Chiminey: Reliable Computing and Data Management Platform in the Cloud

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***Abstract*—The enabling of scientific experiments that are embarrassingly parallel, long running and data-intensive into a cloud-based execution environment is a desirable, though complex undertaking for many researchers. The management of such virtual environments is cumbersome and not necessarily within the core skill set for scientists and engineers.**

We present here *Chiminey*, a software platform that enables researchers to (i) run applications on both traditional high-performance computing and cloud-based computing infrastructures, (ii) handle failure during execution, (iii) curate and visualise execution outputs, (iv) share such data with collaborators or the public, and (v) search for publicly available data.

Demo video: http://youtu.be/Twi-d2WT94A

I. Introduction

Researchers have been using computing resources such as desktops and supercomputers for running their experiments. In order to use such resources, researchers are expected to know how to set up their execution environment, run their experiments and collect and optionally share the output of their experiments. When executing computational experiments on a local desktop machine, performing these tasks may not be challenging. However, if an experiment's resource requirements exceed those of a single workstation, then computing environments such as cluster, grid or cloud can be considered.

Cloud computing [3] presents a unique opportunity for users: it enables researchers to acquire very large numbers of computing and storage resources quickly. Moreover, researchers with relatively modest requirements for parallelisation of existing code may be able to avoid learning high-performance computing (HPC) infrastructure concepts. Researchers still need to learn how to work within a cloud-based environment, which itself presents its own challenges. They need to to create and set up virtual machines (VMs) in the cloud, collect the results of their experiments, and then release the VM resources. Furthermore, cloud-based environments are more prone to failure than HPC environments due to network and third-party software issues [13], and these environments expect researchers to handle such failures themselves.

The rate of technological change and innovation for compute environments is ever increasing. When a new technology is introduced, both opportunities and challenges are presented. As a researcher migrates from desktop to cloud computing, new computing capabilities may be realised; but new skills are required: there needs include not only operational but also fault tolerance and recovery skills. Such challenges distract the user from focusing on their core goals such as research discovery through creating domain-specific software.

In this paper, we present *Chiminey* platform, designed to enable the user to focus on their domain of investigation, and to delegate the platform to deal with the detail that comes with accessing high-performance and cloud computing infrastructure, as well as the data management challenges it poses. Researchers are not expected to have a deep technical understanding of cloud-computing, HPC, fault tolerance, or data management in order to leverage the benefits provided by Chiminey. Users may interact with Chiminey via a web-based graphical user interface or a scriptable API.

We have conducted a number of case studies, applied Chiminey across to two research disciplines in order to assess its practicality: physics and structural biology. The domain experts appreciated Chiminey's features and noted the time savings for computing and data management. We believe that Chiminey will have a strong positive impact on the research community, because it gives an opportunity to focus on the main research problems and takes upon itself solving of the major part of the infrastructure problems.

II. Chiminey

The *Chiminey* platform (cf. Fig. 1) is a computing and a data management platform that enables researchers to perform complex computation on cloud-based and HPC facilities, handle failure during the execution of their application, curate and visualise execution outputs, share such data with collaborators or the public, and search for publicly available data. Chiminey provides a data management platform both as a source and sink of data coming from instruments and being processed through Chiminey, and as a curation and storage repository for data to utilised by future tools, published and then cited. Whenever HPC computation is completed, its output is transferred to user-designated locations including a data curator. For curating

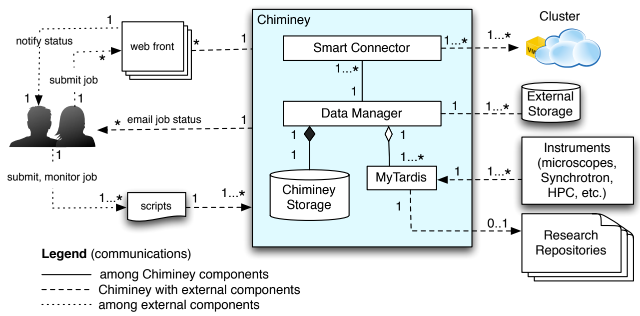

Fig. 1. UML-based reference architecture of Chiminey platform

data, Chiminey uses *MyTardis* [2], an application for cataloguing, managing and assisting the sharing of large scientific datasets privately and securely over the web. MyTardis is currently deployed at various labs and institutions around Australia to capture, manage and provide access to data in research areas such as x-ray crystallography [8], microscopy, medical imaging, genomics, and HPC. The Chiminey platform was created as part of the Bioscience Data Platform project [12], which is an agile software collaboration between software engineering and natural sciences researchers. Python was chosen as the development language due to its rapid prototyping features, integration with the MyTardis data curation system, and due to its increasing uptake by researchers as a scientific software development language. However, the domain-specific calculations could be written in any language (the choice depends on the domain and the concrete research task).

Software engineering challenges: One of the main challenges is the development of *Smart Connector* (SC) components of Chiminey. An SC is a core Chiminey component that interacts with a cluster or a cloud service on behalf of the user: it sets up the execution environment (creates the VMs, configures then for the upcoming simulation, etc.), runs a computation, and then transfers the output of the computation to the user's desired location. SCs handle the provision of cloud-based and HPC infrastructures, as well as give special importance to resource access abstraction and fault tolerance. The user does not need to know about how VMs are created and destroyed, how a simulation is configured and executed, or how the final output is transferred. With respect to the execution environment, the only information that is expected from the user is to specify the number of computing resources she wishes to use, credentials to access those resources, and the location for transferring the output of the computation. With respect to configuring and executing the simulation, the user may set the value of domain specific parameters. .

SCs vary from each other by the type of computation to be supported and/or the specific computing infrastructure to be provisioned. Chiminey provides a set of APIs to create new and customise existing SCs. The APIs enable research software engineers to focus on developing the variation point of the new connector rather than access abstraction and/or fault tolerance support. Chiminey allows to specify ranges of input parameter values for a given SC, and subsequently automatically creating and executing multiple instances of the given connector to sweep across ranges of values. This allows the researcher to quickly explore a parameter space, and the results to then be visualised.

Another challenge was to develop a user interface which is intuitively clear to the research scientists, who do not have a deep technical understanding of cloud computing, fault tolerance, etc. The present interface was created on the basis of contextual interviews with the physics and biology researchers. Fig. 2 shows a web interface for the specification of an SC execution. Fig. 3 shows an example of visualisation: two- and three-dimensional graphs are automatically generated as physics simulation data is curated.

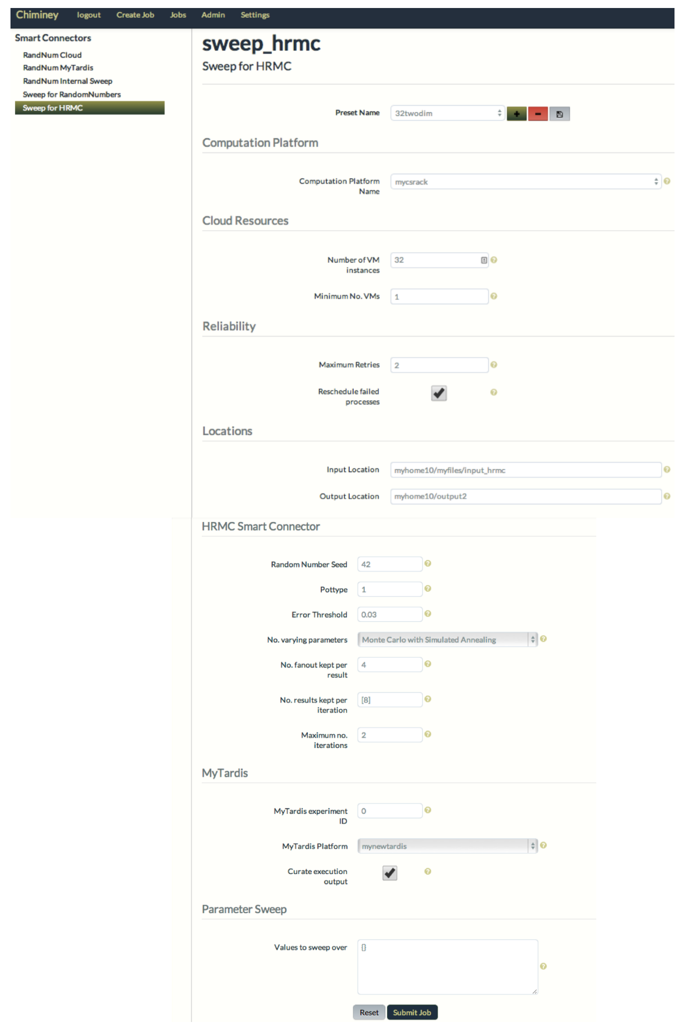

Fig. 2. Chiminey interface: specification of an SC execution. The user defines a name of the SC, chooses the computational platform from a given list, specifies required cloud resources (desired and minimal number of required VMs), reliability requirements (maximum number of retries of a failed computation and whether a failed computation should be rescheduled), input/output locations, and domain specific characteristics. Finally, the user selects whether the execution output should be curated and where.

Example of a Smart Connector: One of the SCs we implemented in Chiminey is a *cloud-based iterative MapReduce*

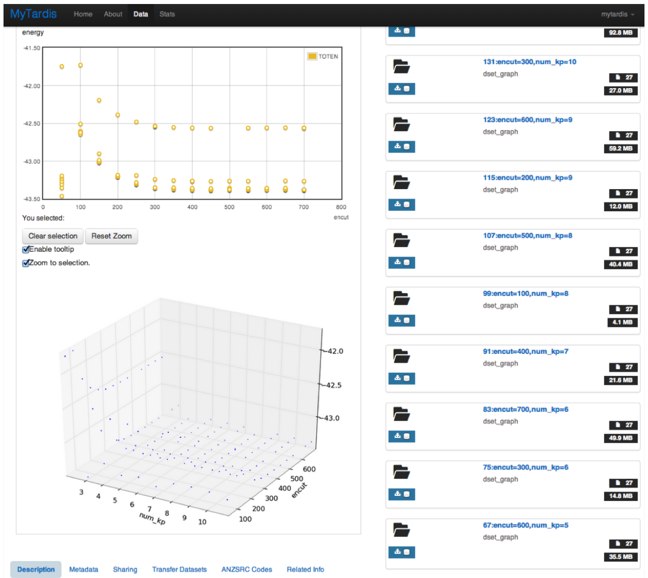

Fig. 3. Visualisation of computation results in MyTardis, using a plug-in developed to provide better usability for the Chiminey platform. The curated datasets are fully accessible and shareable online.

Smart Connector (MRSC), which is suitable for long-running data-parallel programs like Monte Carlo simulations. These simulations are computational algorithms that rely on repeated random sampling to obtain numerical results: simulations (so called *MapReduce computations*) should be run many times over, until a predefined criteria are met, in order to obtain the distribution of an unknown probabilistic entity. Monte Carlo simulations are often used in solving physical and mathematical problems, especially for optimization, numerical integration and generation of draws from a probability distribution.

The communication and computation pattern of the MRSC is shown on Fig. 4. Since VMs need to be created and configured before execution commences, the execution time of applications should be long enough to justify the use of cloud resources. The MapReduce computation is performed iteratively until the predefined criterion is met. The output of each task is sent to a MyTardis instance for both generic data access, and domain-specific visualisation.

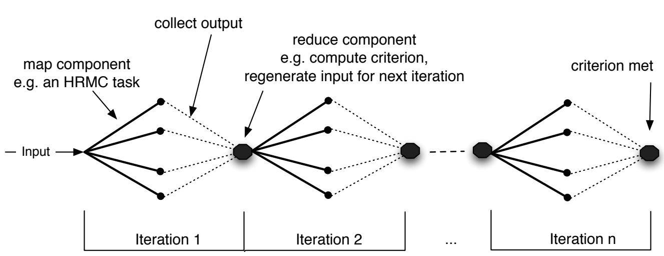

Fig. 4. The communication and computation pattern of the cloud-based iterative MapReduce Smart Connector

III. Evaluation

We have evaluated our system by running a number of case studies, involving experiments in physics (material characterization) and structural biology (understanding materials at the atomic scale). The domain experts noted the time savings for computing and data management, as well as usability aspects of the Chiminey platform.

The *user interface* allows flexibility in the initial setup, with most parameters easy to change from their default values for a new exploration of the parameter space available to the platform. Finally, the ability to index and store the increased volumes of data stemming from this new tool are also of high value; academic research is often conducted under conditions requiring the storage and/or accessibility of data for several years following the actual work. Chiminey user interface, combined with the MyTardis data curation module, allows for flexible handling of data according to its completion and significance. Files can be transferred between computational resources while the work is in progress, and can be curated when the workflow slows naturally, such as when the solution to a problem involving many calculations is found.

In addition, the inclusion of *automated graphing software* means that the user can easily trace the flow of the calculations through the several sequential parallel executions that are often required to reach reasonable convergence to the experimental data. This diagnostic information allows the user to cope with the increased flow of information available, and judge whether the model is converging adequately or requires further tweaking. Where the methods can involve simulated annealing to varied temperatures in an effort to locate the correct solution, the pathways leading to the best candidate are also of interest, and the graphs can easily be used for presentations or in written documents.

In the rest of this section we discuss the application of our tools to execute Monte Carlo simulations. As these simulations give the basis for modelling of a material's porosity and the size distribution of its pores, they are of recent interest in the material characterization community. One such modeling methodology is the Hybrid Reverse Monte Carlo (HRMC) method [10]. This method aims to produce three dimensional atomic coordinates of disordered materials which are consistent with a variety of experimental data (e.g., electron, x-ray and neutron diffraction, porosity information) while ensuring a low energy local bonding environment. Together with the the Theoretical Chemical and Quantum Physics group at RMIT University, we have identified the requirements for a cloud-based execution and deployed this using the MapReduce Smart Connector (cf. Section II). The connector was configured to run the HRMC program on the cloud and to manage the output of that execution. The main requirements are (cf. also Fig. 4):

1) To exploit the randomness inherent to the HRMC method for executing multiple tasks, each with unique input data, in parallel bursts: this data parallelism can be satisfied by using the the *map* component of the SC.
2) To automate a decision-making process to prune the

calculations in accordance with pre-defined criteria, as well as to regenerate a new batch of parallel tasks based upon the outcomes of the previous tasks: this requires computation to be performed on the outputs of all map tasks. These computations are equivalent to the *reduce* component of the MRSC.

3) To visualise output of each task to indicate the progress of the calculations with respect to the criteria at a glance: to satisfy the fourth requirement, the output of each task are sent to a MyTardis instance for both generic data access, and domain-specific visualisation.
4) To organise and store each output persistently, i.e. to provide data curation: this is achieved by transferring all data to either a MyTardis, or a user designated location.

In a process reliant on the random nature of Monte Carlo simulation, the abilities to rapidly process simulation results, make decisions based on outcomes, and generate new calculations when necessary are of high value. Here, the automation of the HRMC package via Chiminey has led to significant speedups in model planning, setup and execution. Where before, the typical modus operandi was to run a calculation and subsequent evaluation of the pore-size distribution in the hope of a random match to experimental data, and then to tweak some initial parameters and try again, now a structured process exists to facilitate and manage these time-consuming tasks. As well as saving time on the low-level evaluation and changes to setup, this also has consequent flow- on effects at the computational level; restarting calculations no longer have to wait for user input, meaning that the available resources can be used more efficiently, with minimal downtime while the problem iterates.

IV. Related Work

There are different types of scientific workflow systems such as Kepler [7], Taverna [9] and Galaxy [1], which are designed to allow researchers to build their own workflows. However, Chiminey provides drop-in components, i.e. Smart Connectors, for existing workflow engines. Researchers utilise and adapt existing Smart Connectors. New types of Smart Connectors would be developed by the Chiminey development team in collaboration with researchers.

There are a number of platforms/applications with similar aims and features. In comparison to them, Chiminey provides more features to make the researchers' work more efficient. Unlike VIVO, a semantic web application for the discovery of research outputs within an institution [6], the data management component of Chiminey focuses on curating data from *instruments*, visualising and publishing these data, and making the research data itself accessible. Unlike Chorus, a web application for managing spectrometry files [5], Chiminey is not restricted to managing a specific type of files: Chiminey not only manages any type of files but also allows the addition of filters to the files for automatic generation of domain-specific metadata. Furthermore, Chiminey provisions a reliable computing capability for data processing. Unlike ReDBox, a software platform for curating and publishing experimental results [11], Chiminey curates and publishes metadata and data collected from instruments. Furthermore, Chiminey provides a reliable computing and data visualisation capability.

Nimrod [4] is a set of software infrastructure for executing large and complex computational processing across several compute resources at a time. It is compatible with the scientific workflow system Kepler, s.t. users can set up complex computational workflows and have them executed without having to interface directly with an HPC system. Incorporation the Nimrod into Chiminey's architecture for the execution of its Smart Connectors is an ongoing work.

V. Conclusion

The nature of many scientific problems today mandates the use of parallel programming to unlock the power of HPC and big data from advanced instruments. This has required researchers to learn HPC, cloud computing and data management skills to address their problems.

We have presented the Chiminey platform, which provides a reliable computing and data management, and be used by researchers without having to learn extensive infrastructure concepts and technologies. Researchers can access HPC, use cloud services, and archive, visualise and publish the result of their computations. In the demo, we have discussed one of our case studies: Monte Carlo simulations. The domain experts appraised Chiminey with these scenarios, and noted the time savings for computing and data management.

Acknowledgement

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