4. SCIPION

Description

Scipion is an application framework developed as a collaboration between many institutions including the Instruct Image Processing Center (I2PC) in Madrid to help the Structural Biology community to process Cryo Electron Microscopy (CryoEM) data. Scipion is developed as a plugin-based workflow management system that integrates many important software packages available in the field. Scipion is a desktop application and the user interacts with it through a GUI developed in python and Java. ScipionCloud, previously offered as an EGI AppDB image, has been converted to a web service that can be used by Instruct users to deploy a cluster in EOSC cloud resources to keep processing data acquired at a CryoEM facility. This cluster has Scipion installed as well as most of the plugins and external packages used by the community, all ready to be used. In this first prototype only a single Scipion node is deployed but the next version will deploy a slurm elastic cluster using one of the core EGI services, EC3. Worker nodes will only be created when the workload requires it, ensuring an optimum usage of cloud resources.

Architecture

The architecture of SCIPION service is shown in figure 14. User acquires images at a microscope facility where some automatic preprocessing is done using Scipion. Raw data and projects are stored locally. Later, a user can access the IM dashboard portal using her ARIA (the identity provider developed by Instruct) credentials on the EGI check-in service and deploy a cluster with all software ready to be used.
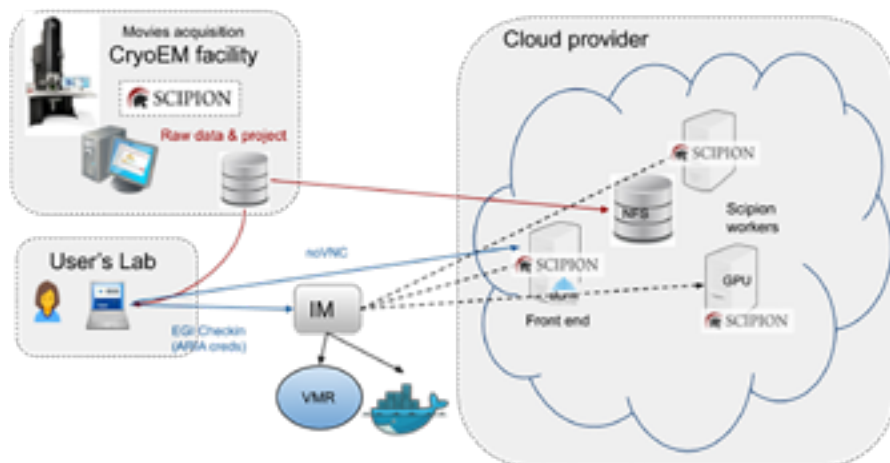

Figure 14 - Architecture of first prototype for the SCIPION Service (only a single node but a slurm cluster will soon be integrated

The cluster comprises a front-end node with Scipion, a shared storage containing data and project (movies raw data might be skipped due to the size) and the required components to send jobs to worker nodes through SLURM batch system. In this first prototype slurm and EC3 are not yet fully integrated and a single node is deployed. Users will interact with the front-end server via noVNC from a web browser.

EOSC Services

SCIPION service has moved from a static image that needed to be deployed directly on a specific site to a fully web service that is easy to use thanks to the integration of some of the EOSC core services. Now INSTRUCT users can access the service at the IM dashboard using her ARIA (the identity provider developed by Instruct) credentials and deploy a cluster on EOSC cloud resources by clicking on a button and providing some input through a guided wizard. All this is accomplished by using the following services:

- **Authentication:** The portal to deploy Scipion service (currently the IM dashboard) integrates the EGI Check-in service that allows INSTRUCT users to keep using her ARIA (the identity provider developed by Instruct) credentials.
- **Elastic cluster deployment:** Currently IM service is used to deploy a single Scipion node but the next version will use EC3 and SLURM to deployan elastic cluster on EOSC cloud resources or public clouds such as AWS EC2. Scipion can send jobs through SLURM which is totally integrated with EC3.
- **EOSC cloud resources:** The cluster might be deployed on EOSC federated cloud if user credentials permit it.

4. SCIPION

Service Endpoint

Scipion service is accessed through the IM dashboard login using EGI Checkin and ARIA credentials. Scipion is available in the IM collection of application templates as an icon to guide users through creation of the node (cluster) as shown in figure 15.

Figure 15 - Scipion available from the IM collection of application templates

In this first version users only need to specify the VNC password to access the remote desktop in the front-end server but a field already present will allow uploading a Scipion project to continue processing in the cloud (see figure 16).

Figure 16 - Scipion connection details

Demonstration Video

A video has been prepared to show the current status of the service. It demonstrates how to access the service using EGI Checkin and deploy a server in the cloud. Then the user can process her Cryo Electron Microscopy (CryoEM) data on a full Scipion installation in cloud resources, including GPU, which is a must for Cryo Electron Microscopy (CryoEM) processing nowadays.

Click the image to view the video