5th October 23

Today is the first day of term, and my first working on my master’s project!

The first aspect of the project I’ve been advised to work on is developing the Tillotson equations of state for a wide variety of minerals that are typical in common rocks. My approach is first to download a database of shock wave experiment data, which will then be imported into Python and presented graphically. As equations of state are too complicated to develop theoretically, they will be formed empirically from a Python-generated line of best fit to the data. I have been warned that the graphs can contain kinks due to high-pressure phase changes. To combat this I plan on forming multiple lines of best fit for the relevant minerals, allowing me to gain a more thorough understanding of how the mineral and its polymorphs behave over a wide range of conditions.

The process of navigating the database has been very simple. The challenge now is to import it into Python. I remember a practical from Simon Matthews course last year when we imported data from a file similar to Excel, so I plan on using a similar method. I cannot remember the exact file type used, so I will revisit the practical to find out.

I have figured out how to import my data into Python by copying it into Excel and splitting it into columns, then using pandas to read the file. I have also refamiliarised myself with using numpy and plt to plot a graph of the data. I have successfully plotted a line to the data and can find the polynomial coefficients of the line, including the Tillotson parameters, A and B.

A red line with blue dots

Description automatically generated

However, the Tillotson equation of state has multiple independent terms in the ‘constant’ term of the polynomial equation. I am unsure of how to extract the remaining Tillotson parameters, a and b, from this term given the current function. I have asked Auriol for advice on this problem, and will hopefully hear back from him shortly so I can continue.

I’ve just spoken to Auriol, he explained that I should substitute the third Hugoniot equation into the equation of state to eliminate the dependence on E. He also mentioned that a is always 0.5, which allows b to be found from the coefficients. He also said that a good sanity check is to use the final Tillotson parameters to give a value for C and S in the linear relationship between particle and shock velocities, and then compare to the values found using linear regression of the available data.

Finally, we discussed the final format of the finished equations, which we agreed would work well as a series of data files containing the experimental data for each mineral, along with the final parameters for the mineral. A program should be produced that can sample specific minerals upon request, producing graphs to display their behaviour, as well as the final parameters.

After taking Auriol’s advice, and a small amount of help from my more Python-literate friend, I have figured out how to use the scipy.optimize function correctly. The program runs as it should, but the calculation is complicated enough that the program times out before the calculation can finish. I can manually input initial guesses and increase the time the calculation can run for, so this should hopefully fix the issue.

Agu table

Johnson 95 table c and s from us up linear relationship

7th October

I added initial guesses and ran the code for 5+hrs but the program still didn’t produce a solution. I ran the program again for a different mineral that had previously defined parameters, but it still couldnt’ find a solution in a reasonable amount of time. As such, I’ve now emailed Auriol to ask for advice on the problem. Hopefully the code can be adapted to solve the problem reasonably simply.

12th October

I had a meeting with Auriol and Oli on Monday afternoon which was very helpful. Auriol and I were able to fix the problem with the code, which ended up being to do with the sign of the b^2 term in the quadratic equation. We also restructured the primary function to make it more legible, which should help me to identify any problems going forward and more easily adjust parameters. The code now runs as it should and is producing reasonable values - yay!

We discussed how to now progress the code to get it into its final form. This week I will;

Implement an automatic filter to remove any anomalies from the datasets;

Develop a second parameterisation code to find A from the linear relationship between shock and particle velocity, which can then be used as a fixed parameter to better constrain E0;

Apply more appropriate bounds to the parameter optimiser;

Get comfortable using isale to run shock simulations by running the planar eulerian example while changing the tillotson parameters of the simulated material;

Understand how to record pressure and temperature data from isale simultaneously.

I’m currently working on the automatic filter - after looking through a few different options I have decided to use a Local Outlier Factor algorithm, as this takes into account the general trend of the data within the space, instead of just restricting the two variables to certain bounds.

So far this method is working well. I am now working on calculating A from the velocity data using the scipy.optimize function that is being used for the main function as well.

13th October

While the values for A using each method are comparable, the one from the velocity data is more similar to the expected values given in Melosh (1989). As such, I’ve decided to use the A value given from this method as a fixed parameter for the second curve fit.

The second curve fit is difficult because it wants to put the parameters unreasonably high, so the values end up automatically being the upper bounds I use to constrain them, which is quite frustrating as it feels like I’m just choosing the parameters instead of them being calculated. As well, the more I constrain the parameters, the higher the error. The upside of this is that all the parameters that I’ve tested so far fit the data very well, so at least the data is consistent with the theory.

E0 is easily the least sensitive parameter, so I’ve decided to fix this value as well, which means b and B don’t need to be constrained as much, so have lower errors.

14th October

I’ve come up with a way of labelling the data files so I can allow the user to input a mineral and analyse all of them using the same code. The only problem with this is that some minerals need specific constraints. I’m therefore trying to add in an extra column for these constraints that can be read and inputted into the curve fit function.

I’ve done this successfully, so the code is now as I’d like it to be. The outstanding problem is that I need to figure out how to constrain the parameters to reduce errors while also giving reasonable values.

I’m running through all the minerals to see if the problem applies more generally and it does. Corundum especially is proving difficult and the algorithm cannot even find a set of parameters to fit the data, never mind ones that also make physical sense. The data itself has minimal amounts of scatter and forms a very obvious line.

The problem with it I think is that the A value calculate is quite high (200) which is forcing the line up, preventing the parameters from keeping the correct shape and putting it in the right location in the space. Bringing A down seems to help, so I will constrain it more in this case.

After inspecting my code for calculating A, I realised that I was using the same rho0 for all minerals instead of having it read from the datafile. This has now been corrected and has fixed the issue with corundum, which now fits very well (RMS= 0.63), but it has not fixed the overall issue.

16th October

Today I spent the morning trying to get the code up to scratch with little success. I think the parameters simply cannot fit in the desired ranges while consistently producing a reasonable fit to the data.

I also tried to experiment with some of the simulation examples on iSALE. I am able to run them very easily, but I’m struggling to figure out how to save the figures produced, as the program is running from the Linux OS installed on my desktop, and I’m trying to save the figures to the Windows desktop.

In the afternoon, I had a meeting with Auriol about the above issues. We’ve managed to fix a problem where the initial guess was being described as infeasible, so this can now have a larger impact on the parameters, which should improve the results of the program. However, when running through some data to check, the best fit still often requires physically odd parameters and can produce strange-looking curves that have a strange horizontal ‘foot’ feature at low densities.

There does not seem to be any obvious solution to this; the experimental data simply does not provide a good fit to the Tillotson Equation of State. It may be that this EOS is simply not appropriate for all minerals, or the methodology behind the data is not suited to this type of analysis. As a result, Auriol and I have agreed that the best way forward is to take the parameters that give the best fit to the data, even if the parameters are slightly odd. Obviously, if two optimal fits exist, I will select the one with the most reasonable parameters.

This approach should be reasonable for the rest of the project, as it is important to run the simulations on iSALE so the synthesised material is as close as possible to the data - but it does place limitations on how versatile the results of the study will end up being. This is quite frustrating as one of the more important results of the project was intended to be a coherent database of mineral data all constructed with a consistent methodology. While this will still be the case, the questionable parameters will make it less useful going forward.

Auriol also suggested ways to help make the initial guesses more accurate - B is usually very similar to A, which I had not fully appreciated before, so A will be put as the initial guess for B, and then the fit will be adapted from here; and the initial guess for E0 should be the vaporisation energy for the given mineral. This itself will have to be calculated for each mineral, where data for it is available.

As such, my plans for this week are as follows:

* unticked

Find and process thermodynamic data for each mineral

* unticked

Use this data to calculate vaporisation energy for each mineral (this will likely be done using Excel for efficiency)

* unticked

Use the results to find best-fit parameters for the minerals

* unticked

Record the parameters in a spreadsheet where they can be retrieved and formatted upon request with a python script

* unticked

Retry running iSALE simulations using the script provided by Auriol

22/10

Oligoclase data does not form a polynomial style curve - vertical line at 2750 kg/m3

Ok, so I’ve spent all day searching for the thermodynamic data online and I’m really struggling. I’m not sure if I’m just not searching for the right thing, but I cannot find the boiling temperature or enthalpy of vaporisation for any of the minerals, apart from one or two. This approach does not seem feasible, which is incredibly frustrating.

I think the way forwards is to more forcibly constrain the data wherever possible to produce reasonable values.

23/10

This morning I went to the downtown site to use the SEM! It was a really exciting experience and will hopefully be really useful to the project. The point of it is to produce a phase map of some shocked samples provided by Auriol (a quartzite and a sandstone), based on relative densities of the grains present, which are obviously primarily quartz, with some feldspars and oxides also present. The scanning process is expected to take 8 hours, so I will go back tomorrow to collect the data from the lab.

After the SEM setup in the lab, I had a chat with Auriol about next steps of the project (once the parameters can be finalised). He talked me through the process of converting the data into tillo files that can be read by iSALE, which was incredibly helpful. I’ve previously had a look at the input files in the eos folder and didn’t understand how to edit them, and I now understand how to use the ‘nano’ function in ubuntu to do this. We also walked through how to construct them using python commands, so this should be reasonably simple to do as part of the param\_finder.py programme I’ve written.

We also discussed making changes to the geometry of the iSALE simulation in order to maximise the amount of data I can record from it. Essentially, the buffer block below the test area should be far down enough so that the maximum peak is achieved in the test area and not interrupted by the boundary between the two. The buffer block should also be the same material as the test area, instead of iron, as is the default, as this will reduce the effect of any reflections at the boundary. For now, the plans seems to be to keep the impactor material as iron, as this is comparable to the composition of certain meteroites. There is definitely scope to change the impactor shape from a plane to a spheroid as well, but this is something that may be confirmed at a later stage.

Expectations for this week are to finalise parameters, produce tillo files, run tillo files in iSALE, and to collect the SEM files.

26/10

Unfortunately when I went to collect the SEM data from the lab on Tuesday there was no one there to ask about where to find the info on the computer. I went again yesterday, and luckily Peter Methley was there, so he talked me through it and copied the data over to the main SEM database for me. This was expected to take a few hours to do, so I went back today to collect the data. Iris was there and I was able to transfer the images onto my USB stick.

This evening I’ve been working on finalising parameters. I’ve found that I can get the function to fit very closely to the data with a very specific shape at low pressures that looks similar to a golf club. However, the parameters are coming out at odd values quite a way out of the expected range of values. A and B parameters seem correct, but b is usually around the value of 50 (should be up to 2.5), and E0 wants to be as low as possible (often as low as 0.01 MJ/g). I don’t know why this is the case, but for now, I’m going to accept these values, as the fit is exceptionally good for all minerals, and the parameters are of a consistent order of magnitude. I will re-inspect the code to check for any errors that may be causing the problem.

29/10

Today I’ve been developing code to put on the end of param\_finder.py to process the parameteres for each mineral and put them into a tillo file that can be read by iSALE. I’ve been able to produce files that replicate those found already in iSALE, but they don’t run correctly, and cause a segmentation error in the program. I don’t really know what this error means, and couldn’t find a relevant sounding explanation online, so I will ask about this in my meeting tomorrow.

30/10

While the new tillo files are providing some difficulty, I thought I’d check to make sure that the normal ones are still functioning properly and that it’s not a separate issue with the version of iSALE installed on the Bullard computer. I can get demo2D to run fine, but planar\_eulerian\_2D won’t run, and gives an error saying ‘permission denied’ which is a concern!

As I wanted to get to grips better with iSALE before my meeting with Auriol and Ollie, I have delayed the meeting until tomorrow afternoon so I can spend this afternoon on the project.

31/10

I have just had my meeting with Auriol and Ollie, which was very helpful. Ollie has suggested that there might be a units issue causing the strange parameter values, so I will look into this when I’m next in the Bullard (hopefully on Thursday morning).

I also mentioned the technical problems I’ve been having getting iSALE to run properly on the Bullard computer, and Auriol has agreed to meet me on Thursday to assist with this.

2/11

Frustratingly, Ollie was correct and there is a units issue with the A parameter. I'm really glad the issue has now been fixed and that I’m generating more reasonable numbers now, but it’s frustrating that such a small error has delayed progress for the last few weeks. At least now I can move on from this section.

Auriol came by as discussed and fixed the problems with the iSALE permissions, as well as talking me through how to create the tillo files in a different way so as to avoid the segmentation error. I have not yet had time to rerun them, as I had to run to the downtown site for a lecture as soon as the meeting finished.

5/11

Today I have rerun all the tillo parameters (for hopefully the final time!), they are all now in tillo files that I can successfully read into iSALE.

I will now spend some time familiarising myself with how to adjust the various input parameters for the geometry of the simulation so that I can minimise the processing time of each simulation while still covering the relevant areas of interest.

6/11

Adjusting the geometry has been a bit challenging, as multiple inputs need to be changed in both the simulation program and the pysaleplot scripts in order to change the outputted visuals as required.

While doing this, I have found that the main plot of interest, the pressure profile, either produces an error message or produces multiple subsequent lines for each timestep. I think the script must be outdated or wrong. I will talk to Auriol about this later in our meeting.

The meeting was very helpful, Auriol talked me through the next steps of the project. One of these will be to adapt the plotting scripts so that they show temperature as well as pressure, and their maximum values. He walked me through how to use tracer particles to track max values so they can be used this way. We also discussed changing the reference frame of the simulation to make it on the correct scale for studying samples, and how the impacter thickness can be reduced to localise the shock wave peak into this smaller region. Hopefully, this will be relatively simple and just require some trial and error. I will also need to increase the impactor speed so that the peak reaches 60GPa, which may need to be offset against the impactor thickness.

I also need to figure out how to make a bitmap that can be used as a simulated material until I meet with Iris to stitch my SEM tiles together.

I also need to find relevant thermodynamic data (heat capacities) to input into my tillo files, as I am currently just using the one for albite in all of them.

A black and white background with grey circles

Description automatically generated

9/11

This morning I have been adjusting the input parameters (impacter thickness, impacter velocity, and simulation scale), as was previously discussed. I think I am getting close to values that I am happy with! The simulation encapsulates a sample height of about 1.2cm, which includes the sharpening of the wavefront, and a drop off to 10-20GPa at the sample base, and the sequence can run for a sufficient time to show the interactions of multiple reflections of the wave with the primary wavefront.

While waiting for some simulations to run, I also produced a bitmap showing a pretend cartoon rock, which will allow me to practice running a shockwave through a real sample while I wait for a response from Iris about stitching my SEM tiles together.

10/11

This morning I finished collecting and processing all of the necessary thermodynamic data. I have found melting points for all but one of the minerals (topaz let me down). From here, I have extrapolated the ratio between melting and boiling points found for Albite, to calculate estimates for the boiling points of the other minerals. I have done a similar calculation to find the heat capacities of the various melts. I realise this will give very rough values, but I believe it is safe to assume that, on average, minerals should all behave in a similar way.

My final calculated values for Eiv are available in both J/kmol and J/kg, as I am not sure which is used in iSALE. I will need to check the iSALE manual to see if this is stated anywhere, if not, I will ask Auriol before Monday.

12/11

Checked the iSALE manual, and the unit used is J/kg. I have inputted all of the values into their respective tillo files

I plan on spending the rest of this afternoon adjusting the plotting scripts in order to prepare them for future simulations and to produce figures that could be used in my project report.

This took a little while, as configuring the position and size of each graph, as well as adjusting labels and colour schemes used, but now they are ready to go for future use:

A diagram of a pressure

Description automatically generated with medium confidence

A diagram of different colored lines

Description automatically generated with medium confidence

A diagram of a graph

Description automatically generated with medium confidence

13/11

This afternoon I had a meeting with Auriol to discuss this week’s progress and the next steps.

We had a great idea to use the enthalpy of formation as an approximation for enthalpy of complete vaporisation, as the two values ultimately represent next to identical atomic processes. I will be checking for these values online and comparing them to those given already in iSALE tillo files to confirm that the two values are on the same order of magnitude as each other, and that this method is a justified one.

If this ends up not working, I suggested that the scaling factor between the calculated Eiv and the iSALE value of Ecv should be applied to all the minerals not already with

Auriol clarified the geometry needed for the simulation, which I seem to have misunderstood last week. The isobaric region should be 1cm in height, and the overall height of the simulation and material should be 4cm. This is because I need the simulated sample region to be the same size as the thin section sample, so that the simulation models an isobaric region across the entirety of the sample, allowing for controlled interpretations of the conditions reached across the sample.

Auriol also walked me through how to input the sample file into iSALE, which can be done using a specific script he wrote, that I will need to adapt to my needs. The script will allow me to specify the different minerals present in the rock according to what shade of grey they are represented by in the bitmap.

When using a natural sample imaged by the SEM, each shade of grey will have an approximately normal distribution around it due to natural variation of densities across the different crystals of that mineral. To remove this effect, I will use a software called ImageJ to threshold the different shades and separate them into a set number of discrete shades.

16/11

Had a busy week so far (had an interview on Wednesday!!) So haven’t been in the Bullard since my meeting on Monday, but hoping to have a productive weekend. I’m downtown today, but have a few spare hours, so I’m going to start researching enthalpy of formation data, which I can do on my laptop.

Having had a look and comparing the values available with those in the iSALE files, the two seem reasonably close. For example, the iSALE Ecv value given for Albite is 18.2D+6 J/kg, and the researched value is 15.0D+6 J/kg, making the two very comparable, as they are only 17.6% different. As a result, I have concluded that the two values can reasonably substituted for one another in this context, as this value only provides a trigger point for vaporisation, which is not the primary phenomena being studied here, and should not have too massive of an effect on the rest of the simulation.

I will now spend the rest of my available time gathering data to input into the Bullard computer when I return tomorrow.

17/11

I have returned to the Bullard and have put in all of the data I collected yesterday (as far as Hematite). I will now spend some time collecting the data for the rest of the minerals.

After spending an hour or two on this, I have collected all of the data and inputted it into the tillo files. I was able to find the enthalpy of formation for all of the minerals apart from Augite, Enstatite and Nepheline, for which I used the average values for the enthalpy of formation in kJ/mol, and then translated these into values in J/kg. I chose to use the mean in kJ/mol, as these values have a smaller standard deviation than those in J/kg, and would more effectively allow the individual mineral to be expressed, as it incorporates its Mr value.

With the rest of the day, I want to readjust the geometry to that discussed in Monday’s meeting, then attempt to run the mock sample I produced on canva last week. The procedure for doing both of these things looks reasonably simple, so I’m hoping this should go smoothly and be finished by the end of the day. One of the key things I need to do during this process is check if the listed materials in the input file are supposed to be in order or lightest to darkest or vice versa.

Success! I was able to increase the depth of the simulation while maintaining the peak pressure, and then convert the bmp to a readable file and run it through iSALE. Turns out the order is darkest to lightest, which I have made a note of for future samples.

A diagram of different colored lines

Description automatically generated with medium confidence

A diagram of different colored lines

Description automatically generated with medium confidence

A diagram of different colored lines

Description automatically generated with medium confidence

A graph of different colors

Description automatically generated with medium confidence

Obviously, there’s a problem with the line graphs for all of these simulations, which I’m not sure how to fix. I had a quick mess around with the script for this and couldn’t quite figure out how to isolate a single or average value to use at each depth in order to be left with a single signal, instead of multiple stacked together. I’m not quite familiar enough with how to manipulate this type of dataset unfortunately, and I couldn’t seem to quite word a google search well enough for it to give me a helpful answer. As such, I will leave this for now and discuss the problem with Auriol on Monday.

Unfortunately, I have a presentation to prepare for next week, so I’m going to take tomorrow off from project work, and resume on Sunday.

19/11

Today I want to get my head round using ImageJ to form discrete shades of grey in order to assign densities in iSALE. Auriol walked me through the general procedure for this in our meeting, so hopefully it won’t be too difficult. I can’t remember exactly which function to use, but hopefully it will be labelled fairly obviously.

Well…

The web browser version of ImageJ is borderline unusable, so I installed FIJI instead! While this was a definite improvement, it’s still pretty horrible to use, and the commands are pretty non-intuitive. After looking through a few different tools for image adjustment, I found the thresholding one, which looks as I remember from the meeting. Using it is quite tricky, and it essentially removes all other shades and puts them into either black or white, depending on which you select for the shades you’re trying to highlight. This is not what I want to do, as it removes large amounts of data, and does not allow the specification of the shade of grey I want for the highlighted shades. After a lot of trial and error, googling and considering other software options (and tears, life is rough right now), I managed to figure out a system:

Import the image

Transfer the image to being a colour image (colour thresholding is a much more helpful tool than normal thresholding)

Colour threshold the brightest shades into white

Duplicate the image, so as to not overwrite this iteration of thresholding when more thresholding is done

Threshold the darkest shades into black

Duplicate

Threshold a grey shade into red

Transfer the image into B&W

Transfer the image back into colour (which maintains the newly established greyscale pallete)

Duplicate

Threshold the remaining greys into red

Adjust the brightness and contrast of the image so that the red-grey shade is now no longer the same shade of grey as the one about to be created upon greyscaling of the current red mineral

Transfer to B&W

Badabing, badaboom

After having finally completed this, I attempted to run it through iSALE, but I got the following error:

A screen shot of a computer

Description automatically generated

I looked in the iSALE manual, and now understand what the error means, but I don’t know where such a value is kept, and therefore how to adjust it to remove the error. I have to write an essay tonight (including reading) for a supo tomorrow, and I haven’t started yet, so I’m going to leave this for now, and pick up just before the meeting tomorrow.

20/11

The essay kept me up until 4am, so I feel like I’m going to die, but we move. I’ve been at the Bullard for the last few hours, but I’m not getting much done at all, as I’m finding it really hard to concentrate.

Had the meeting with Auriol. He fixed the error shown above - apparently you can just input an unstated parameter into asteroid.inp, which is handy to know!

He also helped me to rectify the line graph, so now an average value is being taken for all depths at a given time.

With the issues from last week sorted, we discussedthe aims for this week, which is the final full week before the end of term. The aim is to choose and run 5 separate simulation for each sample, with pressures ranging from 10 to 50GPa in increments of 10GPa. For each simulation, I need to produce the previously setup plots displaying the spatial changes in P and T, as well as a new one showing these changes with another displaying the mineralogy at different points in the sample. For each of the simulations, I should also produce histograms showing the responses of each mineral to the shockwave, which is the ultimate aim of the project, as this will allow me to interpret the behaviours of each mineral more easily.

Another aim for myself in the near future is to get caught up with reading the literature. I spent a decent amount of time before the start of the year studying the key pieces suggested by Auriol, but have had little time to continue this through term time. As such, I would like to do this more during the Christmas break in a few weeks.

27/11

Today I’ve had a slow start but want to spend a few hours doing the following:

1. Determining the impact velocities needed to achieve isobaric regions at 10GPa, 20GPa, 30GPa and 40GPa (50GPa is already determined at 4.5D+3)
2. Running the simulations for each of these pressures through sample SS l3\_c0\_crop
3. Finish processing the images for the other samples using FIJI
4. Create appropriate folders for all of these samples and simulations, ready to be run

Have determined necessary velocities: make a note of them here!!

Simulations all run

Found that when producing the histograms, the s.mat numbers are in reverse order to the list in additional.inp - 1 = void, 2 = quartz, 3 = clay, 4 = magnetite

I have succesfully set up and run simulations for l3\_c0 and run the primary plotting scripts for them, including TrPMat, the main visualisation showing the sample structure, and histograms showing the peak pressure achieved by each tracer in the sample, categorised by mineral. There is a particularly interesting feature in the clay and magnetite 50GPa histograms that show three distinct regions of peak pressure, with no frequency in between: low pressure, high pressure, and the initial pressure of the system. I will discuss this observation in the meeting with Auriol this afternoon.

Add an example histogram here!

The meeting with Auriol was very helpful. We discussed the pattern in the histograms mentioned above and he suggested that there’s the possibility it has arisen due to a sampling bias caused by the radial geometry of the simulation. To combat this effect, I intend on adding a weights term into the histogram function dependent on the tracer volume varibale given in the jdata file. Auriol also suggested it could be helpful to add a linear measure of the pressure variation on top of the histogram, called a Gaussian kernel density estimate, which I hadn’t heard of before. As I will be copying this first sample directory to be used for other samples, I would like to perfect it first, so I will start by adjusting the histogram script.

After this, I intend to copy the directory, select sample images to be used in subsequent trials, and image process them to be used.

After I have finished running simulations on real samples, I want to expand the study to consider generated sample images of more varied rocks, as I’m currently only considering quartz-dominated sedimentary lithologies, which limits the application potential of the study’s results. I would like to incorporate all of the major lithologies like basalt, granite (G5a fo course), andesites, as well as some common metamorphic rocks like greenschists. To do this, Auriol has sent me a script for generating bmps of such samples.

We also discussed adapting the current simulations of the samples to mimic the experimental setup they were produced in, including having the same material and size impactor (as seen in Kurosawa 2022), as an extensions to the study. This would allow me to directly compare the predicted outcome to the sample (any phase changes and textures), to what is directly observed under a microscope, as we are hoping to have thin section samples ready for me to examine by next term.

Finally, we discussed ideas for the poster and what layouts generally work best. We both agree that a landscape poster is more engaging. Obviously at this point, the poster needs to be ready in 6/7 weeks, but once the figures have been prepared, putting them together will not take too long, so this is where my focus will be for now.

My mental health has been pretty poor for the last two weeks, so I’m going to take some time off from work now, as it is basically the end of term. I have a job interview on Thursday, and after this I will be focusing on recovering, including at least a week’s rest once I go home on the 9th.

6th December

I had a meeting with Ollie this morning to update him on progress from my project, as we haven’t seen each other since week 5. He seemed happy with the progress made since then and the next steps I’ll be taking over the holiday. He emphasised the importance of getting as much of the project written as possible (mainly the method and the motivation section of the introduction and abstract), as well as the motivational paragraph for the top of the poster. He encouraged finding inspiration for this from literature when needed.

In terms of the actual research, he suggested it could be interesting to add a fabric to some of the simulated samples I plan on producing to assess the effect of anisotropy in the sample. I agree that this would be an interesting investigation as it would allow for better determination of the effect that heterogeneous grain boundaries has. Unfortunately it is not possible to incorporate this into the real samples, as the bedding textures in the sandstone is on too large of a scale to be at all noticeable on the scale used in the simulations, although they are visible in hand specimen. It would be good to create bedded sandstones, foliated metamorphic rocks, and flow-banded igneous rocks, in order to maximise the scope of the study.

Therefore, going forward my to-do list is:

1. Finish image-processing selected sample files
2. Copy the bmps across to the appropriate directories and run the established simulation and plotting scripts
3. Produce non-fabriced simulated lithologies, image process them, run them through simulations and plotting scripts
4. Produce fabriced simulated lithologies, image process them, run them through simulations and plotting scripts
5. Combine datasets for a given pressure across all sample types to produce more rigorous histograms with larger sample sizes, for each given mineral
6. Produce a poster template showcasing all major steps in the research process
7. Choose the most appropriate figures to display
8. Complete the poster

19th December

I’ve been working on image processing the selected samples, but forgot that the final versions are only supposed to be 100x100 pixels, meaning for the more zoomed in ones, barely any of the sample would be included. To fix this problem, I would have to reduce the image quality of the images and re-process the colouring, which would change the granular structure and make the simulation less accurate to the actual sample. As such, I will instead stick to the more zoomed out scans, cropping them to a higher magnification scale when appropriate.

I will now go through and select more sample images to run, I think 3 per lithology is appropriate, two l3, and one l4.

8/1

It’s my first day back in the Bullard after Christmas, adn I’m excited to get cracking with the to-do list above!

Today, I want to finish points 1 and 2, but unfortunately, there’s an IT problem with the whole building and I can’t access my desktop, not even remotely. As a result, I can’t get going with point 2 yet, but I can finish image processing and develop a poster template. I started a template over the holiday, butI’m not very happy with it. There are a few scientific posters in the room, so I’m going to have a look at them for layout inspiration.

Lunch update:

I’ve made good progress with the poster and have a solid layout that I’m happy with. So far, the plan is to have the following headings:

1. Determining mineral behaviour
2. SEM images of shocked samples
3. Shockwave simulations
4. Anisotropy and shockwaves
5. Comparison to shocked samples/further work (depending on progress)

I’ve also added a QR code so that people can watch animation videos of the impact simulations, which I thought could add an extra element of interest (it looks v cool).

I’ve been able to add some figures in, and I have a plan for what I want each section to look like, but I currently can’t access all of my figures, so I’ve hit a wall with it for today.

Evening update:

They got the computers back online! I was able to finish image processing while I ran simulations in the background, and have just set the final ten simulations running before I leave for the day. I’ve managed to run several of the plotting scripts for the simulations I did earlier today, so I have a few figures ready to go.

9/1

I’ve now run into the problem of running out of space on the department system, and can no longer copy over the simulation directories needed to produce more simulations. I’ve emailed Neil about this and I think he’s addressing it. Hopefully this will be sorted by tomorrow morning and it won’t hold me up too much! Unfortunately, I can’t seem to move any files onto my USB stick, as there is a permission error, so I can’t solve the problem myself.

I’ve taken the opportunity to backup my directories on google, and to familiarise myself with Latex, which I would like to use for writing my report. I’ve also revised the introduction on my poster, which I will use as a base for my report introduction as well.

My main focus today has been generating images of fictitious samples to further the study. Auriol gave me a script for this, so I’ve been adapting this for my purposes with the use of chatgpt to help me to understand the commands involved. I’ve managed to adjust the proportions of each region produced, and the elongation of the regions, in order to make foliated metamorphic rocks, as well as igneous. I would like to simulate the following lithologies:

* unticked

Granite (G5a)

* unticked

Basalt

* unticked

Lewisian gneiss

Obviously, I will run 3 samples of each lithology with varying modal mineralogy, in order to balance any sampling bias, such as that observed so far in the peak pressures experienced in clay in sample SS\_l3\_c0.

I have decided that to save time I will no longer write this journal in prose! You will now function as a glorified to-do list.

10/1

Need to redo elongated samples for fabric - those produced yesterday as tests look unrealistic and too fine, which could reduce simulation accuracy

This took a while to figure out, as the code is not the most clear

11/1

Having a rough time personally this week - don’t feel like goin to the bullard, especially when i don’t have a functioning working directory at the moment. Will read a paper instead - Wittmann et al, 2021

12/1

Have spoken to Neil about fixing the directory problem. He will look into fixing it next week. Will focus on course content revision until then.

15/1

Had a meeting with Auriol to go over poster planning. It was very helpful and I felt more confident about structuring it. This will be the focus this week. Have also spoken about organising training for the optical microscope in 007. Will need training from Norbert and a safety session from Oli.

Neil fixed directory problem with an extra hard drive, so I now have an extra working directory. Unfortunately i cannot access it directly, which I’m expecting to slow my progress.

19/1

Taken a few days out for personal reasons. I’m not expecting to be as productive as I’d like for the near future.

Had the safety session with Oli this morning, everything made sense, looking forward to microscope training at some point soon.

20/1

Run more plots today, will write poster sections tomorrow

21/1

Writing poster info at the mo, will move to making histograms/kdes this afternoon

22/1

Have arranged to see Norbert for microscope training on thursday

Poster is taking shape well, but still need to put together a spiel. Spent the day polishing off figures i’m using

23/1

Generated an animation to go on the poster as a qr code

Key things to include in spiel:

Numerical simulations on cylindrically symmetrical grid

Solves for conservation of momentum, mass and energy

Emphasise importance of tillo results

Just sorting some final formatting and adding acknowledgments

26/1

poster session went well but had a severe confusional migraine immediately after

Took thursday off and have rescheduled training to next week

Still feel very tired

29/1

Spent the weekend reading and catching up on missed lectures from thursday

Want to continue with generating bmp files for samples today.

Training with norbert went well! The microscope is very similar to a normal one, but isjust a bit biger and has better magnification options and higher resolution. It also connects to the computer so I can take scans of a whole thin section. This will be very useful. In the process of booking time in the SEM with Iris, so will need to finish here before then due to carbon coating

1/2

Struggling organise my work into a reasonable structure for the report, going to start seriously thinking about that this week.

What conclusions am i drawing from the experimental samples? Surely just compositional

For testing grain size - how do i exclude other effects? Thought about cropping it in a certain way to maintain the impact site structure.

2/2

I think cropping like this is the best way forward. Will test how this needs to be done as the samples seem to rotate when imported into the simulation setup.

Now figured this out!

This seems like a good test to use a granite for, as there are multiple minerals i can include from my database.

5/2

Sem will be on 19th

Spent today running grain size simulations, making plots at the moment but will not finish them today

Met with Auriol and put a firm plan in place for report organisation. Extra sims will be run of homogeneous samples and simple heterogeneous ones in order to build up the examiner’s understanding of the simulations. Voronoi samples will then go before the natural ones, which will go before the kurosawa ones. This structure will be kept for methods, results and discussion for clarity. One set of samples will be reunr for 10,20,30,40,50GPa to see if certain parameters have greater significance at higher/lower pressures, all others will just be 30GPa.

6/2

Starting to think about how to best represent statistical variation in distributions across samples.

Finished plots for grain size, next is fabric!

8/2

Finished sorting the sample images for fabrics

I’m limited in metamorphic lithologies due to the lack of micas - thinking a lewisian gneiss? I have enstatite and garnet so this should be doable

Have setup the directories for this and will leave sims running overnight to come back to at the weekend. Read North et al 2023 today, thought their approach was very good and might struggle to criticise it at all in my literature review

10/2

Working on the microscope today to look at shocked samples. Light is giving me a headache, but it’s going well. The obvious two are 592 for sandstones and either 584 or 586 for quartzites. Quartzite samples aren’t great generally, the impact site is quite off-centre

11/2

Chosen 592 and 584

Been taking pics of them literally all day

The scanning function is really fiddly and can fail for no reason. Has taken many attempts to get a full one of both

12/2

Meeting with auriol - realised that the kde plots include qz from the sample and buffer/runoff sections. Need to figure out how to fix this. He mentioned masking is a function, so will try that this evening! Also realised i should have been using circular polarisers for my scans, so will need to redo them. Very annoying as i’ve already sunk a full weekend into them.

Couldn’t figure it out, was here til 10pm trying 🙁

It seems to result in the two arrays (s.mat and TrP) being different sizes but not sure why

14/2

Redone the scans. Took literally all day. Have dropped off the samples for carbon coating.

16/2

Had a look at the arrays by saving them to excel files - TrP is a column instead of a 2d representation of the setup geometry. This seems like a stupid way to format the data but oh well. Will ask Auriol about this.

17/2

Apparently there’s a tracer filer for materials, s.TrM

Haven’t been recording this because i din’t know it existed, so will need to rerun all my simulations again. yay

I will update once this is done

19/2 got my sem done

22/2

Finished redoing sims  - now have homogeneous, simple heterogeneous, grain size, fabric, composition (porosity vs qz vs plag in nat samples), and need to do the kurosawa sims. Will make tillo params for polycarb and titanium for this

Have started putting figs into a latex file to structure the results section

23/2 i did a stupid

So in rerunning my sims i seem to have accidentally rearranged the order of materials in some of the input files 🙁

I need to rerun half of them again

Having a tough week generally, this is not helping

26/2 had a full weekend fixing this

Sorted now

This has also fixed the kurosawa simulations which was behaving ridiculously before an basically causing the stup to explode - but sorted now and looking very sensible, with the kurosawa setup hemisphere of pressures, so very happy with this

28/2

Now need to use the new sims to sort the hist problem from last week - masking is still being weird, but using np.where as before, but for s.ymark is working much better! Will use this to only consider sections in the isobaric region.

1/3

Finished sorting the hists

Now want to determine how i’m representing statistical variation

Standard deviation seems obvious, but there are a lot really high values that are far from the mean peak pressure - maybe only considering the interquartile range of values would help this?

Going to start writing a python script to extract the data needed from the output files

2/3

These scripts have actually been really easy to sort out! Huge contrast to my ability at the start of the year lol

Still taken a while just because of the amount of info needed to assess data across all 5 pressures run.

4/3

Have been working on these plots

Have decided to run: std dev, norm std dev, iqr std dev, norm iqr std dev, ratio of stde dev/ iqr std dev (no clue if this will have any meaningful pattern, but could say something about peak broadness), mean with std dev error bars, and norm mean with norm std dev error bars. Norm - normalised to impact pressure (10, 20, 30, 40, 50)

6/3

Plots are all sorted for these!! There’s actually a lot of interesting trends that i’ll be able to talk about in the discussion, so i’m excited for that!

Need to redo hists so kde extends to 0 and up to flat for all minerals in a sample will do this today and tomorrow hopefully (what even are lectures?)

7/3 it’s crunch time, we be writing! will no longer need this journal for research! Can’t wait to be done with this now, it’s all i’ve been doing at this point and i’m really drained by it. In retrospect, i wish i’d have gotten to grips with python and isale last term, as it would have made everything much easier this term.