CURTIN UNIVERSITY

RESEARCH, LEADERSHIP AND ENTREPRENEURSHIP IN SCIENCE 2

NPSC3000

Portfolio

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1 Reflections

AHHH just stuff - working w/ supercomputers - files, files, files -> backing up and working with them - working with a codebase -> importance of documentation and open source code - being honest about progress and not understanding this

1.0.1 Finding a comp chem workflow

1.0.2 Pawsey Tour

On Thursday March 30th the Curtin Computational Chemistry group, along with three visiting Italian Masters students, toured the Pawsey Supercomputing facility in Technology Park near the Curtin University Campus. The visiting students were being introduced to the prospect of studying a PhD in Australia and shown what Curtin has to offer. I found it valuable chatting with these students. They seemed open to the idea of completing a PhD in Australia, Perth specifically. They liked our mild weather and location. I think the location of study is important in reinforcing positive learning and feeling towards studying. I haven't properly considered studying or working oversear. I'm definitely not opposed to it, but chatting with the students has made me concious that I need to consider the town and surrounds of a possible place I might move to. I have ideas about countries that I would like to study in, but countries are so vast in culture, climate and people that I now know I have to be specific in my search for a host town or city (if or when I choose to look seriously at oversear study!).

The tour started with a presentation about the history and current specifications of the Pawsey supercomputers and the precinct itself. This was a fairly generic presentation, but interesting nonetheless. I was particularly intrigued by the centers used of an underground aquify to aid in watercooling the supercomputers. This is an ingenious way of reducing grid power requirements for the supercomputers. I can tell that a lot of planning went into developing the Pawsey center. After this we got to peer through the windows to where the supercomputers (and a small quantum computer) were housed. Figure ??? shows a photograph of my view. While the supercomputers are much larger than any other computer I've seen in person, they also appeared quite small. A few students on the tour gave a small snicker upon seeing it for the first time. I suppose we were expecting an super-sized computer! I'm somewhat glad at seeing how compact the system was, given its power output (and power requirements). It is an impressive feat of engineering.

After gazing at the black boxes that make my project possible I chatted with one of the Pawesy technicians. I'd read a recent article for a seperate university unit. The article covered the consequences and worries about computer processor manufacturing in Taiwan with the current tension surrounding China trying to gain ownership of the country. With all of the processors that are necessary for the supercomputer, I asked the technician whether Pawsey has any risk mitigation or plans if issues in Taiwan escalated and crippled the worlds primary computer processor manufacturer. The conversation was short, but the technician said that the processor vendors would be directly effected and Pawesy was well equipped with stores of spare parts for the current supercomputer outfit. They mentioned that while it wasn't a current concern for Pawesy, it would be beneficial to add it to the centers discussions. I was pleased to have potentially add a possibly important point to the centers discussions. I am a stakeholder after all! While I wouldn't consider myself politically literate or focussed, I think this reminds me why knowing what is going on around the world is important, even for just using a supercomputer for a university project.

1.0.3 Learning a codebase

1.0.4 Super Computer vs. Laptop Computer

I had to run a computer simulation for my project, but it was actually several simuations that would be run in a sequence. This was going to be orchestrated using a shell script, but a may have misheard my supervisor at some point because I thought they said I had to run this simulation on my laptop, not the supercomputer. I thought I heard that the shell script was written for the Z shell and not Bash and that the supercomputer did not have Z shell, but my personal computer did. I ran the simulation. It took three days to finish with my laptop fans and processor going full tilt. When I saw my supervisor after this, they said that running it on the supercomputer was fine, so we reran the simulation. It finished that same day. This comparison shows me the computing power difference of a laptop and a supercomputer - a lot! I already knew this, but having an unusable laptop for three days wasn't ideal when I still have things I could be doing on it. I have a new found appreciation of being able to connect remotely to a machine to complete a job or simulation and having the perfomance of my host machine be untouched.

1.0.5 Making Mistakes

1.0.6 Supervisor being away

1.0.7 Mid-year Presentations

1.0.8 My Understanding of Chemistry

1.0.9 Plain Text talk and TeXMacs

1.0.10 Slumps vs. Pumps

I have struggled throughout this year with my motivation in my university work and my project. I sometimes find it difficult to find meaning and passion in the work that I should be doing and it feels like a cloud is covering how I really feel (that I do trully enjoy this work!). These struggles also enxtend to my personal activities. Thankfully, I've been inspired by the great bodybuilder Arnold Shwartzenegger to strive for somethink called "the pump." The pump is the feeling of your body being extremely strong and tight when working out and it feels great. This was what I think about when I'm struggling to be active - that I could get the pump - and it's typically the nudge I need to get back into doing physical activity that I like and makes me feel good. So, recently when I've been struggly with my work, I've considered "the pump" in terms of working my brain. This has helped me transition out of slumps of being unproductive to getting work done. Hard work of any kind doesn't seem attractive at first glance, so it's easy to brush it off, but just starting with something small makes it easier to continue and try and find the elusive pump.

1.0.11 Thinking about Honours

1.0.12 Wrinting Units vs. science

1.0.13 Conducting Peer reviews

1.0.14 Being in a new cohort

Having to redo NPSC3000 this year meant that I was a part of a new cohort of Advanced Science students. Previously, a change like this would have caused me significant anxiety, but I'm

happy to say that this wasn't the case. A was already familar with the Advance Science chemistry major students from this cohort, so this eased any tension I had. While I haven't has any ground-breaking chats with my fellow students, they all seem pleasant to be around and engaged with science throught their projects. I feel as though this experience is important for building my adaptability for working with new people as I will have to join a workplace in the future and meet a new team of people (a cohort in a way).

1.0.15 ChatGPT

1.0.16 Working Remotely

This winter and autumn has been quite strange weather-wise. Cold, miserable days followed by a glimmer of warmth before more rain and cold. I'm happy to have found it possible to work from home for my project on these more miserable days when a commute under a gloomy sky to universitay is very unappealing. Although, it occurs to me that since I'm using the supercomputer to run my simulations remotely, my project technically doesn't need me to be present at university. However, I definitely see the value in seeing my peers and supervisor in person for quick queries, instead of sending emails back and forth. Also, I find the environment at university more conducing to getting work done which helps me with keeping on track. I'm not going to stop going to university to do my work, but it's nice to know that I can still get some things done from home if the weather is particularly miserable (or my mood for that matter). Hello, this is indeed a test to see whether or not using dictation is a viable way of trying to type place and you expend less energy while doing my portfolio task.

1.0.17 Coffee Chemistry

1.0.18 Different Processing Unit Technologies

1.0.19 Futureness of this Research

1.0.20 Sustainability of Chemistry Research

1.0.21 Backing up big data

Running molecular dynamics simulations requires a lot of disk space on a computer. The largest output file is usually ta trajectory file for a simulation. It is a binary file with all of the values for the positions and velocities of particles in a a simulation for every time step. These files for my simulation are typically in the tens of gigabytes in size, so personal storage on my user on the supercomputer is quickly filled. I took it apon myself to ask my supervisor about transferring and backing up lots of data before it would become a problem. It turns out that Pawsey has a system called Banksia for storing data from discs to tape, which is a highly efficient method for storage, but comes at the cost of being slow to retrieve stored data later. Understanding has been important when backing up my data and retrieving parts of it to back up locally on a large solid-state drive that I own, for easy access. I wonder what I will do with this data once I have concluded my project. Will I keep a single copy of my whole project repository on Banksia? If so, how long will Pawsey allow it to stay there? Should I keep a copy for myself? If I keep a copy for myself, I wonder if my supervisor has strategies for archiving and/or compressing large amounts of data. Producing, using, and storing big data is a new concept for me and I'm interested in gaining knowledge in how to deal with it because I feel as though lots of data stored today is redundant, but with how cheap access to storage is, this issue doesn't seem to bother some people. It bothers

me though. I wonder how much power and resources are given to storage mediums that are storing redundant data and the greater impact this could have in the future.

1.0.22 Group Meetings

1.1 Feedback

1.2 Workshop Material

1.3 Meetings

1.4 Topics

1.5 Supervisor Report

2 Software

2.1 Emacs

2.2 GPTA

2.3 DynamicEntropy

3 Network

4 Entreprenuership

5 Peer Reviews

6 Literature