Contribution ID: **56**   Type: **Oral Presentation**

Science Gateway on GARUDA GRID for Open Source Drug Discovery (OSDD) community

Thursday, 22 March 2018 16:00 (30 minutes)

Scientific applications are moving to the distributed environment like grid computing and cloud to take advantage of the high-end computational power availability with reduced cost. Large datasets and compute intensive analysis needs compute infrastructure. The researchers/users want a platform/gateway where they have ease of submitting their experiments accessing a web browser to run them on high end computational resources and if required to share them with other researchers. Science gateways allow science & engineering communities to access shared data, software, computing services, instruments, educational materials, and other resources specific to their disciplines.

In this paper we describe, how the open source Galaxy Workflow is customized to provide a science gateway for Open Source Drug Discovery community on GARUDA GRID. GARUDA grid is an aggregation of heterogeneous resources which aims to bridge gaps between the researchers and accessibility to high computational power. Galaxy is an open source web based workflow system for data intensive biomedical research. Open Source Drug Discovery (OSDD) is a CSIR led team India Consortium and platform for drug discovery which brings together informaticians, scientists and research organizations.

Galaxy based Science Gateway for OSDD is enabled with secure access to GARUDA through in-house developed Login Service, job runner for the Gridway metascheduler, seamless access to the storage server, web services of bio-informatics tools that are added as tools and deployed and hosted on GARUDA over internet. Firstly, we describe extending the pluggable architecture of Galaxy workflow for execution on the grid with the grid middleware-Gridway. Gridway metascheduler is the GARUDA workload manager that performs job execution management and resource brokering. For managing jobs submission with Garuda grid, a Gridway runner was developed which will be managing the execution of jobs. It will include, preparing the jobs for submission and creating a job wrapper, putting it in a queue to be submitted, capturing the Job Id, monitoring the Job Id – watches the jobs currently in the queue and deals with the state change (queued to running and job completion), and finishing the job - Get the output/error for a finished job, pass to JobWrapper class finish method and cleanup all the temporary files.

The paper also talks about the integration of Garuda Login service with the Science Gateway and how the authentication is managed by the Digital certificates for rights delegation.

Science Gateway for OSDD community is designed to support the large distributed community involved in drug discovery. The users are freed from the issues of maintenance and cost and can focus on large data analysis experiments more. There has been substantial increase of resources after the release of gateway mainly due to ease of usage. Also, the implementation of job runner was specifically done for the Gridway metascheduler, but can be extended to support other types of grid systems.

Summary

Science Gateway for OSDD community is designed to support the large distributed community involved in drug discovery. The users are freed from the issues of maintenance and cost and can focus on large data analysis experiments more. There has been substantial increase of resources after the release of gateway mainly due to ease of usage. Also, the implementation of job runner was specifically done for the Gridway metascheduler, but can be extended to support other types of grid systems.

Primary author: PRASAD, Karuna (C-DAC)

Co-authors: Mrs CH, Janaki (C-DAC); Mrs N, Mangala (C-DAC)

Presenter: Mr J, Santhosh (C-DAC)

Session Classification: Distributed & Parallel Computing Applications Session

Track Classification: Science Gateways, Long Tail of Science, and Volunteer and Massively Distributed Computing