HemeWeb: Blood flow simulation in the cloud using docker

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Declaration

I declare that this thesis was composed by myself, that the work contained herein is my own except where explicitly stated otherwise in the text, and that this work has not been submitted for any other degree or professional qualification except as specified.

(*Steven Steven*)

Table of Contents

List of Figures

Chapter 1

Introduction

Software are increasingly complex. Our everyday software are packed with features that makes its usage difficult. To people without familiarity with the product, it will be a barrier of entry to use it even when it helps them tremendously.

This also ties in to the complexity of a research that use these softwares. Open science dictates that research should be reproducible or replicable for it to better validate the research. However, recent findings have shown that not many research in psychology or even computation are replicable easily.

1.1 Motivation

To study how blood flow in a given vessel, Mazzeo and Coveney [2008] developed a fluid dynamic simulation software named HemeLB. Currently, it is actively developed and used by researchers to help their study. For example, Itani et al. [2015] used HemeLB for automated ensemble simulation of blood flow for a range of exercise intensities, Bernabeu et al. [2015] used it for detecting difference of retinal hemodynamics with regards to diabetic retinopathy, and recently Franco et al. [2015, 2016] used it to understand branching pattern of blood vessel networks.

As I have written in the proposal for this dissertation [Steven, 2016], HemeLB works by calculating fluid flow in parallel by using lattice-Boltzmann method [Mazzeo and Coveney, 2008]. This calculation allows HemeLB to simulate blood flow within a given blood vessel structure. Unfortunately, the calculation part is only a small part of the workflow to run the simulation. There are multiple pre-processing and post-processing steps needed to run the simulation from start to the end. These includes of preparing the input so HemeLB can work on it, and also processing the output so it is

ready to view.

These long pipelines of steps needed to run simulation, coupled with complexity of configuration of the software created a high barrier of entry for scientists and doctors to use HemeLB. Furthermore, as observed previously [Steven, 2016], interesting simulation will require parallel computing resources like ARCHER supercomputer which might be difficult to get access to by interested parties. While smaller simulation instances can run on typical laptop, most of the problems will require more powerful machines.These facts might prevent usage of the software by interested parties. More importantly, it shows there are still improvement that can be done to lower the barrier of entry for users to use HemeLB. This is important for HemeLB, especially when it is envisioned to be an integral part of future medical decision [Green, 2014].

Another aspect that HemeLB workflow can be improved is with regards to its reproducibility aspect. Researches that used HemeLB embrace reproducibility as one of its concern. As observed before [Steven, 2016], There are steps that are in place to make sure HemeLB and its simulation result are reproducible. First, the entire code base are publicly available on Github. Second, in running simulation with HemeLB, version of the software is automatically recorded. Lastly, in addition to the version used, input files and configurations are also recorded automatically. These facts can be seen from the publications mentioned above [Bernabeu et al., 2015; Itani et al., 2015; Franco et al., 2015, 2016] that include all these information. These information allow researchers interested to replicate the simulation to do it manually. Automation of these steps could further improve HemeLB's reproducibility and allow peers to replicate, duplicate, and audit its simulation results quickly and easily. This automation will be important, in addition to being usable, for HemeLB to become integral part of medical decision in the future.

1.2 Objectives

Based upon the needs to improve the usability. reproducibility, and auditability aspect of HemeLB project, I will develop a prototype web interface for HemeLB. This prototype web interface will lower barrier of entry in using HemeLB software compared to the current approach of using command line interface. In addition to that, using web interface will also allow features to be added to the simulation workflow which might not be essential to the HemeLB core itself. For example, automating packaging, sharing, and reproducing simulation result. These features are not essential for the

HemeLB core, but definitely help the overall workflow of blood flow simulation.

Using the dynamic capabilities of cloud computing vendor, the web backend should be able to dynamically scale without much efforts. On top of that, these infrastructures are available to everyone with a costs, allowing its user to access it without having to get access to supercomputers. Its user should be able to run a blood flow simulation without having to deal with the complexity of running each steps of the workflow manually.

In addition to the web interface, I will also develop deployment script so that peer could deploy its own instance of the web interface. This will ease up deployment process for individuals or organizations intending to use HemeLB for its own purposes. This script will be developed as part of the project.

1.3 Outline

I provide a brief introduction to the topic of this dissertation in this chapter. The rest of the chapters will be organized as follow:

- **Chapter 2**. I will provide background information that are necessary for readers to understand the concepts, technology and implementation that are done in this dissertation. HemeLB, containerization technology, cloud computing, High-Performance computing infrastructure, and other topics will be discussed in details in this chapter.
- **Chapter 3**. I will discuss the bulk of the work in this chapter. Implementation details and design of the proposed solutions will be provided and discussed in details.
- **Chapter 4**. Evaluation
- **Chapter 5**. Analysis
- **Chapter 6**. Future work

Chapter 2

Background

In this chapter, I will discuss about various background information that are used as a basis for the work presented in this dissertation. I will discuss about how HemeLB currently works, High-Performance Computing (HPC) infrastructure, and docker.

2.1 Current HemeLB workflow

Currently, running a blood flow simulation consists of multiple steps that needs to be run in sequence. These steps are done in a variety of interface, from command line to graphical user interface. Additionally, these steps also require various level of computing resources to work efficiently. In order to understand how the proposed work will improve the current conditions, I will elaborate on how HemeLB currently work. Also, discussion on computing resources and interface for each steps will be provided.

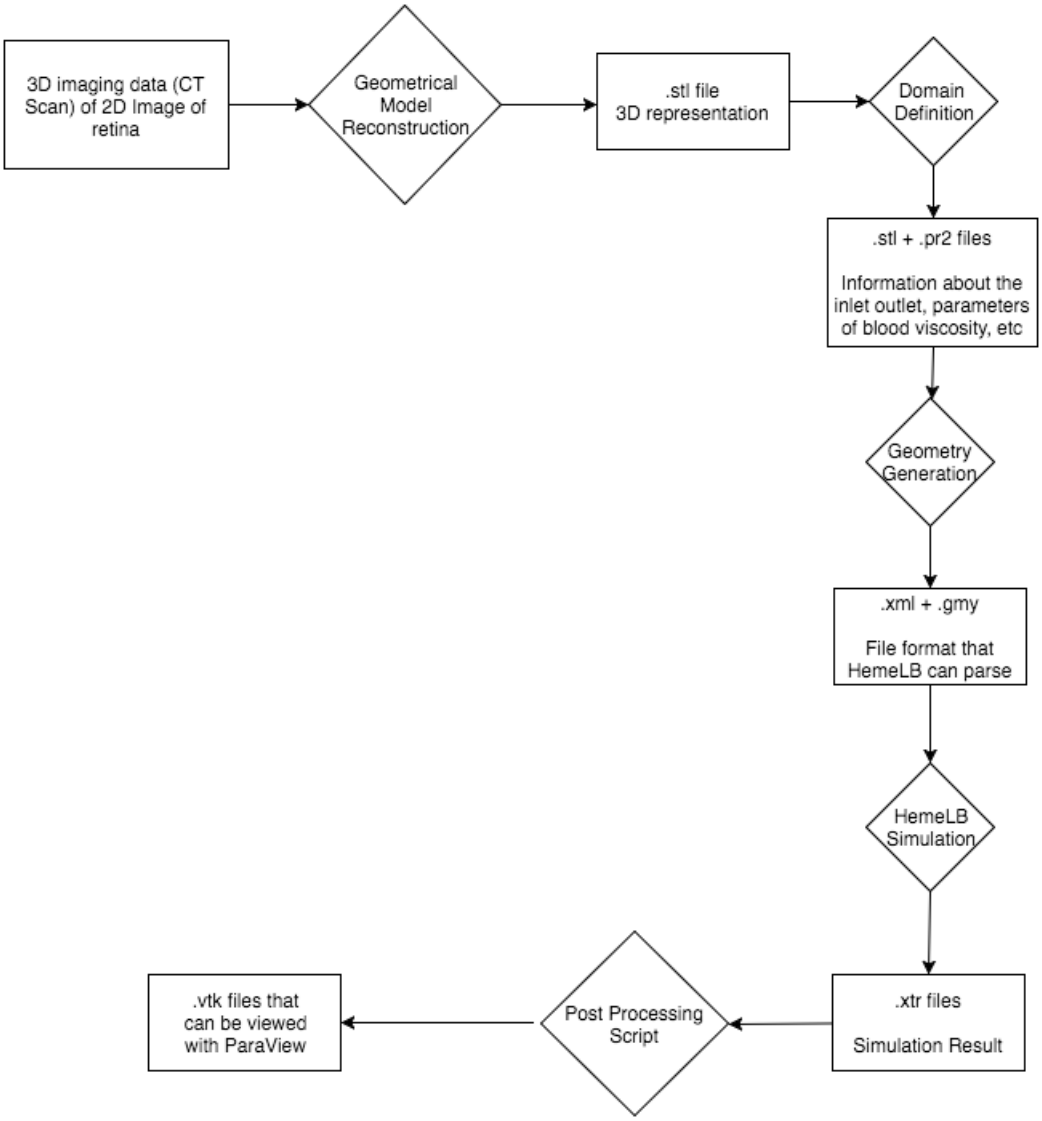

Figure 2.1: Current HemeLB workflow taken from Steven [2016]

Figure 2.1 illustrates steps involved in running HemeLB workflow. These steps will be discussed in details below:

1. **Geometrical model reconstruction**

   In this step, a 3D model of vascular system is constructed from the raw microscopic image of it. Alternatively, the 3D model can also be constructed from CT scan with its 3D imaging data. From this step, a 3D geometry file are generated in the form of .stl file. This process can run in a regular workstation just fine. However, it is highly problem dependent as the tools needed to parse and generate the 3D model are dependent to the problem experts try to simulate.

2. **Domain definition**

   3D geometry model generated from the previous step is now used as an input for the domain definition step. In this step, a graphical user interface is used to add domain information to the 3D model. Information like blood viscosity, inlet outlet placement, and blood pressure will determine how the simulation will run. The HemeLB setup tool was developed for this particular needs. The setup tool provides a graphical user interface for domain experts to add these parameters. All parameters are then saved in a profile file with .pr2 format. This step can run on standalone commodity hardware and should not require a highly parallel computing resources.

3. **Geometry generation**

   This step will take the encoded information from domain definition step and the 3D model of the vascular system to generate files that can be understood by the main HemeLB program. These files contain similar information with the previous 3D model and the profile file. However, both of them are now formatted in a HemeLB parseable format, an XML configuration file and a GMY geometry file. This geometry generation step can also run on a commodity hardware. However, it requires users to use command line interface to operate with the files. The process is done with piping the input files to a python script which is part of HemeLB setup tools.

4. **HemeLB simulation**

   The main heavy computations of the workflow are done in this step. Configuration and geometry files that are generated in the previous step are feed into the HemeLB binary as input files. HemeLB will then run calculations that govern how blood will flow inside the provided vascular system for a number of iterative steps. The number of steps is defined in the configuration file that is generated in the domain definition steps.

   As observed in the proposal of this work [Steven, 2016], HemeLB can scale up from 1 up to 32,000 cores in running the simulation [Groen et al., 2013]. This means that a typical problem could run in a commodity hardware with a small number of cores. However, bigger and scientifically challenging problems will require a higher number of cores that requires high-performance computing resources as portrayed in Franco et al. [2016, 2015] and Bernabeu et al. [2015].

In addition to that, users of HemeLB have to use command line interface to configure, run HemeLB simulation, and interact with the output files.

Output files generated by this step are written in parallel into output directory which is set when running the simulation. These output files represent the state of blood flow in the vascular system at a given step count. The interval in which HemeLB writes an output is also set from the domain definition step.

5. **Post processing**

   The output files generated by the HemeLB simulations are not easily viewed by domain experts. The files are generated in a fashion that is efficient to write in parallel, however, it will need further conversion to make it easy to be interpreted. This is where the post-processing step comes in.

   In this step, the output files are piped into two python scripts that are included in HemeLB tools to convert them into a .VTU files. These .VTU files are viewable in a separate software called ParaView. With it, domain experts could visualize the result of the simulation in a graphical user interface which ParaView provided. This step can be run on commodity hardware without problems. However, to do this step, users will require to interact with command line interface.

All of these steps requires users to configure and install the tools required for each step by themselves. However, the target audience of HemeLB are biologists, clinician, researchers, and medical professionals, which might not have the capabilities and the technical know-how to do it. This is one of the motivating reasons for the proposed work in this thesis.

2.2 High performance computing infrastructure

Researchers increasingly use complex mathematical and computational approaches in doing their research. In understanding complex phenomenon, researchers use interdisciplinary approaches in providing insight into the problem. Bioinformatics and computational biology are examples of this interdisciplinary discipline.

The problems that these disciplines tries to understand require computational approaches that are not cheap. The smaller size of these problems would probably run on a commodity hardware, more complex one will require highly parallel computing resources. These resources are often be found in the form of a supercomputer like

ARCHER supercomputer. HemeLB software package is the prime example of these computational approach that requires highly parallel computing resources.

Traditionally, there are two paradigm that tackles large computing processes. These are High Performance Computing and High Throughput Computing (HTC). HPC involve using many similar computing nodes to perform tightly coupled computations. These nodes are often placed in the same room and connected with high bandwidth network. These network allow the nodes to communicate between each other in doing the computations [13]. An example for this type of resources are computer clusters, GPUs, and supercomputers. In contrast, HTC allow heterogeneous computing resources to cooperate for common goals. These resources are often distributed geographically and varies in type and performance. These resources will then do different independent computations that independently scheduled [13]. Based on these distinctions, HPC is a correct categorization of HemeLB.

However, running these simulations requires access to HPC infrastructures that might not have reproducibility of research as a priority. Facilities that operate these infrastructure often give out computing hour usage to projects based on the merit of their peer-reviewed proposal, for example how PRACE [14], the Partnership for Advanced Computing in Europe, and EPSRC [15] give access to their infrastructure to researchers. This means that those seeking to reproduce computation of a research have to compete with other projects for the limited computing hours that are given out by these institutions. Most likely, it will not be the top priority, hence creating barrier for reproducing computational research.

Furhtermore, most biology and biomedical research fall outside the remit of these organizations and their counterpart in these domains, e.g. BBSRC, HRC, do not provision HPC resources at the time of writing. Not having access to these facilities create a barrier for HemeLB to become more open because reproduction of simulation is non-trivial. This is where cloud computing infrastructure enter the picture.

2.3 Cloud computing

In response to the huge demand for computational power by researchers and academics, a concept called grid computing was envisioned in 1990s [16, 17]. This vision considered computing resources analogous to power grid, where user should not care from where the resources are acquired and how it is delivered to the user. This paradigm was mainly developed with the interest of researchers and academia that the

business models caters to the most [18]. Grid computing typically give CPU hours based on the proposal that is vetted by the institutions. Example of this institution is TeraGrid which operates until 2011 [19].

Cloud computing shares similar vision with the grid computing paradigm, in that the computing resources are acquired and delivered are invisible to the users, but different on the execution of the business model. It is massively scalable, allows abstract encapsulation of computing resources, dynamically configured and delivered on-demand and most importantly, driven by economies of scale [18]. Since it is driven by economies of scale, it is in the interest of cloud providers to provide features that users actually need and want to pay for, therefore creating a tight feedback loop between users and the providers to develop the platform better than how grid computing handle feature developments.

This has allowed cloud vendors to grow significantly, for example in 2013 it was noted that some cloud vendors could reach more than 90% growth per annum [20]. This growth further fuels demand and allow them to cut pricing for their service multiple times [21, 22, 23] and create more demands. This development has allowed businesses and institutions to offload their computational need to the cloud vendors for a price rather than building their own infrastructure. This scenario could also be used for our purpose of performing or reproducing computational research without needing to have access to large HPC systems.

Cloud vendors like Amazon also capitalize on the need for computing resources for HPC applications [13]. Running HPC applications on cloud platforms, while incurring performance overhead, can be a viable alternative to supercomputers as shown by the Nekkloud project [24], NASA HPC Applications [25], and HPC applications benchmark in cloud case study [26]. Also, part of this project is to demonstrate that HemeLB can run acceptably on a cloud platform.

2.4 Containerization Technology

2.5 Other High Performance Computing

In the past few years, many complex HPC software packages have been deployed to the cloud. In this section, I will highlight these projects to learn how they solve similar issues.

One similar project is Nekkloud [24]. In this case, Nektar++, a complex high-order

finite element code, face similar usability problems. Their original workflow was so complex that only few people can run it. People without computer expertise had a hard time to actually run computations with it. Furthermore, one should also get access to a HPC infrastructure to run it, which may not be easy. Nekkloud project is their answer to these problems. It was developed to encapsulate most difficulties in using the software package. Using a web application to provide high level interface instead of using the command line. Making it more accessible to more people without computing expertise. In addition to that, it ran on cloud infrastructures. Allowing people without dedicated HPC infrastructure to run high-order finite element computations.

Another project that is tackling similar space is Galaxy [27]. Galaxy, a web-based reproducible research platform, uses cloud infrastructure to run its HPC applications. In illustrating its use, the developers have developed a super-resolution spark (SRS) model. This modeling process needs a supercomputing resources to execute the cloud infrastructure provides. These capabilities are also encapsulated in an easy to use web interfaces, making it easy for scientists to run, and share simulations.

Above examples illustrate that a web application can be a viable alternative interface for complex applications. However, this implementation on the cloud also has a negative impact on the applications. Raw performance is lower than dedicated HPC infrastructures. These performance penalty was observed in the projects mentioned already [24, 25, 26]. Nekkloud authors considered the performance penalty acceptable, because the cloud infrastructures allow flexibility. This flexibility and the benefit of making it more usable will sometimes outweigh the performance penalty.

Pros and cons of web application for complex HPC projects are area that are often discussed. But, deployment scenario for these HPC projects in cloud infrastructure are rarely discussed. More specifically, the use of containerization technology in helping tools deployment.

Deploying HPC applications is considered as a time-intensive process [28]. For example, the ARCHER support team has 36 members [29] to support this process. One approach to reduce these problems is software containerization. Containerization technology is developed to run applications or tools in an isolated environment within a kernel. It is more lightweight than traditional virtualization technology that use hypervisors to manage virtual machines [30]. Containerization technology has been discussed in high performance computing area. For example how Docker, one of the more popular implementation of containerization technology, is abstracting software environment in the HPC infrastructure [31] and used to build virtual HPC clusters [32].

Also, the shifter project [33] is trying to unleash Docker on HPC infrastructure. Meaning, allowing their HPC infrastructure to use Docker capabilities. To date, I am not aware of any discussion on the effect of containerization in running HPC application in cloud.

One of the above projects, Galaxy, support containerization technology for their tools packaging. They used Docker, one implementation of linux container software. Galaxy claimed that using Docker allow efficiency, isolation, and portability of their tools [34]. These are good traits that could also be helpful for HemeLB. Docker, in particular, are often discussed as a promising technology to support reproducible research [35]. Usage of containerization technology, however, are sparsely detailed in the literature.

Chapter 3

Implementation

In this chapter, I will discuss HemeWeb's project implementation. This will consist on how the HemeLB core container is developed, how it is deployed, and how the web application itself is being implemented.

3.1 HemeLB core docker container

In this section I will explain how I developed the HemeLB core docker container. This part is the most straightforward of the project. There has been effort to make HemeLB portable by packaging it with the setup tools and a portable desktop environment using docker. It is done with the rationale to be shared with peers without having them to configure their work station too much.

In this phase, I modified the previous available image to handle few problems I found when trying to run HemeLB with it. 1) The size is big because it consists of the setup tools, not only the HemeLB binary, and 2) It cannot be run as a daemon. To solve this issue, I used a different base image than the previous. I used the ubuntu base provided by phusion. This image handle services correctly and allow the container to be ran as a daemon with SSH service running. This allows HemeLB to run with multiple containers. Also, I purged all package that are not needed for the container, resulting in a minimal sized container image.

3.2 Deployment

In addition to have a working prototype available. I also wanted to make sure that the process of deploying the web application is as painless as possible. Therefore,

I developed a deployment script for automatically configuring the architecture with minimal manual intervention. The script is made with the help of a configuration management and orchestration tools called ansible (https://www.ansible.com).

The goal of the script are as follow: 1. Provision the required master instance 2. Configure the master instances with the correct security and network settings 3. Configure and Install the HemeWeb correctly 4. Configure and install all the services needed by HemeWeb 5. Provision required compute instance 6. Configure the compute instances with the correct security and network settings 7. Configure the compute instances to run HemeLB core docker container

In the development of the script, I faced few problems in regard of orchestrating the infrastructure. Mainly with regards to cloud vendors having non-similar application programming interface to access or control the resources. This led to some part of the deployment needing manual intervention. One of this part is creating an image from the running instance so the master instance can request a new pre-configured instance instead of configuring from the start.

I developed the script as modular as I can so that it can be refactored easily. I separated the cloud vendor specific instruction into its own folder for each vendor. This part mainly deal with the provisioning, security, and network configurations. The more common part, like installing softwares and services needed, are abstracted into the common scripts that are called by the vendor specific script after provisioning instances are done. With this in mind, I had been able to run the deployment script on three different cloud vendors. They are Google Cloud Platform, Amazon Web Service, and Digital Ocean. After the deployment script is done, the architecture will be ready to run HemeLB simulation on the cloud.

This script is online as part of the codebase that is published on github. It is available on https://github.com/SeiryuZ/HemeWeb/tree/master/deployment .

3.3 HemeWeb

This section will discuss the bulk of the work that is developed for the project. The main interface for users to interface with HemeWeb, the web application. I developed this web application using django web framework for my familiarity with the framework, so I can focus my time on developing the web application.

3.3.1 Architecture

3.3.1.1 Web application components

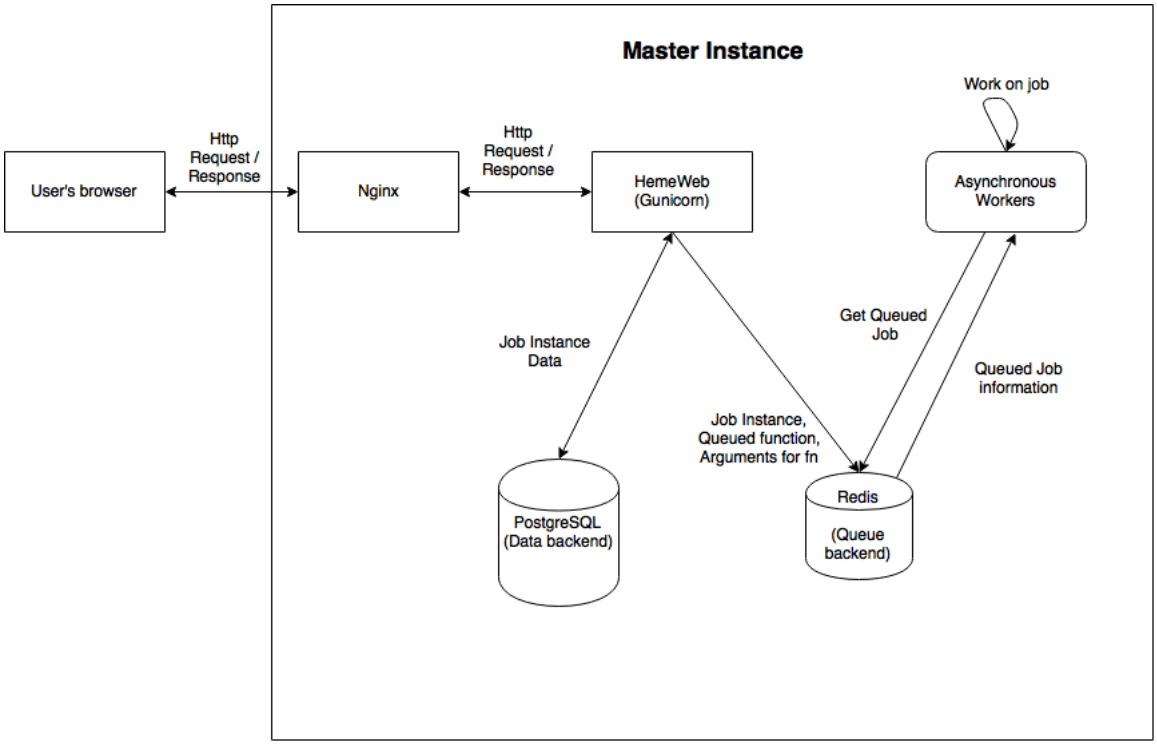

Figure 3.1: HemeWeb architecture

Figure 3.1 above illustrate how HemeWeb interacts with the other components on the master instances. HemeWeb, a django web application, lives on the master instance with various components that it interacts with.

User's browser will send a HTTP request to the master instance, in which nginx frontend will handle. It will act as a reverse proxy, and proxy those Http request towards the web application server process, which is handled by green unicorn python library. This library will run the HemeWeb python code to process the HTTP request by the user, it will server a static HTTP response, or handle job related logic that might interact with the PostgreSQL database service. The database will persist job information locally on the instance and will be wiped out when the master instance is terminated.

Another way the HemeWeb application can interact is to submit a job into the queue which use Redis datastore as the queue backend. HemeWeb use third party library called django-rq that handles asynchronous background tasks handling. It uses the pub

/ sub mechanism that Redis has to create a light weight background job workers. It will store the function to be executed, the job instance, and parameters to used by the function. A background worker that is called using cronjob at an interval will look at the queue and work on a job if there's any. The worker will execute the function and update the instance with relevant job execution result. The worker then will go back to idle until next invocation.

3.3.1.2 Docker components

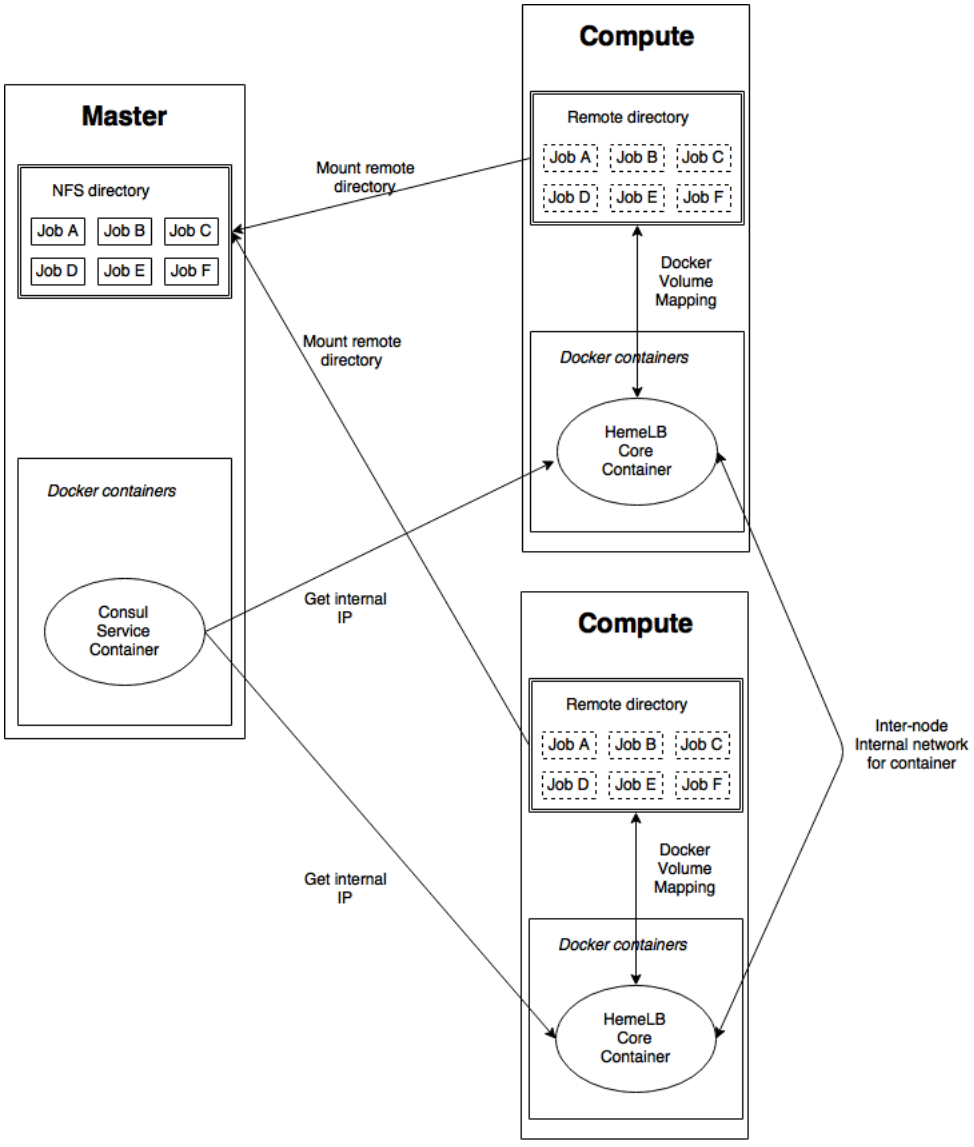

Figure 3.2: HemeWeb docker component

In this section, I will discuss how the docker components interact with its host and each other as illustrated on figure 3.2. In the master instances, job directories are required to be exported via the Networked File System service. These directories need to be exported for the purpose of sharing the folders and files with the compute node. The web application actually do not really interact with the Networked File System, it create or modify the folder, but configuration is handled during deployment process.

Also, in the master instance we have one docker containers running at all time. This container handle the consul service. This service is used by docker service to co-ordinate inter-host communication. With this service running, docker service running on other hosts will be able to coordinate with the master instance with regards to container network, give its container non-conflicting internal IP. In a nutshell, containers on different hosts can communicate as if they are on a local network. This feature is key in allowing HemeLB simulation to be run inside docker container on multiple host on the cloud platform.

On the other hand, the compute node will first mount the job directory from the master instance. This is done in order to allow HemeLB containers to have shared access on the input and output folders they are going to use. The container will gain access to the folder on the host by using the docker volume mapping features.

Docker containers on the compute node will only run HemeLB core containers. The compute node will pull the appropriate HemeLB core version from docker hub, but if specified version is locally cached on the instance, no network activity will be made. When running the container, the compute unit will coordinate with the consul service on master instance with regards to internal network configuration. Allowing multiple HemeLB core containers on different hosts to communicate with each others.

After this configuration is done, then the job execution will be done by one of the compute node. It will execute an mpi job for HemeLB with internal IP of all hosts that are started for this particular job.

3.3.1.3 Job instance structure

HemeWeb use django python library to handle the heavy weightlifting with regards to web functionalities. The way job instance is created is also dependent on django's model hierarchy. **Job** is a class that represent one instance of job simulation. It inherits from django.db.models.Model class that exist within django infrastructure. Django's model class handles the interaction with the database and with the django environment and HemeWeb's job class only need to extend this class to add its own functionality.

HemeWeb's Job class has the following attributes:

- id: This is a unique UUID field that represent the Job ID. UUID field was chosen because it is appropriate for the possibility of sharing the job simulation files between different deployment of HemeWeb. UUID can prevent clashes of ID between these instances.
- input_file, stl_file, profile_file, output_file, configuration_file: These attribute keep track of the files that are used by the job. It is stored as path to the file in the local file system, but with django functionalities HemeWeb can work with the file as an object.
- container_image: This attribute determine which container of HemeLB core will be used in the simulation. Currently, this field is set manually on the code.
- instance_type: This determines which compute node type will be started for the simulation.
- instance_count: This attribute determines how many compute node will be started for the simulation. Currently, this is also set manually on the code.
- status: The attribute to determine Job's status, whether it is *queued, added, done, failed, etc*
- created: Attribute to keep track when the job is created
- updated: Attribute to keep track when the job is updated

3.3.1.4 Job instance directory structure

HemeWeb structure each job's files and configurations into its own folder. I will discuss how it is structure to provide clearer picture on how the application package and work with the job's files.

<UPLOAD_FOLDER_DIR>/<JOB_ID>
<UPLOAD_FOLDER_DIR>/<JOB_ID>/inputs/*
<UPLOAD_FOLDER_DIR>/<JOB_ID>/logs/*
<UPLOAD_FOLDER_DIR>/<JOB_ID>/outputs/*
<UPLOAD_FOLDER_DIR>/<JOB_ID>/metadata

HemeWeb installation can change the upload folder directory as the basis of all job's folder will be located. Job ID will be generated by the web application using UUID4 scheme, so ID's generated by different instances of HemeWeb should theoretically have really low chance of clashing. This is also why adding previous job to the HemeWeb instance is not problematic, because using auto increment ID will be a problem for multiple installation.

Next, we have the inputs folder inside the job folder. This is where all the inputs and configurations are stored by the web application. There's also logs folder, where the job stdout, stderr, and HemeLB logs are stored. The web application will read from this folder and make it available on the web interface. Outputs folder will be used by the HemeLB simulation to output files on this folder. One final file is the metadata file. This file is used by the web application to store the state of the job. The job is pickled into this metadata file so when it is downloaded, the web application can unpickle the state of the job instance and it is preserved, ready to be used for another simulation.

3.3.2 Simulation workflow

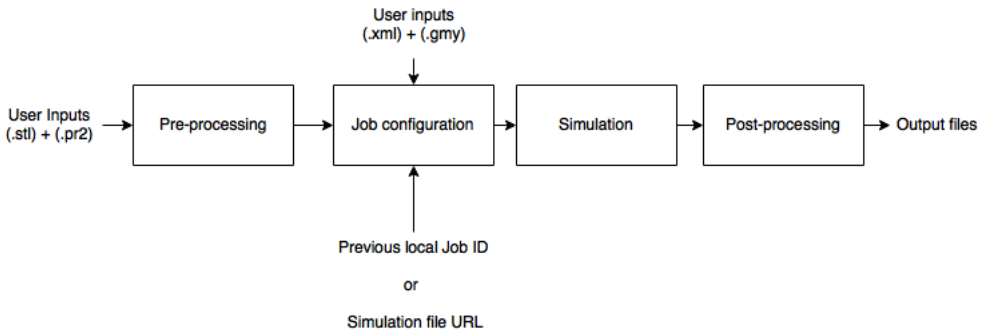

Figure 3.3: HemeWeb flow

Figure 3.3 illustrate how the HemeWeb web application works. it consists of mainly 4 core activity that will be discussed in details in the following section.

3.3.2.1 Pre-processing

HemeWeb handle pre-processing of inputs that are needed so that HemeLB simulation can parse the files. User provide a geometry file (.stl) and a profile file (.pr2) to the web application. HemeWeb will then create a job instance with these two files, save

them locally on master instances and queue the pre-processing job.

The asynchronous worker on master instance will then pick up the job whenever they are free. It will run the pre-processing python script to generate the geometry files and HemeLB configuration file. These files will then be saved on the master instance, and HemeWeb will track these files by recording the path to these files on the job instance. Now the job instance is ready for the next step. of the workflow.

3.3.2.2 Job configuration

In this step, HemeWeb application will take a job instance with correctly set geometry file (.gmy) and HemeLB configuration (.xml). However, there are multiple ways that HemeWeb can get this correctly set job instance. As illustrated on Figure 3.3 , there are 4 possible entry points for this step. They are:

- **From the post-processing step.** These files are generated from the previous pre-processing step. The job instance is directly used in this step
- **User's provided geometry and configuration file.** User have pre-processed their own file locally, or have their own geometry and configuration files available. HemeWeb will create a new job instance, save both files and keep them tracked with the job instance.
- **User's provided previous job ID.** There are two possible case when user specify previous job ID. First, the previous job is available locally on the HemeWeb instance. Second, the previous job is cached on the persistent storage on the cloud vendor and are not available locally. HemeWeb will download the previous file from the persistent storage if it is not available locally. It will then create a new job instance that copy the previous job's geometry file and configuration file to be used for further configuration.
- **User's provided simulation file URL.** The last alternative is for user to provide the simulation file URL. Simulation files are uploaded to a persistent storage at the end of the workflow. These files, if made public, can be used by other instance of HemeWeb to download the simulation files and use it as a basis to create a new job instance. The way the system work is the same as using previous job ID, but its source is not its own persistent storage, but other people's simulation files.

After the job instance is created from one of the four way possible discussed above, HemeWeb will then ask users for the job configuration. This entails on configuring how many instances should be started, what are the type of the instance, and the hemelb-core container version. After configuring all these parameters, then the user can queue the job into the queue system.

3.3.2.3 HemeLB simulation

Once job instance are queued into the simulation queue, free asynchronous workers will pop the queue and run the job. The worker will start up the configured amount and type of server instance from the cloud provider. These instances will then be further reconfigured by an ansible script so that it points to the correct master instance address. Next, input files are shared via Networked File System(NFS), the compute units will mount the input folders to their instance.

HemeLB core container will be pulled from docker hub in the next step. This step will skip the download if the container asked are already cached in the image for compute unit which are prepared on the deployment part. After all of these are done, then the simulation can finally begin. Master node will issue an mpi command to be run by the leader of compute nodes. The leader of compute node then will run this mpi command in the docker container. This command will be run on multiple compute node if it is configured as such in the previous steps.

The HemeLB simulation will run until outputs are produced. The output will be written back to the correct output folder in the shared folder. This means that the master instance will have access to the outputs file and can do further processing. This step ends with the termination of the instances.

3.3.2.4 Post-processing

After HemeLB simulation is done, HemeWeb web app will do some post-processing steps to make sure the output files can be viewed easily. The output from HemeLB simulation is structured in such a way that makes it efficient to write in parallel. However, these output cannot be viewed by visualization system like Paraview. What HemeWeb will do is to pipe the output to two scripts that will format the output into a format that can be understood by paraview.

However, the post-processing steps are not done until converting the output. There are further steps that HemeWeb took to make sure that the simulation files, configura-

tions, and results are preserverd. HemeWeb will package the job directory, compressed it, and upload it into persistent storage that cloud vendors provide. As the time of writing, HemeWeb only support amazon S3. The simulation file are uploaded to this storage and made available for public for other HemeWeb instance to use. Also, with the job files persisted on persistent storage. The next HemeWeb instance deployed can take advantage of these files that it can download them as previous job available.

3.3.3 Implementation Challenge

In this section, I will try to outline and discuss the challenges in implementing this project, and if any, the solution that I choose.

3.3.3.1 Cloud vendors features and API difference

Cloud vendors each have their own API and features. This has led to some problems when trying to create a common API to do certain task. One notable problem is that the absence of image creation from running instance task from one of the cloud vendors.

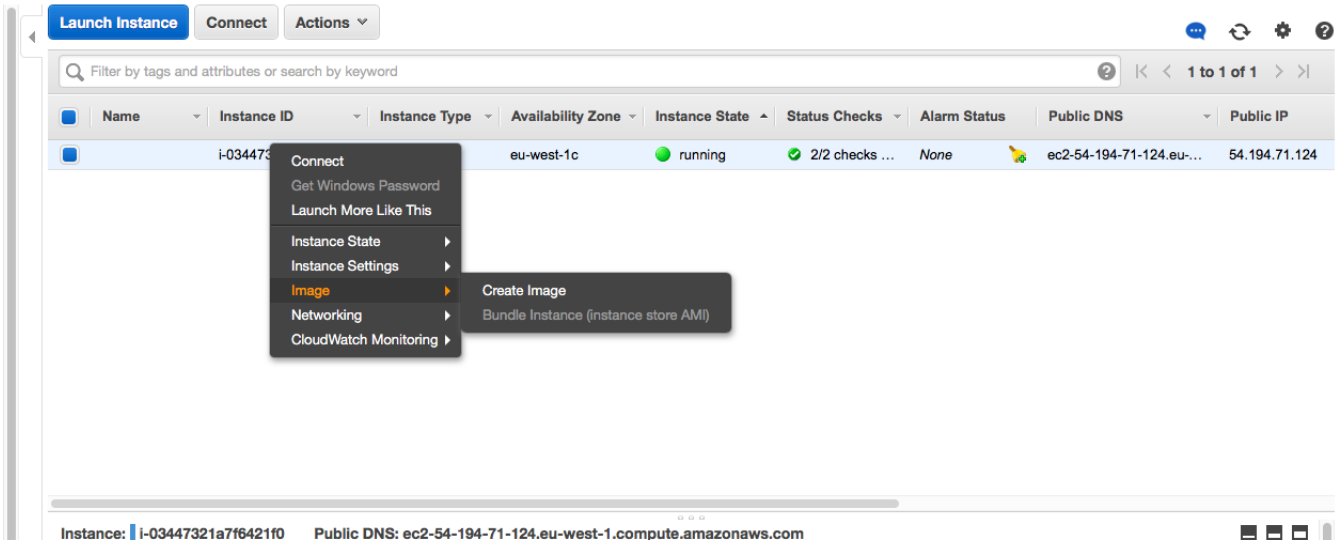

Figure 3.4: Manual image creation

Figure 3.4 shows how I decided to solve the problem. By instructing users to manually create image from running instance. Users have to go the web interface of cloud vendors, right-click on the running instance, and create image from it. This is a simple workaround which is less complicated than accommodating different features

and API from different cloud vendors.

Another problem is time constraint. Due to the time constraint, I cannot achieve full compatibility with all cloud vendors. The development time is mainly focused on amazon web service because it has all the features HemeWeb need. However this means that the codebase is currently tied to one cloud vendors. Features like automatically reading past simulation files from cloud storage and uploading simulation files are tied to amazon infrastructure. It is possible to refactor this functionalities out to become more generic, however for the interest of time, I decided not to.

3.3.3.2 Security

Another challenge that I face during the development of HemeWeb is to handle the security of the application. However, security is not the main focus of this work and is apparent in the development of the application. I will still discuss the security issues so that I can give an objective assessment on the application.

The first security issues that I found is with regards to the compute node security in some cloud vendors. Digital ocean for example, does not provide a ”real” private networking option within compute nodes. They have a ”shared” private networking options that allow other compute nodes, which are not even under your account have network access to your node. Theoretically, this allow other people access to your private compute node if they have the credentials. In this case, I made sure that all the compute nodes have a sensible access policy to deter unauthorized access to the nodes. I only allow ssh with public key and disabled password access to ssh. Also, it is also much better to choose cloud vendors that have real private networking like AWS. In which, the compute nodes are not accessible to other nodes that are not part of your own private network. This is much more secure and sensible.

Another security issue is on how the compute nodes and master node share simulation job’s files. It currently use Network File System without any security measures towards the nodes that try to mount it via the private network. There is an opportunity to secure these communication by encrypting the job files, but it is not currently done.

3.4 Development process

The development process is divided into 5 phases. The planned phases are as follow:

1. Separate HemeLB core into its own container

2. Orchestrate the deployment of HemeLB cluster / infrastructure
3. Develop HemeWeb to accept user input
4. Extends HemeWeb to handle geometry generation workflow
5. Extends HemeWeb to handle domain definition step or Viewing of HemeLB simulation result

The development process loosely follow the agile method in which I regularly meet with the stakeholders every week to give an update and gather feedback on the project. The phase are designed in such a way to minimize the risk of having nothing at all during the end of the project phase. This is due to that HemeWeb can work on its own after finishing step 3. The HemeLB simulation can be done on its own. The rest of the steps are there to extend the functionalities of the HemeWeb to cover more functionalities.

During the first week of the development, I focused more on stripping the HemeLB core container into its own. I researched on how Docker and dockerfile work, and finding out what are the issues with the current container. After identifying the issues, which are ssh service and full of functionalities which are not essential, I stripped down the image and changed the base image so that the container could avoid the mentioned problems. I end up with smaller container size and it is available online on https://hub.docker.com.

However, one particular issue with what i have currently is that the Dockerfile is published as a part of the HemeWeb source code. It should be tied down to the HemeLB development instead of HemeWeb. Currently the development model of HemeLB is that there is an internal private repository where the less than stable build is pushed to it, and there are public repositories where only stable builds are pushed into. The release process should include adding the dockerfile towards the core HemeLB source code repository and tagging the release correctly. HemeLB core containers should then be built automatically on docker hub with regards to additional tags being pushed to the public repository.

After the HemeLB core container, I then focused on how the architecture could be primed for the HemeLB simulation. It involves on configuring the servers and all supporting infrastructures on cloud vendors to be ready for HemeLB simulation. Network configuration, security configuration, docker configuration, and other should

be handled automatically. I elect to choose ansible orchestration software because it is closely related to python language that I used.

In this phase, I successfully achieve the provision and deployment process that with the correct credentials and authorization, the script could provision and configure the architecture correctly so it is ready for HemeLB simulation. In addition to that, I successfully created the script so that it will be cloud vendors agnostic. I can deploy the architecture to google cloud vendors, amazon web service, and digital ocean.

However, it is to be noted that the deployment process that I achieve can only run HemeLB simulation from the command line. I have not considered the web application installation and configuration at this point of the deployment. I am only considering the infrastructure being build and configured for HemeLB simulation.

Next, I started developing HemeWeb web application. I choose django web application framework due to my experience with it. I created a basic interface, where job simulation is listed on the index page on the home interface. After that, I added a basic interface to add new job with a geometry file and hemelb configuration file. The web application will then add those input files into a newly created job instance and configure the job instance in the job configuration step. Job will then be submitted.

Here I developed a separate ansible script that will be called when a queued job is being worked at. The ansible script is responsible for starting up compute nodes needed by the job and executing HemeLB simulation. After the simulation is done, the script is also responsible for correctly terminating the compute node.

After the basic HemeWeb web application is achieved, I extends it to handle preprocessing. I added an extra form in the adding new job form to handle a profile file and geometry file. These two files will be converted into a geomtery file and HemeLb configuration file that the job configuration steps expect. In addition to adding the interface, I also added a new function on the job instance that will run this preprocessing step on the background.

Lastly, due to the limited time, I can only manage to run a small post-processing step on HemeWeb. What I did was adding post-processing step that convert the Extracted results from HemeLB output into a format that can be viewed by third party software, ParaView. The results are piped into two scripts that will output a .vtu that is compatible with ParaView. This is done during the background activity after simulation result is outputted. However, currently this is done on the master node.

In addition to that, I also managed to add persistence capability to HemeWeb application. What I did was to package the job simulation folder into a compressed archive

and upload it to persistent storage service of cloud vendors. These archives can be queried by another instance of HemeWeb to get previous job IDs available for the particular cloud vendor account used to deploy HemeWeb. Also, the job simulation file URL is also showed on the web interface. Making it easy for the users to share the simulation file with their peers.

Chapter 4

Evaluation

In this chapter, I will discuss on the system's evaluation. Success will be measured by answering these questions:

- Can users run a simulation using our system ?
- Can users reproduce past simulations using our system ?
- Are users satisfied in using our system ?
- Are users more likely to run a simulation using our system compared to command line ?
- How does it perform compared to the existing infrastructure ?

In answering above questions, I conduct two sets of evaluation. First, an online questionnaire was conducted to measure user's experience and system's usability. And secondly, a performance analysis comparing the performance of HemeLB between dedicated hardware against cloud vendor's. Questionnaire will answer most of the questions related to user experience and usability above, while the performance benchmark will be the basis for performance evaluation and justification in using HemeWeb.

4.1 Questionnaire

In measuring user's experience, I created a questionnaire for HemeWeb using google form. The questionnaire was live for a week, from 3rd of August 2016 until 10th of August 2016.

At the start of the questionnaire, respondents are asked about their background information. This information will be used to provide demographic insight on the respondents and how it affect the type of answers the respondents will most likely give. Respondents will be asked to fill out their age, gender, job, discipline, and level of familiarity with various software tools. From their responses, I can determine whether the sample population is representative of the target audience.

The questionnaire is set to make tester run specific scenarios that HemeWeb is developed for. These scenarios are running a simulation using the web interface and reproducing past simulation with it. Testers running the scenario are given an option to skip the scenario and go straight to the questions below it to measure their experience if they find it too difficult.

The first scenario asks testers to run a simulation with given inputs. The questionnaires list two input files, a geometry file and a HemeLB configuration file that testers will need to download to their computers. After downloading the input files, testers are asked to open their browser and go to a specific URL where HemeWeb was deployed for the evaluation purposes. In that URL, testers will then add a new simulation job with the downloaded files, configure the job, and submit the job to the queue. The scenario ends when the job is submitted.

The second scenario asks testers to reproduce past simulation with a given URL that contains past simulation files. It asks testers to create a new job from the given URL instead of using files that are downloaded in the past scenario. After creating a new job, testers then will change some configuration and parameters from the past scenario and submit the job. The scenario also ends when the job is submitted.

Following each scenario are questions to measure whether users skip the scenario and an after-scenario questionnaires that users have to answer. The after-scenario questionnaire is based on the usability measurement at IBM developed by James R Lewis [Lewis, 1995]. It measures users' usability satisfaction with the system with regards to given scenario. The questionnaire give 3 statements which testers should agree or disagree, they are:

- Overall, I am satisfied with the ease of completing the tasks in this scenario
- Overall, I am satisfied with the amount of time it took to complete the tasks in this scenario
- Overall, I am satisfied with the support information (online-line help, messages, documentation) when completing the tasks

In addition to above questions, there are some questions about the tester's willingness to do exactly the same tasks as the scenario, but with the command line. This question will measure user's willingness in using the command line interface compared to the web interface.

After running both scenarios, testers are then redirected to the final questionnaire. The Post Study System Usability Questionnaire which is based on the same work by James R Lewis [Lewis, 1995]. In this questionnaire, testers are given 19 statements where they should agree or disagree, they are:

- Overall, I am satisfied with how easy it is to use this system
- It was simple to use this system
- I can effectively complete my work using this system
- I am able to complete my work quickly using this system
- I am able to efficiently complete my work using this system
- I feel comfortable using this system
- It was easy to learn to use this system
- I believe I became productive quickly using this system
- The system gives error messages that clearly tell me how to fix problems
- Whenever I make a mistake using the system, I recover easily and quickly
- The information (such as online help, on-screen messages, and other documentation) provided with this system is clear
- It is easy to find the information I needed
- The information provided for the system is easy to understand
- The information is effective in helping me complete the tasks and scenarios
- The organization of information on the system screens is clear
- The interface of this system is pleasant
- I like using the interface of this system

- This system has all the functions and capabilities I expect it to have
- Overall, I am satisfied with this system

In addition to the above questions, testers also will be asked to list the most negative aspects and positive aspects of the system if they have any. These questions will measure users satisfaction with the overall system, whether it is useful, whether the information given by the system is any good, and the interface quality.

4.2 Performance benchmarks

The second part of the evaluation is the performance benchmark. HemeWeb is running HemeLB simulation outside its original scope of being used on a highly parallel computing resources like a supercomputer. This could have an interesting impact on the performance of the system because cloud vendors, being much more easily accessible and provisioned, have an underlying difference with the stand-alone infrastructure. This performance benchmarks will then measure whether the impact on the performance justify the claimed usability benefit that we measure on the first half of the evaluation.

The performance benchmark will be done by the internal tooling that is baked inside HemeLB. Every HemeLB simulation will produce a report file that measures the performance of said simulation. On this evaluation, I will compare the performance of HemeLB simulation on four different scenarios to measure the performance impact on having HemeLB simulation on the cloud with docker containers. They are:

- ARCHER supercomputer
- Highly parallel computing resources
- Cloud computing with docker
- Cloud computing without docker

The benchmark on ARCHER supercomputer will be the gold standard of the performance. It's a gold standard because the infrastructure has a clear purpose of being used for the HPC application. It has the necessary resources and components that are tailored for it. It should be the ideal performance scenario. Next, the local computing infrastructure. This paints a picture if how HemeLB will perform on a private local

infrastructure which is built to run highly parallel jobs. This will be the measure that can be used if HemeLB is to run on private infrastructure.

The next two benchmark will be done to measure the performance of HemeLB simulation compared to the local infrastructure. Cloud computing vendors have an underlying difference with regards towards how the infrastructures are structured and connected together. This could have an inherent performance different with a standalone infrastructure. However, an analysis will be made with regards to running HemeLB simulation with another overhead, which is docker. While docker is used for easily swapping of the HemeLB version, it might affect the performance of HemeLB simulation. With this benchmark, we can answer whether the flexibility of docker container can justify the performance that we get. It is also interesting to see whether there are performance penalties that we incur when using docker.

Chapter 5

Analysis

5.1 Usability result and analysis

5.2 Performance result and analysis

Chapter 6

Conclusion

Chapter 7

Future work

To better support HemeLB simulation workflow, HemeWeb can be further improved. I suggest the followings area to be further developed in the future:

1. Handle geometry generation step of HemeLB simulation workflow

   There are some steps which are not included in this project due to time constraints. One of them is the profile generation step. In this step, the domain experts should generate a profile file by pointing out how the simulation will run. They need to point where the blood will flow into the 3D model of the vascular system, where it will flow out, the blood viscosity, and other various parameters that will affect the simulation result. This process will most likely require a graphical user interface for the domain experts to interact with.

2. Viewing simulation result on the browser.

   HemeLB simulation outputs are in a format that is viewable by a third party tool, ParaView. It will be ideal if HemeWeb can be one stop solution for HemeLB simulation that domain experts do not have to bother with all other tools to view the output of it. A ParaView integration can be done in the next step of the development so that simulation result can be directly viewed on the browser so users do not have to bother with an extra tool to configure and install.

3. HemeLB simulation security

   As outlined in the implementation challenge of the project, security was not the main focus of this project. However, if this project is to be an essential part of the future medical decision, security will need to be addressed seriously. After

all, the patient's private health information will be used for the simulation. A system using such highly private information should be better secured.

4. Cloud vendor abstraction on web application

   One challenge of the project was the difference between cloud vendors. Due to the time constraint, the developed web application is tied down to amazon web services only. It would be ideal if HemeWeb could work on any cloud vendors with minimal changes. This is going to be more of a reconciling the difference between cloud vendors and make an abstraction layers that HemeWeb will need to call whenever it needs to interact with the cloud vendors' feature.

   The project did achieve cloud vendor abstraction for the deployment scripts. The infrastructure can be deployed to three different cloud vendors easily. They are google cloud platform, amazon web service, and digital ocean. However, the web application needs more work to achieve the similar feat. Infrastructure can be deployed on these infrastructures, but HemeWeb still cannot work.

Bibliography

Bernabeu, M. O., Lu, Y., Lammer, J., Aiello, L. P., Coveney, P. V., and Sun, J. K. (2015). Characterization of parafoveal hemodynamics associated with diabetic retinopathy with adaptive optics scanning laser ophthalmoscopy and computational fluid dynamics. In *2015 37th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC)*, pages 8070–8073. IEEE.

Franco, C. A., Jones, M. L., Bernabeu, M. O., Geudens, I., Mathivet, T., Rosa, A., Lopes, F. M., Lima, A. P., Ragab, A., Collins, R. T., et al. (2015). Dynamic endothelial cell rearrangements drive developmental vessel regression. *PLoS Biol*, 13(4):e1002125.

Franco, C. A., Jones, M. L., Bernabeu, M. O., Vion, A.-C., Barbacena, P., Fan, J., Mathivet, T., Fonseca, C. G., Ragab, A., Yamaguchi, T. P., et al. (2016). Non-canonical wnt signalling modulates the endothelial shear stress flow sensor in vascular remodelling. *Elife*, 5:e07727.

Green, C. (2014). Computer simulation could become 'integral' in the diagnosis of.

Groen, D., Hetherington, J., Carver, H. B., Nash, R. W., Bernabeu, M. O., and Coveney, P. V. (2013). Analysing and modelling the performance of the hemelb lattice-boltzmann simulation environment. *Journal of Computational Science*, 4(5):412–422.

Itani, M. A., Schiller, U. D., Schmieschek, S., Hetherington, J., Bernabeu, M. O., Chandrashekar, H., Robertson, F., Coveney, P. V., and Groen, D. (2015). An automated multiscale ensemble simulation approach for vascular blood flow. *Journal of Computational Science*, 9:150–155.

Lewis, J. R. (1995). Ibm computer usability satisfaction questionnaires: psychometric evaluation and instructions for use. *International Journal of Human-Computer Interaction*, 7(1):57–78.

Mazzeo, M. D. and Coveney, P. V. (2008). Hemelb: A high performance parallel lattice-boltzmann code for large scale fluid flow in complex geometries. *Computer Physics Communications*, 178(12):894–914.

Steven, S. (2016). Hemeweb: Container based high performance computing scenario in cloud infrastructure for hemelb. Informatics research proposal, University of Edinburgh.