Using Cloud Computing for Scalable, Reproducible Experimentation

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ABSTRACT

Whether it be data generated from genomic sequencers, telescopes, or other laboratory instruments, technology apparent in many scientific disciplines is generating data at rates never witnessed before. Scientists in the area of bioinformatics are among the many who perform inductive experiments and analyses on these data with the goal of answering scientific questions. These computationally demanding experiments and analyses have become a common occurrence, resulting in a shift in scientific discovery, and thus leading to the term *eScience*.

Reproducing controlled eScience experimental conditions is a challenging task. To reproduce an eScience experiment, the investigator must be able to recreate the original conditions, including operating system, software installations and configurations, and original data set. The challenge of reproducibility is compounded when the experiment must be run in a distributed manner.

In this work, we create a reproducible framework for the construction of large-scale computing environments on top of cloud computing infrastructures. We demonstrate how this framework can reduce the challenges of experimental reproducibility in large-scale eScience applications.

Categories and Subject Descriptors

H.4 [**Information Systems Applications**]: Miscellaneous

General Terms

Design, Performance

Keywords

Cloud Computing, eScience, Reproducibility

1. INTRODUCTION & MOTIVATION

Data-intensive science is considered part of a relatively new paradigm in the scientific discovery process [19]. The term *eScience* [27] has been coined to help explain the common themes and processes found in this new shift in scientific thought. One common need across all domains of eScience research is to have an infrastructure available with software configured to process large-scale data and perform simulations to produce scientific insight.

As a researcher investigating a scientific paper within a particular eScience domain, it can be challenging to reproduce the controlled conditions of the original authors' experiments. To fully reproduce the experiments in the paper, one must have both the infrastructure and software configured in the same manner, as well as have access to the data used within the original experiment. In many cases, having access to all these items is not possible [42].

Even if the original data are not available, it should be a reasonable expectation within the scientific community for the experimental environment be reproducible. If the infrastructure setup and the software installation and configuration can be performed in a reproducible manner then eScience researchers, who are traditionally not system administrators, are much more enabled at replicating or extending the experiments being investigated.

Therefore, in this work, we demonstrate through the use of cloud computing along with infrastructure and software automation the concept of scalable, reproducible experimentation is an achievable goal. To this end, this work enables eScience researchers to spend less time on the system administration processes of recreating a previous experiment and more time on enabling and advancing scientific thought in his/her particular domain. Towards the goal of performing reproducible eScience experiments in the cloud, we demonstrate the following:

- The construction of computing framework, which enables scalable, reproducible experimentation.
- A fully reproducible eScience experiment built on top of the framework performed in academic or commercial clouds.

2. BACKGROUND & RELATED WORK

2.1 Virtualization & Cloud Computing

Virtualization technology has opened the door to many advances in computing. A virtual machine (VM) [26] is a running instance of a computer where resources such as memory and central processing units (CPUs) are allocated through virtualization software. Cloud computing has emerged in recent years because of advances in virtualization software. Companies such as Amazon, Google, and Microsoft provide services to customers for use of the virtual resources owned by them. The definition of cloud computing has taken many forms in the academic community and industry. For this work, we use the definitions and terms discussed in [16].

Cloud computing refers to the software, platforms, and infrastructure services provided over the Internet as well as the data centers offering these services. The hardware and virtualization software running on top of this hardware is termed a *cloud*. Providers of cloud computing services offer application programming interfaces (APIs) as means with which customers subscribe and interact. The lowest level of service available with a cloud is termed *Infrastructure as a Service* (IaaS). At this level, users provision virtual resources such as a VM or a virtual block storage device. We consider this the infrastructure layer whereabouts our framework interacts with the cloud.

2.2 Experimentation & Reproducibility

Four properties of good experimentation are outlined in [45]: 1) reproducibility, 2) extensibility, 3) revisability, and 4) applicability. An experiment exhibits the property of *reproducibility* if another researcher is able to perform the experiment and produce the same result. The properties of *extensibility* and *revisability* both dictate that changes to conditions and modifications must be possible for the experiment. Those changes may be necessary for future expandability or if a modification is needed for corrections to the original experiment. Lastly, experimental parameters must be of realistic in nature and resembling real-world conditions while allowing for changes to thus promote *applicability*.

The limits of reproducibility were reviewed in [22]. In this work, the author provides details of how stochastic methods, such as the use of genetic algorithms, can prevent an experiment from being fully reproducible. Moreover, the finite nature of floating point precision also limits numerical simulation reproducibility. Relative to this work, our framework demonstrates that even if an exact numerical value cannot be reproduced, the experimental conditions and execution should be reproducible.

Experimental complexity and scalability are discussed in [21]. In order to answer more difficult scientific questions, both of these conditions must increase. Therefore, by advancing the processes for managing experiments will lead to improvements in reproducibility and experimental integrity.

2.3 Appliances & Clusters

Several works [23, 28] have outlined how virtual appliances can provide a reproducible environment for researchers. In [23], the authors propose reproducibility as a two step process. First, by storing scientific datasets in the cloud more researchers have access to the data. Second, the authors introduce a concept called Whole System Snapshot Exchange (WSSE) where the entire computer system, including the operating system, is copied so that other researchers can fully replicate the *in silico* experiment. This same sentiment is shared in [28]. The author states that by providing a pre-installed, pre-configured virtual machine the original "laboratory" is provided in tact for future researchers.

Our framework achieves the same outcome of reproducible computational experiments; however, only a generic, "golden" machine image is maintained within a cloud. Then utilizing a configuration management tool, VMs are fully installed and configured software installation scripts at deployment run-time. Through this approach, we are able to use the same software installation and configuration scripts within the software layer in separate clouds. Moreover, using an automation approach to software installation and configuration management provides the ability to build scalable architectures in the cloud. The properties of scalability and elasticity have gained much of cloud computing's attention, which has led to work in building virtual clusters.

A *virtual cluster* (VC) [25] is a set of VMs and any corresponding storage, which operate as a whole to create the presence of a single computational entity. The ability to quickly provision a VC within a cloud computing infrastructure is useful in many scenarios within eScience experiments. For example, a researcher can build the necessary environment closer to the data, especially as more public datasets are being stored in the cloud [35]. Both [31, 15] discuss the how as the size of data sets grow, and if the construction of a VC can be performed in a straightforward manner, then it is possible to move the computing infrastructure to the data. This is in contrast to moving the data to the location of a dedicated high performance computing (HPC) cluster, such as a research university's supercomputer.

Other researchers have worked on bridging the gap between dedicated physical clusters and the elasticity of the cloud [30]. The concept of *cloud bursting* allows one to utilize dedicated compute resources such as high performance computing cluster or grids first before taking advantage of elasticity of the cloud.

2.4 Genomic Sequencing in the Cloud

Scientists in the area of genomic sequencing have been performing research work in the cloud to provide the necessary scale in both computing power and storage [17]. The National Institutes of Health (NIH) announced in late March 2012 the 1000 Genomes Project [11] data are now available on the Amazon Cloud as a public data set [35]. There are many recent works on the use of cloud computing for bioinformatics and genomic sequencing analyses [47, 40, 43].

2.5 Cloud Computing Technologies

Research work is also being performed tools, technologies, and applications to create as well as manage cloud infrastructures. Eucalyptus [37] is an open-source cloud computing platform that provides IaaS capabilities. Using Eucalyptus, one can create a cloud with a compatible API to that of Amazon's EC2 and S3. During this research, our framework was implemented and tested both on Amazon as well as FutureGrid's Eucalyptus cloud.

There are several configuration management tools available for use in automating software configurations and installations. Tools such as CFEngine [6] and Puppet [9] have been created to manage and configure infrastructures and systems. In this work Chef [5] was chosen as one of the open source software products to aide in the framework implementation.

Other projects have built on top of these configuration management tools to help launch and configure independent VMs on IaaS clouds. One such tool is cloudinit.d [20].

3. REPRODUCIBLE FRAMEWORK

3.1 Separation of Concerns

The foundation to our reproducible framework is the separation of interactions between an IaaS cloud computing infrastructure (the infrastructure layer) and the interactions of of a running virtual machine (the software layer). This separation of concerns allows for the reuse of software installation and configuration management scripts between clouds. Moreover, any differences in the IaaS cloud application programming interface (API) are handled at the infrastructure layer.

Figure 1 details how a client machine interacts with these two layers. For the infrastructure layer, the client interacts with the IaaS cloud provider's API whereas within the software layer the client is executing commands directly on the running virtual machine.

3.2 Software layer

The software layer is the one in which a researcher interacts with the most often. This is where the scientists interacts with applications and the operating system.

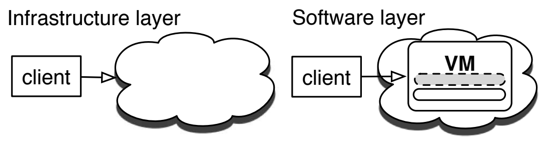


Figure 1: Client interactions between the infrastructure and software layers.

Figure 2 provides details of the software layers necessary for a researcher to have a fully-configured running virtual machine to execute an experiment. Each layer within this running VM has a version associated with it.

The base layer is the operating system. Installed on the VM's operating system layer are platform languages and software. For example, compiled languages such as C, C++, and Java as well as interpreted languages such as Perl, Python, and Ruby are foundational languages to many researchers work.

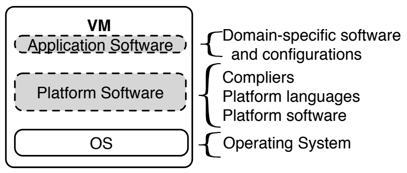


Figure 2: Operating system and software layers

Additionally, installed and configured on top of the running operating system, the VM has platform software and filesystems, which provide foundational components for distributed systems. HPC/HTC scheduling software, distributed file system software, and distributed computing frameworks such as Hadoop [7] are all examples of platform technologies that domain-specific researchers use perform distributed computing experiments.

The final layer in the application stack is domain-specific software. Domain-specific software is dependent on both the operating system and the platform technologies to be installed correctly.

When installing and configuration distributed systems, application configuration files must be populated with values to allow machines to interact with one another. For example, when configuring a Condor [44] pool a file named *condor_config.local* must be configured on each node of the cluster. This configuration file indicates which node in the pool is designated with the role of `Central Manager`. Reproducing an experiment that uses Condor as its scheduler must have its *condor_config.local* file be populated with a different value than the `Central Manager` of original experiment. Figure 3 displays a Condor pool with an example of the `CONDOR_HOST` variable populated in the *condor_config.local* file.

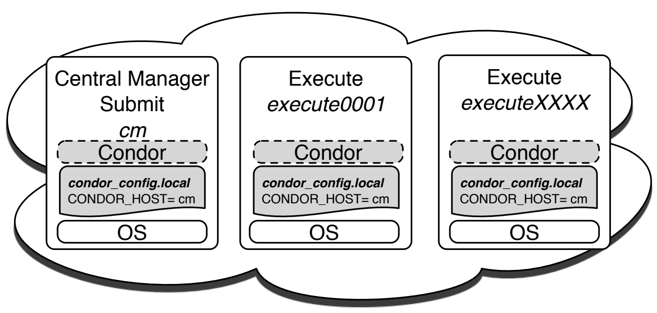


Figure 3: Condor pool with configured condor_config.local file

3.3 Framework Implementation

To implement the framework, two equivalent machine images were created. The first, a Eucalyptus Machine Image (EMI) was created in FutureGrid's Eucalyptus cloud. The second, an Amazon Machine Image (AMI) was created in Amazon Web Service's cloud. The following steps were performed in each cloud to make the software layer consistent between the clouds.

- Launched a base CentOS 5.8 machine image (MI).
- Installed software configuration management open source software (specifically, the `chef-client` version 0.10.10).
- Registered the new machine image, which is considered the "golden" machine image within that cloud.

Figure 4 provides a visual representation of the two machine images created in separate IaaS cloud.

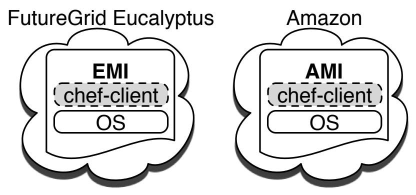


Figure 4: Equivalent machine images (MI) were built in IaaS separate clouds.

As opposed to storing fully configured virtual appliances in the cloud, we store several other persistent objects that can be used to recreate the entire environment. Figure 5 presents the three objects that are persisted in the cloud: 1) the "golden" machine images, 2) a volume containing the software source code (e.g., tar.gz files) and packages (e.g., RPMs), and 3) the software installation and configuration management scripts.

Figure 6 demonstrates how the persistent objects are used to reproduce eScience environments at scale. The volume storing the software source code, software packages, and any data is attached to a deployment web

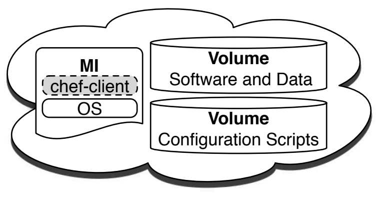


Figure 5: Persistent objects stored in the cloud.

server. This web server distributes the software to all of the running virtual machines. The second server hosts the scripts for installing and configuring these specific versions of software. This is the Chef server. Therefore, a snapshot of a scalable eScience application is persisted in the software artifacts and deployment installation and configuration scripts stored through this framework. In the next section we use the implementation of this framework to test both scalability and reproducibility.

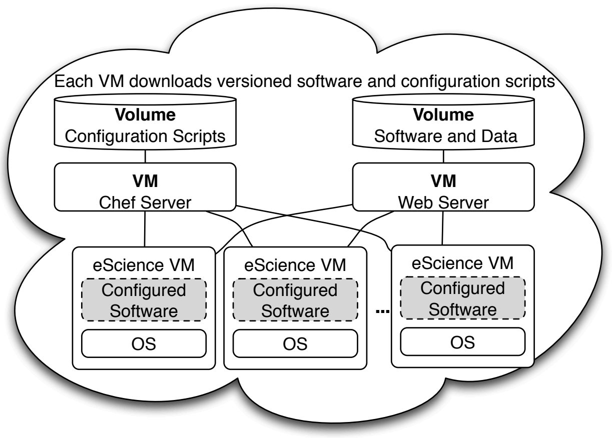


Figure 6: Chef server and software web server install and configure VMs.

4. EXPERIMENTS

4.1 Scalability

The first set of experiments test the feasibility and scalability of our framework outlined in Figure 6. The Condor pool pictured in Figure 7 was created in FutureGrid's Eucalyptus cloud with four different execute node counts: 10, 25, 50, and 100. For each of these pool sizes, we performed the cluster deployment three times.

Figure 8 displays two charts. The top graph presents the deployment run-time average and standard deviation for each of the twelve deployment tests. As witnessed from this graph, the more nodes requested for the pool, the longer the deployment time to configure the virtual cluster.

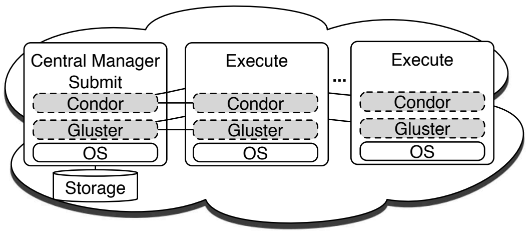


Figure 7: Scalability tests created a Condor pool.

The bottom chart begins to investigate the reasons for the additional deployment time. A result of creating a "golden" image (with no pre-configured software), is that each individual node must download, install, and configure software at deployment run-time. The result of this on-the-fly configuration is longer deployment times as the cluster size increases. Specifically because the software must be transferred over the cloud's network from the web deployment server to each individual node.

For clusters of size 10, the deployment on average takes just over 40 seconds whereas for a 100 node cluster the average deployment for a node is around 120 seconds. The second chart in Figure 8 presents the total received network traffic of the 100 execute nodes during a deployment. As witnessed by the large spikes, there are seconds during the deployment (around the 70 second mark, 80 second mark, and 120 second mark) where as a whole, the entire pool is receiving over 200 MB of software.

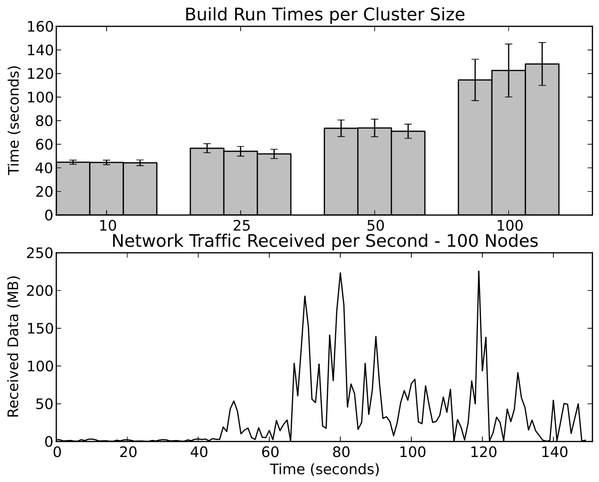


Figure 8: Node deployment times and network traffic received

Another item of note in Figure 8 is the larger standard deviation among the three tests of deployment 100 node clusters. Figure 9 delves into the details of one 100 node deployment.

The individual deployment times for each of the 100 nodes is presented in the top graph of Figure 9. The length of the horizontal lines provides the total run time for that particular node's deployment. Some of the first execute nodes begin completing their deployment as quickly as 80 seconds whereas the last nodes to complete take up to 70 seconds longer. This chart demonstrates why there is a larger standard deviation for the 100 node deployments.

The second chart in Figure 9 demonstrates when the Condor central manager recognizes the execute host has been registered in the Condor pool. The Condor installation is the last step in the node deployment process because all other software needs to be configured before the scheduler is to be enabled on the execute node. Therefore, this second chart provides another view into how many nodes have completed their deployment. One can see the association between the deployment completion time and the Condor central manager registering a new execute node in the pool. This bottom chart demonstrates the elasticity or cloud-bursting capability of the cloud. In this particular case, a 100 node cluster has been created in 150 seconds.

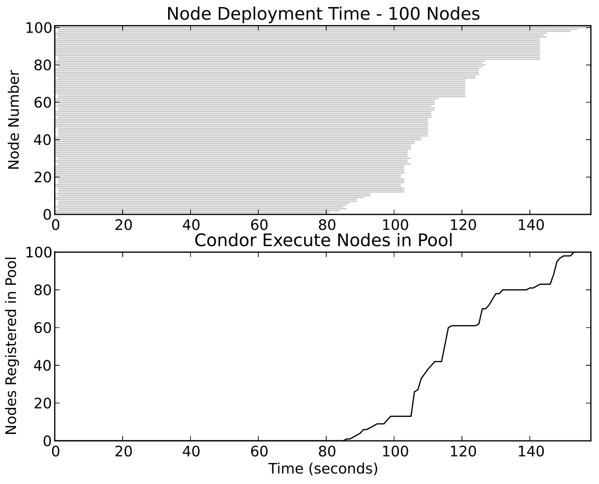


Figure 9: Individual deployments times and Condor node counts.

These deployment experiments have demonstrated that the framework can install and configure software up to 100 nodes. The upper limit of 100 was chosen only because of the amount of resources available within the FutureGrid Eucalyptus cloud. Additionally, each of the virtual machines created in these deployment experiments were single core. Larger multi-core instance types can also be chosen during deployment to increase the scalability. For example, Amazon provides a variety of instance types. One instance, named `m2.2xlarge`, which is categorized as a high-memory instance has 13 EC2 Compute Units and 32 GB of memory [12]. A

100 node Condor pool with default configurations would have 1,300 available slots and over 3 TB of total memory among the execute nodes.

The goal in these first set of experiments was to demonstrate that the framework could install and configure software at scale. The experimental goal for the second set of experiments is to show how the framework can be used to reproduce an eScience experiment, and in particular in separate IaaS clouds.

4.2 Genomic Sequencing Use-Case

This experiment reproduces a specific genomic sequencing use-case in two separate clouds. Specifically, the experiment will reproduce the transcription start sites (TSS) detailed use-case [13]. The transcript start sites use-case makes use of a dataset from a ChIP-Seq analysis paper on histone methylations in the human genome [18]. Details on the software and steps performed to produce the experiment will be provided to help bring clarity to details of the experiment.

There are four genomics applications used in this experiment. The first is a Python module named HTSeq, which is used to analyze high-throughput genomic sequencing assays [14]. The second is the Burrows-Wheeler Aligner (BWA) [32], which is used for aligning a genome to the reference genome. The SAM (Sequence Alignment/Map) Tools application [33] is used for creating SAM formatted files, and their binary counterparts, BAM files. Lastly, the Sequence Read Archive (SRA) Toolkit [34] is used for data conversion out of the SRA file format.

Table 1 lists the application software discussed above as well as the other installed and configured software needed to perform this experiment. This table does not include the platform components such as operating system packages or compilers necessary. All operating system packages were hosted on the deployment web server, as seen in Figure 6. The volume attached to the deployment web server stored a snapshot of operating system packages for the CentOS yum[10] repository as well as the Extra Packages for Enterprise Linux (EPEL) [39] yum repository. To control the experimental conditions on the operating system packages, the deployment web server in both clouds contained the same snapshot of operating system packages from repositories on the Internet.

Each application listed in Table 1 was also downloaded from its original site on the Internet to the deployment web server in each individual cloud. All software installation and configuration scripts were created to accept configurable URLs for downloading software during deployment. This implementation allowed for controlling the version of application software.

The installation and configuration scripts were created and stored in the Chef server hosted in each cloud.

Software	Version
BWA [32]	0.6.1
Condor [46]	7.8.0
Cython [4]	0.16
HTSeq [14]	0.5.3p6
Python [38]	2.7.3
Matplotlib [29]	1.1.0
NumPy [36]	1.6.2
SAMtools [33]	0.1.18
SciPy [41]	0.10.1
SRA Toolkit [34]	2.1.10

Table 1: Software Installed and Configured.

File Name
Homo_sapiens.GRCh37.67.gtf.gz [1]
Homo_sapiens.GRCh37.67.dna.chromosome.1.fa.gz [2]
SRR001432.sra [3]

Table 2: Datasets

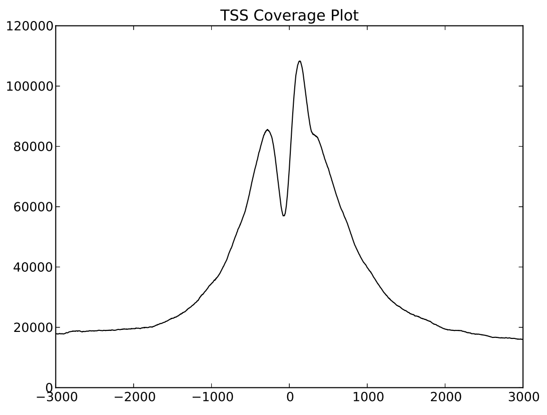
These software automation scripts provide the details of every configuration value, and installation command run to reproduce the installed environment. For example, to configure and install the numerical Python module NumPy [36], a Fortran compiler must be installed. Determining the correct Fortran compiler and making sure the flags are set accordingly when compiling NumPy is but one example of how installation and configuration of the entire software stack can be challenging toward the goal of experimental reproducibility. Through the use of software configuration management, this complexity is reduced anyone needing to reproduce the experiment.

The final piece of reproducing the experiment is having access to the original data. Table 2 lists the original files used to produce the charts. Similar to the software applications above, each of these files were downloaded to the deployment web server within each cloud from the original site on the Internet so that they could be deployed to the execute nodes when necessary. The sample numbered SRR001432 from the Short Read Archive [8]. This sample is one of the H3K4me3 samples from [18].

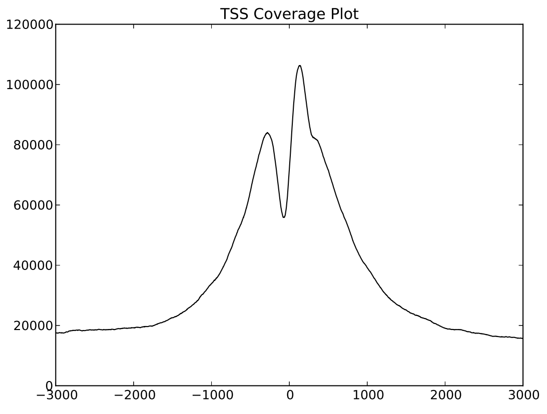
Table 3 outlines the high-level workflow executed to produce the charts in Figure 10. The applications were installed, and the workflow was executed in both the FutureGrid Eucalyptus and Amazon to produce the two TSS plots. Validating the data, we annotated one of the plots with a gray box from $-200 \leq x \leq 50$ because of a "significant dip in the signal was observed between -200 to $+50$ for H3K4me3" [18].

1. Convert SRR001432.sra file to SRR001432.fastq
2. Gunzip Homo_sapiens.GRCh37.67.gtf.gz → Homo_sapiens.GRCh37.67.gtf
3. Extract chromosome 1 features from Homo_sapiens.GRCh37.67.gtf → Homo_sapiens.GRCh37.67_chrom1.gtf
4. Gunzip Homo_sapiens.GRCh37.67.dna.chromosome.1.fa.gz → Homo_sapiens.GRCh37.67.dna.chromosome.1.fa
5. Index Homo_sapiens.GRCh37.67.dna.chromosome.1.fa
6. Align SRR001432.fastq to Homo_sapiens.GRCh37.67.dna.chromosome.1.fa
7. Create SRR001432.sam
8. Create SRR001432.bam
9. Sort SRR001432.bam → SRR001432.sorted.bam
10. Index SRR001432.sorted.bam
11. Extract chromosome 1 from SRR001432.sorted.bam → SRR001432_head.bam
12. Use HTSeq[13] with Homo_sapiens.GRCh37.67_chrom1.gtf and SRR001432_head.bam → TSS plot

Table 3: Steps to producing TSS plots



(a) TSS plot produced in AWS



(b) TSS plot produced in FutureGrid Eucalyptus

Figure 10: TSS plots produced in separate clouds

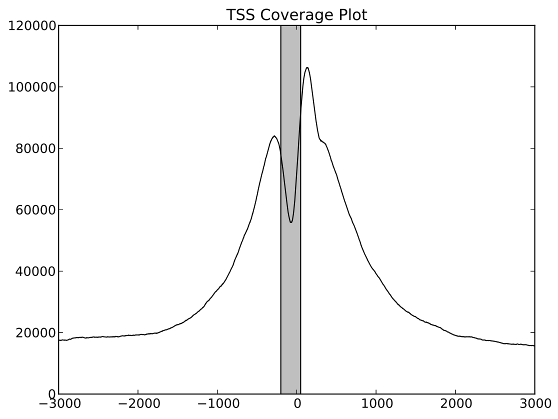


Figure 11: TSS plot annotated to confirm the significant dip in signal between $-200 \leq x \leq 50$.

5. CONCLUSIONS & FUTURE WORK

We made evident in this work through the use of cloud computing infrastructures and the automation of software installation and configuration, that a researcher can control experimental conditions to reproduce scalable eScience experiments and applications. Two sets of experiments were performed. The first tested scalability by deploying a virtual cluster with 100 execute nodes. The second reproduced a genomics experiment in two separate clouds. Through these experiments, we demonstrated the ability to construct scalable computing environments in different clouds, which opens the opportunity for researchers to use our work in academic or commercial clouds.

In the future we plan to extend this work in the following directions. First, we plan to expand further into the next generation sequencing pipelines to enable bioinformaticians to embed workflows into our framework so that these workflows can be constructed in separate clouds. Additionally, we plan to extend this framework into educational uses to help lower barriers for people to use distributed environments. Incorporating our framework in with other monitoring tools like Ganglia[24] to provide researchers with the ability to monitor the experiment.

6. ACKNOWLEDGMENTS

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[3] ftp://ftp-trace.ncbi.nlm.nih.gov/sra/sra-instant/reads/ByRun/sra/SRR/SRR001/SRR001432/.

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[5] Chef | Opscode. http://www.opscode.com/chef/.

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