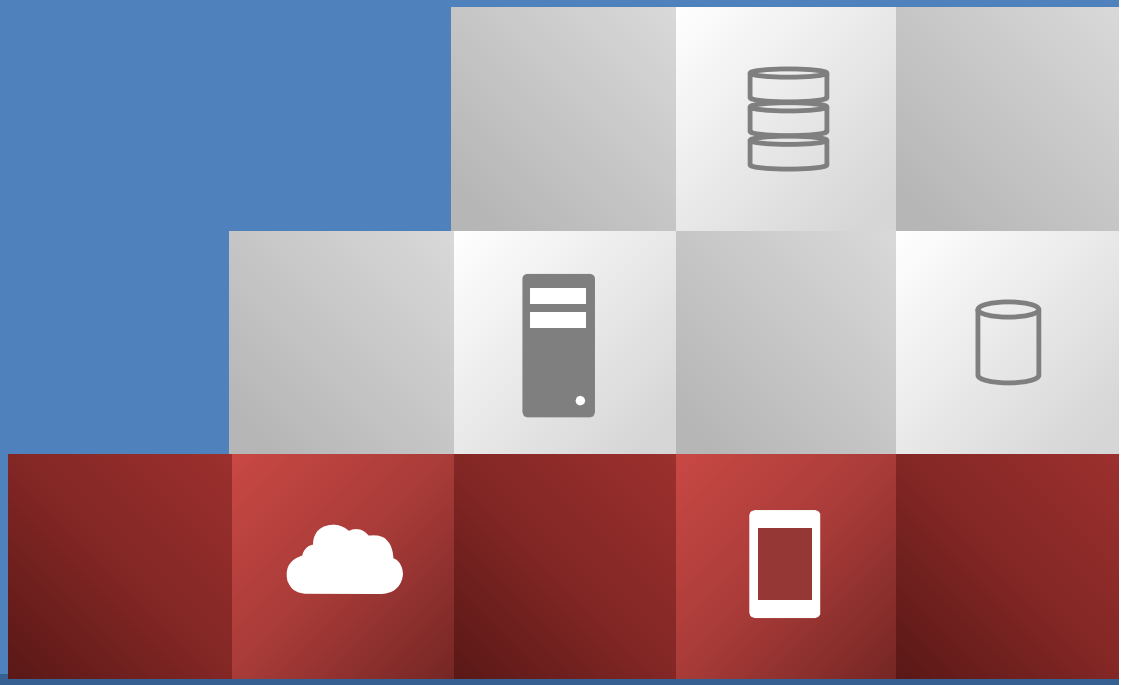
Science Gateways



Suresh Marru, Indiana University

Outline

- Introduction to Science Gateways
- Ushering Scientific Software to “as-a-service” model
- Containers and Gateways
- Hands-on tutorial
- Q&A
- Advanced Gateway Topics

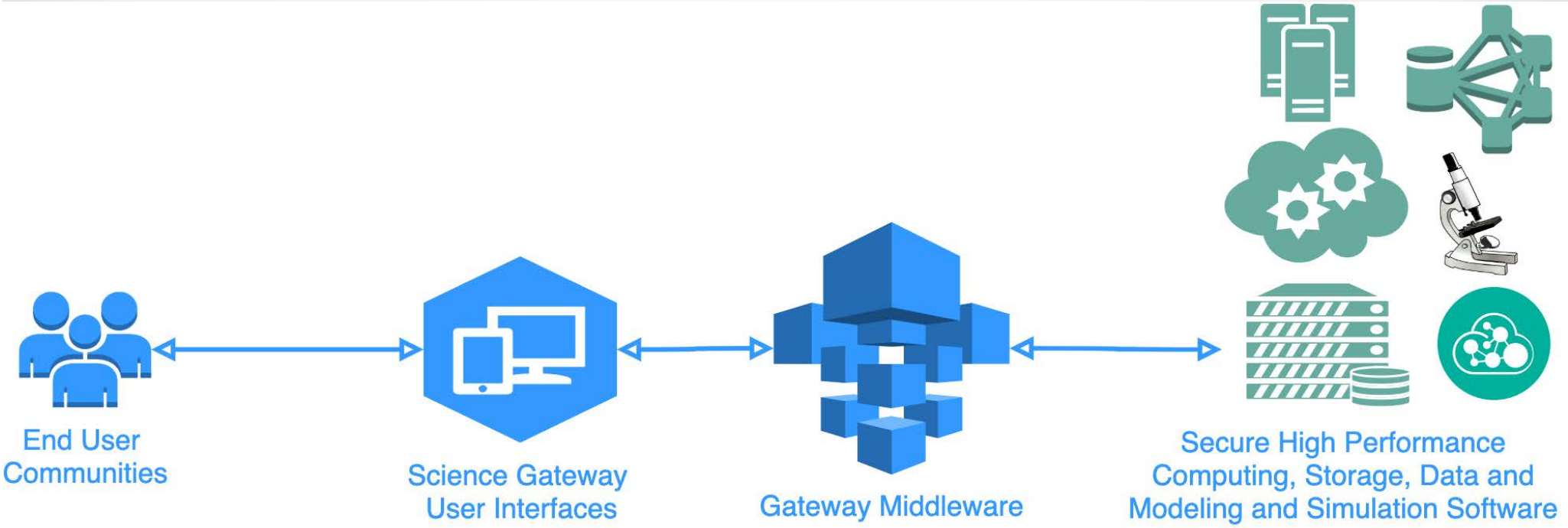
WHAT ARE SCIENCE GATEWAYS?

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

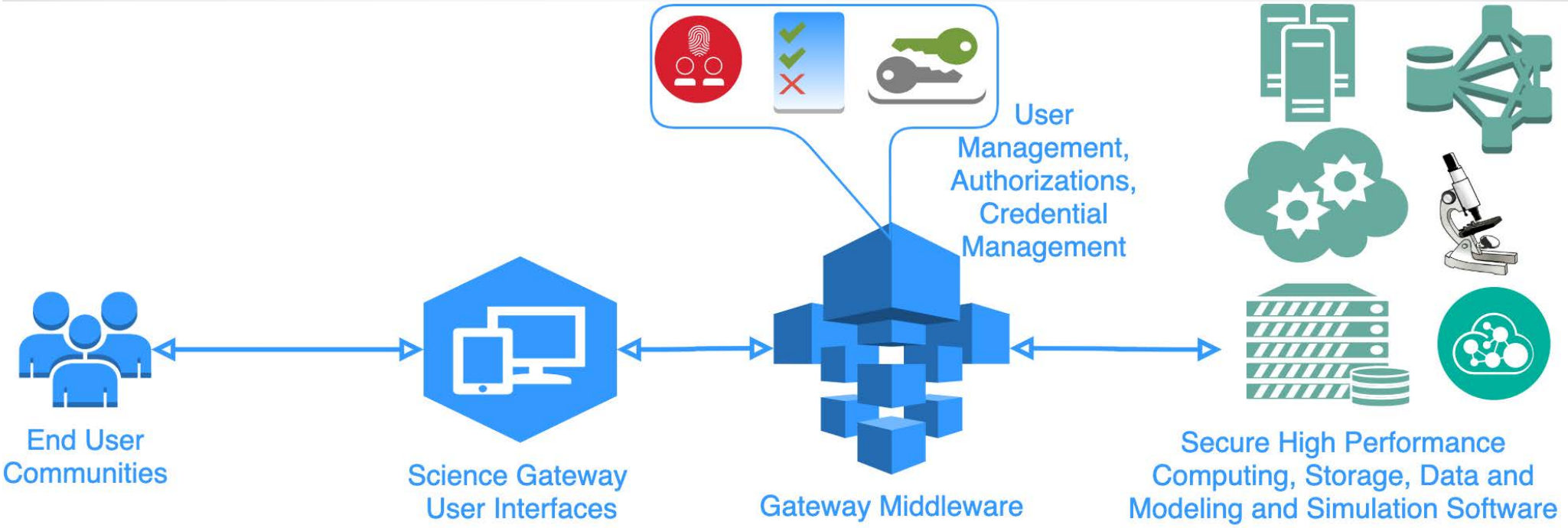
Learn more at https://sciencegateways.org/

Serving Targeted Communities

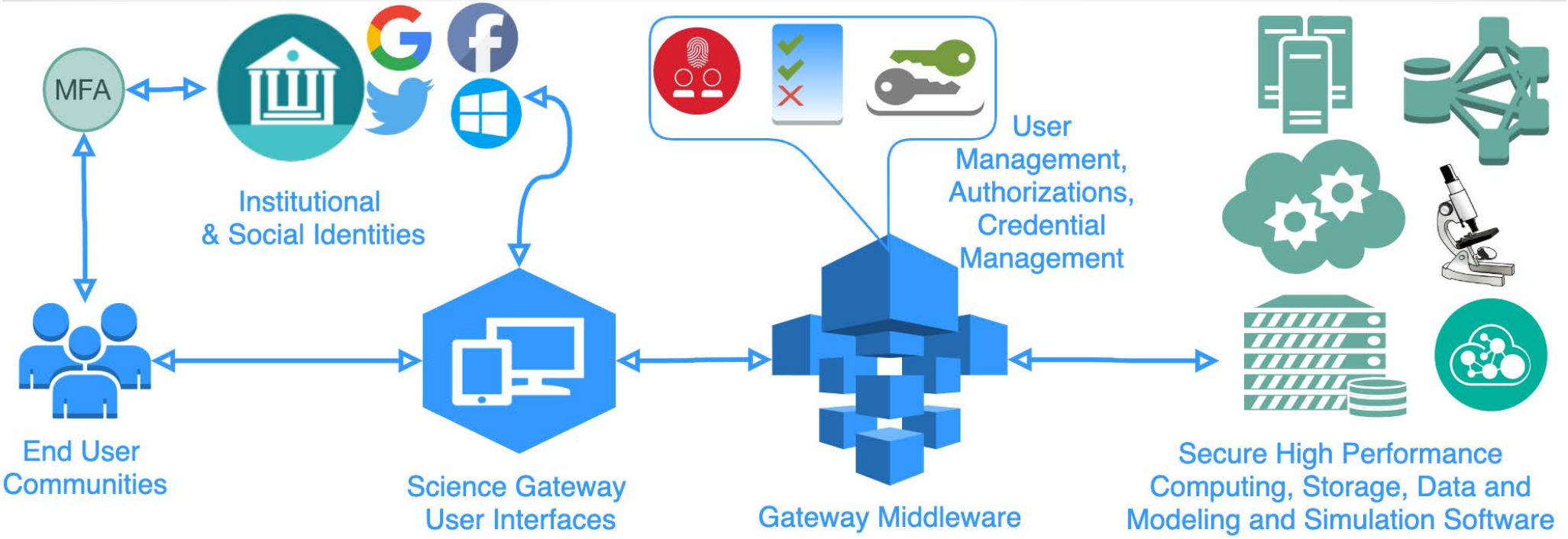
Resource-centric view --> Science-centric view



Secured access & Controlled sharing of digital artifacts

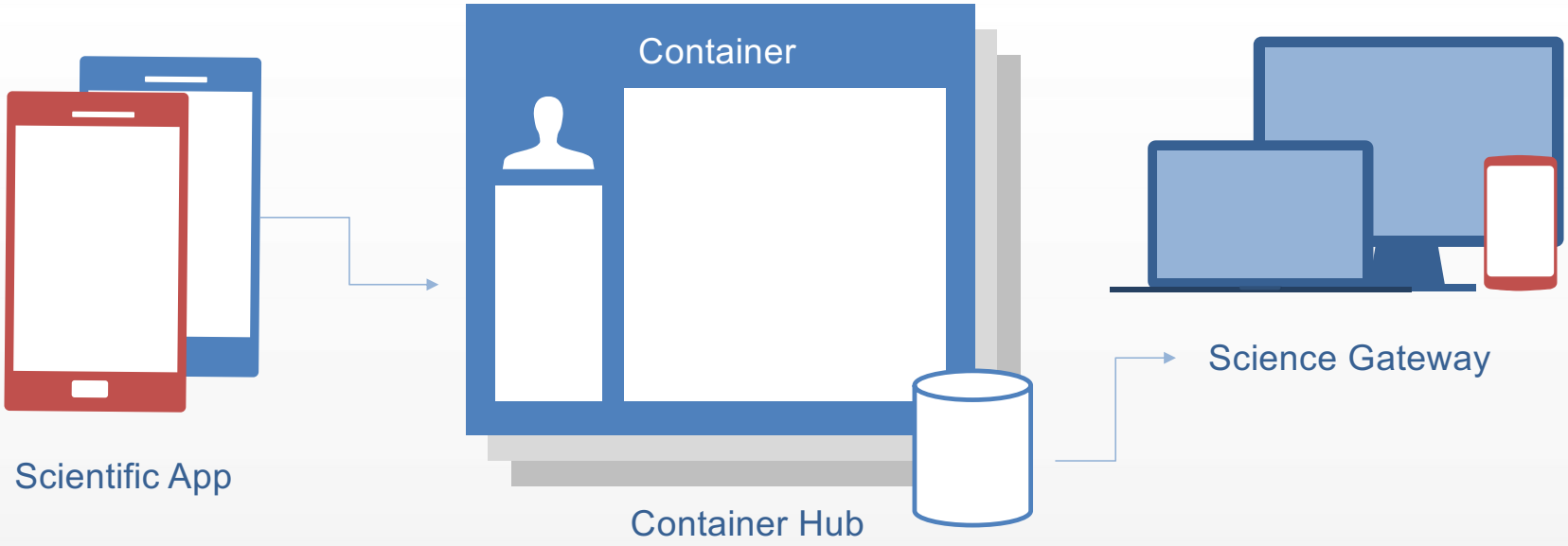


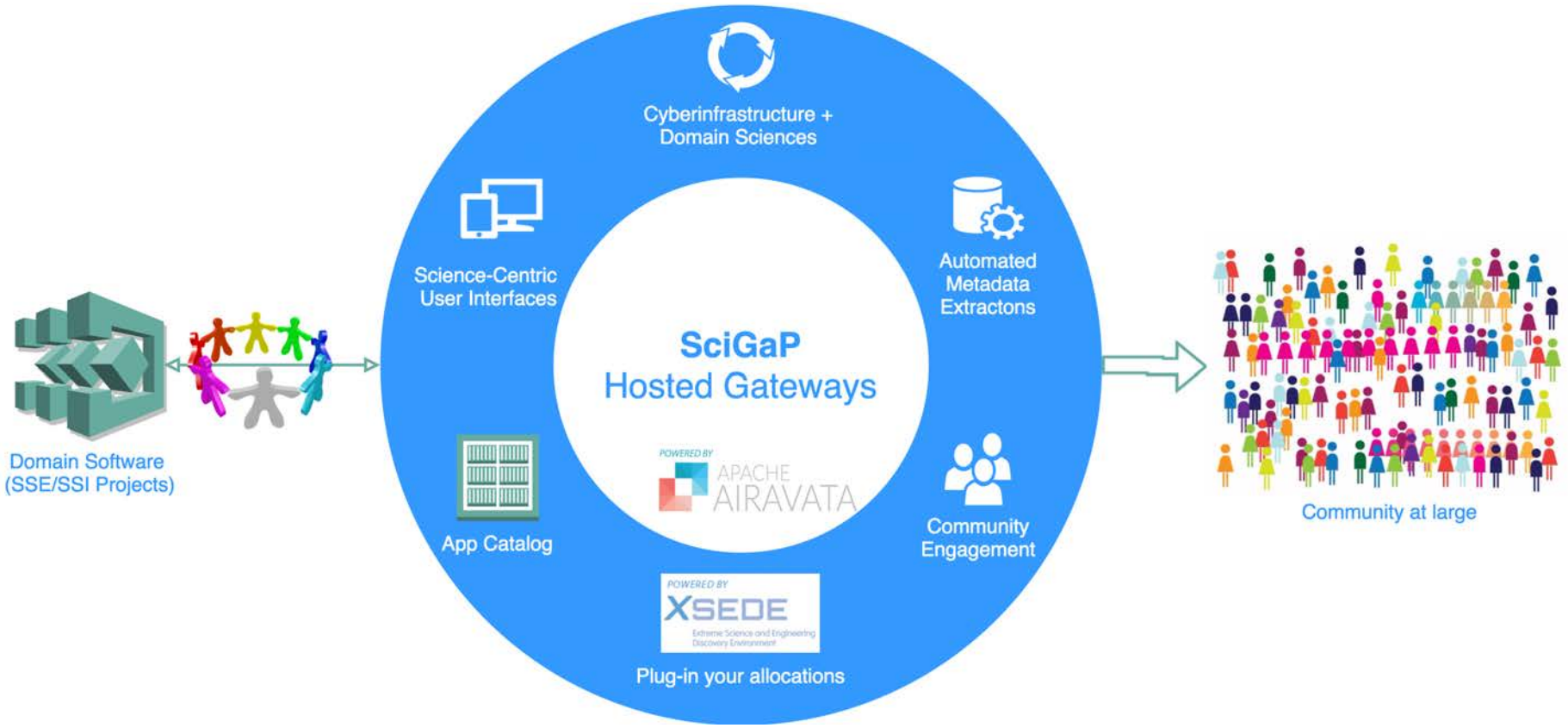
Federated Authentication



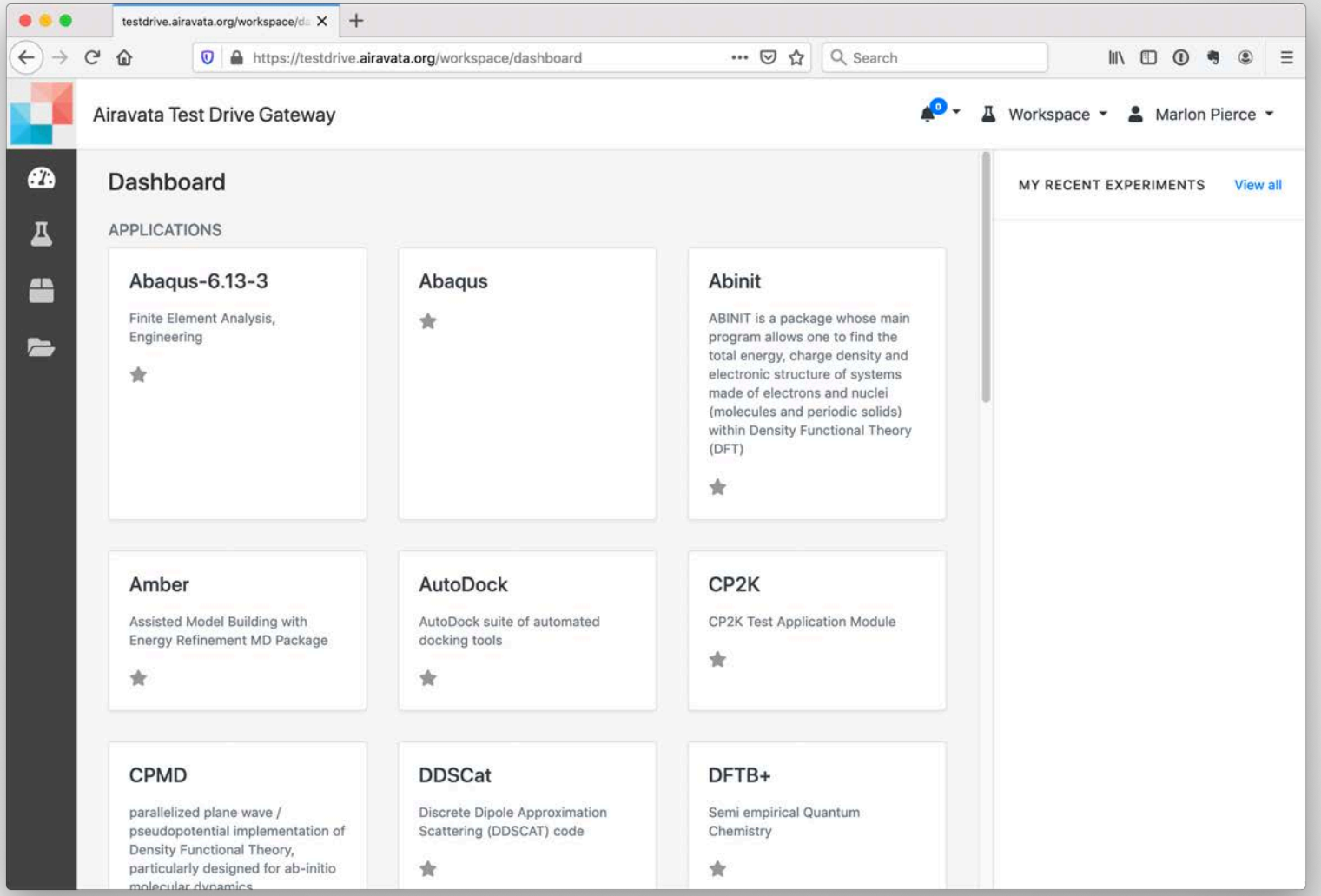
CONTAINERS & GATEWAYS

Scientific App to a Gateway Interface

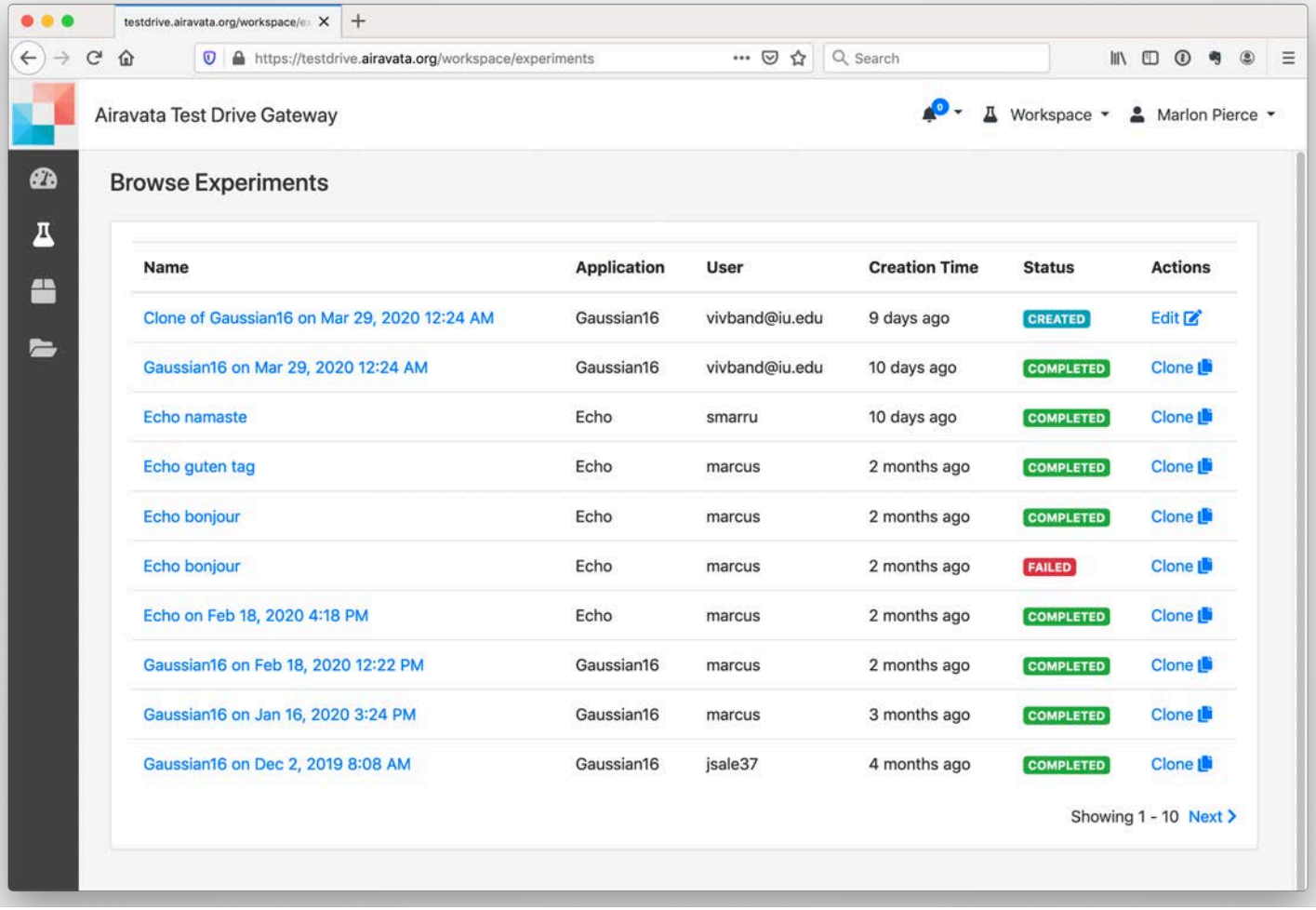



Cyberinfrastructure +
Domain Sciences
Science-Centric
User Interfaces
Automated
Metadata
Extractons
SciGaP
Hosted Gateways
POWERED BY
APACHE
AIRAVATA
App Catalog
Community
Engagement
POWERED BY
XSEDE
Extreme Science and Engineering
Discovery Environment
Plug-in your allocations
Domain Software
(SSE/SSI Projects)
Community at large

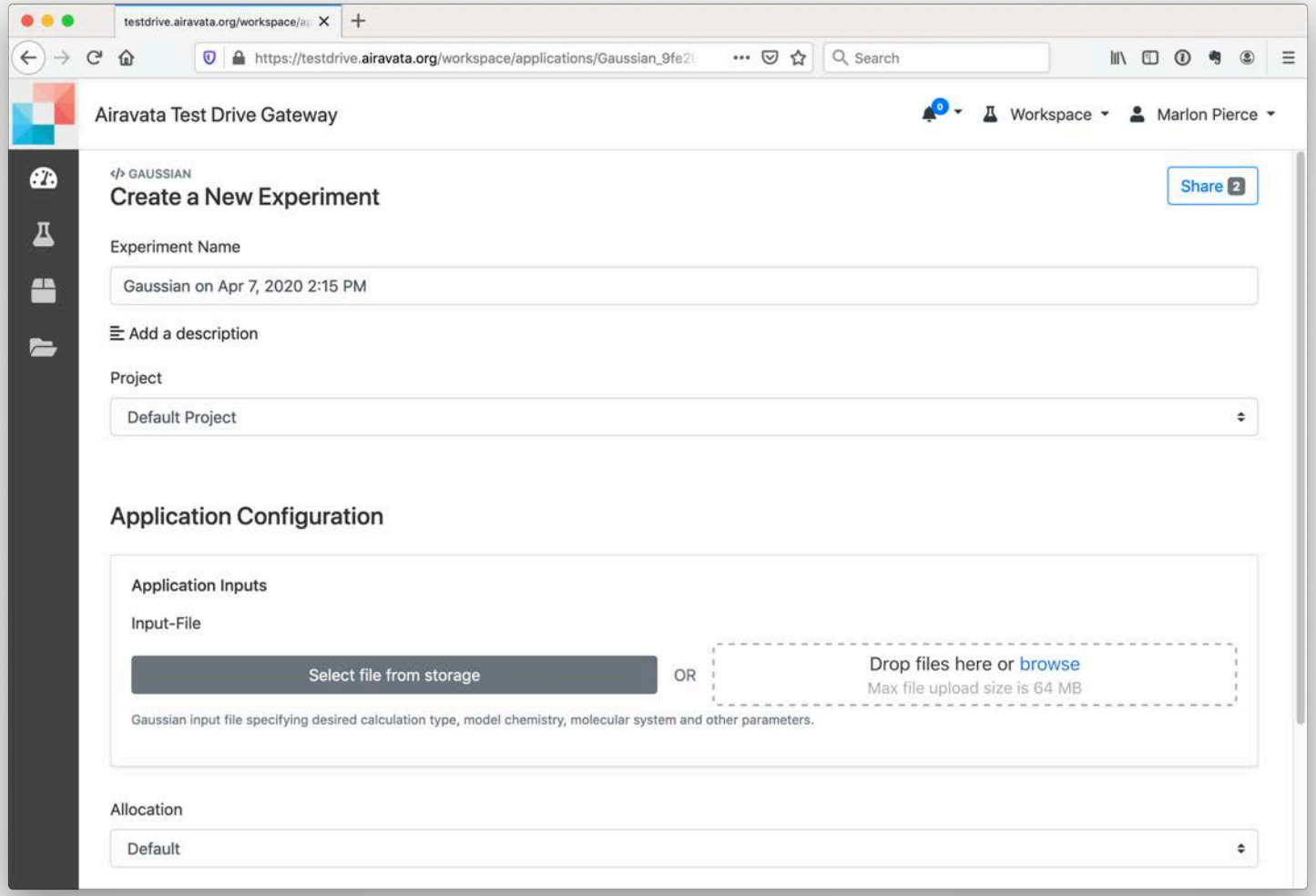
Gateways can enable “Scientific app-store”

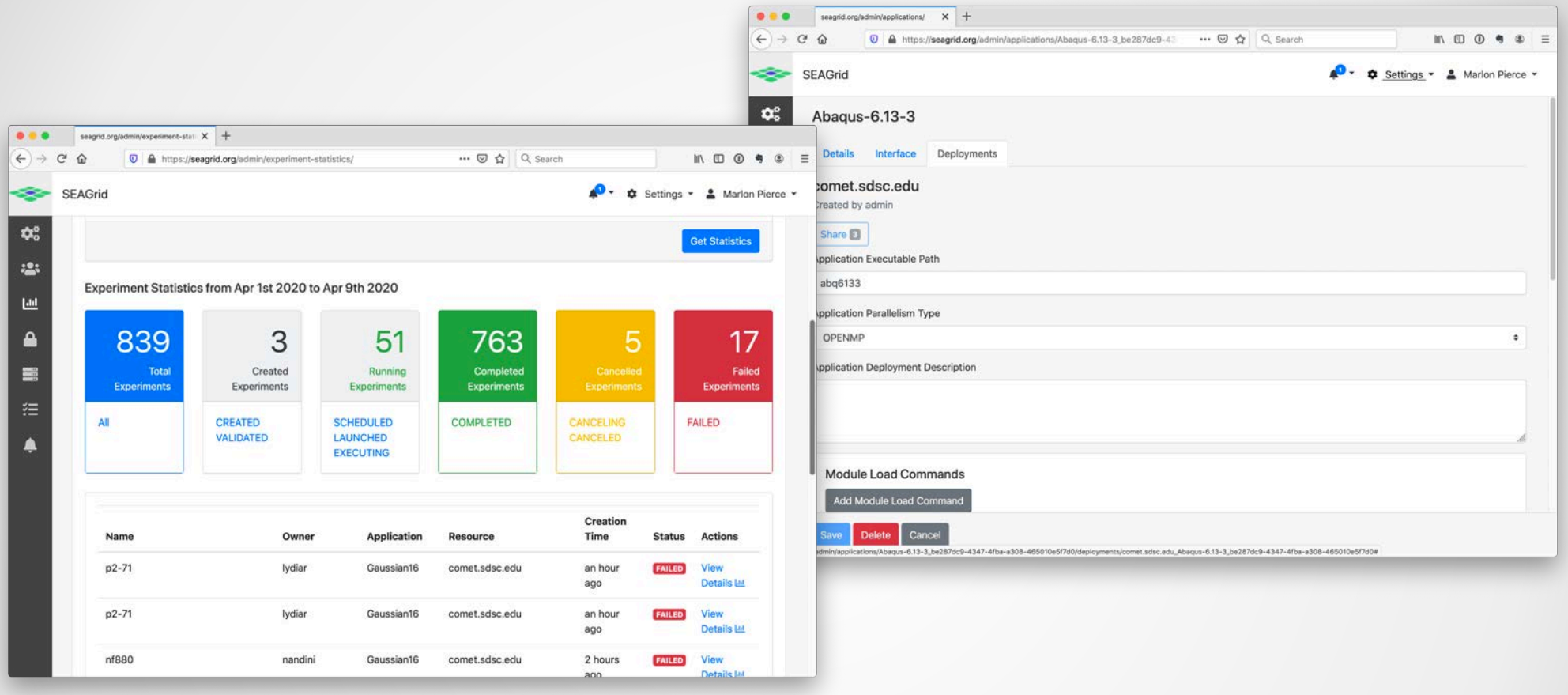


Dashboard of Scientific Experiments



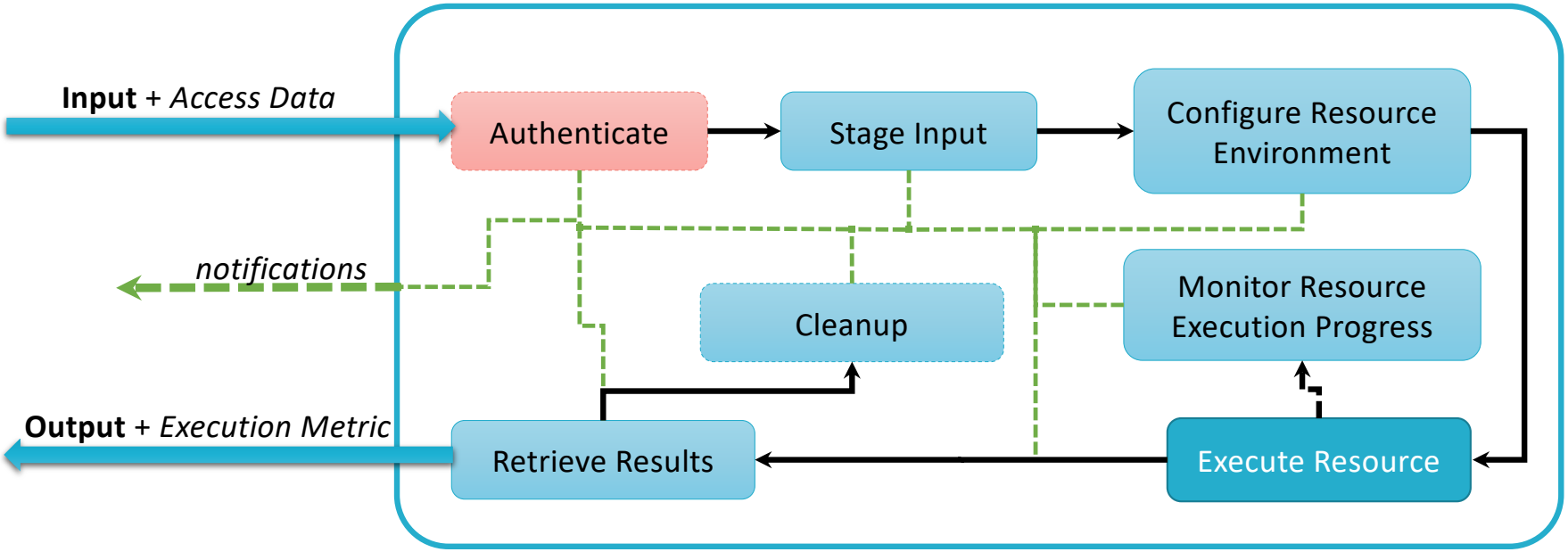
Launch “Experiments”

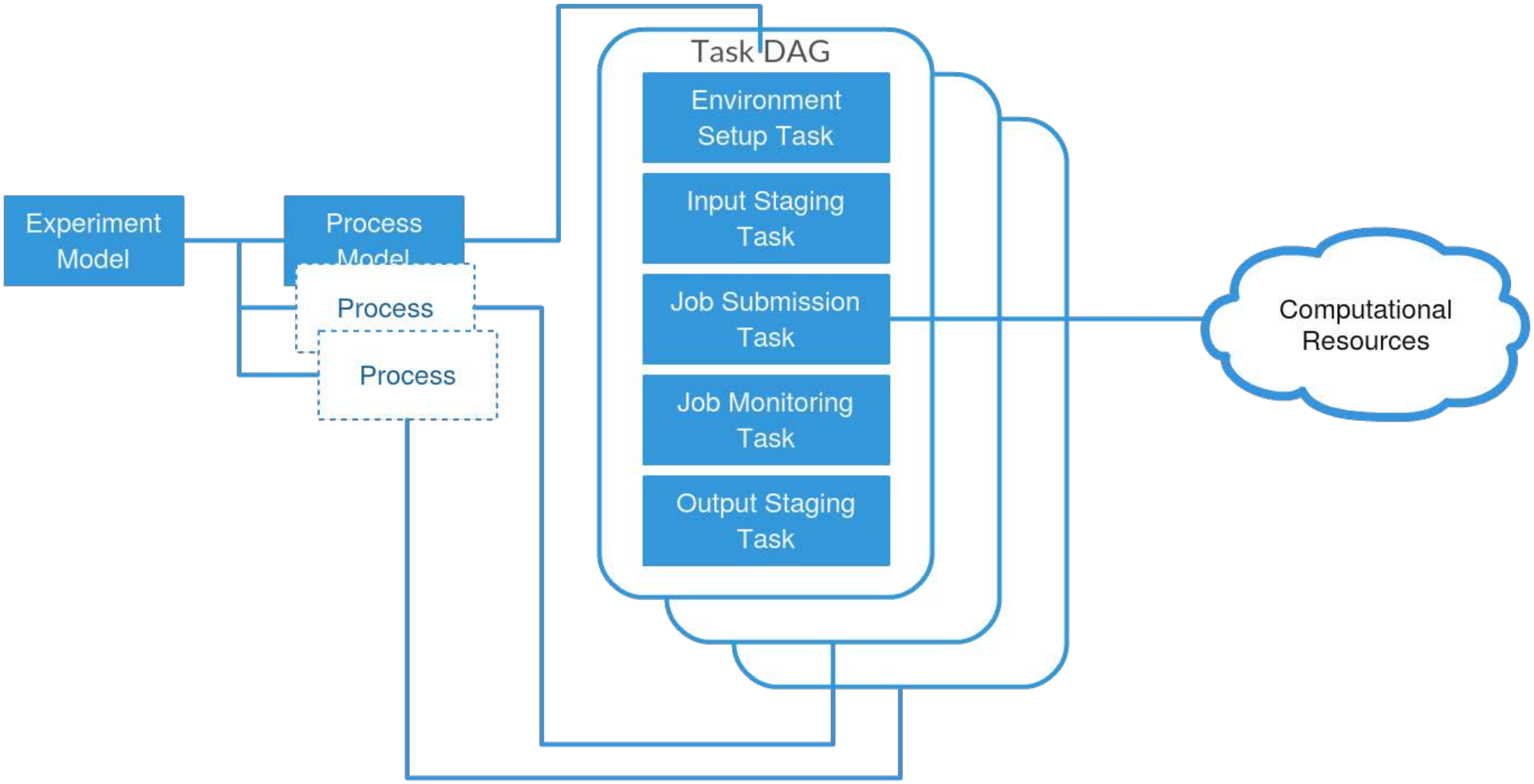


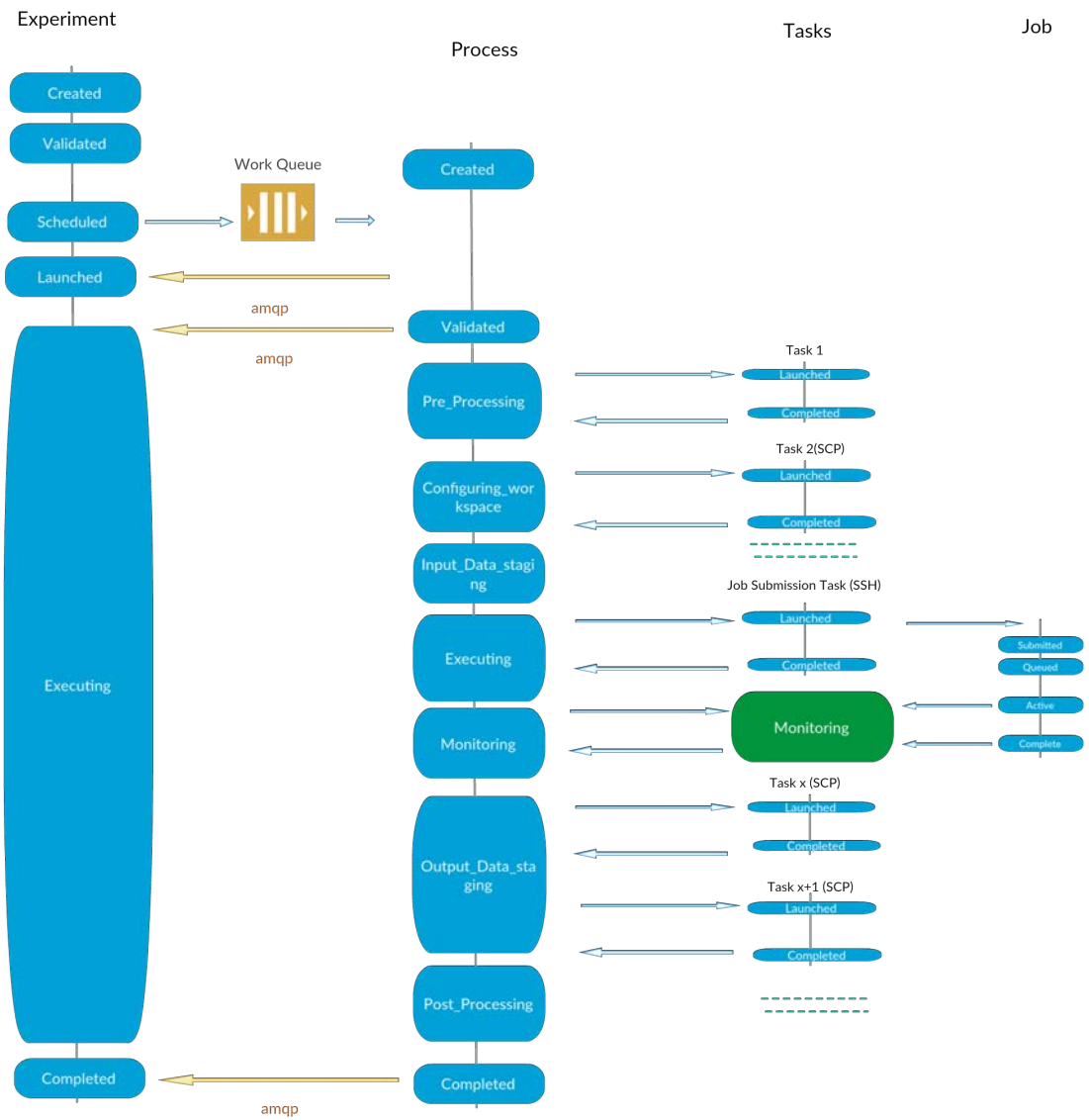


Administrative Dashboards

Abstracting HPC and Cloud Job Management




Experiment Model
Process Model
Process
Process
Task DAG
Environment Setup Task
Input Staging Task
Job Submission Task
Job Monitoring Task
Output Staging Task
Computational Resources


Experiment
Process
Tasks
Job
Created
Validated
Scheduled
Launched
Executing
Completed
Work Queue
amqp
amqp
amqp
Created
Validated
Pre_Processing
Configuring_workspace
Input_Data_staging
Executing
Monitoring
Output_Data_staging
Post_Processing
Completed
Task 1
Launched
Completed
Task 2(SCP)
Launched
Completed
Job Submission Task (SSH)
Launched
Completed
Monitoring
Submitted
Queued
Active
Complete
Task x (SCP)
Launched
Completed
Task x+1 (SCP)
Launched
Completed

ADVANCED TOPICS

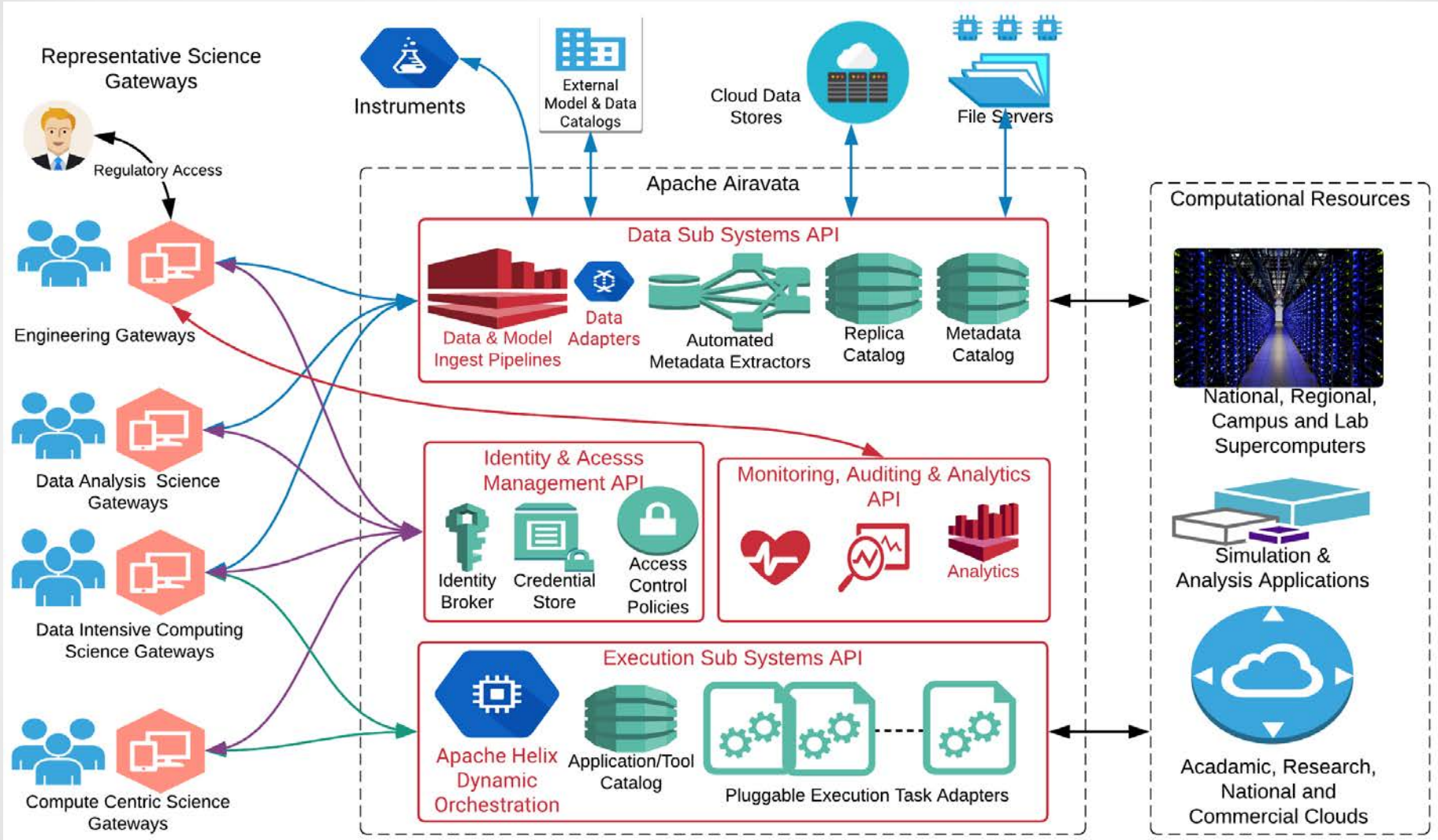
Apache Airavata

- **Gateway Developers:** Open source software for building science gateways
- **Users:** Use it to transfer data and execute remote applications and pipelines on distributed resources
- **Teams:** Create, organize, clone, and share computational experiments
- **Software Providers:** Make scientific software available as a service

Science Gateways Platform as a Service: SciGaP

Powered By

Registered SciGaP Gateways	40
Supported Applications	118
Integrated Computing Resources	50
Registered Users	3500+
Number of applications run (3 years)	>136,000
Computing Hours (3 years)	> 22.8 M


Representative Science Gateways
Regulatory Access
Instruments
External Model & Data Catalogs
Cloud Data Stores
File Servers
Apache Airavata
Data Sub Systems API
Data & Model Ingest Pipelines
Data Adapters
Automated Metadata Extractors
Replica Catalog
Metadata Catalog
Engineering Gateways
Data Analysis Science Gateways
Data Intensive Computing Science Gateways
Compute Centric Science Gateways
Identity & Acesss Management API
Identity Broker
Credential Store
Access Control Policies
Monitoring, Auditing & Analytics API
Analytics
Execution Sub Systems API
Apache Helix Dynamic Orchestration
Application/Tool Catalog
Pluggable Execution Task Adapters
Computational Resources
National, Regional, Campus and Lab Supercomputers
Simulation & Analysis Applications
Acadamic, Research, National and Commercial Clouds

Key Points

- Apache Airavata is open source, open community software
- CIRC runs a hosted Apache Airavata deployment for clients: SciGaP
- We integrate campus clusters, XSEDE resources, computational clouds, and international resources for gateways
- We use best of breed software subsystems and DevOps operations practices
- Subsystems for security, data management can be used independently