Charge Detection Mass Spectrometry

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A Charge Detection Mass Spectrometry research application is used to show the benefits of using Cloudmesh and Ansible Galaxy to deploy software on one or more Virutal Machines in the Cloud. Previously, this properitery research application was installed and run by hand on local servers or Supercomputers which turned out to be cumbersome for the domain scientists. Furthermore, transfering the input data to remote systems as well as aggregating and visualizing the results is difficult and tedious. Improving this research workflow by automating the deployment of the necessary software subsystems in the Cloud assists in building 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

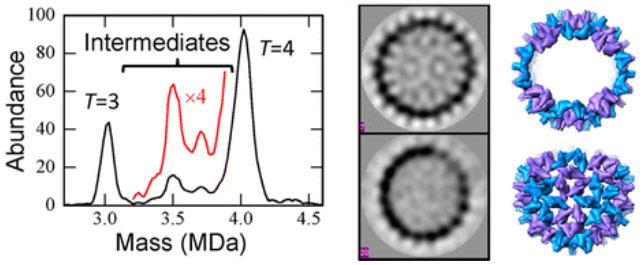

Fig. 1. The chart to the left displays an accurate measurement of the Hepatitis B virus (HBV) created by the research group's Charge Detection Mass Spectrometry research application [**?**]. This detailed mass information is used to create the images shown in the middle and to the right, which show 2-D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

1. INTRODUCTION

1.1. Research Background

The Martin F. Jarrold research group studies Charge Detection Mass Spectrometry (CDMS). Their general day-to-day workflow consists of conducting many scientific experiments using a Mass Spectrometer. This expensive instrument creates raw frequency data throughout each experiement. They have developed a Fast Fourier based application written in Fortran to processes this raw frequency data in order to determine detailed mass information of the substance used in the aformentioned experiment. The detailed mass information outputted from the application is then used to solve important research topics such as the measurement and classification of the the Hepatitis B virus. The mass information can be straightforwardly plotted to determine interesting peaks and valleys when comparing the mass/abundance of ions and can be used to create graphical representations of the ions, shown in Figure 1.

1.2. General Problem

The Martin F. Jarrold research group generates a lot of raw data that needs to be processed. For instance, a typical day conducting research will consist of 8 to 10 one hour experiements with each experiement generating 2 MB of raw frequency data every half second. Therefore, a single day of experiements can 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 for the data generation or they will quickly get inundated in piles of raw data. This day-to-day research workflow typically strains the research groups local compute resources. And furthermore, the research group makes algorithmic changes to the CDMS research application from to time to time which requires a bulk reprocessing of months or even years worth of raw data. In this case, the limited compute resources available to the group becomes a significant limitation to their research.

1.3. General Solution

The research group is composed of domain scientists who do not necessarily have backgrounds in Computer Science. Therefore, a scalable, efficient, and reproducible solution must be generated to handle their day-to-day research workflow as well as bulk reprocessing of months or even years worth of raw data. The solution to their compute limitations consists of leveraging

Cloudmesh and Ansible Galaxy to deploy their research application and the required software subsystems on one or more Virutal Machines in the Cloud. The ability to dynamically modify the number of Virutal Machines and even the number of Clouds will ensure a scalable, efficient, and reproducible solution that meets their compute needs. Furthermore, the usage of Ansible Galaxy will ensure a simple solution that these domain scientists will be able to master while spending the majority of their time and effort on their actual research problems.

2. EXECUTION PLAN

The following subsections act as a timeline regarding how I broke the project up week-by-week in order to complete the entire project 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 VM's. I also wrote the project proposal, which will eventually become the 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 VM's using Ansible Galaxy. I did not expect significant progress to be made during this weeek given that I was out of town for Spring Break.

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. This required connecting to Indiana University's VPN from the command line.

2.4. March 27, 2017 - April 2, 2017

This week I deployed the Charge Detection Mass Spectrometry along with the required input data on one or more Chameleon Cloud VM's using 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 application to leverage Hadoop Streaming.

2.6. April 10, 2017 - April 16, 2017

This week I benchmarked both the deployment and the analysis on at least one cloud (i.e. Chameleon Cloud). I also created a method to aggregate the output from one or more VM's 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 the report.

3. ANSIBLE GALAXY

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

Fig. 2. CDMS Pipeline

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.

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. CDMS RESEARCH PIPELINE

5. LICENSING

5.1. Deployment and Benchmarking Source Code

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

5.2. 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.

5.3. 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.

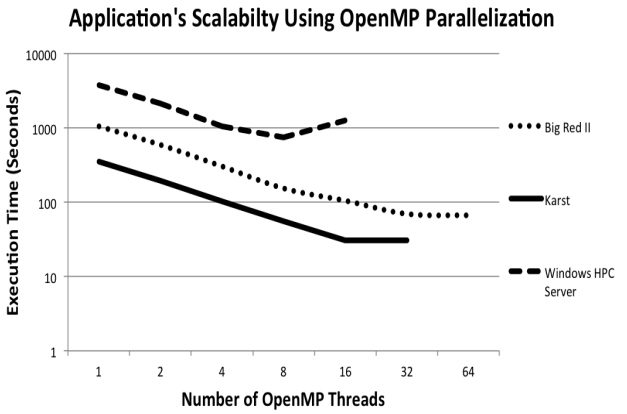

Fig. 3. The figure above shows the scalability (i.e. reduction in time-to-solution) as the number of OpenMP threads increase on local servers, Supercomputers and Clouds.

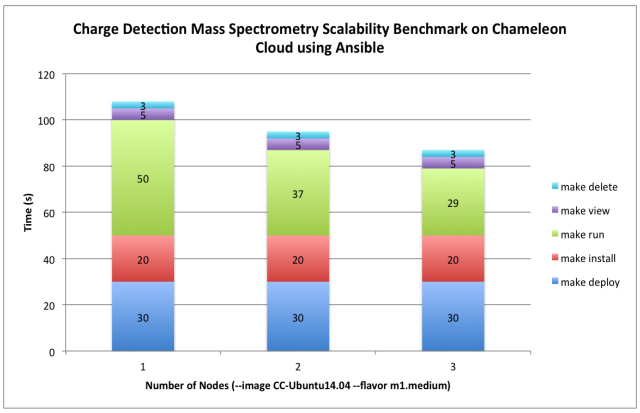

Fig. 4

6. BENCHMARK

As discussed in section 3.2, the application is parallelized using OpenMP. Therefore, this application utilizes the avaialable computational power available. Figure 3 compares the performance 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 4. This benchmark includes the time required for the installation of the software subsystems as well as the time required to run the application.

Add timing information for one or more clouds (i.e. Chameleon) to Figure 3 and compare the results (if possilbe).

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, as the table below indicates, the runtime remains consistent for all clusters.

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 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 6 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 command:

```
>> make [deploy/install/run/view/delete]
```

8. CONCLUSION

8.1. 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, reproduciblity and scalability.

8.2. Performance

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.

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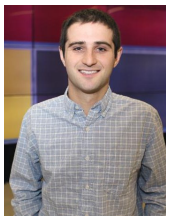
AUTHOR BIOGRAPHIES



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 CDMS 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/