Thesis Plan

** Denotes sections that have already been drafted.

Work on the Thesis Format

I Need to decide on the visual layout of the thesis and the font that I want to use. I also need to actually get the Latex (I've decided to write it in Latex) document structure in place to write the thesis.

Timeline:

- ***27th December 2015 - 2nd January 2016***

Chapter 1 - Introduction

Subheading - Introduction to crystallography

This section will contain a general introduction to crystallography.

- Why we do it
- What is involved
- Limitations and alternatives - XFELS, Cryo-EM. Include radiation damage so it flows nicely into the next section.

Subheading - Radiation Damage

- Explain global and specific damage
- Mitigation of Radiation Damage
  - **Pre experiment**
    - Improving data collection strategies with RADDOSE-3D (DWD) along with a discussion about the history of RADDOSE.
  - **During experiment**
    - Cryo-cooling
    - Scavengers
  - **Post experiment**
    - Zero Dose Extrapolation/Damage modelling
- Section on Radiation damage in SAXS experiments (SAXS automation improving, scavengers).

Subheading - Summary of section

Brief summary of the chapter (X-ray crystallography and radiation damage)

Subheading - Thesis Layout

Explain how the thesis is laid out.

Timeline:

- ***18th January 2016- 31st January 2016***: Write the bulk of the section
- ***1st June 2016 - 15th June 2016***: All main research chapters need to be finished so I can come back to this section and write the final piece on the Thesis layout

Chapter 2 - Dose Metric Analysis

Subheading - The Hamburg Experiment

- Aim of the experiment (uniform irradiation) **
- Crystallisation protocol **
- Data collection **
- Data processing - RADDOSE-3D/Sliding window **

Subheading - Analysis of DWD metric.

- Dose Decay Models for η **
- Sensitivity of η to data processing **
- Comparison of DWD performance with and without η **

Subheading - Chapter Summary

Summarise the main points of the chapter.

Timeline:

- ***1st March 2016 - 14th March 2016***: Write the section for the thesis

Chapter 3 - Radiation Damage Correction in MX

Subheading - Structure Factor Correlations

- Give overview of the algorithm
- Results
- Conclusions about structure factor correlations

Subheading - Regression based RD correction model

- Explain the algorithm **
- Results
- Limitations of the correction model. **

Subheading - Machine Learning based RD correction model

- Explain the algorithm **
- Results
- Limitations of the correction model.

Subheading - Chapter Summary

Summarise the main points of the chapter.

Timeline:

- ***Now - 30th November 2015***: Work on machine learning algorithm code
- ***19th May 2016 - 30th May 2016***: Write the section for the thesis

Chapter 4 - RADDOSE-3D

Subheading - Error analysis in RADDOSE-3D

- Explain the expected effect that various factors have on the dose values **
- Results **

Subheading - Extensions to SAXS experiments

- Model of the experiment implemented
- Scavenger work - Rebecca's results

- Feedback from users of the SAXS software (Adam Round, Rob Rambo, Sean McSweeney)

Subheading - Beam deconvolution/image processing

- Diamond beam profile measurements (summer project) **
- Image analysis for background subtraction **

Subheading - RADDOSE-3D GUI

- Design of the GUI
- Strategy comparisons
- Strategy optimisation

Subheading - Chapter Summary

Summarise the main points of the chapter.

Timeline:

- ***1st December 2015 - 7th December 2015***: Write RADDOSE-3D tests for SAXS code.
- ***1st February 2016 - 14th February 2016***: Finish work on Beam image analysis
- ***15th February 2016 - 15th March 2016***: Write optimisation algorithm for Data collection strategy
- ***16th March 2016 - 31th March 2016***: Write section for thesis

Chapter 5 - Gas Analysis

Subheading - Background

Mini literature review of the state of knowledge about the gas produced in MX experiments

Subheading - Experiment

- Dialysis tubing protocol
- Beamline modifications for the experiment

Subheading - Chapter Summary

Summarise the main points of the chapter.

Timeline:

- ***1st April 2016 - 30th April 2016***: Attempt another experiment to capture gas and get analysis done.
- ***1st May 2016 - 19th May 2016***: Write up section in thesis.

Chapter 6 - Conclusion

- Summary of the major results of the thesis.
- Limitations
  - Data correction models
  - RADDOSE-3D - fluorescence escape, photoelectron escape.
- Future work to be carried out as a result of the thesis.

Timeline:

- ***16th June 2016 - 30th June 2016***: Write up section in thesis.