

# Science Gateways



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## Outline

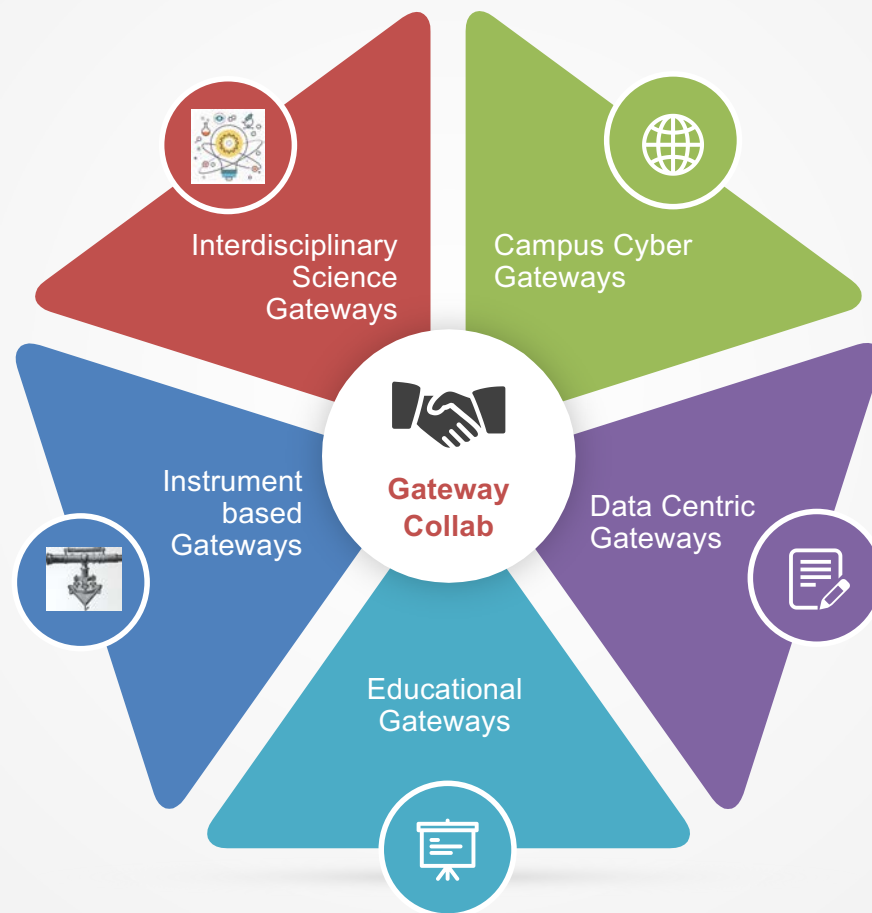
- Introduction to Science Gateways
- Ushering Scientific Software to “as-a-service” model
- Containers and Gateways
- Hands-on tutorial
- Q&A
- Advanced Gateway Topics

# WHAT ARE SCIENCE GATEWAYS?

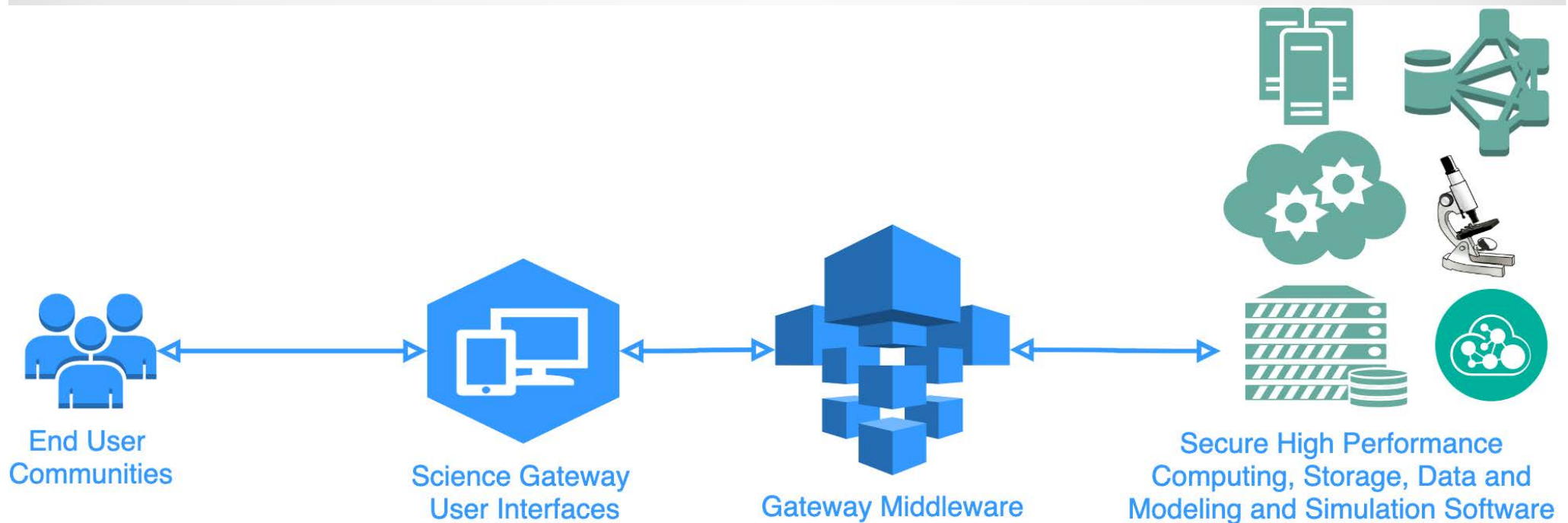
Web interfaces and middleware for integrating distributed computing and data, automating expertise, controlling access, managing results, and speeding up your critical computational workflows

Learn more at <https://sciencegateways.org/>

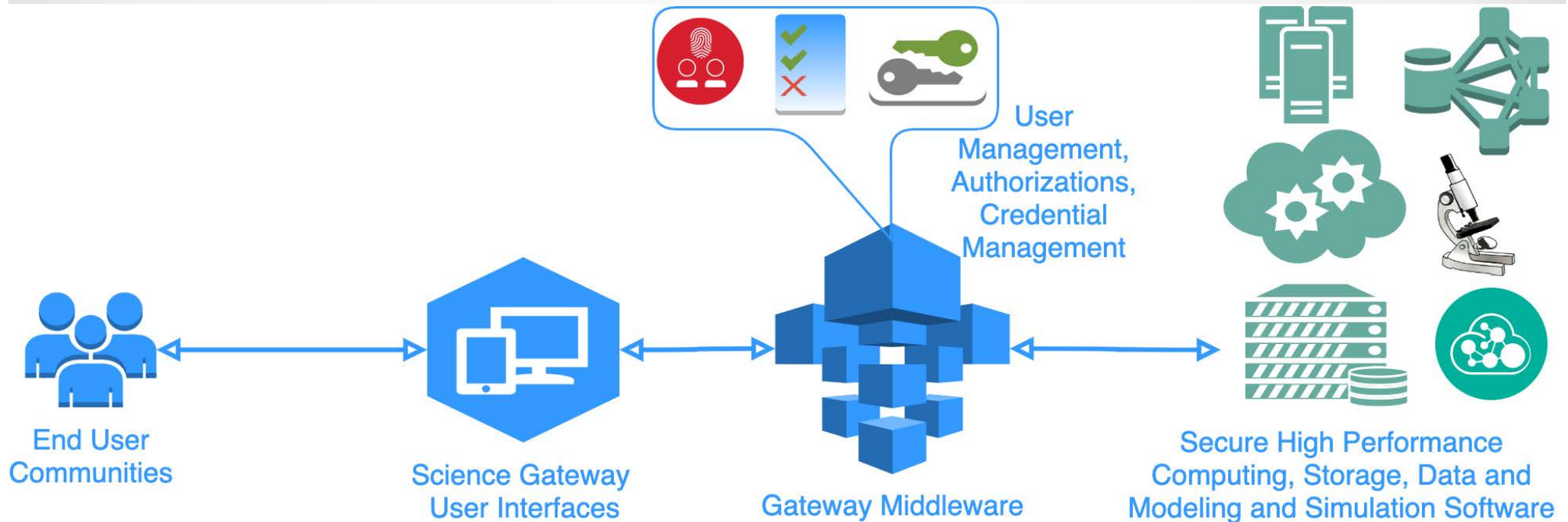
# Serving Targeted Communities



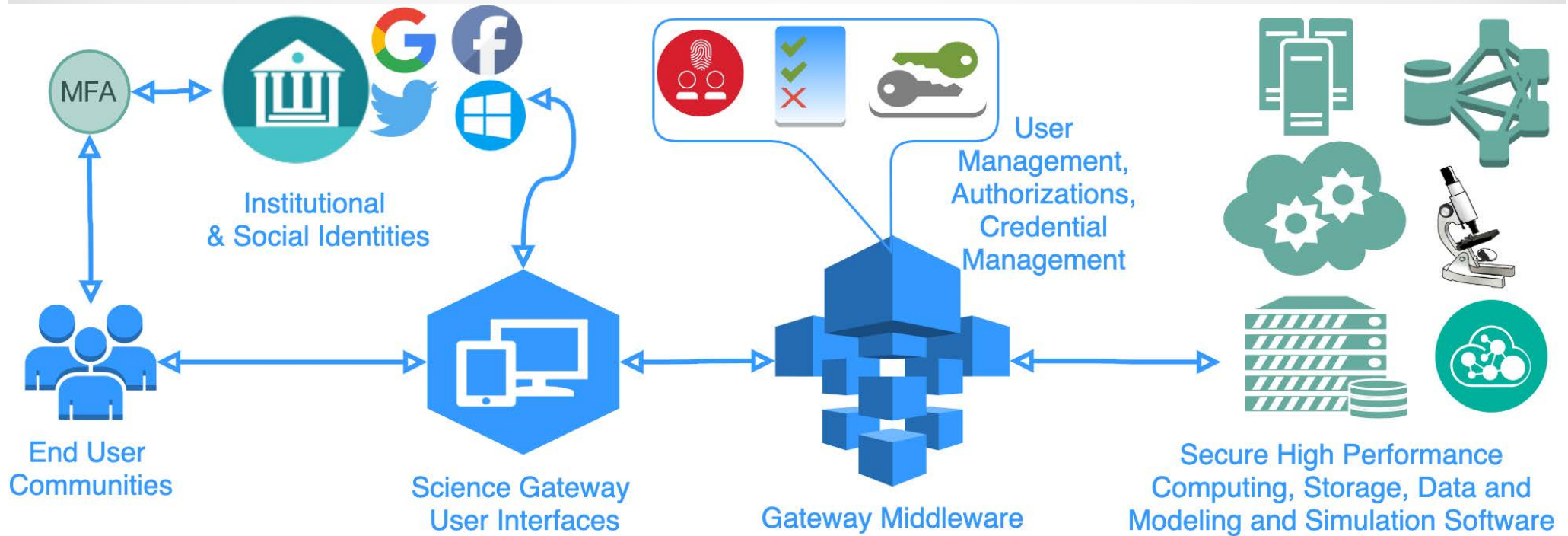
## Resource-centric view --> Science-centric view



# Secured access & Controlled sharing of digital artifacts



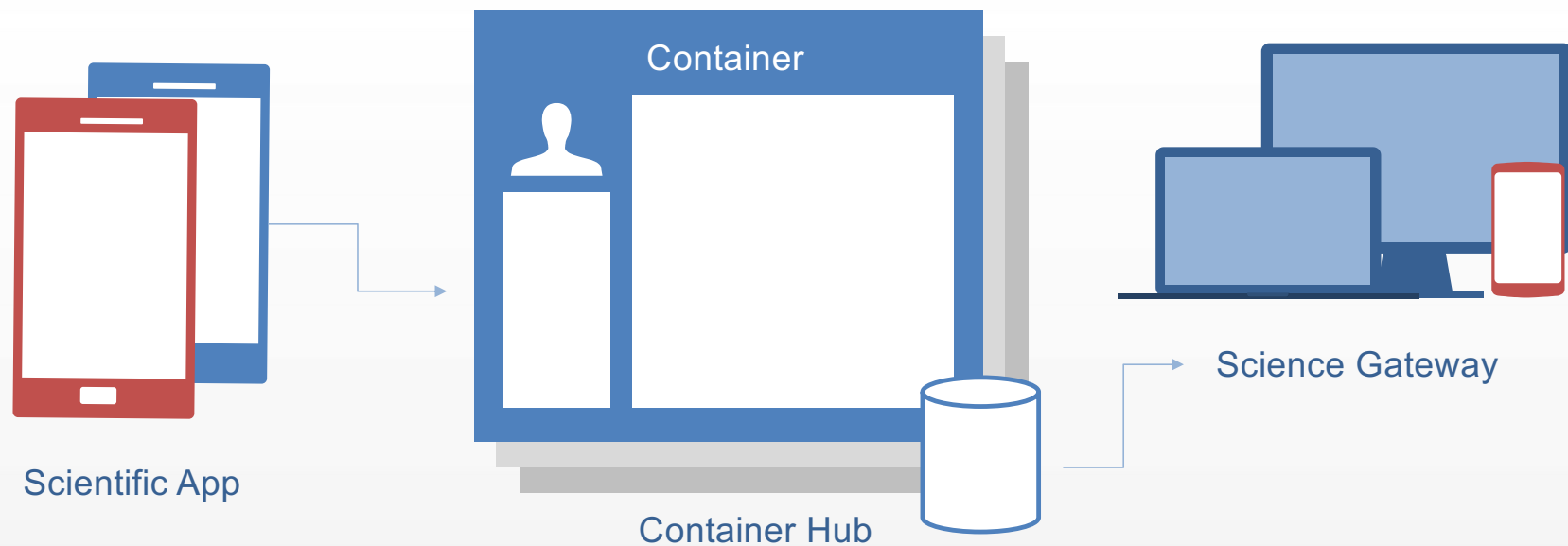
# Federated Authentication

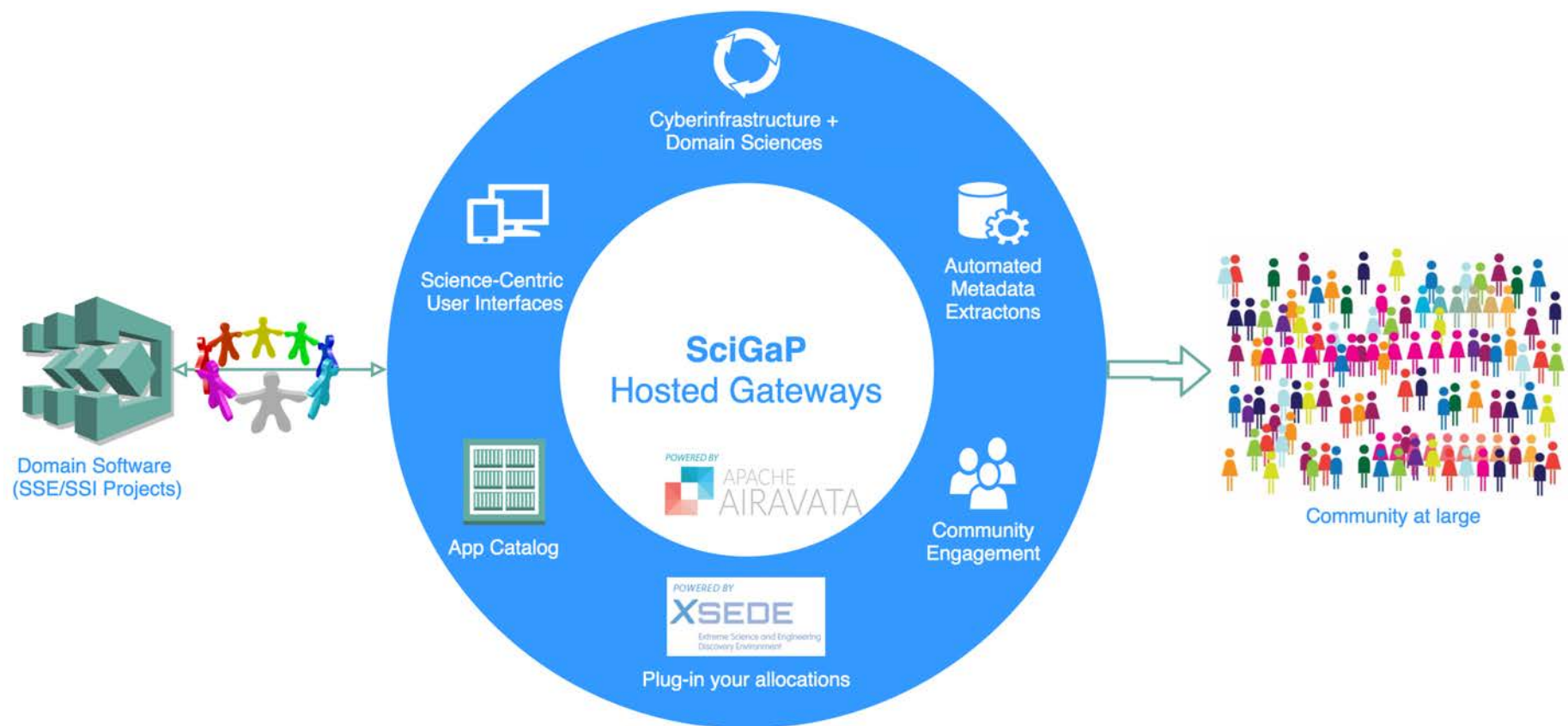


# **CONTAINERS & GATEWAYS**



## Scientific App to a Gateway Interface





Gateways can  
enable “Scientific  
app-store”

The screenshot displays the Airavata Test Drive Gateway dashboard in a web browser. The browser's address bar shows the URL `https://testdrive.airavata.org/workspace/dashboard`. The page header includes the Airavata logo, the title "Airavata Test Drive Gateway", and user information for "Marlon Pierce". A left sidebar contains navigation icons for dashboard, applications, workspace, and files. The main content area is titled "Dashboard" and features a section labeled "APPLICATIONS" with a grid of application cards. Each card includes the application name, a brief description, and a star icon for favoriting.

Application Name	Description
Abaqus-6.13-3	Finite Element Analysis, Engineering
Abaqus	
Abinit	ABINIT is a package whose main program allows one to find the total energy, charge density and electronic structure of systems made of electrons and nuclei (molecules and periodic solids) within Density Functional Theory (DFT)
Amber	Assisted Model Building with Energy Refinement MD Package
AutoDock	AutoDock suite of automated docking tools
CP2K	CP2K Test Application Module
CPMD	parallelized plane wave / pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics
DDSCat	Discrete Dipole Approximation Scattering (DDSCAT) code
DFTB+	Semi empirical Quantum Chemistry

On the right side of the dashboard, there is a section titled "MY RECENT EXPERIMENTS" with a "View all" link.

# Dashboard of Scientific Experiments

The screenshot shows a web browser window with the URL `https://testdrive.airavata.org/workspace/experiments`. The page title is "Airavata Test Drive Gateway". The user is logged in as "Marlon Pierce". The main section is titled "Browse Experiments" and displays a table of experiments.

Name	Application	User	Creation Time	Status	Actions
<a href="#">Clone of Gaussian16 on Mar 29, 2020 12:24 AM</a>	Gaussian16	vivband@iu.edu	9 days ago	CREATED	<a href="#">Edit</a>
<a href="#">Gaussian16 on Mar 29, 2020 12:24 AM</a>	Gaussian16	vivband@iu.edu	10 days ago	COMPLETED	<a href="#">Clone</a>
<a href="#">Echo namaste</a>	Echo	smarru	10 days ago	COMPLETED	<a href="#">Clone</a>
<a href="#">Echo guten tag</a>	Echo	marcus	2 months ago	COMPLETED	<a href="#">Clone</a>
<a href="#">Echo bonjour</a>	Echo	marcus	2 months ago	COMPLETED	<a href="#">Clone</a>
<a href="#">Echo bonjour</a>	Echo	marcus	2 months ago	FAILED	<a href="#">Clone</a>
<a href="#">Echo on Feb 18, 2020 4:18 PM</a>	Echo	marcus	2 months ago	COMPLETED	<a href="#">Clone</a>
<a href="#">Gaussian16 on Feb 18, 2020 12:22 PM</a>	Gaussian16	marcus	2 months ago	COMPLETED	<a href="#">Clone</a>
<a href="#">Gaussian16 on Jan 16, 2020 3:24 PM</a>	Gaussian16	marcus	3 months ago	COMPLETED	<a href="#">Clone</a>
<a href="#">Gaussian16 on Dec 2, 2019 8:08 AM</a>	Gaussian16	jsale37	4 months ago	COMPLETED	<a href="#">Clone</a>

Showing 1 - 10 [Next](#)

# Launch “Experiments”

The screenshot shows a web browser window with the URL `https://testdrive.airavata.org/workspace/applications/Gaussian_9fe2l`. The page title is "Airavata Test Drive Gateway". The user is logged in as "Marlon Pierce". The page is for creating a new experiment using the "GAUSSIAN" application.

**Create a New Experiment** Share 2

Experiment Name  
Gaussian on Apr 7, 2020 2:15 PM

Add a description

Project  
Default Project

**Application Configuration**

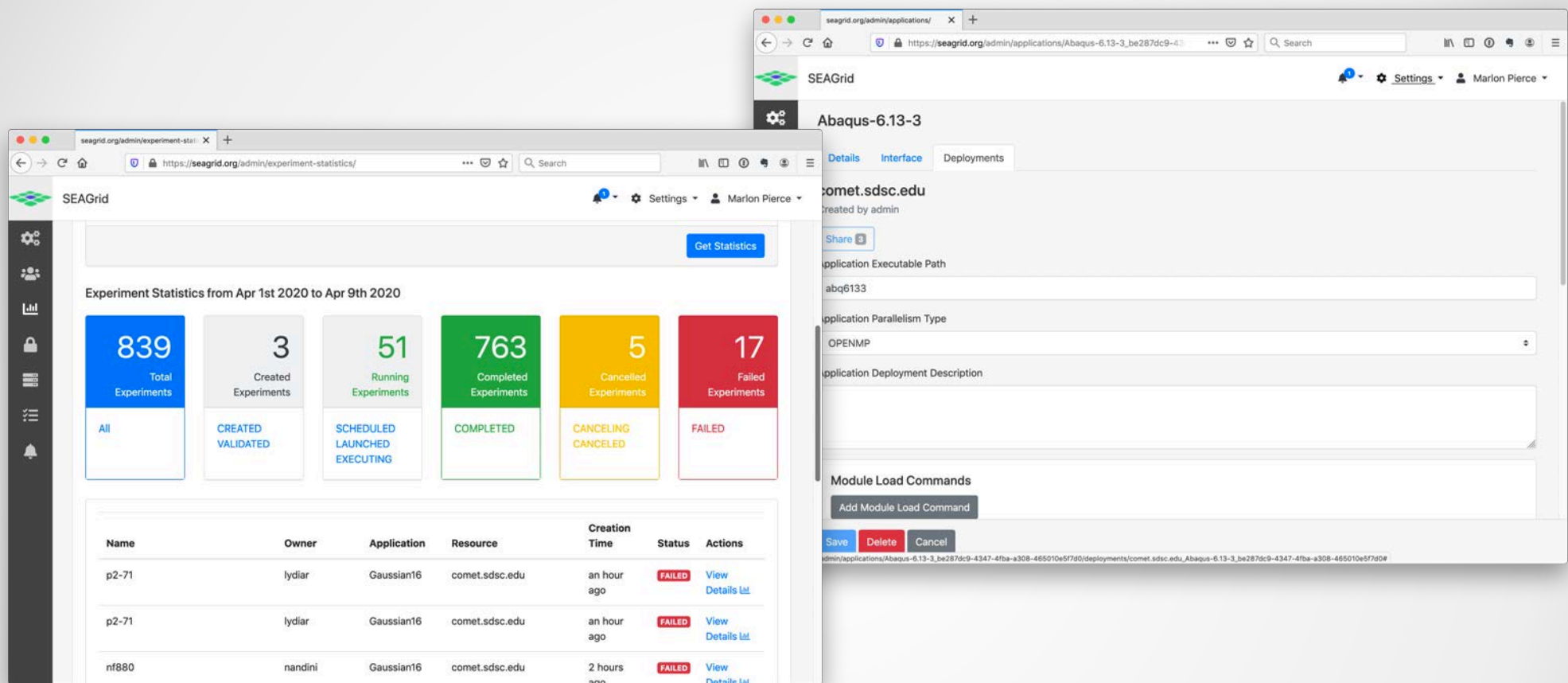
**Application Inputs**

Input-File

Select file from storage OR Drop files here or [browse](#)  
Max file upload size is 64 MB

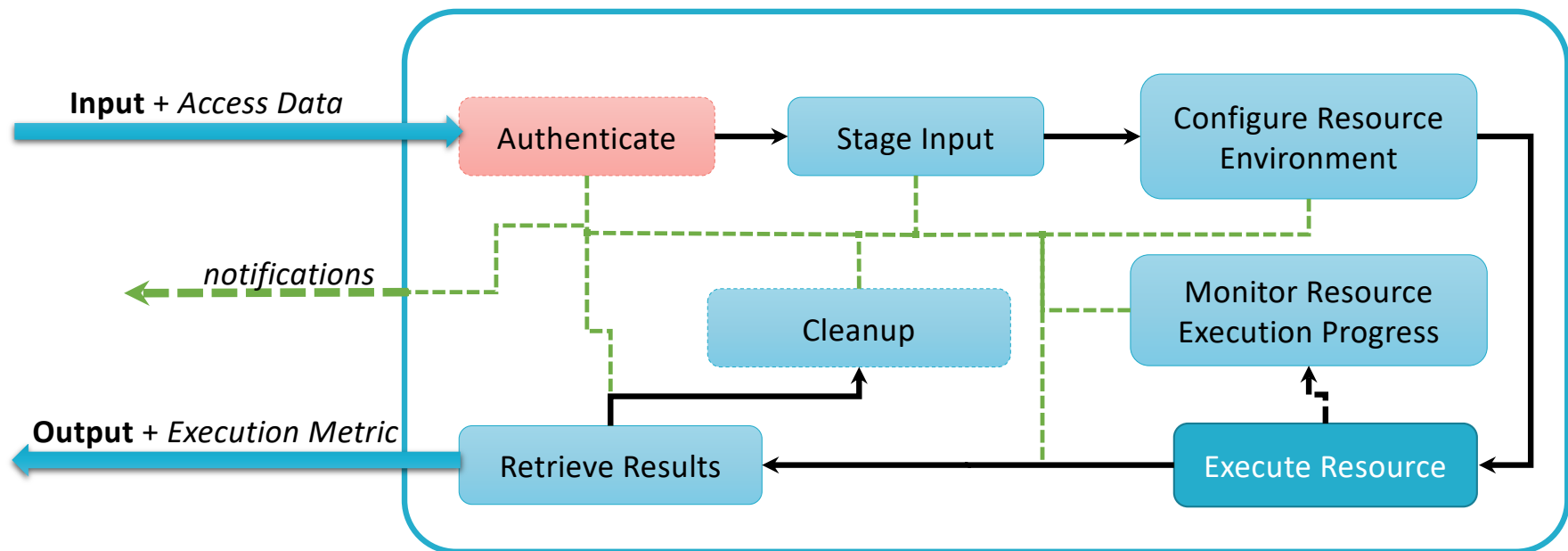
Gaussian input file specifying desired calculation type, model chemistry, molecular system and other parameters.

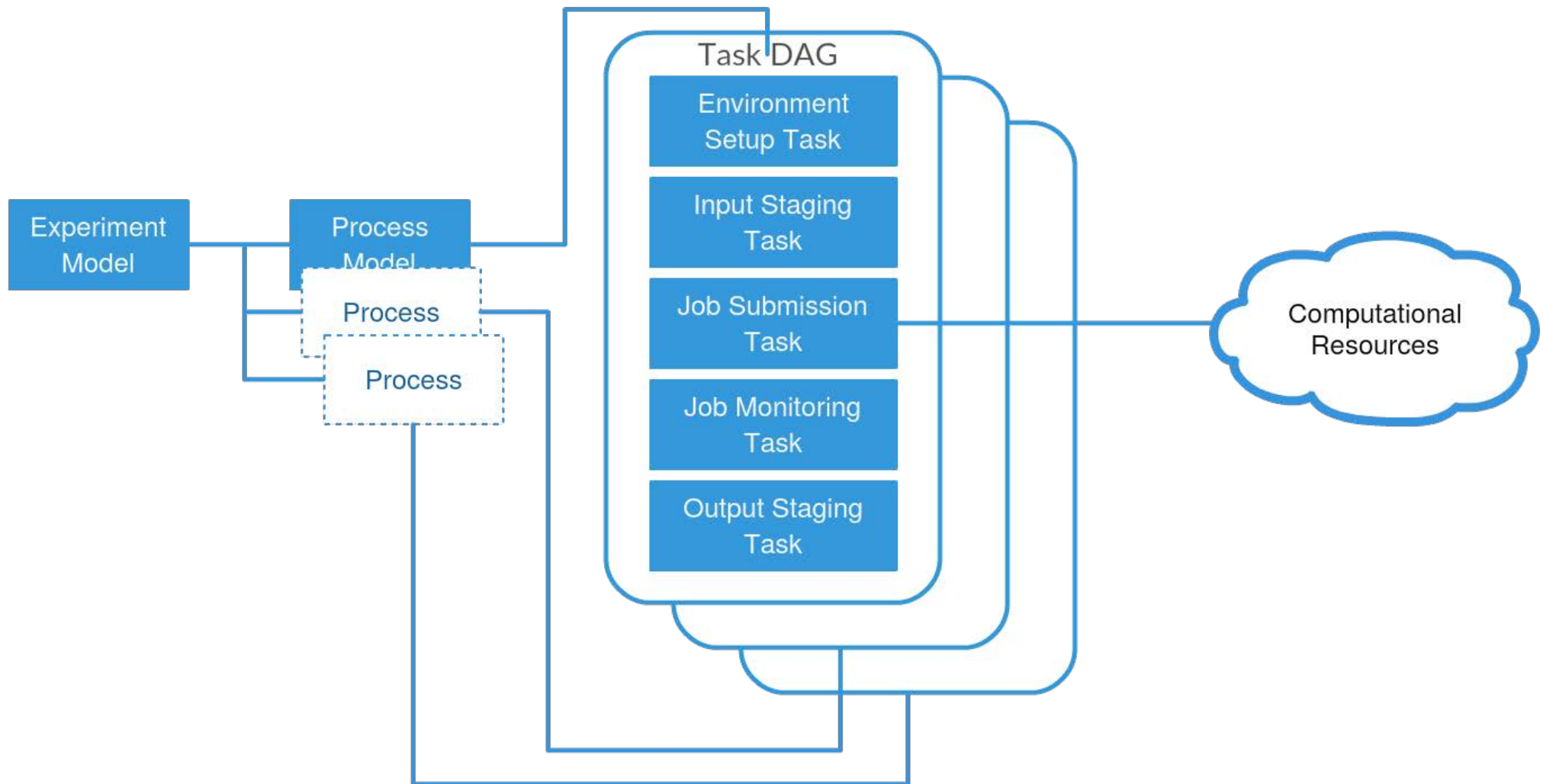
**Allocation**  
Default



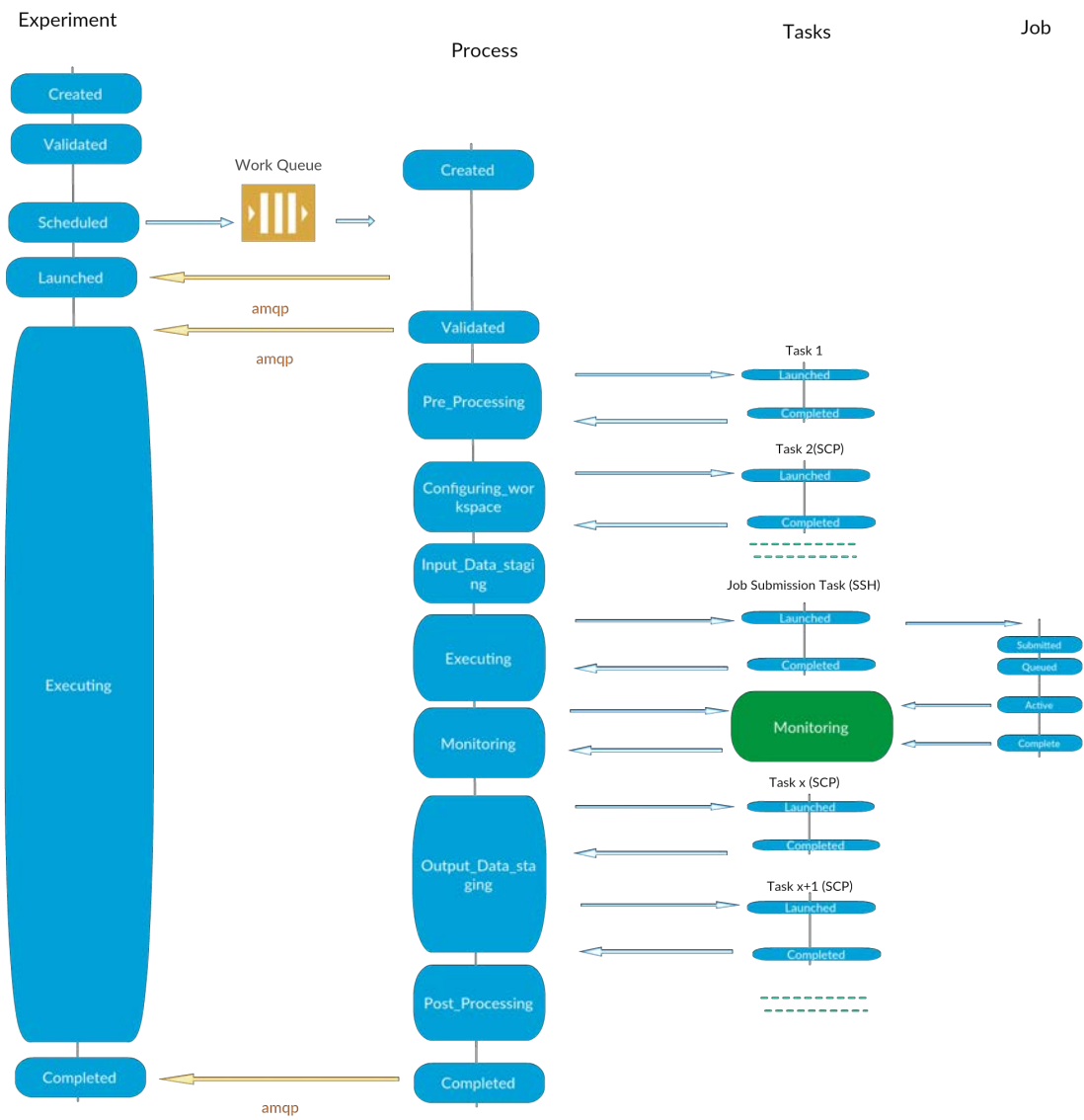
## Administrative Dashboards

# Abstracting HPC and Cloud Job Management









# **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

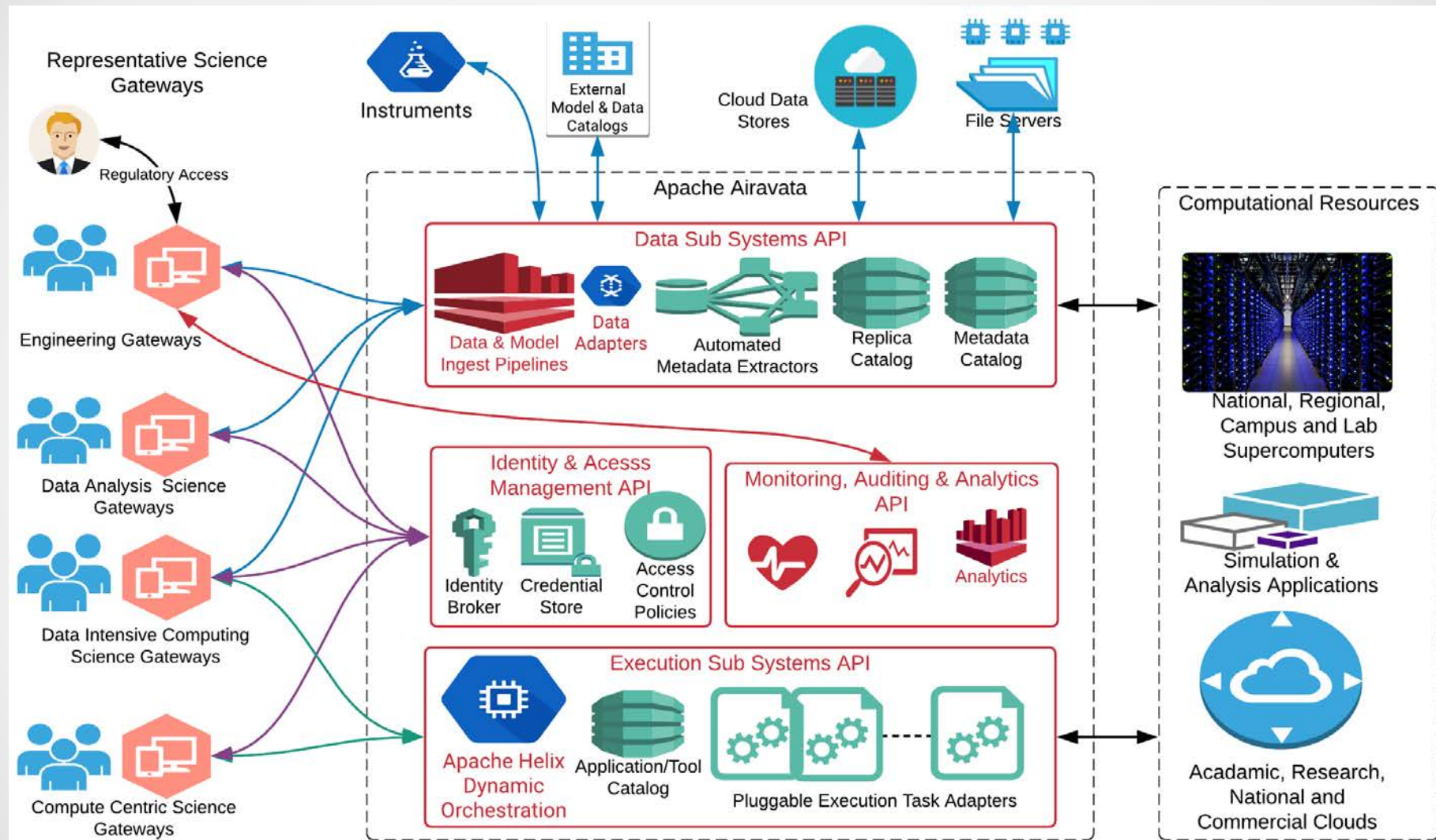
# Science Gateways Platform as a Service: SciGaP



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



## 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