

# Science Gateways



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# Outline

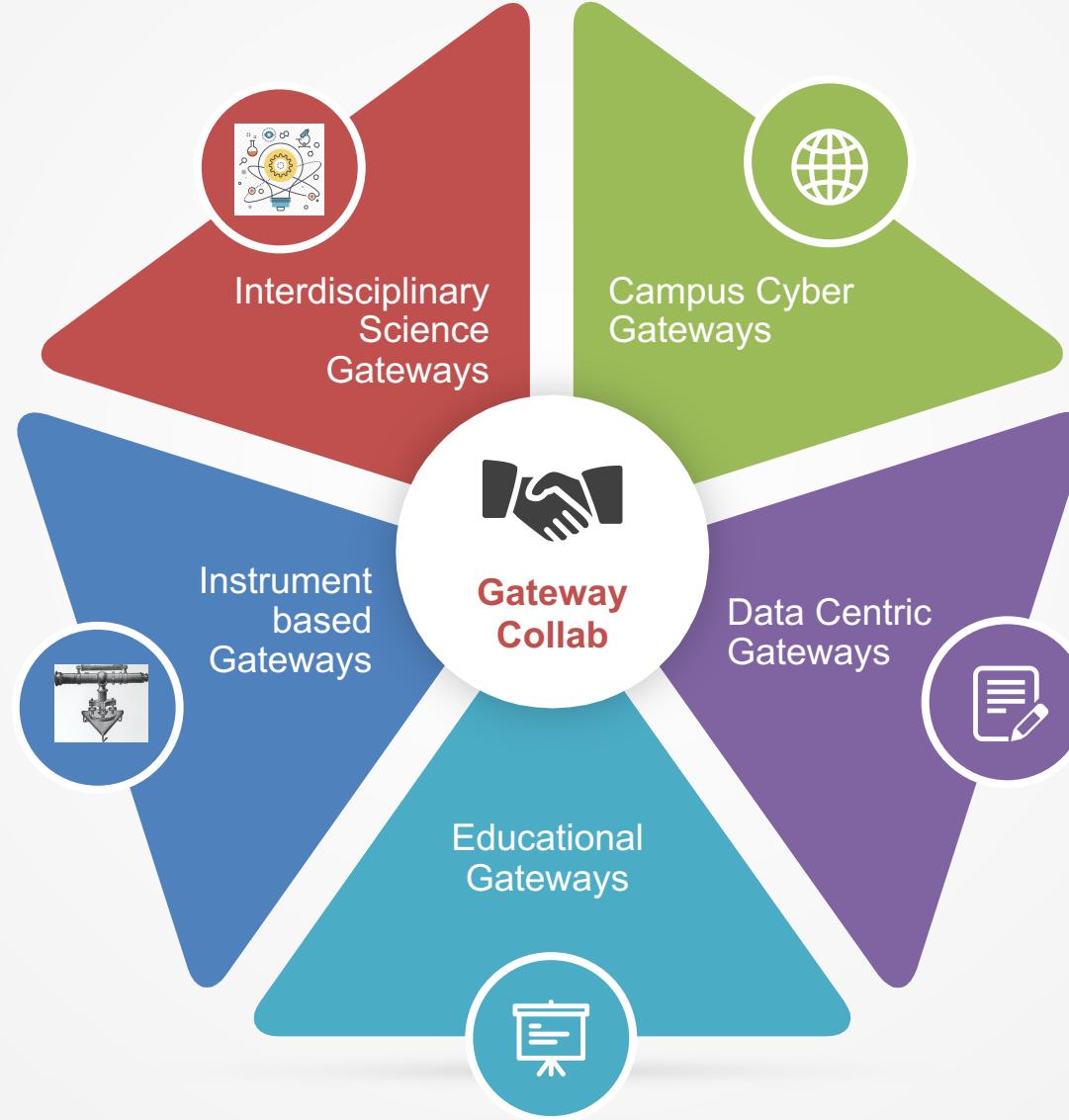
- Introduction to Science Gateways
- Ushering Scientific Software to “as-a-service” model
- Containers and Gateways
- Hands-on tutorial
- Q&A
- Advanced Gateway Topics

# WHAT ARE SCIENCE GATEWAYS?

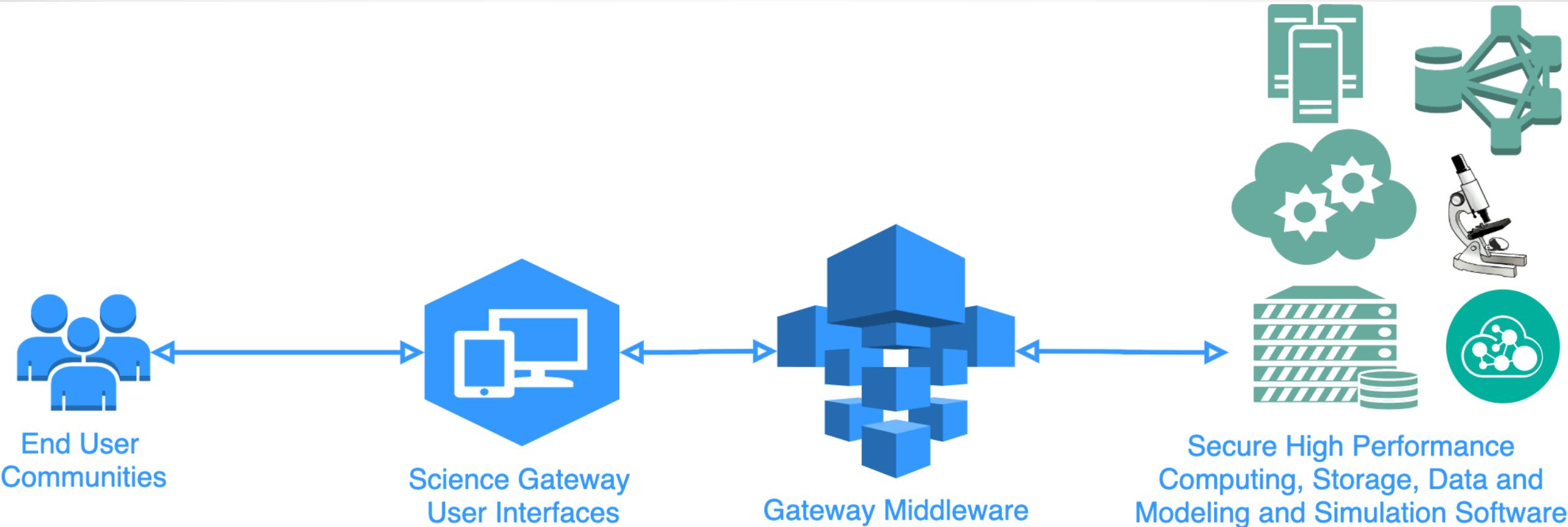
Web interfaces and middleware for integrating distributed computing and data, automating expertise, controlling access, managing results, and speeding up your critical computational workflows

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

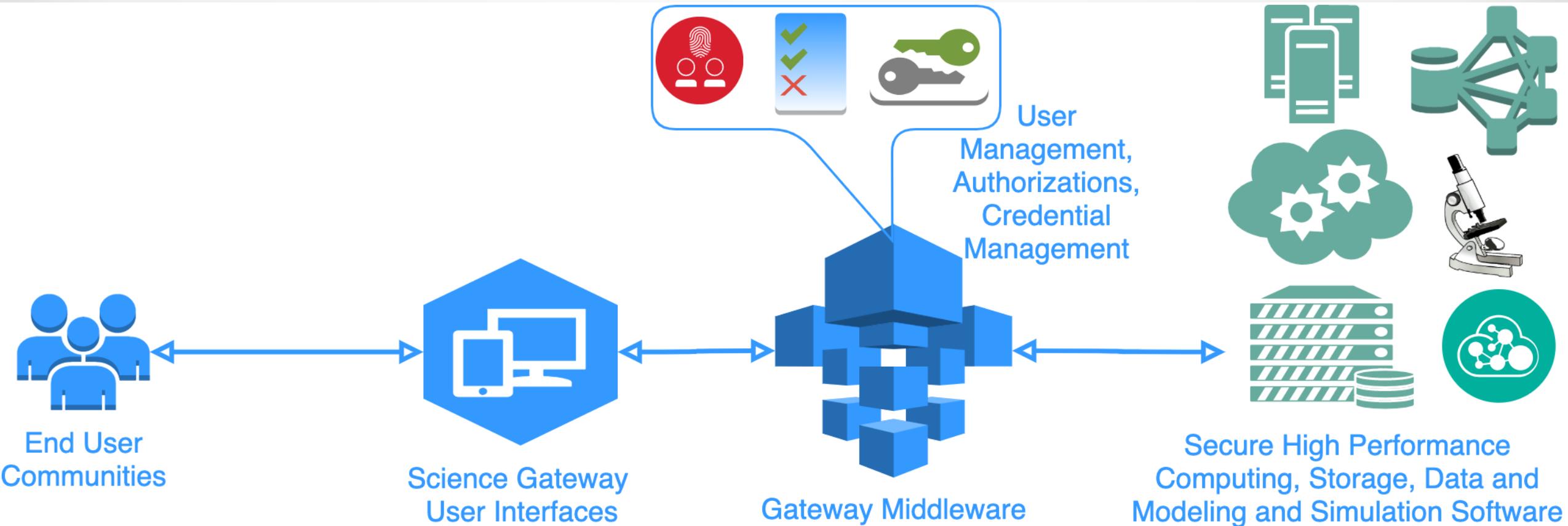
# Serving Targeted Communities



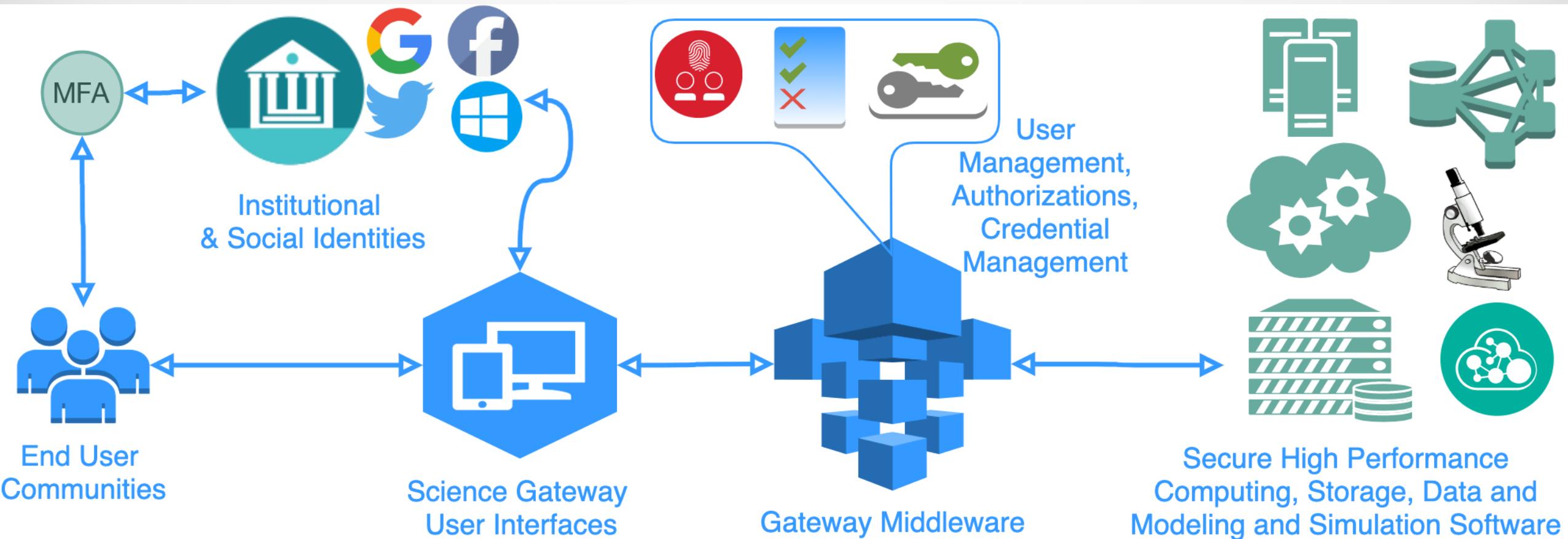
# Resource-centric view --> Science-centric view



# Secured access & Controlled sharing of digital artifacts

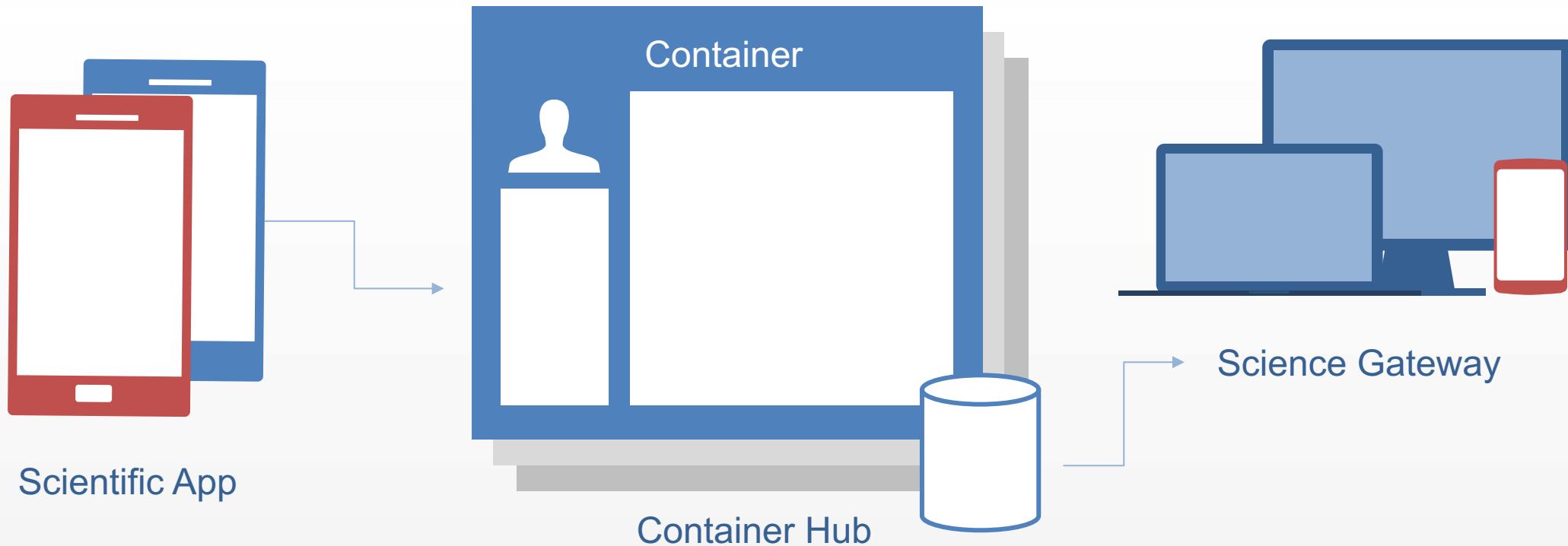


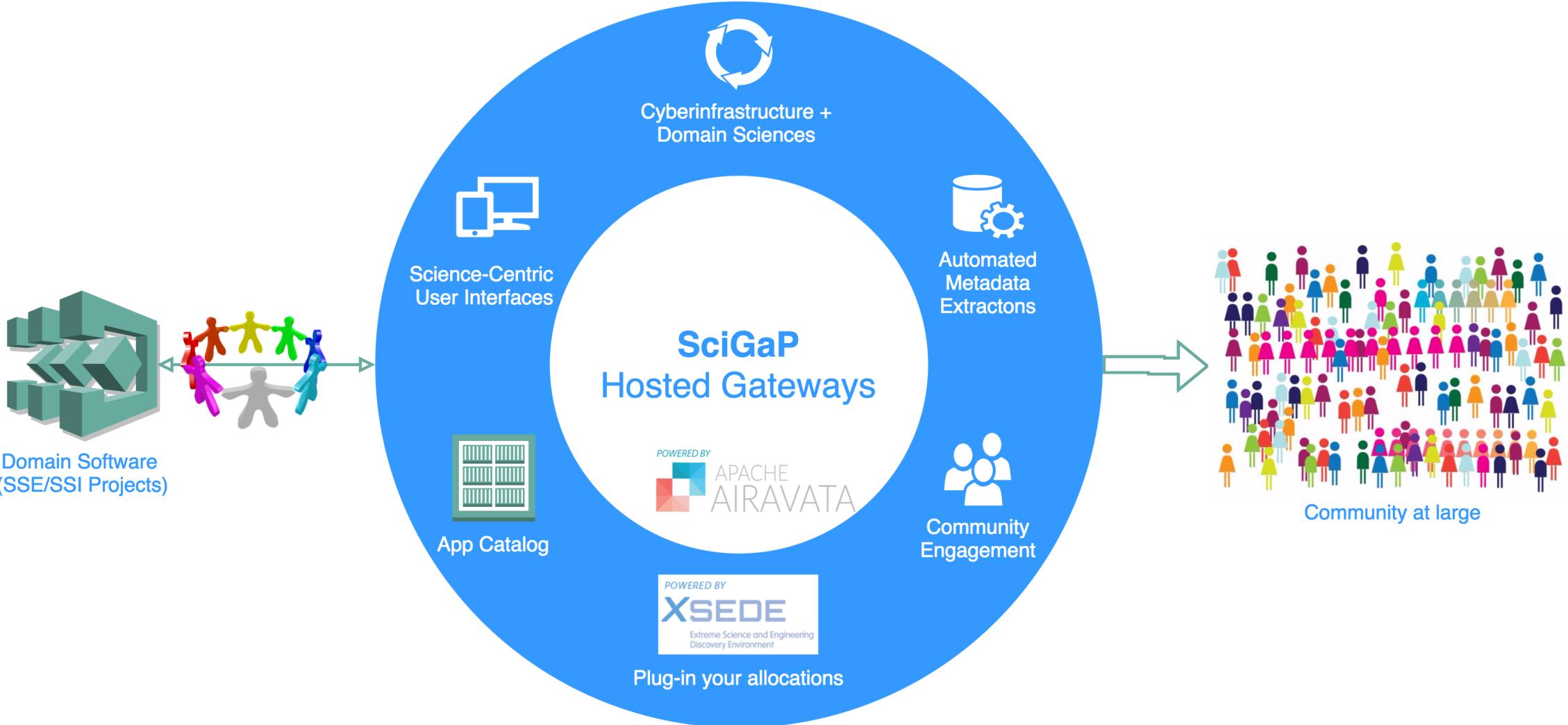
# Federated Authentication



# **CONTAINERS & GATEWAYS**

# Scientific App to a Gateway Interface





Gateways can enable “Scientific app-store”

The screenshot shows the Airavata Test Drive Gateway dashboard. On the left is a sidebar with icons for Home, Applications, Projects, and Files. The main header bar includes the URL https://testdrive.airavata.org/workspace/dashboard, a search bar, and user information for Marlon Pierce. The dashboard has a title "Airavata Test Drive Gateway" and a "Dashboard" section. Below it is a "APPLICATIONS" section containing nine cards:

- Abaqus-6.13-3**: Finite Element Analysis, Engineering. Status: Available.
- Abaqus**: Status: Available.
- 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). Status: Available.
- Amber**: Assisted Model Building with Energy Refinement MD Package. Status: Available.
- AutoDock**: AutoDock suite of automated docking tools. Status: Available.
- CP2K**: CP2K Test Application Module. Status: Available.
- CPMD**: parallelized plane wave / pseudopotential implementation of Density Functional Theory, particularly designed for ab-initio molecular dynamics. Status: Available.
- DDSCat**: Discrete Dipole Approximation Scattering (DDSCAT) code. Status: Available.
- DFTB+**: Semi empirical Quantum Chemistry. Status: Available.

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

# Dashboard of Scientific Experiments

The screenshot shows a web browser window titled "testdrive.airavata.org/workspace/ex" with the URL "https://testdrive.airavata.org/workspace/experiments". The page is titled "Airavata Test Drive Gateway" and features a sidebar with icons for Home, Recent, Applications, and Help. The main content area is titled "Browse Experiments" and displays a table of experiment details. The table has columns: Name, Application, User, Creation Time, Status, and Actions. The "Actions" column contains links for "Edit" (pencil icon), "Clone" (clone icon), and "Delete" (trash icon). The experiments listed are:

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

At the bottom right, it says "Showing 1 - 10" and "Next >".

# Launch “Experiments”

The screenshot shows a web browser window for the Airavata Test Drive Gateway at [https://testdrive.airavata.org/workspace/applications/Gaussian\\_9fe2b](https://testdrive.airavata.org/workspace/applications/Gaussian_9fe2b). The title bar indicates the current application is Gaussian.

The main content area displays the "Create a New Experiment" form. On the left, a sidebar menu includes icons for Home, Applications, Projects, and Help.

**Create a New Experiment**

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

The screenshot displays two overlapping browser windows from the SEAGrid platform.

**Top Window (Details View):**

- Title:** Abaqus-6.13-3
- Sub-Header:** comet.sdsc.edu
- Owner:** Created by admin
- Buttons:** Share, Get Statistics
- Text Fields:** application Executable Path (abq6133), application Parallelism Type (OPENMP), application Deployment Description (OPENMP)
- Module Load Commands:** Add Module Load Command, Save, Delete, Cancel

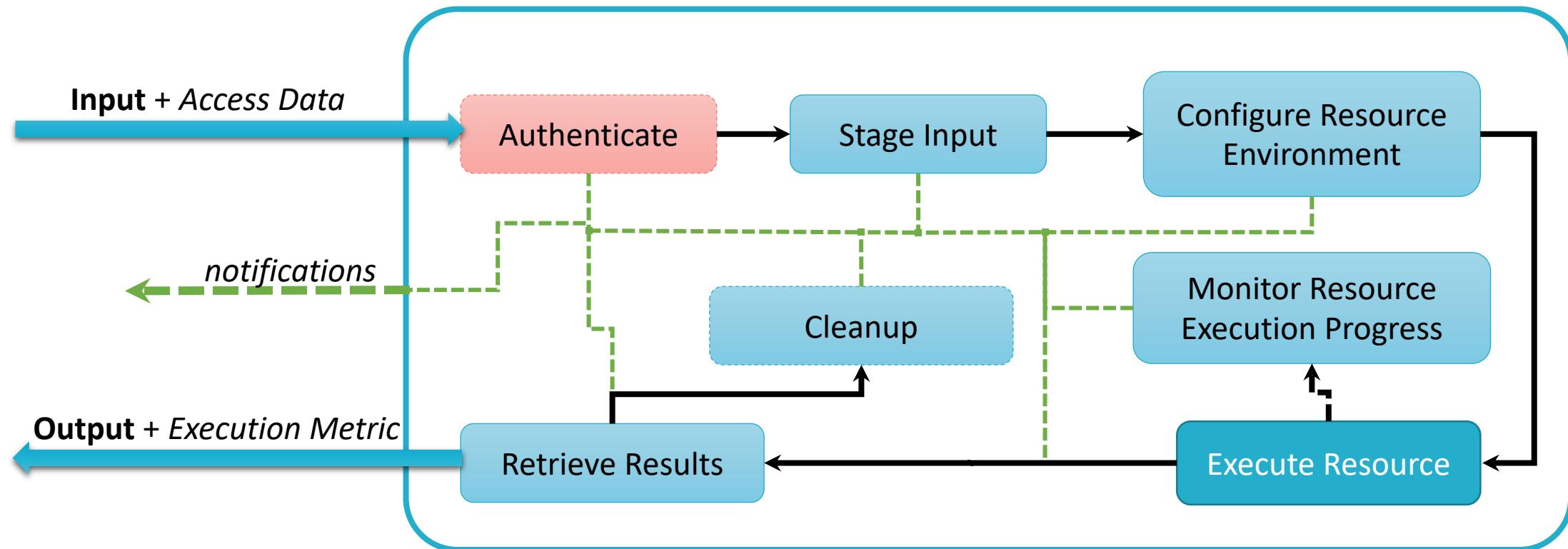
**Bottom Window (Experiment Statistics):**

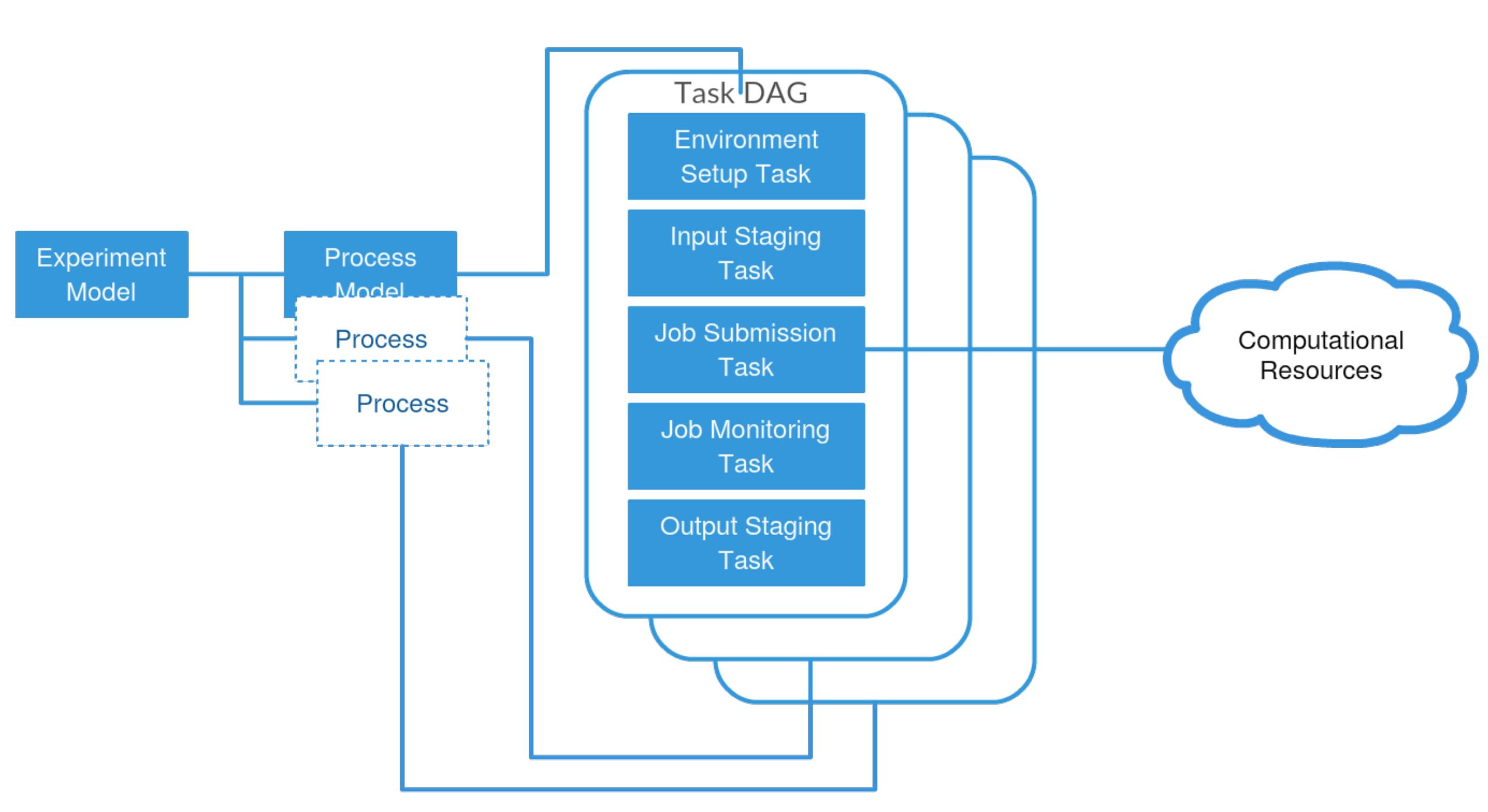
- Title:** Experiment Statistics from Apr 1st 2020 to Apr 9th 2020
- Summary Metrics:**
  - Total Experiments: 839 (All)
  - Created Experiments: 3 (CREATED VALIDATED)
  - Running Experiments: 51 (SCHEDULED LAUNCHED EXECUTING)
  - Completed Experiments: 763 (COMPLETED)
  - Cancelled Experiments: 5 (CANCELING CANCELED)
  - Failed Experiments: 17 (FAILED)
- Table:** A list of experiments with columns: Name, Owner, Application, Resource, Creation Time, Status, Actions.

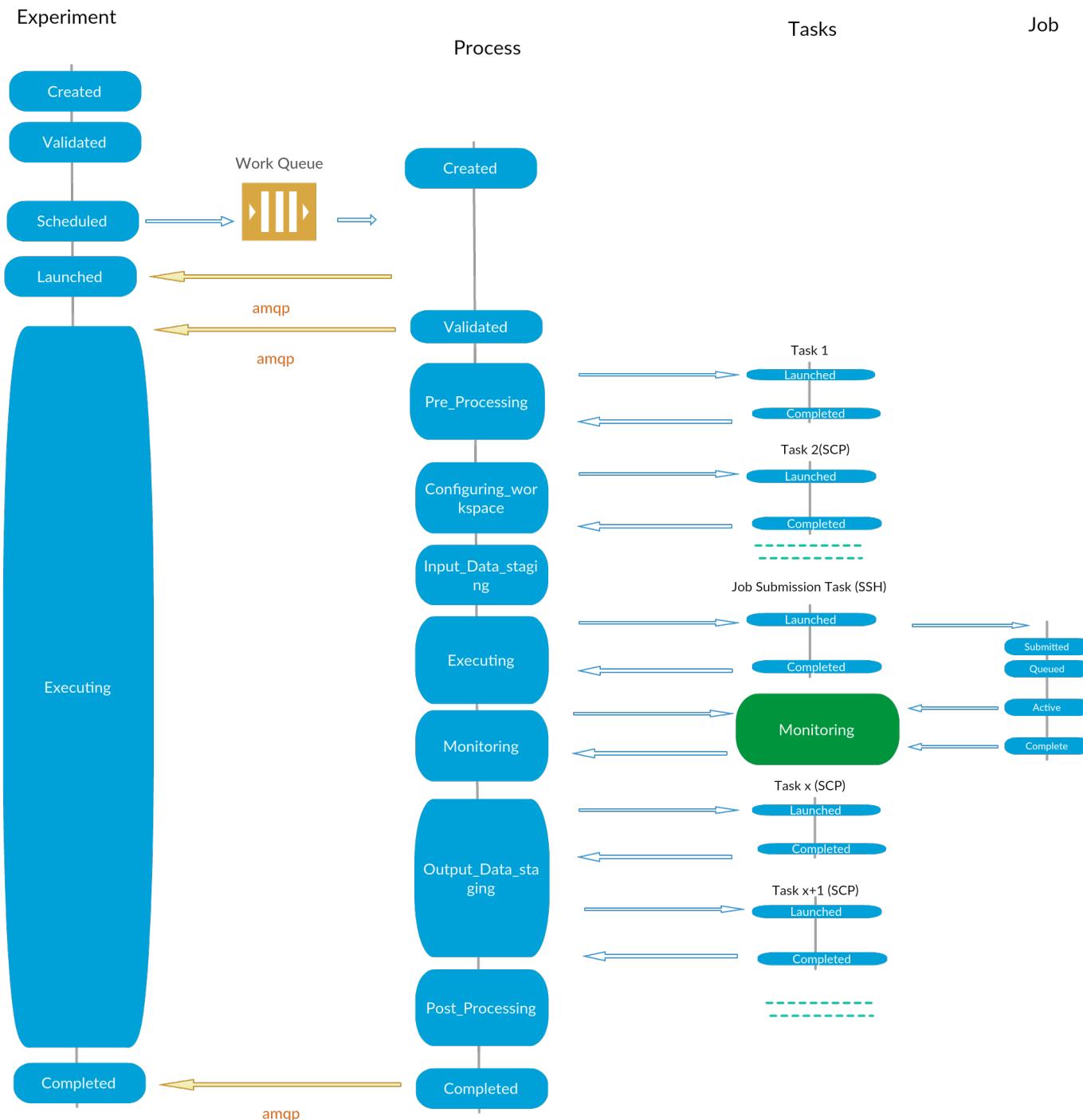
Name	Owner	Application	Resource	Creation Time	Status	Actions
p2-71	lydiar	Gaussian16	comet.sdsc.edu	an hour ago	FAILED	<a href="#">View Details</a>
p2-71	lydiar	Gaussian16	comet.sdsc.edu	an hour ago	FAILED	<a href="#">View Details</a>
nf880	nandini	Gaussian16	comet.sdsc.edu	2 hours ago	FAILED	<a href="#">View Details</a>

# Administrative Dashboards

# Abstracting HPC and Cloud Job Management







# **ADVANCED TOPICS**

# Apache Airavata

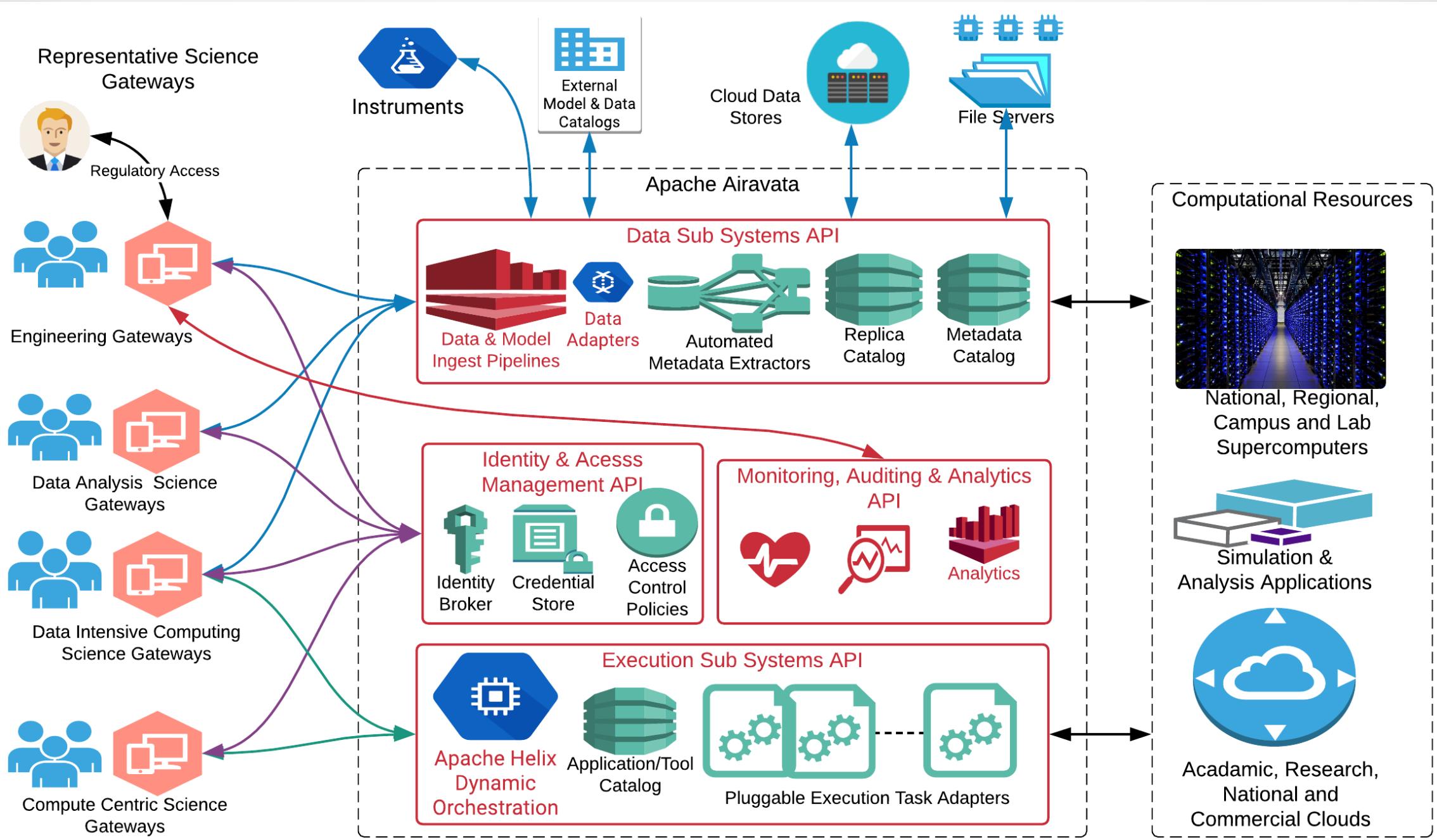


- **Gateway Developers:** Open source software for building science gateways
- **Users:** Use it to transfer data and execute remote applications and pipelines on distributed resources
- **Teams:** Create, organize, clone, and share computational experiments
- **Software Providers:** Make scientific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

# Science Gateways Platform as a Service: SciGaP



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