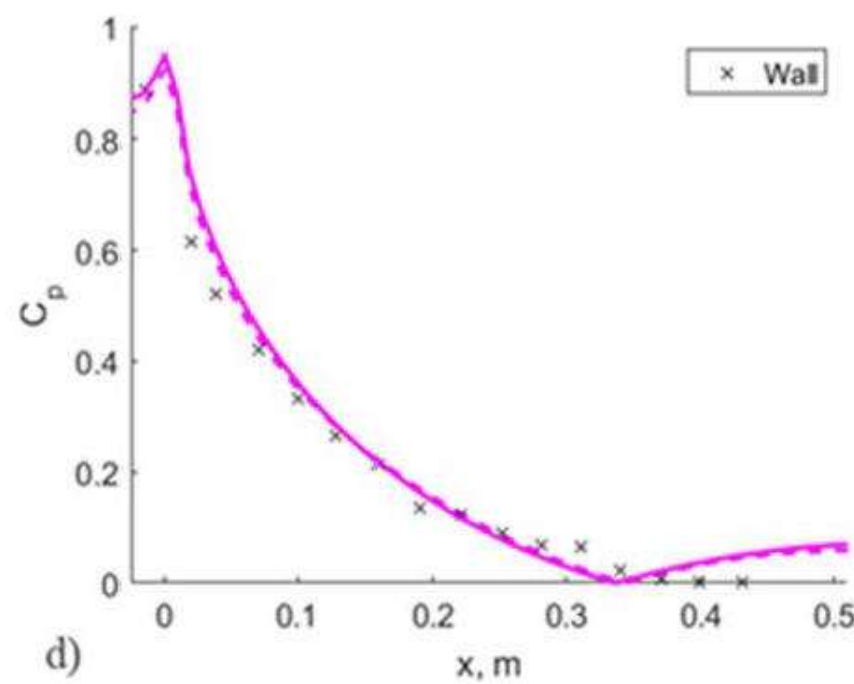
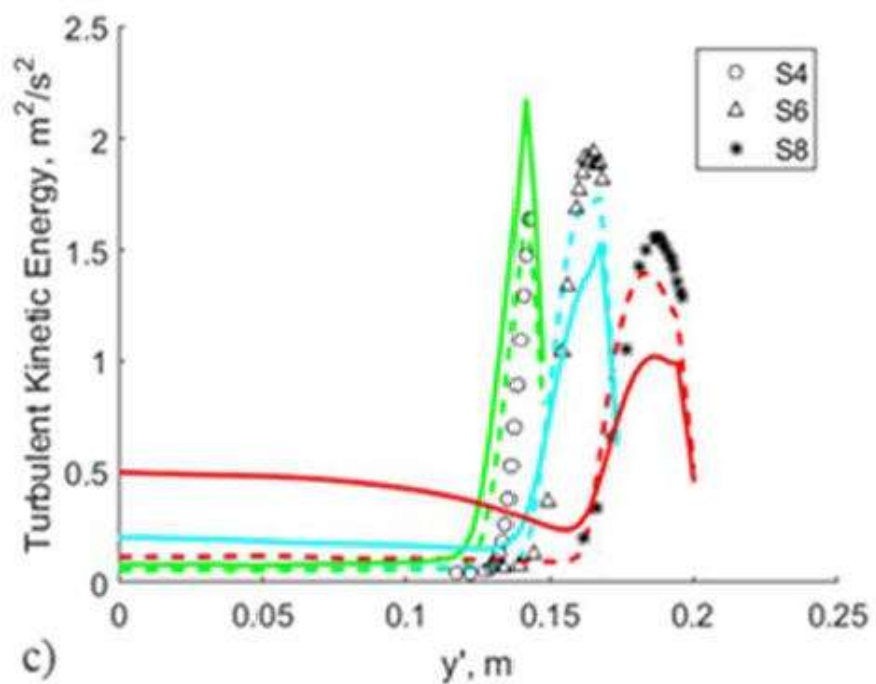
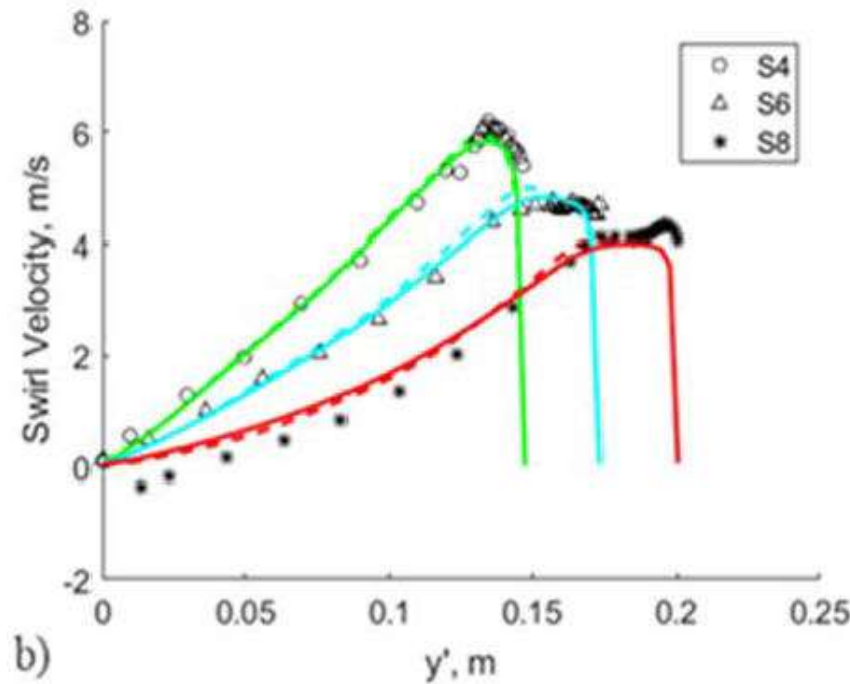
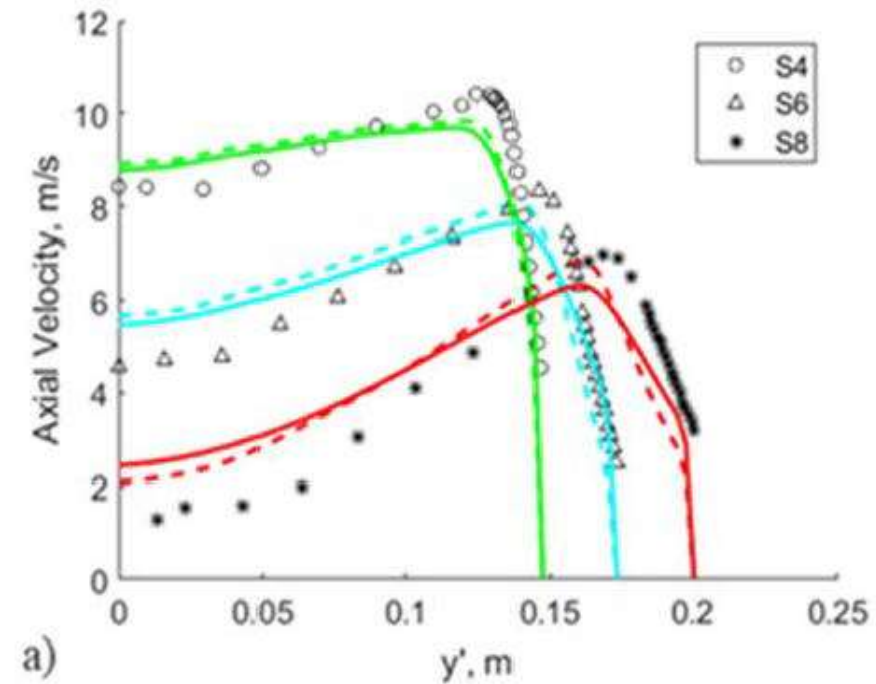
Anatomy of an Application Execution

Apache Airavata-Apache Helix Throughput



We can also create more flexible and elaborate execution patterns with the Airavata-Helix integration





Hartl and Crossley compared two different formulations of Navier-Stokes equations to simulate turbulence.

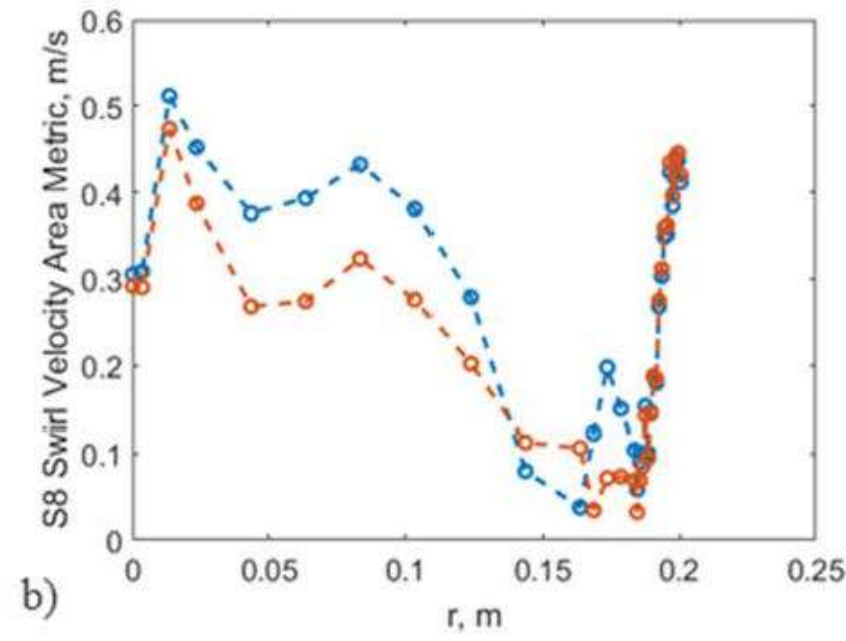
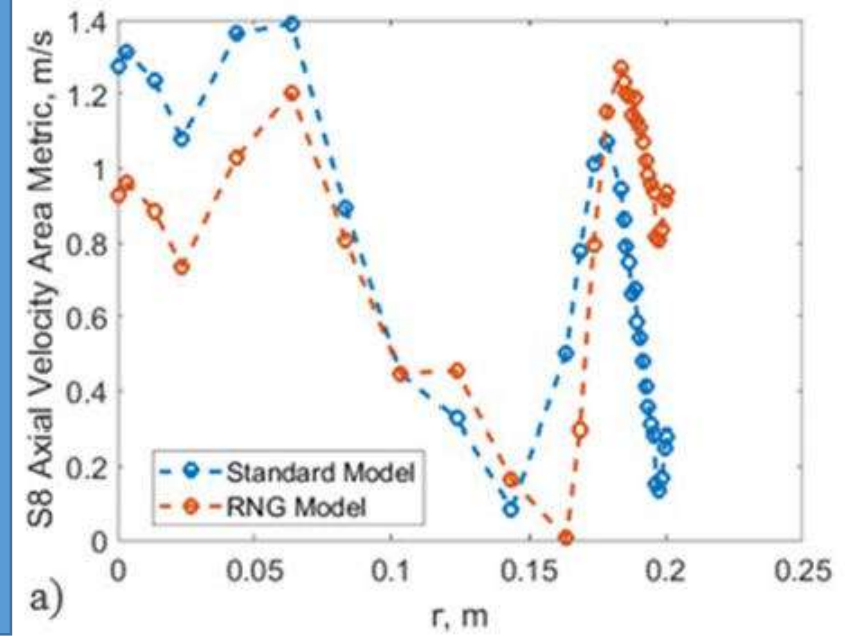
- Dashed lines are Method 1
- Solid lines are Method 2
- Symbols come from experiments

Can you “eye-ball” this and make conclusions?

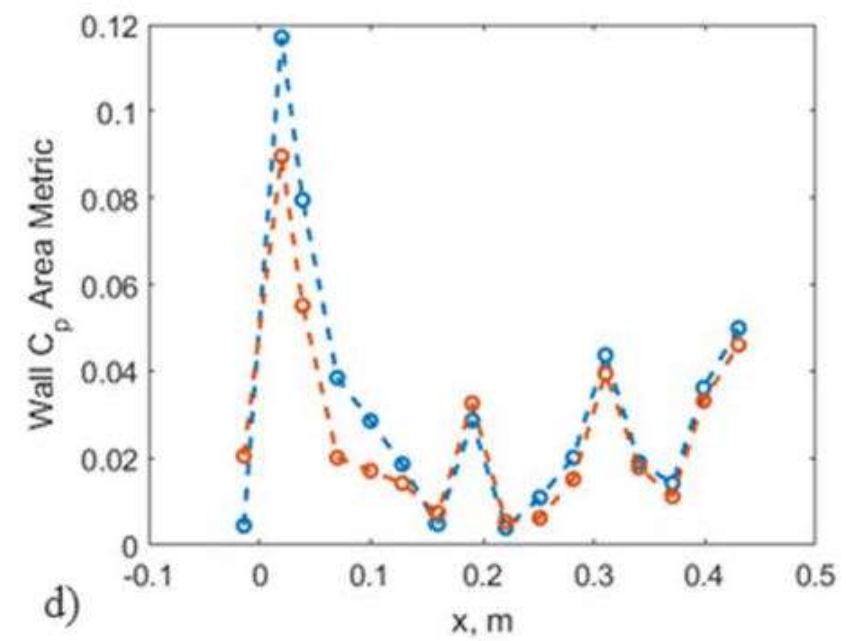
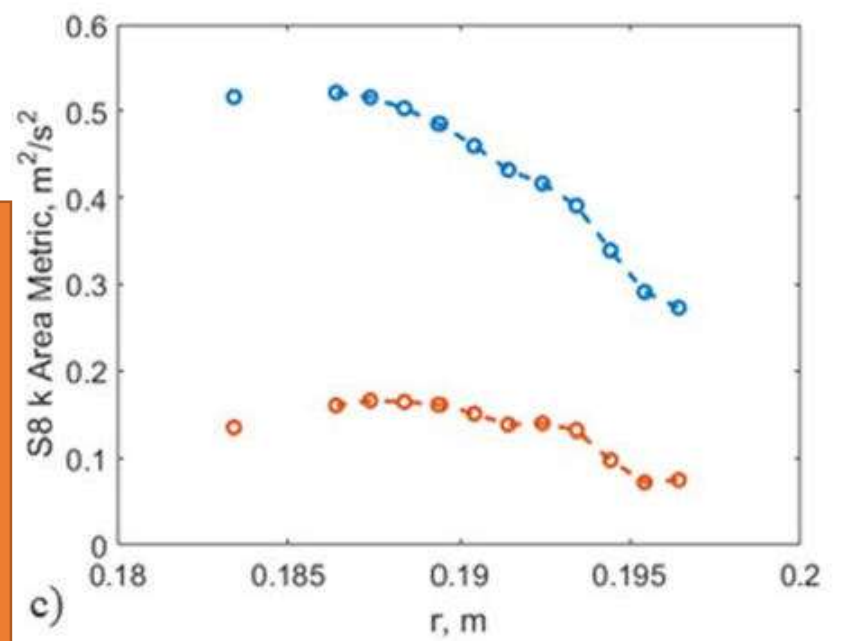
- A: No

Hartl, J. and Crossley, W.A., 2019. Application of a Verification and Validation Framework for Turbulence Modeling of Swirling Diffuser Flow. In *AIAA Scitech 2019 Forum* (p. 0501).

Area Metrics emphasize differences between experiment and simulation, incorporate uncertainties, maybe less susceptible to presentation obscuration.



VVUQ requires a lot of bookkeeping to manage numerous simulations and their post-processors. This is what science gateways do.



Private Sector Considerations

- “On premise” deployments for clients with strong IP and security considerations
 - “On premise” includes cloud providers
 - Integrate vendor’s authentication mechanism
- Hybrid platform/on-premise approach
 - Run agents on target resources that directly manage application executions and data.
 - More work, but more interesting

Conclusions

- Science gateways can be used to simplify access to modeling and simulation applications.
- Building gateways from scratch is difficult.
- We have developed a hosted, multi-tenanted platform to simplify building and operating gateways
 - “Shared nothing” architecture
 - Integrates third party components (KeyCloak, Helix, etc) for major capabilities
 - But sometimes we have to build it ourselves (Sharing Service).

More Information

- My email: marpierc@iu.edu
- Apache Airavata: <https://airavata.apache.org/>
- SGRC: <https://sgrc.iu.edu/>



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