

Science Gateways



Suresh Marru, Indiana University

Outline

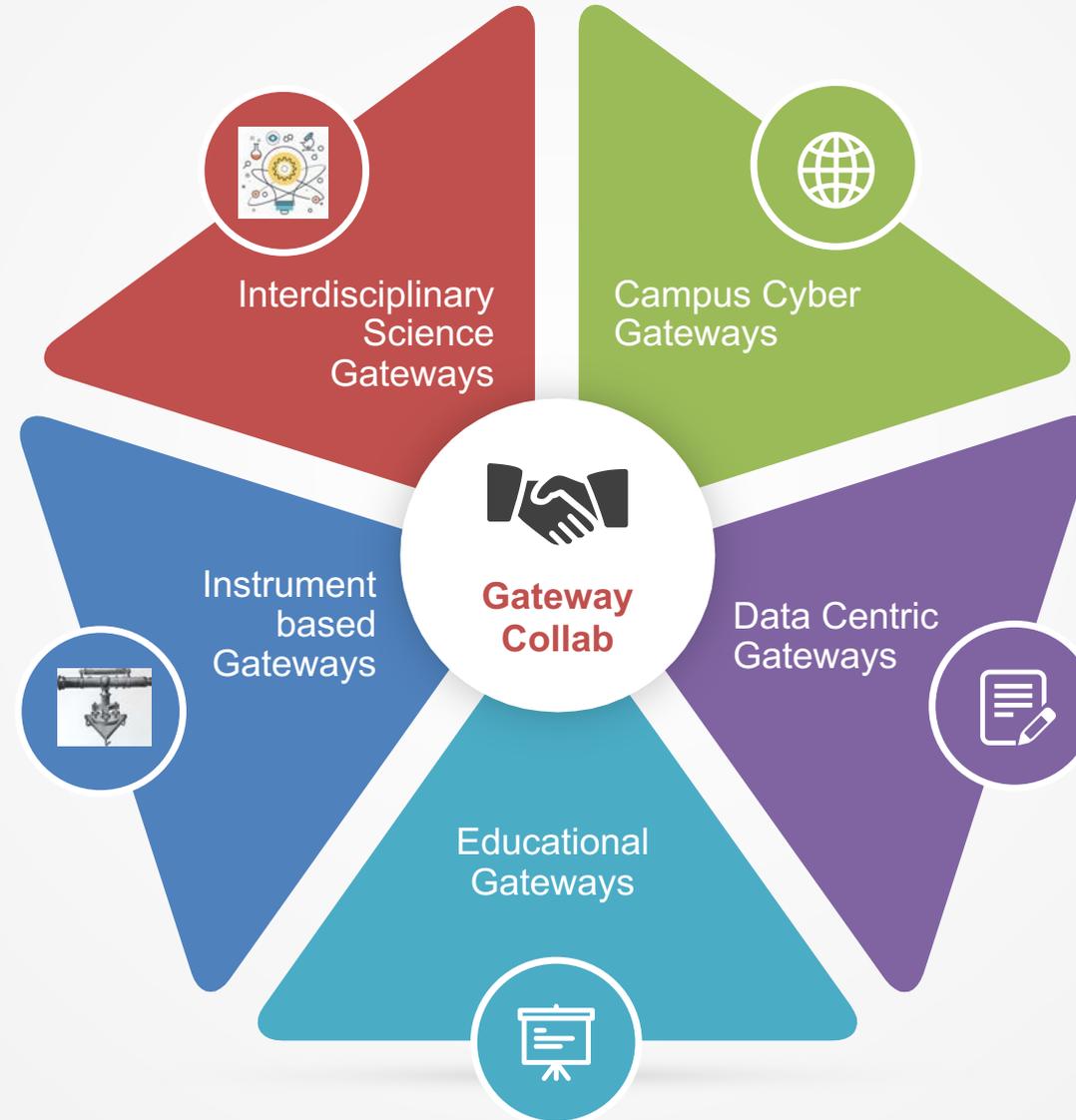
- Introduction to Science Gateways
- Ushering Scientific Software to “as-a-service” model
- Containers and Gateways
- Hands-on tutorial
- Q&A
- Advanced Gateway Topics

WHAT ARE SCIENCE GATEWAYS?

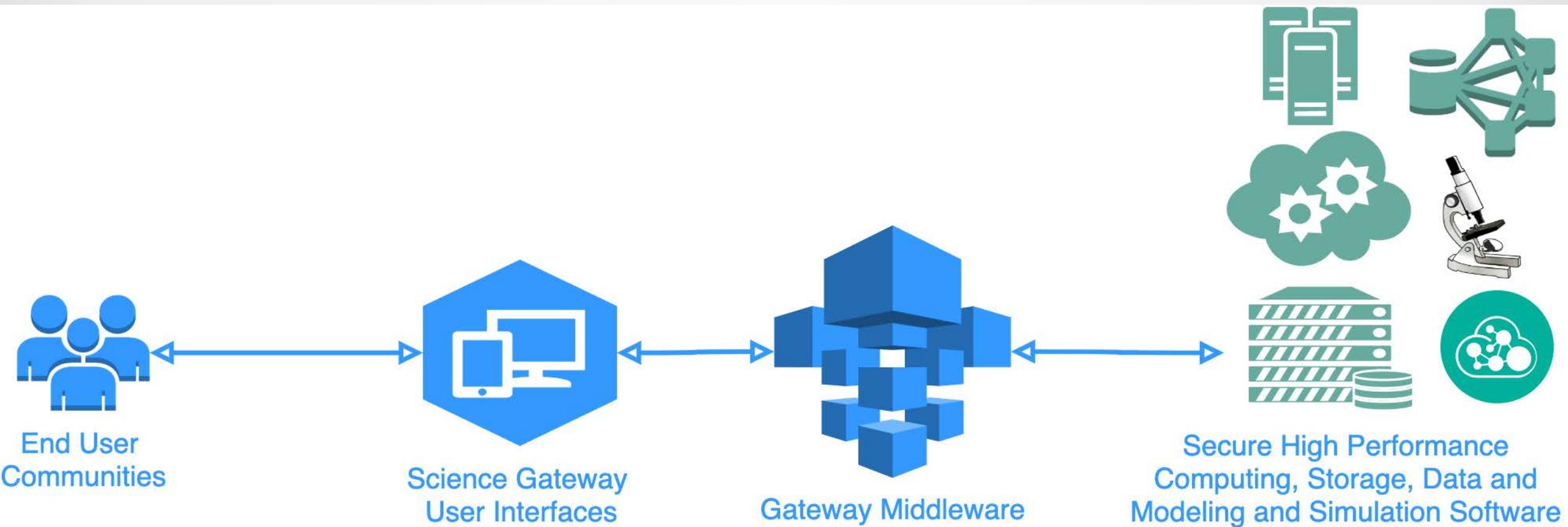
Web interfaces and middleware for integrating distributed computing and data, automating expertise, controlling access, managing results, and speeding up your critical computational workflows

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

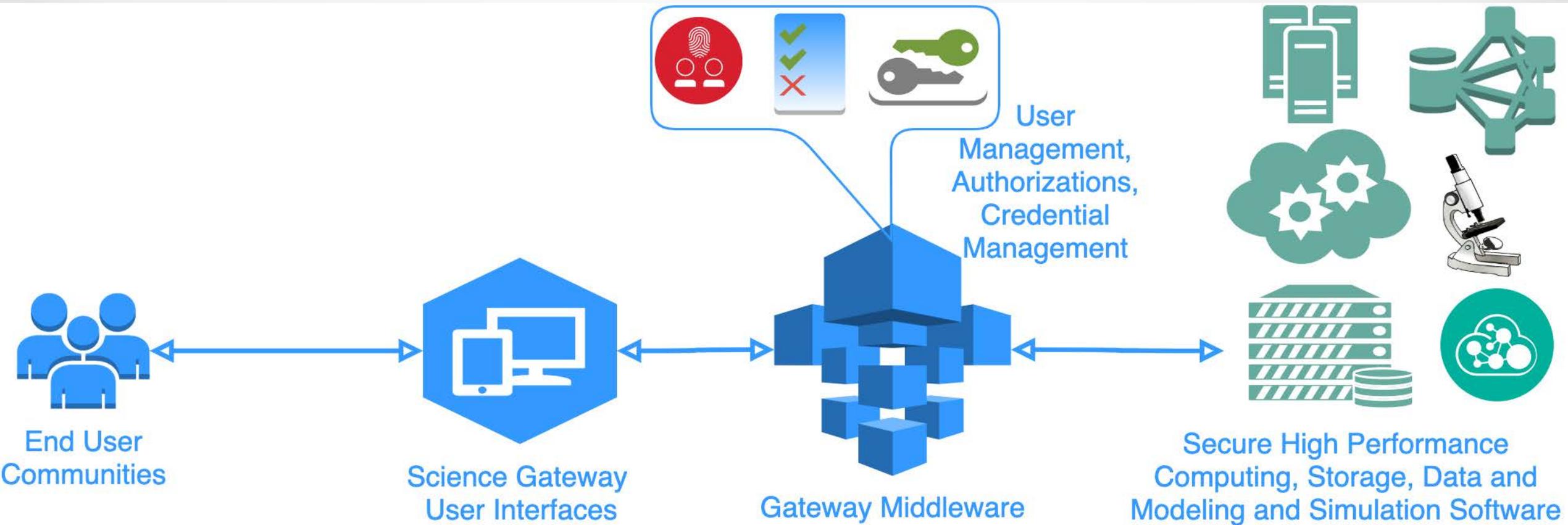
Serving Targeted Communities



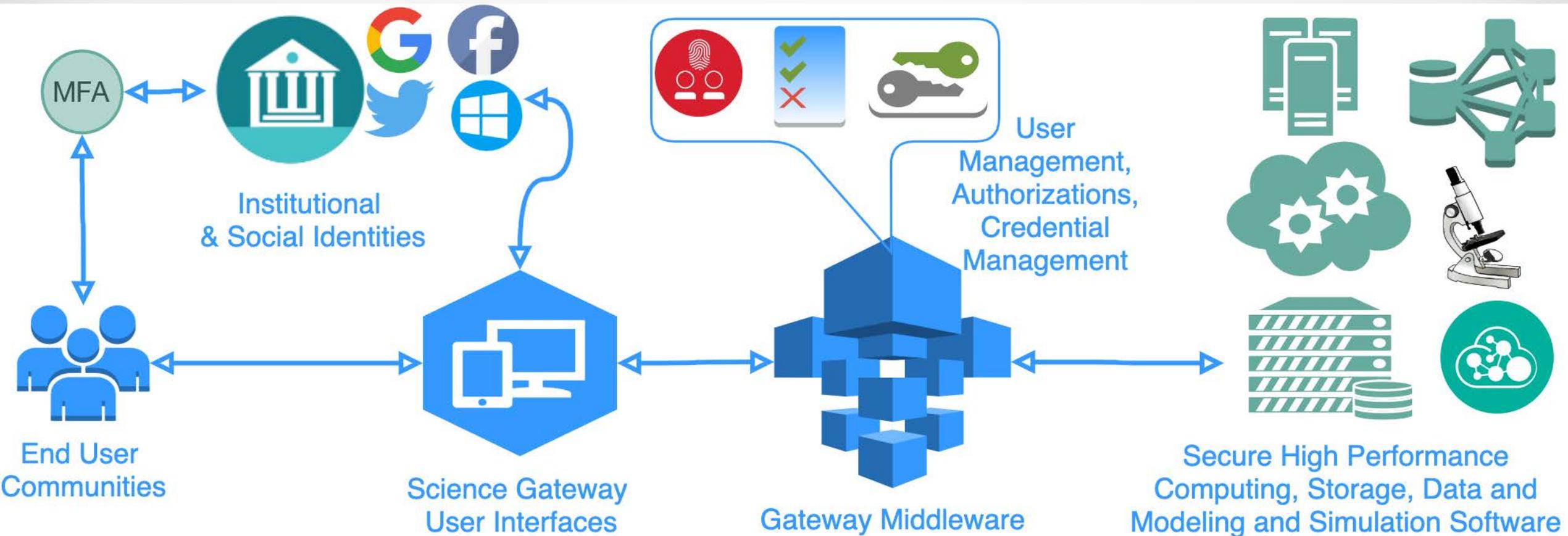
Resource-centric view --> Science-centric view



Secured access & Controlled sharing of digital artifacts

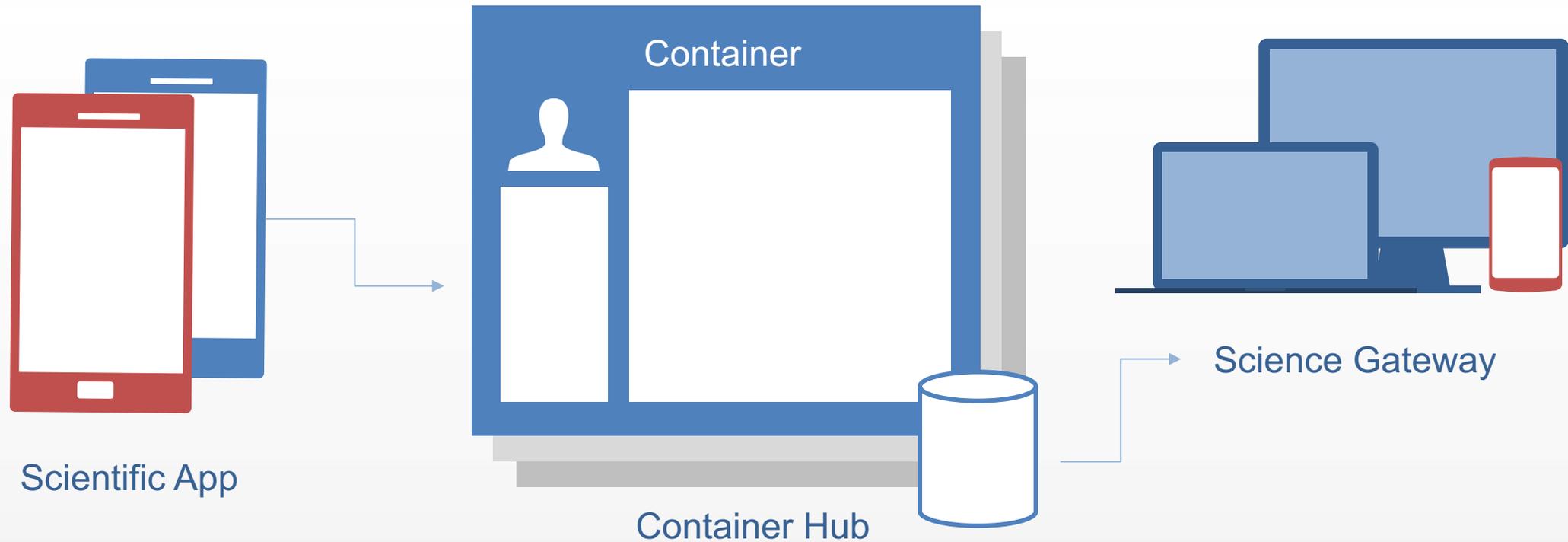


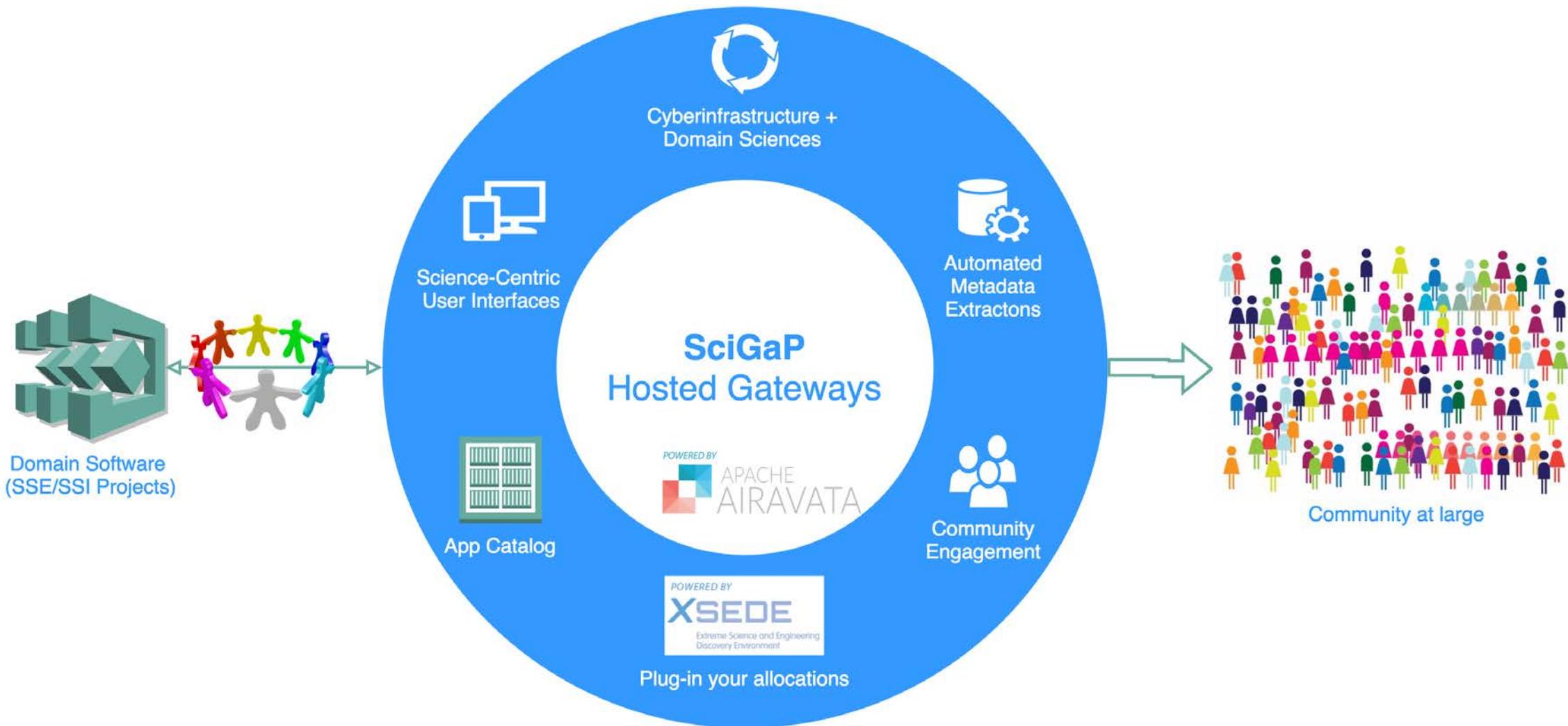
Federated Authentication



CONTAINERS & GATEWAYS

Scientific App to a Gateway Interface





Gateways can enable “Scientific app-store”

The screenshot shows a web browser window with the URL `https://testdrive.airavata.org/workspace/dashboard`. The page title is "Airavata Test Drive Gateway". The user is logged in as "Marlon Pierce". The dashboard is titled "Dashboard" and features a sidebar with navigation icons. The main content area is labeled "APPLICATIONS" and displays a grid of application cards. Each card includes the application name, a brief description, and a star icon. The applications shown are:

- 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" and the user is logged in as "Marlon Pierce". The main content area is titled "Browse Experiments" and displays a table of experiment records.

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
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

Showing 1 - 10 [Next](#)

Launch "Experiments"

The screenshot shows a web browser window with the URL `https://testdrive.airavata.org/workspace/applications/Gaussian_9fe2t`. The page title is "Airavata Test Drive Gateway". The user is logged in as "Marlon Pierce". The main content area is titled "Create a New Experiment" and includes a "Share 2" button. The form contains the following fields:

- Experiment Name:** A text input field containing "Gaussian on Apr 7, 2020 2:15 PM".
- Add a description:** A section with a hamburger menu icon.
- Project:** A dropdown menu currently set to "Default Project".
- Application Configuration:**
 - Application Inputs:**
 - Input-File:** A section with two options: "Select file from storage" (a dark button) and "Drop files here or browse" (a dashed box). Below the dashed box, it says "Max file upload size is 64 MB".
 - Gaussian input file specifying desired calculation type, model chemistry, molecular system and other parameters.
- Allocation:** A dropdown menu currently set to "Default".

SEAGrid

Experiment Statistics from Apr 1st 2020 to Apr 9th 2020

Get Statistics

839 Total Experiments All	3 Created Experiments CREATED VALIDATED	51 Running Experiments SCHEDULED LAUNCHED EXECUTING	763 Completed Experiments COMPLETED	5 Cancelled Experiments CANCELING CANCELED	17 Failed Experiments FAILED
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Name	Owner	Application	Resource	Creation Time	Status	Actions
p2-71	lydiar	Gaussian16	comet.sdsc.edu	an hour ago	FAILED	View Details
p2-71	lydiar	Gaussian16	comet.sdsc.edu	an hour ago	FAILED	View Details
nf880	nandini	Gaussian16	comet.sdsc.edu	2 hours ago	FAILED	View Details

SEAGrid

Abaqus-6.13-3

Details Interface Deployments

comet.sdsc.edu

Created by admin

Share

Application Executable Path
abq6133

Application Parallelism Type
OPENMP

Application Deployment Description

Module Load Commands

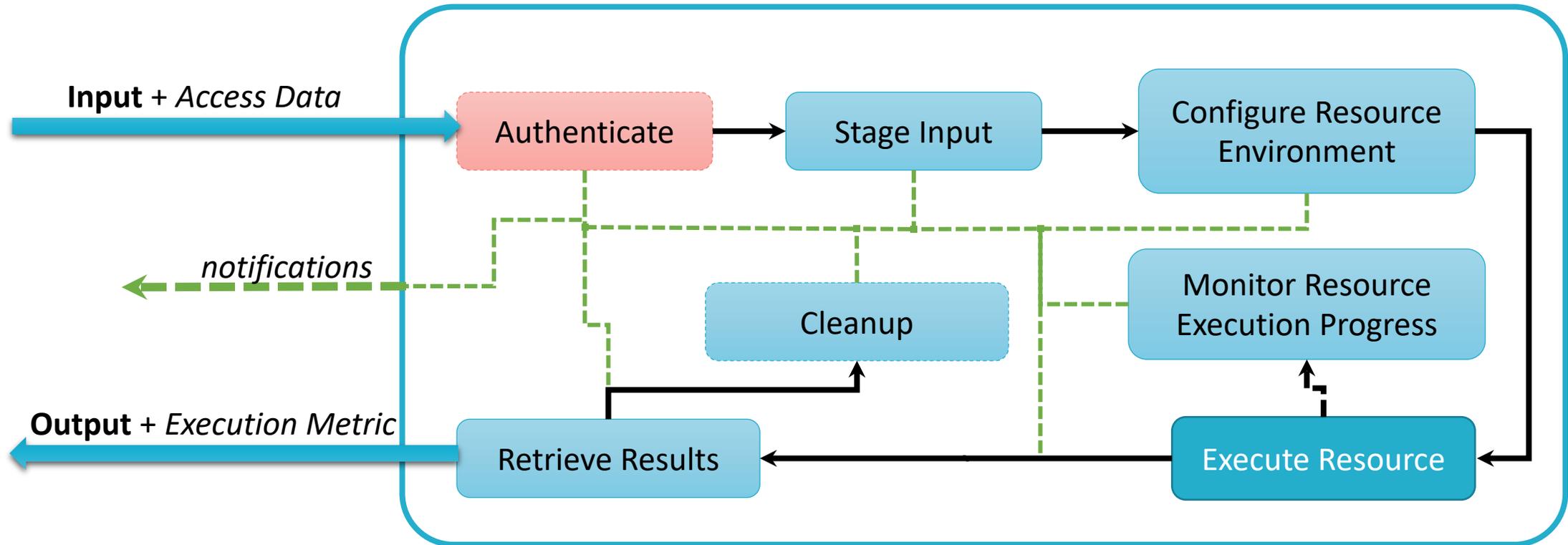
Add Module Load Command

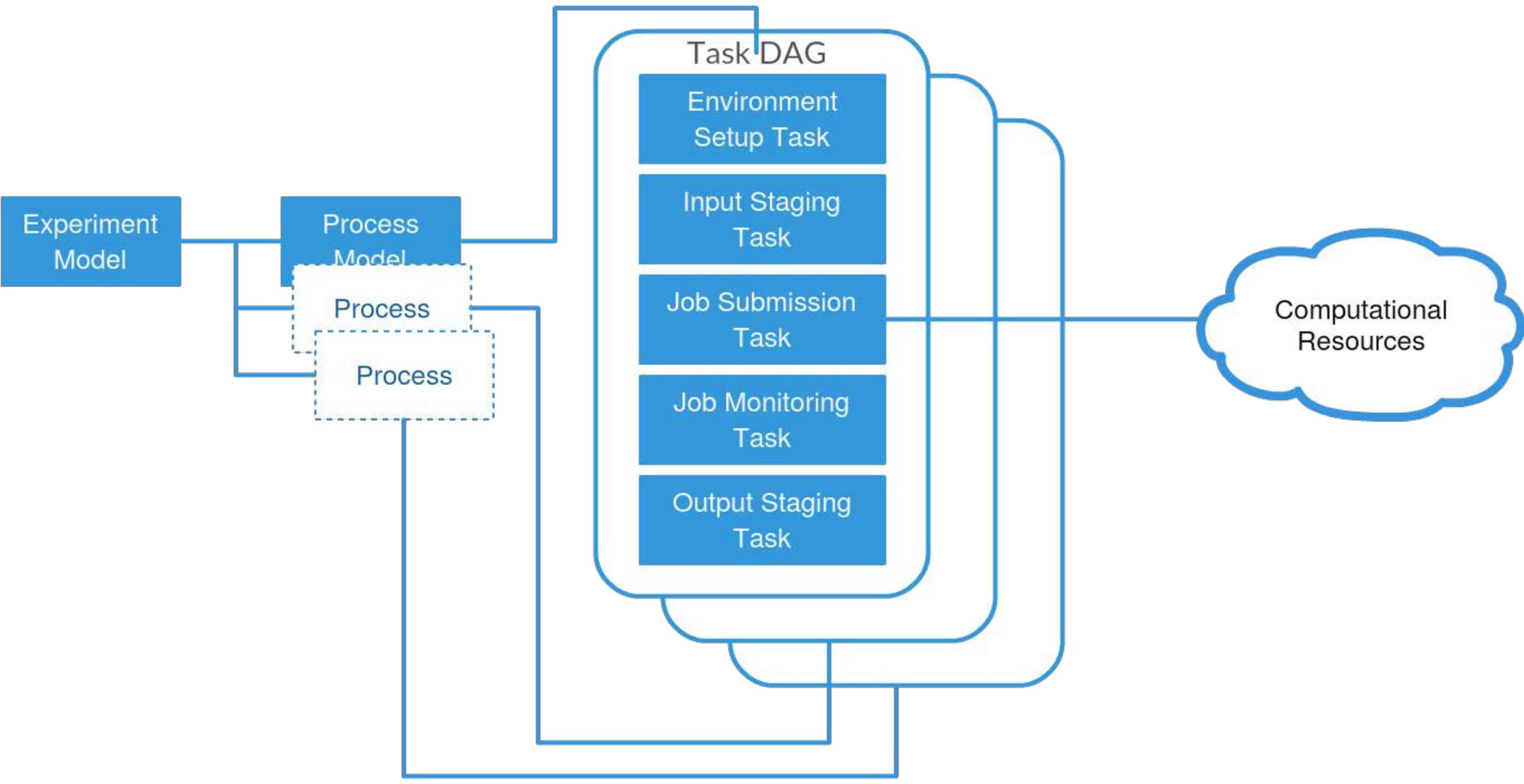
Save Delete Cancel

admin/applications/Abaqus-6.13-3_be287dc9-4347-4fba-a308-465010e5f7d0/deployments/comet.sdsc.edu_Abaqus-6.13-3_be287dc9-4347-4fba-a308-465010e5f7d0#

Administrative Dashboards

Abstracting HPC and Cloud Job Management

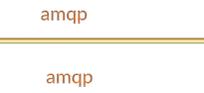
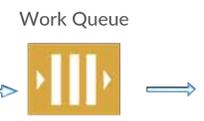
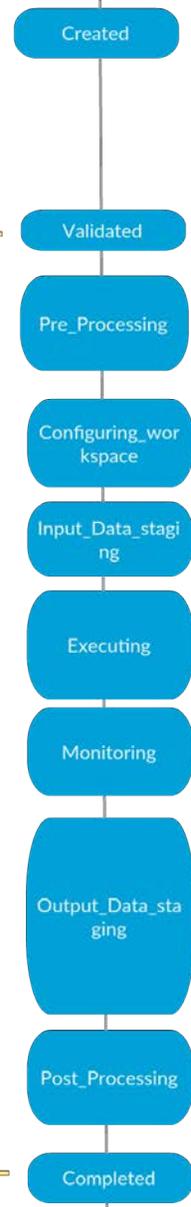




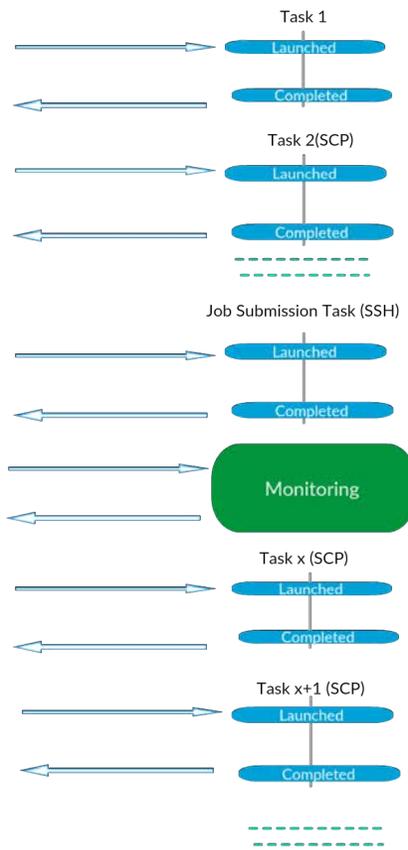
Experiment



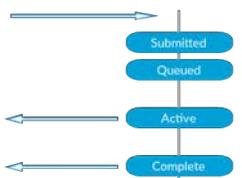
Process



Tasks



Job



amqp

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

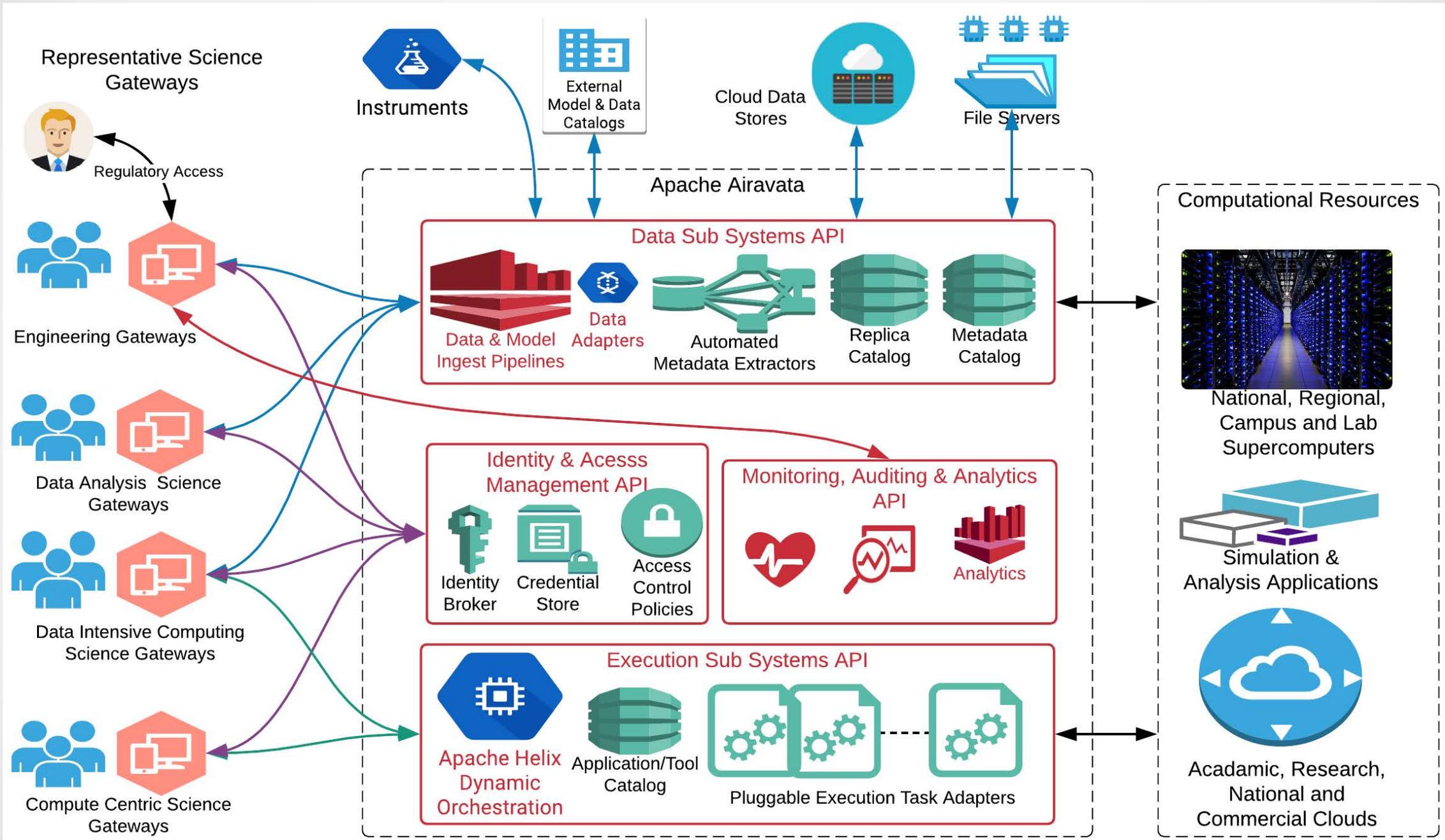
Science Gateways Platform as a Service: SciGaP



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