Apache Airavata

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Apache Airavata provides an alternative to running and monitoring large-scale scientific applications from the command line. The Apache Software Foundation's Airavata software framework allows developers to create what are known as Science Gateways. These Graphical User Interfaces are desktop-based and/or web-based applications, which allow researchers to compose, manage, execute and monitor their research workflows in a user-friendly manner. Apache Airavata simplifies the process of accessing the large-scale computational power of local clusters, supercomputers, computational grids and computing clouds.

Keywords: Cloud, Gateway, HPC, I524, Middlware, Workflow

https://github.com/cloudmesh/sp17-i524/blob/master/paper1/S17-IO-3011/report.pdf

1. INTRODUCTION

Apache Airavata is an open-source software framework designed to diminish the learning curve and reduce the inherent complexity of conducting large-scale scientific computing. Therefore, scientific researchers leverage the Apache Airavata software framework in order to obscure the intricacies of running large-scale applications or workflows on local clusters, powerful supercomputers or distributed clouds. The expertise and interests of a given researcher likely revolves around their specific area of research (i.e. Computational Chemistry, Molecular Dynamics and etc.). The Apache Airavata technology allows these researchers to focus their time, effort and grant money on the science rather than the details of the computing. In addition to executing and monitoring large-scale scientific applications, managing the input and visualizing the output from the command line can be complicated on distributed compute resources. Apache Airavata provides the technological infrastructure to make these complicated tasks simple. The general idea is to wrap command line-driven applications (i.e. Gaussian, Amber, NAMD and etc.) with Apache Airavata in order to create simple, effective and efficient Science Gateways. The Apache Airavata software framework provides the infrastructure to allow Science Gateway developers to abstract away the described complexity so that end-users can simply "compose, manage, execute, and monitor large-scale applications and workflows" with the click of a button [1].

2. ARCHITECTURE

Figure 1 depicts the architectural details of Apache Airavata. From this diagram one can see how end-users are able to interact with the Apache Airavata services (API Server, Workflow Interpreter, Orchestrator, Messaging System and etc.) via Science Gateways. The Apache Software foundation provides a detailed description of the architectural diagram shown in figure 1 [2].

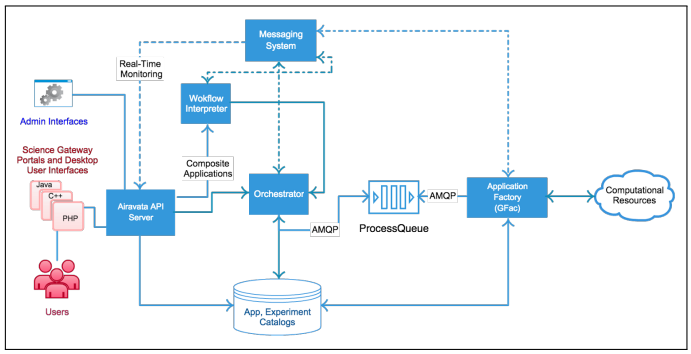

Fig. 1. The image above depicts the architectural details of Apache Airavata [2].

2.1. API

As introduced in section 4 and shown with multiple real-world examples in section 5, researchers leverage Science Gateways to interact with Apache Airavata. In order to promote simplicity, Apache Airavata's application programming interface (API) is intentionally obscured from these end-users. Therefore, the Airavata API is generally intended for Science Gateway developers who are specifically interested in using Apache Airavata as a middleware service between a user interface and one or more compute resources, as shown in figure 2. Airavata API is written

using apache thrift [2]. This allows Science Gateway developers to use the programming language of their choice (e.g. Java, PHP, JavaScript, C++, etc.). The Apache Software Foundation provides an in-depth overview of the API for those interested in learning the details of this service [3].

2.2. Shell Access

As section 1 thoroughly explained, Apache Airavata's purpose is to simplify the typical command line driven process of composing, managing, executing, and monitoring large-scale scientific applications on powerful distributed computing resources. Therefore, end-users of Apache Airavata should not rely on shell access. Instead, section 2.3 explains that end-users interact with Apache Airavata through graphical interfaces (i.e. Science Gateways). Shell access is contained to the Science Gateway developer level of the technological ecosystem, shown in figure 2.

2.3. Graphical Interface

Apache Airavata leverages a Graphical Workflow Composer, known as XBaya, which helps "create workflows, submit and manage multiple applications ... [and] also has a web-based interface ... where users can ... register, run and monitor applications " [2]. Furthermore, the Apache Airavata's thrift-based API, introduced and discussed in section 2.1, allows developers to create their own desktop and web interfaces using Airavata as the technological foundation.

2.3.1. Science Gateways

Science Gateways are the resulting reward of leveraging Apache Airavata. As explained in 4, Science Gateways are an instrumental piece of the Apache Airavata ecosystem that allow end users to compose, manage, execute, and monitor scientific research workflows on distributed (and potentially complex) compute resources. Science Gateways simplify workflows and allow researchers to focus their expensive time and effort on science. Furthermore, Science Gateways promote reproducibility, which is an important piece of scientific research as well as publication. In other words, it is beneficial to researchers to have the ability to easily reproduce results from an experiment in the past and Science Gateways typically ensure this functionality. Section 5 describes many of the prominent and currently available Science Gateways built on top of the Apache Airavata software framework.

3. LICENSING

Apache Airavata is open source software [4]. Therefore, anyone can download, install, modify and improve this software framework using the popular "fork and pull" model. As part of an introductory tutorial, one can create an Airavata Test Drive account, which is free as well. Note, this free Airavata Test Drive account will need to be approved by an Airavata Test Drive Administrator before one can use the system. Once this approval occurs, one can simply create and run "experiments" (i.e. Gaussian, Amber, Trinity and etc.) via a Science Gateway on local clusters, supercomputers, computational grids and computing clouds.

4. ECOSYSTEM

Figure 2 depicts the ecosystem developed around Apache Airavata for SEAGrid. Apache Airavata plays an important role as the middleware between the end-users (Science Gateways) and the compute resources. As discussed above, the placement of Apache Airavata in between the compute resources and the science gateways allows for the abstraction of the complexity of composing, running, executing and managing applications and workflows.

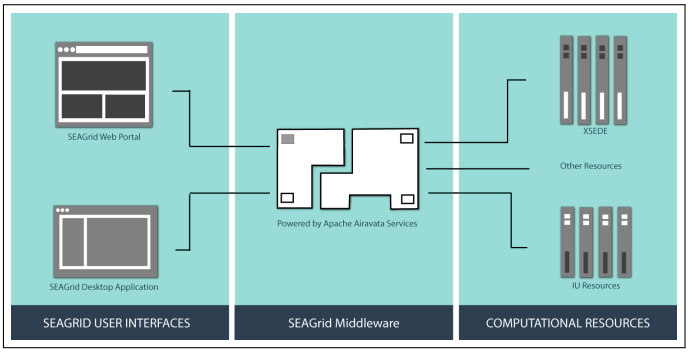

Fig. 2. The image above depicts an example of the technological ecosystem developed around Airavata [5].

5. USE CASES

Ultrascan [6], SEAGrid [7] and GenApp [8] are instances of Science Gateways that leverage Apache Airavata to perform computations [1]. Each of these services is in place to simply bridge the gap between scientific applications on large-scale compute resources and domain specialists. In other words, these Science Gateways are examples of Apache Airavata enabling science.

5.1. SEAGrid

The Apache Airavata services allow Science Gateways such as SEAGrid to simplify the use of "scientific applications deployed across a wide range of supercomputers, campus clusters and computing cloud" [7]. SEAGrids bridges the gap between domain specialists and scientific applications on large-scale compute resources using both a desktop client and web application. SEAGrid currently promotes research in Computational Chemistry (e.g. Gaussian, Gamess, etc.), Molecular Dynamics (Lammps, Amber, NAMD and etc.), Structural Mechanics (e.g. Abaqus and etc.), Fluid Dynamics (e.g. Nek5000, OpenFOAM and etc.) and much more. SEAGrid abstracts away the fine-grained details of running such scientific applications on large-scale compute resources and therefore allows the domain specialists to focus on the fine-grained details of their scientific research. Additionally, SEAGrid enables scientists to create model inputs, visualizations of outputs and archives for simulation data" [7].

5.2. Use Cases for Big Data

The One-Degree Imager (ODI) "is a gigapixel mosaic camera ... built by [the] WIYN Observatory with a pixel scale of 0.1 arcseconds for the 3.5-meter telescope" and is the newest instrument at the WIYN 3.5m Observatory in Sells, AZ [9, 10]. Similarly to the SEAGrid Science Gateway, the Apache Airavata software framework is at the foundation of ODI's Pipeline, Portal and Archive (PPA) system which "execute[s] the NOAO High Performance Pipeline System (NHPPS) pipelines on XSEDE resources" [9]. The large amount of data generated by the ODI demonstrates that the ODI-PPA Science Gateway and therefore

the Apache Airavata software framework can handle big data software projects.

6. EDUCATIONAL MATERIAL

There are multiple ways to find out more information about the Apache Airavata software framework [1]. In order to cater to varying audiences and learning styles there is online documentation [2], a course provided at Indiana University, Bloomington [11] as well as online tutorials [12]. The online documentation is entirely sufficient for motivated users to teach themselves. The online tutorials provide everything from quick-start to extended tutorials and everything in between. Historically, there has been a basic Airavata course at Indiana University offered during the Fall semester and a more advanced version of the course is offered during the Spring semester.

7. CONCLUSION

Apache Airavata appeals to a wide range of scientific researchers since the technology allows researchers to focus their time, effort and grant money on the science rather than the details of the computing. Apache Airavata has enabled researchers to compose, manage, execute and monitor workflows on large-scale systems with the click of a button. Gateways such as Ultrascan, SEAGrid and GenApp are clear and defined examples of how Apache Airavata has been leveraged to improve and optimize scientific research workflows. As compute resources get more complicated and/or distributed over time, the Apache Airavata software framework will continue to promote the ease of use with Science Gateways.

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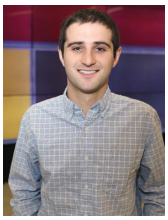
AUTHOR BIOGRAPHIES



Scott McClary received his BSc (Computer Science) and Minor (Mathematics) in May 2016 from Indiana University and will receive his MSc (Computer Science) in May 2017 from Indiana University. His research interests are within scientific application performance analysis on large-scale HPC systems. He will begin working as a Software Engineer with General Electric Digital in San Ramon, CA in July 2017.

WORK BREAKDOWN

The work on this project was distributed as follows between the authors:

Scott McClary. He completed all of the work for this paper including researching and testing Apache Airavata as well as composing this technology paper.

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