Charge Detection Mass Spectrometry

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A Charge Detection Mass Spectrometry research application, developed at Indiana University by the Martin F. Jarrold research group, is used to indicate the performance and simplicity benefits of using Cloudmesh and Ansible Galaxy to deploy and run big data software on one or more virtual machines in the cloud. This proprietary research application was initially installed and run by hand on local servers and remote Supercomputers. The research application performed well on these powerful systems; however, the manual process of deploying and running the application turned out to be inefficient and too cumbersome for the domain scientists. Therefore, Cloudmesh and Ansible Galaxy were leveraged in order to automate the deployment of virtual clusters and execution of this research application in the cloud. This modification abstracted away the need for explicit human interaction while maintaining an efficient, reproducible and scalable Charge Detection Mass Spectrometry research workflow.

Keywords: Chemistry, Cloud, Hadoop Streaming, HPC, I524, Parallel Computing

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

1. INTRODUCTION

1.1. Research Background

The Martin F. Jarrold research group at Indiana University studies Charge Detection Mass Spectrometry (CDMS) [1]. Their general day-to-day workflow consists of conducting many scientific experiments using a Mass Spectrometer. This expensive scientific instrument creates raw frequency data at a rate of four (4) MB/s throughout the duration of each experiment. The research group has developed a Fast Fourier based application written in Fortran to processes this raw frequency data. The Fortran application generates human interpretable output, which assists the domain scientists in understanding the substances analyzed in the aforementioned experiments. The outputted results contain detailed mass information of the many ions discovered, which is used to solve important research topics such as the measurement and classification of the Hepatitis B virus. The mass and the abundance of the ions discovered by the application can be plotted to determine *Intermediates* that exist between definitive peaks in the plot, shown in Figure 1. This mass information can also be used to generate two and three-dimensional graphical representations of the ions, which help the domains scientists visualize the underlying structure of the Hepatitis B virus, shown in Figure 1.

1.2. General Problem

The Martin F. Jarrold research group has the ability to generate a lot of raw data, all of which needs to be processed by their Fortran application, as shown in Figure 2. A typical day conducting research consists of eight (8) to ten (10) one (1) hour experiments with each experiment generating raw frequency data at a rate of four (4) MB/s. Therefore, a single day of experiments has the ability to generate up to one hundred and forty four (144) GB of data. The research group must be able to process this data in a similar amount of time as the time required to generate the raw data. If their collection of compute resources is not powerful enough, they will quickly become inundated with piles and piles of raw data. This day-to-day research workflow typically strains the research group's local compute resources. Further-

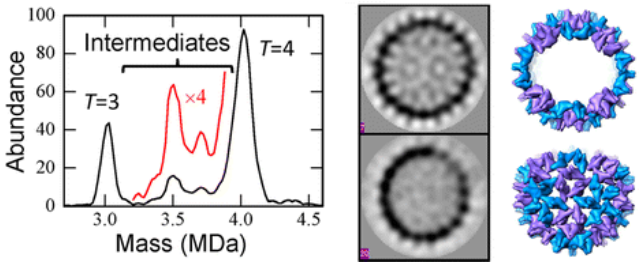

Fig. 1. The chart to the left displays an accurate measurement of the Hepatitis B virus (HBV) created by the research group [2]. This detailed mass information is used to create the images shown in the middle and to the right, which show 2-D and 3-D models of ions within the HBV. [2]

Fig. 2. The Martin F. Jarrold research group's pipeline is shown above. This pipeline includes a one (1) hour experiment, which creates approximately seven thousand (7,000) two (2) MB raw frequency files. Each of these files need to be transferred to the remote compute resource(s) and processed with a Fortran application to generate four (4) human interpretable output files.

more, the research group frequently makes algorithmic changes to the CDMS research application. When a significant change occurs, the research group must conduct a bulk reprocessing of months or even years worth of raw data. When a bulk reprocess is required, the limited compute resources available to the group become a significant limitation to the efficiency of their research. Additionally, when the application is run on remote systems, the raw input data must be transferred to the remote systems and the resulting output must be aggregated and then plotted in order to visualize and interpret the results. The process of moving data around by hand is time consuming and the process to aggregating results is tedious.

1.3. General Solution

The research group is composed of domain scientists who do not necessarily have backgrounds in Computer Science [3]. Therefore, a simple (i.e. automated) and reproducible solution must be developed in order to satisfy their day-to-day research workflow and their bulk reprocessing requirements.

1.3.1. Cloud Computing

Leveraging virtual clusters in the cloud to conduct their CDMS analysis increases their available compute power while simultaneously removing the need to explicitly manage a collection of compute resources. Furthermore, the ability to dynamically scale up or down the number of virtual machines aligns well with the evolving compute needs of the research group. The software tools Cloudmesh Client and Ansible Galaxy are at the foundation of this cloud computing solution [4, 5]. These two software tools collectively provide the ability to abstract away the technological details of the deployment and installation of virtual clusters in the cloud as well as automate the execution of the CDMS research application. These general modifications to their research workflow will ensure scalability, simplicity and reproducibility. These improvements allow the domain scientists in the Martin F. Jarrold research group to spend the majority of their time, effort and money on their research and not on the technological challenges of running the CDMS application.

2. ARCHITECTURE

The underlying architecture of this cloud computing research workflow is explicitly designed to facilitate automation. Cloudmesh and Ansible Galaxy are software tools that enable the creation of a virtual cluster, facilitate the deployment of software/data and automate the execution of the CDMS research application.

2.1. Software

2.1.1. Cloudmesh Client Toolkit

The Cloudmesh Client Toolkit provides an application programming interface (API), which allows users to simply manage a set of cloud resources (i.e. virtual machines, virtual clusters and etc.) [5]. The Cloudmesh Client Toolkit abstracts away the technological details of managing cloud computing resources.

2.1.2. Ansible Galaxy

Ansible is an information technology automation service designed for software deployment and execution [6]. Ansible Galaxy is an Ansible community, which "provides pre-packaged units of work known to Ansible as roles" [4]. Ansible Galaxy's pre-packaged units of work are essentially shared solutions to common automation tasks. This is a representation of the open source style of the Ansible Galaxy community. Ansible Galaxy promotes fast development since the wheel does not need to be reinvented for the automation of common tasks.

2.1.3. CDMS Application

The Martin F. Jarrold Group has written a Fast Fourier based application written in Fortran in order to conduct their CDMS research. This application is composed of approximately fifteen thousand (15,000) lines of Fortran code. Depending on the input, about 60% to 70% of the total compute time is spent within the external Intel Math Kernel Library (MKL) conducting the required Fast Fourier Transformations (FFT) [7].

2.1.4. Intel

The CDMS source code is compiled with the Intel compiler [8]. The CDMS application relies on the Math Kernel Library (MKL) to leverage efficient Fast Fourier Computations [7]. The application also leverages the Intel OpenMP parallel framework in order to divide the work amongst available CPU's [9]. Therefore, the Intel software is a fundamental piece of the architecture, which provides the compiler, MKL, and OpenMP functionality.

2.1.5. Hadoop

Apache Hadoop "is a framework that allows for the distributed processing of large data sets across clusters of computers using simple programming models" [10]. Therefore, Hadoop must be installed at the foundation of each virtual machine in the cloud in order to leverage multiple virtual machines during the CDMS processing phase of the workflow shown in Figure 2.

2.2. Data

The CDMS application requires a set of raw two (2) MB files as input. In order to develop and test the efficiency of the deployment, a small dataset was used to generate all of the performance results. This small test dataset, composed of two hundred (200) files has a total size of four hundred (400) MB and is a representative sample. A typical dataset for the research group is approximately fourteen (14) GB in size. In a single day, up to ten (10) datasets are created and need to be processed.

3. LICENSING

3.1. CDMS Deployment Scripts

The source code (i.e. Bash, Ansible, Python) presented here is licensed under the Apache License, Version 2.0 [11].

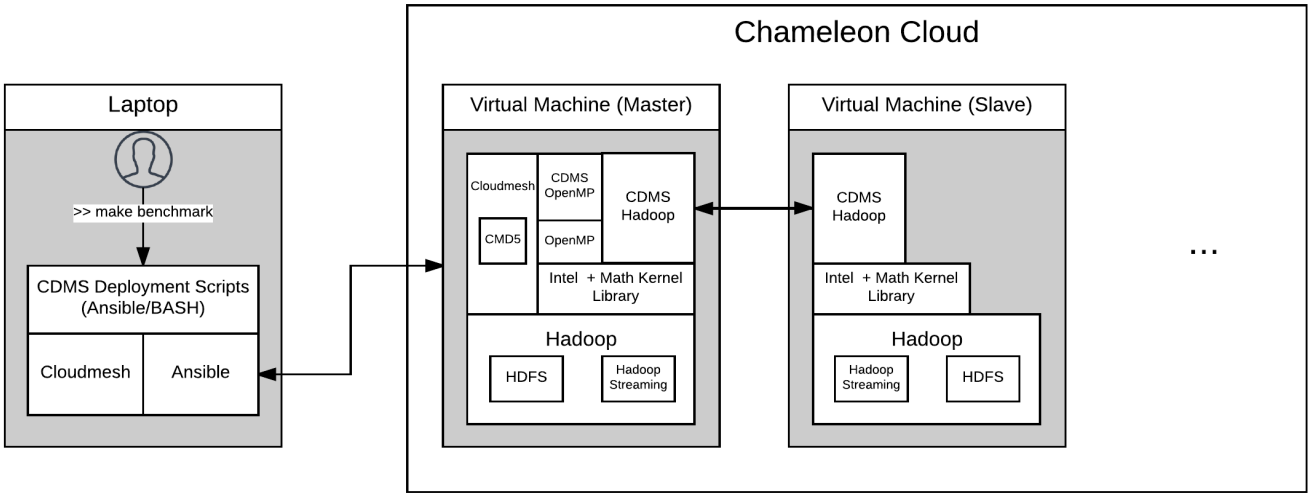

Fig. 3. The figure above provides a visual representation of the underlying architecture required for the Charge Detection Mass Spectrometry Cloud Computing workflow. The necessary software (i.e. Cloudmesh, Ansible, Hadoop, Intel, and etc.) and compute resources (i.e. Laptop and Virtual Machines) are explicitly shown above.

3.2. CDMS Application

The Martin F. Jarrold Group research group owns all of the rights to the Fortran Source code and data [1]. All distribution of the application and data must be consented by the research group.

3.3. Intel

The Intel software requires a license in order to complete the installation [12]. A student license is obtainable for free with an *EDU* email address; however, the leveraging the Indiana University Intel license server would provide a more complete and reproducible solution. In order to use the Indiana University Intel license server, the Virtual Machines must reside in the Indiana University IP address space. This can be achieved by connecting each virtual machine to Indiana University's Virtual Private Network (i.e. VPN) [13]. In order to connect to the VPN, one must connect via DUO Authentication (i.e. use a phone or token to validate) [14]. Given the complexity and reliability concerns with connecting to Indiana University's VPN simultaneously on multiple virtual machines, the Intel software is activated with the free Intel student license in order to promote simplicity and reproducibility.

3.3.1. Student License Limitations

The CDMS Deployment Scripts that were developed for this project leverage a free Intel student license to compile and link the CDMS application. While anyone can use this student license, it is registered to the author of this paper. This student license is *System Locked* and therefore can be installed on at most five (5) virtual machines. Once this threshold has been passed, the Intel software (i.e. compiler, MKL and OpenMP) can no longer be activated. This limitation somewhat inhibits the reproducibility and scalability of the research workflow. If a license registration error occurs during the Intel build phase of the deployment of the software, please contact the author of this paper. The author has the ability to uninstall the license from the currently registered hosts using Intel's Registration Center [15].

4. PARALLELIZATION

The Charge Detection Mass Spectrometry input data is split into many two (2) MB files. Conveniently, the data within each file is entirely independent to the data in the other input files. Therefore, the input data files can be processed simultaneously (i.e. in parallel). Parallel processing may not seem important when working on our sample dataset composed of two hundred (200) files; however, when a large collection of data requires reprocessing, parallel processing becomes critical to the efficiency of the Martin F. Jarrold research group.

4.1. OpenMP

OpenMP is a shared memory parallelization framework that is specified with simple compiler directives [9]. The shared memory parallelization structure limits the scalability of the application to a single node or virtual machine. This is in contrast to distributed memory parallelization, such as Message Passing Interface (MPI) or Hadoop, which enables multi-node parallelization [10, 16]. The original developers of the CDMS application decided to leverage OpenMP parallelization in order to exploit the natural data independency and improve overall performance of the application. However, this design choice limited the parallelization (i.e. scalability) to a single node or virtual machine.

4.2. Hadoop

In order to improve the overall performance and scalability, a distributed processing framework such as Hadoop must be integrated into the foundation of the CDMS application. Such an enhancement would allow for parallelization across multiple virtual machines. As discussed in Section 2.1.3, the source code is composed of fifteen thousand (15,000) lines of legacy Fortran code that interfaces with the Intel Math Kernel Library. In order to leverage the Hadoop MapReduce framework, the source code would need to be rewritten in a compatible programming language such as Java or Python.

4.2.1. Hadoop Streaming

Hadoop Streaming provides an alternative to rewriting the application in a compatible programming language. Hadoop Streaming allows one to "create and run Map/Reduce jobs with any executable or script as the mapper and/or the reducer" [17]. In Hadoop Streaming, "the mapper and the reducer are executables that read the input from stdin (line by line) and emit the output to stdout" [17]. The CDMS application is designed to read and write data to local files on disk; therefore, source code modifications were required in order to ensure the application read from stdin and wrote to stdout. The overall structure of the application and its data, which is naturally split into many relatively small files, allowed for a straightforward transformation from OpenMP parallelization Hadoop Streaming parallelization, as shown in Figure 4. Altering the way in which data was inputted to and outputted from the CDMS application was the only modification that was required in order to integrate Hadoop Streaming parallelization.

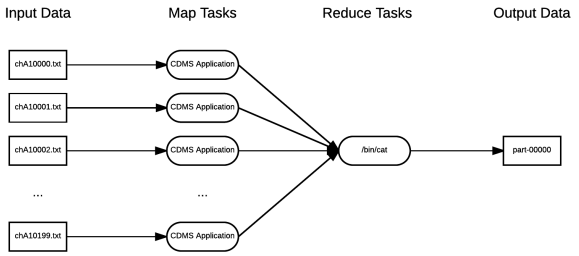

Fig. 4. The diagram shown above indicates the MapReduce style analysis of the CDMS Hadoop Streaming version of the application. Each two (2) MB input file is processed independently by the CDMS application and the results are aggregated with a single *cat* reduce task.

5. GETTING STARTED

The CDMS Deployment Scripts were specifically designed to promote simplicity and reproducibility. The following subsections describe how to use the CDMS Deployment Scripts to install and run the CDMS application in the cloud with as little as one simple command.

5.1. Requirements

In order to execute the CDMS Deployment Scripts, one must have the Cloudmesh Client installed and configured on their local system. This includes having a valid ∼/.cloudmesh/cloudmesh.yaml configuration file, registering Chameleon as the default cloud, registering a profile, uploading a ssh key and uploading a secgroup.

5.2. Fetch Code

The CDMS Deployment Scripts are hosted using GitHub [18]. A single repository contains the required Ansible and Bash scripts used to launch the CDMS research workflow [19]. See the following Bash commands:

```
>> git clone [REPOSITORY]
>> cd sp17-i524/project/S17-IO-3011/code
```

5.3. Benchmark

A single command will deploy the Hadoop virtual cluster, install the required software, run the three versions (i.e. Serial, OpenMP and Hadoop Streaming) of the CDMS application, aggregate the results, create plots of the output and delete the Hadoop virtual cluster. Timing information for each of these stages is printed to the screen once the benchmark has completed. The performance of this benchmark is plotted and explained in Section 7. See the following Bash command:

```
>> make benchmark
```

By default the benchmark will be run on a virtual cluster containing a single virtual machine. You can modify the maximum number of virtual machines to be used in the benchmark by passing in an optional argument to the *benchmark* Makefile option. The example shown below will run the entire benchmark with one, two and three virtual machines. See the following Bash command:

```
>> make benchmark num_nodes=3
```

5.4. Additional Commands

In case one would like to break up the aforementioned benchmark into individual pieces, there are separate Bash commands available. See the following Bash commands:

```
>> make deploy [num_nodes=n]
>> make install
>> make run
>> make view
>> make delete
>> make clean
```

5.4.1. Deploy

The *deploy* Makefile option leverages Cloudmesh Client to deploy a Hadoop virtual cluster in the Chameleon Cloud [20]. By default one (1) virtual machines will be created with the *deploy* option. The specific number of virtual machines deployed can be configured by passing in num_nodes=n, where n is the number of virtual machines requested to be deployed in the virtual cluster.

5.4.2. Install

The *install* Makefile option installs necessary software (i.e. Intel Compiler, Intel MKL, Python, Pip, Cloudmesh, Git, Charge Detection Mass Spectrometry application, and etc.) on the master and slave virtual machines of the active virtual cluster.

5.4.3. Run

The *run* Makefile option runs the serial, OpenMP, and Hadoop Streaming versions of the CDMS application on the active virtual cluster using the small test dataset containing two hundred (200) input files.

5.4.4. View

The *view* Makefile option aggregates the output data from the virtual machines in the active cluster, plots the results using Python's matplotlib and transfers a subset of the plots to the local system in order to visually validate the accuracy of the application [21].

5.4.5. Delete

The *delete* Makefile option deletes all of the virtual machines associated with active virtual cluster.

5.4.6. Clean

The *clean* Makefile option removes all of the local output files, if any exist.

6. COMPUTE RESOURCES

The CDMS OpenMP parallel version application was tested on multiple compute resources, as explained in Section 7. Each resource has unique architectural qualities that impact the performance, scalability and degree of parallelism. While the degree of parallelism (i.e. number of CPUs) may not be indicative of application performance, it certainly provides a baseline understanding of some architectural differences amongst the four (4) available systems.

6.1. Windows HPC Server

The Martin F. Jarrold's local Windows HPC Server has eight (8) CPUs; therefore, the Charge Detection Mass Spectrometry OpenMP version application can process up to eight (8) input files in parallel.

6.2. Karst

Indiana University's Linux Supercomputer, named Karst, has sixteen (16) CPUs per node; therefore, the Charge Detection Mass Spectrometry application can process up to sixteen (16) input files in parallel [22].

6.3. Big Red II

Indiana University's Linux Supercomputer, named Big Red II, has thirty-two (32) CPUs per node; therefore, the Charge Detection Mass Spectrometry OpenMP application can process up to thirty-two (32) input files in parallel [23].

6.4. Chameleon Cloud

The Cloudmesh Client allows one to specify different flavors of virtual machines to be deployed in the Chameleon Cloud [5, 20]. These flavors come in various sizes (i.e. Memory, vCPUs, and etc.). As shown in Table 1, these flavors can be used strategically to specify the number of virtual CPUs allocated to each virtual machine. As an example, the Chameleon Cloud m1.xlarge flavor provides eight (8) vCPUs. This allows the Charge Detection Mass Spectrometry OpenMP application to process up to eight (8) input files in parallel. Additionally, the virtual machines deployed in the Chameleon Cloud are running version 14.04 of the Ubuntu operating system.

Chameleon Cloud Virtual Machine Flavors

# Flavor	# of vCPUs
m1.medium	2
m1.large	4
m1.xlarge	8

Table 1. The table above indicates the number of virtual CPUs allocated to the various virtual machine flavors in the Chameleon Cloud [20]. The number of vCPUs indicates the maximum degree of parallelism for the CDMS application.

7. PERFORMANCE RESULTS

The following subsections describe the performance of the OpenMP and Hadoop Streaming versions of the application. These performance results only include the time-to-solution of the application processing the two hundred (200) input files. Perforamnce results including the entire deployment, installation and execution will be explained in Section 7.3.

7.1. OpenMP Scalability

As discussed in Section 4.1, the application was initially parallelized using OpenMP. This version of the application attempts to utilize the computational power available on a single node or virtual machine. Figure 5 compares the time-to-solution performance of the OpenMP version of the application on the available compute resources (i.e. local servers, Supercomputers and clouds) introduced in Section 6. As expected the time-to-solution (i.e. execution time) of the CDMS OpenMP version of the application decreases as amount of compute resources increase, as shown in Figure 5. For instance, on Karst the application running with sixteen (16) OpenMP threads completes in 9.4% of the time required for the application running with one (1) OpenMP thread.

The application performs most efficiently on Karst when using sixteen (16) CPUs (i.e. OpenMP threads). However, when the application is run using one (1), two (2), four (4) or eight (8) CPUs, the best performance exists on the Chameleon Cloud, as shown in Figure 5. Specifically, the application performs 18% faster on a single Chameleon Cloud virtual machine when compared to running the application on eight (8) CPUs of Karst.

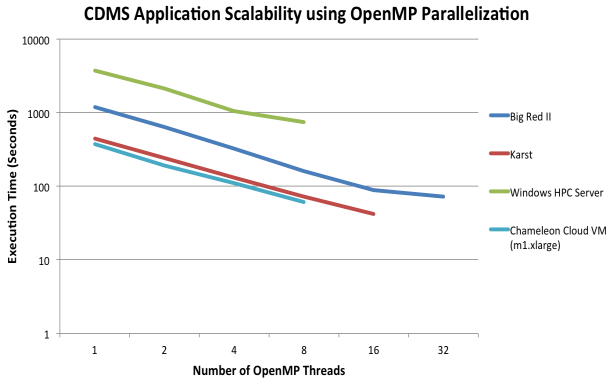

Fig. 5. The figure above shows the scalability (i.e. reduction in time-to-solution) as the number of OpenMP threads increase on local servers, Supercomputers and Clouds.

7.2. Hadoop Streaming Scalability

Unfortunately, the performance results for the Hadoop Streaming version of the CDMS application are not as promising as the performance results for the OpenMP version of the application. The Hadoop Streaming application does not exhibit the desired scalability. Since the application is essentially a map only Hadoop application, the performance (i.e. total runtime) of the application should decrease linearly as the number of virtual machines increase. However, the performance results shown in Figure 6 indicate that the execution time remains relatively consistent when one (1), two (2) or three (3) virtual machines are

used to process the two hundred (200) raw input files. Interestingly, the performance of the application significantly increases as the flavor of the virtual machine changes from smaller (i.e. less vCPUs) to larger (i.e. more vCPUs). Figure 6 shows that the Hadoop Streaming version of the application run on a m1.xlarge flavor requires only 43% of the execution time as the same application run on a m1.medium flavor.

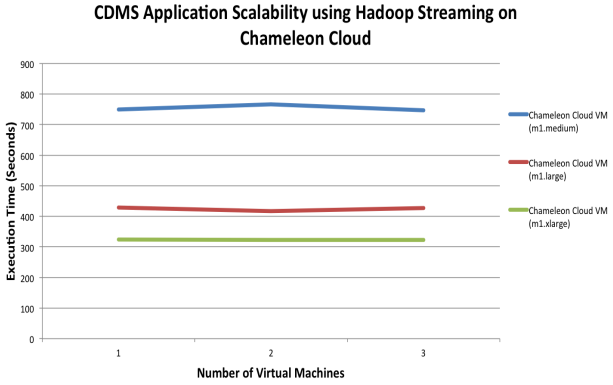

Fig. 6. The image above shows the scalability (i.e. reduction in time-to-solution) of the Charge Detection Mass Spectrometry Hadoop Streaming version of the application in a Chameleon Cloud virtual cluster. The performance information includes timing results for three (3) different virtual machine flavors.

7.3. Benchmark Scalability

The benchmark including the deployment of the virtual cluster, installation of the required software, execution the serial/OpenMP/Hadoop Streaming versions of the CDMS application and the aggregation of the results was tested using one (1), two (2) and three (3) virtual machines in the Chameleon Cloud. Interestingly, this benchmark required increasing time as the number of virtual machines increased, as shown in Figure 7. This performance information indicates that the deployment overhead outweighs the potential benefits of leveraging multiple virtual machines. The lack of scalability shown in the Hadoop Streaming version of the application and the small dataset are major factors, which contribute to the overall performance results. Specifically, if the Hadoop Streaming version of the application exhibited linear scalability and the dataset was significantly larger, the overhead incurred would not be as impactful as shown in Figure 7.

8. FUTURE WORK

Future work includes analyzing the performance of the CDMS Hadoop Streaming application to understand the poor scalability when running on a virtual cluster containing multiple virtual machines. Once the scalability issue has been fixed, larger flavors and more virtual machines will be utilized in order to increase the performance of the Hadoop Streaming application.

Future work includes figuring out how to leverage Indiana University's Intel license server. This will increase reproducibility by allowing the Intel Compiler and Intel MKL to be installed on an unlimited number of virtual machines.

Future work includes dispersing the raw input data across multiple virtual machines and running an instance of the CDMS OpenMP version of the application on each virtual machine and

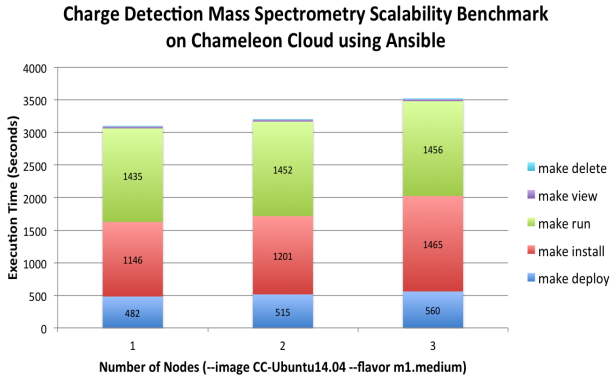

Fig. 7. The figure above indicates the time-to-solution for a full benchmark of the deployment of one (1), two (2) and three (3) virtual machines in the Chameleon Cloud. This benchmark includes depoying the virtual machines, installing all of the software, running the serial, OpenMP and Hadoop Streaming versions of the application and aggregating/plotting the results.

then aggregating the results. This modification will increase scalability for the shared memory parallelization.

Future work includes integrating Message Passing Interface (MPI) as the parallelization structure of the application rather than OpenMP or Hadoop Streaming [16]. This will allow for a dramatic increase in the scalability of the application.

9. CONCLUSION

The use of the Cloudmesh Client and Ansible Galaxy software to automate the execution of the Charge Detection Mass Spectrometry research application in the cloud improved the simplicity, efficiency and reproducibility. The automation allows the Martin F. Jarrold research group to focus on the details of their specific research rather than on the details of managing the software subsystems, executing the application and managing the input/output data. This automated cloud computing solution benefits the Martin F. Jarrold research group with respect to both simplicity and performance of the application. Streamlining the research workflow will inevitably result in an increase in productivity for the research group. An increase in research productivity may also result in an increase in grant funding and/or an increase in publications for the Indiana University research group.

The performance of the CDMS OpenMP version of the application performed favorably on a single Chameleon Cloud virtual machine when compared with a single node of the Indiana University High Performance Computing clusters (e.g. Karst and Big Red II). This unexpected result has sparked future work in optimizing the OpenMP version of the application for the Chameleon Cloud. However, the overhead included with deploying the virtual cluster and installing the necessary software causes the overall time-to-solution to increase dramatically.

The Hadoop Streaming version of the CDMS application did not exhibit optimal performance on a Chameleon Cloud virtual cluster. If the execution time reduced when more virtual machines were used, then this version of the application would become a viable solution for the research group's need to bulk reprocess raw input data. The Hadoop streaming version of the CDMS application is a step in the right direction; however, additional work must to be done to ensure scalability across

multiple virtual machines.

10. EXECUTION PLAN

The following subsections act as a timeline regarding how the project was divided up in order to complete all of the work by the desired deadline. The project execution plan is simply a guide and was followed diligently; however, some items were pushed slightly forwards or backwards as technological challenges were faced.

10.1. March 6, 2017 - March 12, 2017

This week I installed Cloudmesh on my local machine, created my first virtual machine on the Chameleon Cloud and tested Ansible Galaxy on remote systems such as one or more Chameleon Cloud virtual machine. I also wrote the project proposal, which eventually became this project report.

10.2. March 13, 2017 - March 19, 2017

This week I tested the deployment of the Intel Compiler on one or more Chameleon Cloud virtual machine using Cloudmesh and Ansible Galaxy. Given that I was out of town for Spring Break, I did not expect significant progress to be made during this week.

10.3. March 19, 2017 - March 26, 2017

This week I attempted to configure the Intel Compiler and Math Kernel Library to use the Indiana University Intel license server. Using this license server required connecting to Indiana University's Virtual Private Network (VPN) and using Two-Step Login (Duo) from the command line.

10.4. March 27, 2017 - April 2, 2017

This week I deployed the Charge Detection Mass Spectrometry research application along with the required input data on one or more Chameleon Cloud virtual machines using Cloudmesh and Ansible Galaxy.

10.5. April 3, 2017 - April 9, 2017

This week I modified the source code of the OpenMP parallel Charge Detection Mass Spectrometry research application to leverage Hadoop Streaming.

10.6. April 10, 2017 - April 16, 2017

This week I benchmarked the Charge Detection Mass Spectrometry research workflow on the Chameleon Cloud. This included varying the number and size of the virtual machines. I also wrote Python scripts to aggregate and plot the CDMS application's output from one or more virtual machines and locally visualize the results.

10.7. April 17, 2017 - April 23, 2017

This week I ensured the reproducibility of my source code as well as wrote and revised the final version of this report.

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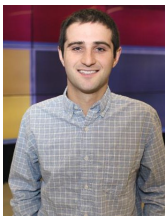
AUTHOR BIOGRAPHIES



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 project including researching, deploying, testing and benchmarking the Charge Detection Mass Spectrometry research application as well as composing this paper.

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