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 virutal machines in the cloud. This properitery research application was initially installed and run by hand on local servers and Supercomputers. The Charge Detection Mass Spectrometry research application performed well on these powerful remote systems; however, the in-depth manual process 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 this research application in the cloud. This modification abstracted away the need for 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

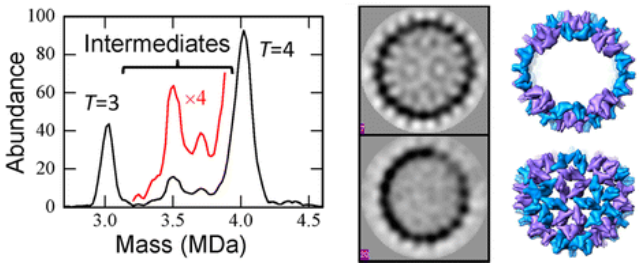

Fig. 1. The chart to the left displays an accurate measurement of the Hepatitis B virus (HBV) created by the research group's Charge Detection Mass Spectrometry research application [**?**]. This detailed mass information is used to create the images shown in the middle and to the right, which show 2-D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

1. INTRODUCTION

1.1. Research Background

The Martin F. Jarrold research group at Indiana University studies Charge Detection Mass Spectrometry (CDMS). 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 experiement. 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 substance analyzed in the aformentioned experiment. 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 experiements with each experiement generating raw frequency data at a rate of four (4) MB/s. Therefore, a single day of experiements has the ability to generate up to 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 are not powerful enough, they will quickly become inundated with piles and piles of raw data. This day-to-day research workflow typically strains the

Fig. 2. The Martin F. Jarrold research group currently employs the research pipeline shown above. This pipeline includes a one (1) hour experiment that creates approximately seven thousand (7,000) two (2) MB raw frequency files. These files need to be transfered to the remote compute resource(s) and processed with a Fortran application to generate four (4) human intrepetable output files.

research group's local compute resources. Furthermore, 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 becomes a significant limitation to the efficiency of their research. Additionally, when the application is run on remote sytems, the raw input data must be transfered 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. Therefore, a simple and reproducible solution must be developed to handle their day-to-day research workflow and their bulk reprocessing requirements. The solution to their limited compute resources consists of leveraging multiple virtual machines in the Chameleon Cloud to conduct their CDMS analysis. The ability to dynamically scale up or down the number of virutal machines will align well with the evolving compute needs of the research group. The software tools Cloudmesh and Ansible Galaxy are at the backbone of the general solution to their difficulties. This software provides the ability to abstract away the technological details of the deployment and installation of virtual machines in the Cloud as well as the explicit need to run the CDMS application by hand. This will ensure a simple and reproducible solution, which allows the domain scientists in the Martin F. Jarrold research group to spend the majority of their time, effort and money on their actual research problems and not on the technogical hurdles of running the CDMS application.

2. 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.

2.1. 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 reoprt.

2.2. 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 weeek.

2.3. March 19, 2017 - March 26, 2017

This week I attempted to configure the Intel Compiler 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.

2.4. 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.

2.5. 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.

2.6. 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.

2.7. 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.

3. CLOUDMESH & ANSIBLE GALAXY

Ansible Galaxy was leveraged in order to automate the deoployment of the required software subsystems, user code and data.

3.1. Software Subsystems

The CDMS application relies on the Math Kernel Library (MKL) to leverage efficient Fast Fourier Computations. The application also leverages the OpenMP parallel framework in order to divide the work amongst available CPU's. Therefore, in order to compile and run the application, the Intel compiler is required, which provides the MKL and OpenMP functionality.

3.2. User Code

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 approximately 15,000 lines of code. Depending on the input, about 60% to 70% of the compute time is spent within external MKL libraries conducting FFT calculations.

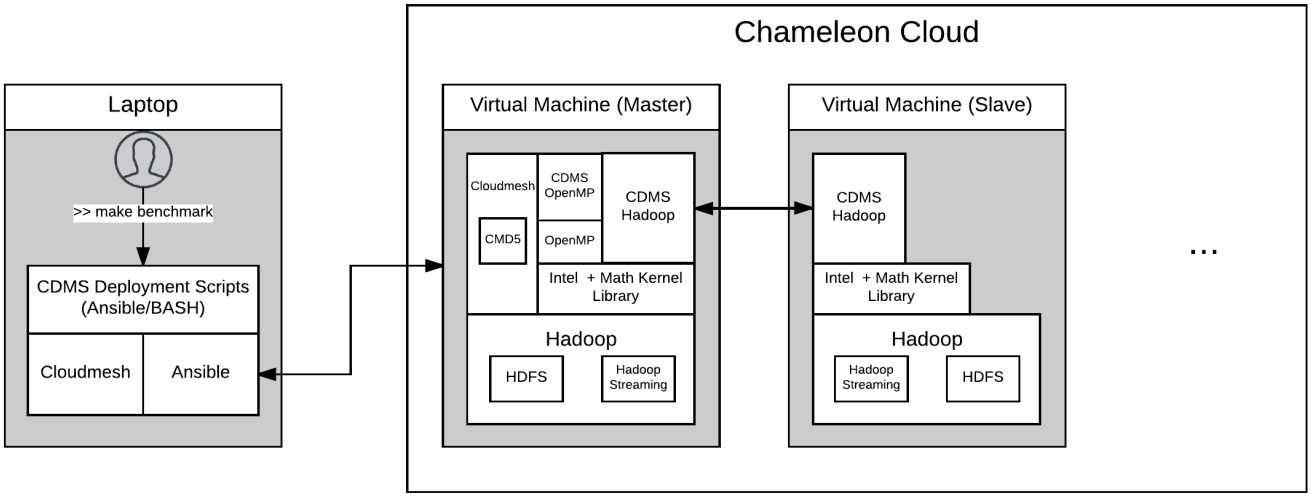

Fig. 3. Architecture

3.3. Data

The CDMS application inputs a set of raw 2 MB files. In order to develop and test the efficiency of the deployment, a small and large dataset was used. The small test dataset (i.e. 200 files) has a total size of 400 MB and the large dataset (i.e. 4,506 files) has a total size of 9.012 GB. A typical dataset for the research group is approximately the size of the large dataset. In a single day, 7 to 10 datasets are created and need to be processed. When an algorithmic change occurs to the research application, a large batch of archived data requires reprocessing. In this case, terabytes of data may be processed. This is why the parallelization and therefore the scalability of the application is critical to the Martin F. Jarrold research group.

4. LICENSING

4.1. Deployment and Benchmarking Source Code

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

4.2. CDMS Source Code

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

4.3. Intel Compiler

The Intel Compiler requires a license in order to complete the installation. A student license is obtainable for free with an EDU email address; however, the leveraginng 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 be 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). In order to connect to the VPN, one must connect via DUO Authentication (i.e. use a phone or token to validate). Connecting to IU's VPN from the command line using Ansible ended up being more of a hassle than it was worth.

4.3.1. Student License Limitations

The Ansible 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, this license is registered to the author of this paper. This student license is *System Locked* and therefore can only be installed on at most five (5) Virutal Machines. Once this threshold has been passed, the Intel compiler and Intel MKL can no longer be installed. This limitatation 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 can uninstall the license from the registered hosts, since the Intel student license is registered to the author of this paper.

5. PARALLELIZATION

The Charge Detection Mass Spectrometry input data is split into many two (2) MB files. Conveniently, this data within each file is entirely independent to the data in the other input files. Therefore, the input data files can be processed in parallel.

5.1. OpenMP

The application contains OpenMP parallelization.

5.2. Hadoop

The source code is composed of ten thousand (10,000) lines of Fortran code that interfaces with the Intel Math Kernel Library. In order to use Hadoop framework, the source code would need to be rewritten in Java.

5.2.1. Hadoop Streaming

The overall structure of the input and application allowed for a transformation of the parallelization interface from OpenMP to Hadoop Streaming.

6. BENCHMARK

As discussed in section 3.2, the application is parallelized using OpenMP. Therefore, this application utilizes the avaialable computational power available. Figure 5 compares the performance

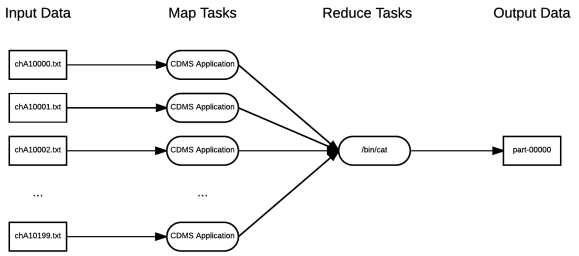

Fig. 4. CDMS Hadoop Streaming MapReduce

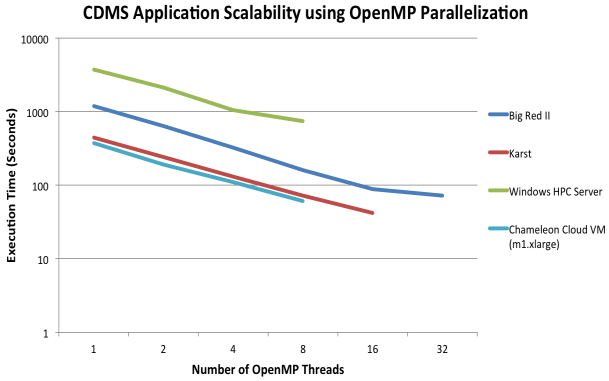

Fig. 5. The figure above shows the scalability (i.e. reduction in time-to-solution) as the number of OpenMP threads increase on local servers, Supercomputers and Clouds.

of the application on difference compute resources (i.e. local servers, Supercomputers and clouds).

The time required to deploy and run the application in the cloud is shown in the figure 7. This benchmark includes the time required for the installation of the software subsystems as well as the time required to run the application.

6.1. OpenMP Scalability

6.2. Hadoop Scalability

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 with an increase in the number of nodes deployed. However, the performance results in Table 1 indicate that the runtime remains relatively consistent when one (1), two (2) or three (3) virtual machines are used to process the two hundred (200) raw input data files. The performance analysis of the Hadoop Streaming application will be conducted as part of the Future Work, as explain in Section 8.

7. REPRODUCIBILITY

This solution was specifically architected in order to be easily reproducible.

7.1. Requirements

Must have Cloudmesh and Ansible installed locally and must have valid ∼/.cloudmesh/cloudmesh.yaml file stored locally. The cloudmesh installation is used to launch and manage VM's

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. The number of vCPUs indicate the maximum degree of parallelism for the CDMS application.

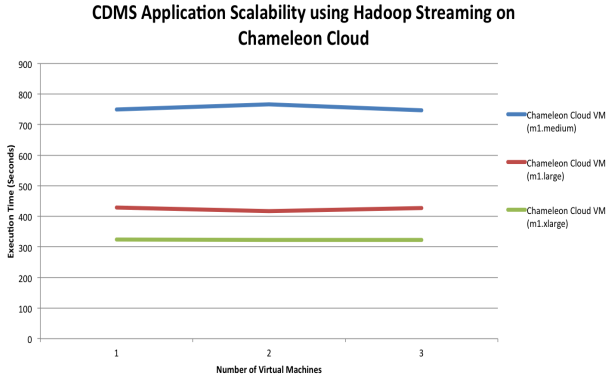

Fig. 6. The table above shows the scalability (i.e. reduction in time-to-solution) of the Charge Detection Mass Spectrometry Hadoop Streaming application as the number of Virtual Machines increase in the Chameleon Cloud Cluster.

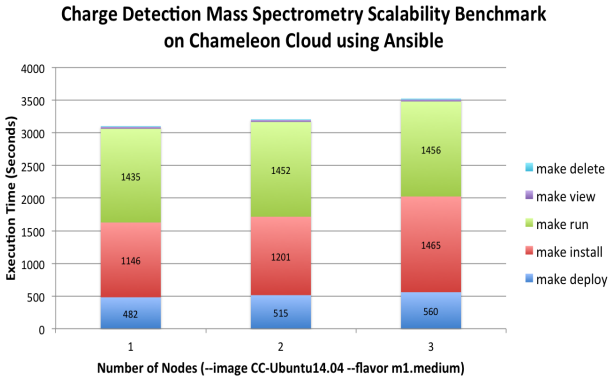

Fig. 7

in the cloud. The ansible installation is the backbone which initiates the deployment of the cluster, installation of the required software and benchmarking of the CDMS application.

7.2. Fetch Code

The source code is hosted using Github [**?**]. This repository contains the required Ansible and Bash scripts used to automate the research workflow. See the following Bash commands:

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

7.3. Benchmark

The benchmark discussed in Section **??** is available for you to reproduce the results. A single command will deploy the Hadoop cluster, install required software, run the three versions (i.e. Serial, OpenMP and Hadoop) of the CDMS application, aggregate the results, create plots of the output and delete the Hadoop cluster. Timing information for each stage will be printed to the screen once the benchmark has completed. See the following Bash command:

```
>> make benchmark
```

By default the benchmark will be run on one, two and three node(s). You can modify the maximum number of nodes (i.e. 5) to be used in the benchmark with the following command. This will run the benchmark with one, two, three, four and five node(s). See the following Bash command:

```
>> make benchmark num_nodes=5
```

7.4. Additional Commands

There are many pieces within the benchmark explained in Section 7.3. In case you would like to break up the benchmark into individual pieces, there are seperate Bash commands available. These commands will deploy the Hadoop cluster, install the required software subsystems, run the application, view the results and delete the Hadoop cluster. See the following Bash commands:

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

7.4.1. Deploy

The *deploy* Makefile option leverages Cloudmesh to deploy Hadoop virutal machines in the Chameleon Cloud. The default number of virtual machines that the *deploy* option will create is three (3). The number of virtual machines deployed can be changed by passing in num_nodes=x, where x is the number of virutal machines you would like to be deployed in your cluster.

7.4.2. Install

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

7.4.3. Run

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

7.4.4. View

The *view* Makefile option aggregates output data from the virtual machines in the active Chameleon Cloud cluster, plots the data using Python's matplotlib and transfers a few of the plots to the local system in order to confirm the accuracy of the application.

7.4.5. Delete

The *delete* Makefile option deletes all virtual machines associated with your username in the Chameleon Cloud cluster.

7.4.6. Clean

The *clean* Makefile option removes all local output files, if they exist.

8. FUTURE WORK

Future work includes analyzing the performance of the CDMS Hadoop Streaming application to understand the poor scalability when running on multiple nodes. Future work on this project includes using larger images and more virtual machines 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 virutal machines. Future work includes dispersing the raw input data across multiple virutal machines and running an instance of the CDMS OpenMP application on each virutal machine and then aggregating the results. Future work includes integrating Message Passing Interface (MPI) as the parallelel backbone of the application rather than OpenMP. This will increase the scalability of the application to more than a single virtual machine.

9. CONCLUSION

The development and analysis discussed above benefitted the Martin F. Jarrold research group with respect to simplicity for the domain scientists and with respect to the performance of the application. Streamelining the entire workflow will inevitably result in an increased in productivity for the research group. This may result in an increase in grant funding and/or an increase in publications for the Indiana University research group.

9.1. Simplicity

The use of Ansible Galaxy and Cloudmesh to run the Charge Detection Mass Spectrometry application in the Cloud (e.g. Chameleon Cloud) imporved the efficiency, reproducibility and scalability.

9.2. Performance

9.2.1. OpenMP

In comparison torunning on the Indiana University HPC clusters (e.g. Karst and Big Red II), the application time-to-solution diminished sigificantly. The most important and useful tool that was developped as a result of this project was the automation of the deployment of the necessary software subsystems, the application itself, the necessary input data and aggregation/visualization of the output. The use of Ansible Galaxy within

this research workflow will allow 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, running the application and managing the input/output data.

9.2.2. Hadoop Streaming

The Hadoop Streaming version of the CDMS application does not exhibit optimal performance for the Martin F. Jarrold research group. 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 CDMS version of the application is a step in the right direction; however, additional work must to be done to ensure scalability across multiple virtual machines.

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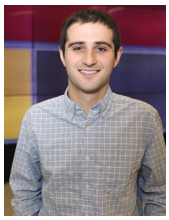
AUTHOR BIOGRAPHIES



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.

REFERENCES

[1] Gregor von Laszewski and Badi Abdul-Wahid, "Big Data Classes," Web Page, Indiana University, Jan. 2017. [Online]. Available: https://cloudmesh.github.io/classes/