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Interactive Visualization for the Design, Prototyping and Development of Research Software






EPSRC RSE Fellow

In Research Computing and Imaging

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What is an RSE?

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Stands for:

Research Software Engineer

New page on Wikipedia

- https://en.wikipedia.org/wiki/Research_software_engineering
- Research software engineering is the use of software engineering practices in research applications. The term started to be used in United Kingdom in 2012[1][2], when it was needed to define the type of software development needed in research. This focuses on reproducibility, reusability, and accuracy of data analysis and applications created for research.

Talk Contents

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- Set up the case study
- Software development models
- The visualization pipeline/model
- A model for the evolution of research software
- Python features that affect interactivity in research software
- The architecture of the visualization pipeline
- Details of the case study
- Importance of interactive visualization in research software development
- Information on RSEs

The Case Study

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- Software not complete – a working case study
- Michelle Peckham and Alistair Curd are biologists at the University of Leeds who develop and use novel imaging techniques.
  - For example, Direct Stochastical Optical Reconstruction Microscopy (dSTORM) is an emerging high-precision technique, for which new data analysis methods are needed, especially for 3D data and they are developing pattern analysis for this type of data.
- Have inherited and developed Python 2 scripts that form a 'messy' software stack. Their script is called **perpl**.
- These scripts need to be turned into an easy-to-use tool for researchers in their lab and for publication.

Traditional Software Engineering

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- Large scale activity
- Generally top down, heavy on administrative roles such as requirements capture and testing that responds to the legal needs of the client's contract
- Fits the legal requirements and framework of the industry that uses the software application
- Uses methodologies and procedures for example the water fall model

The Waterfall Model

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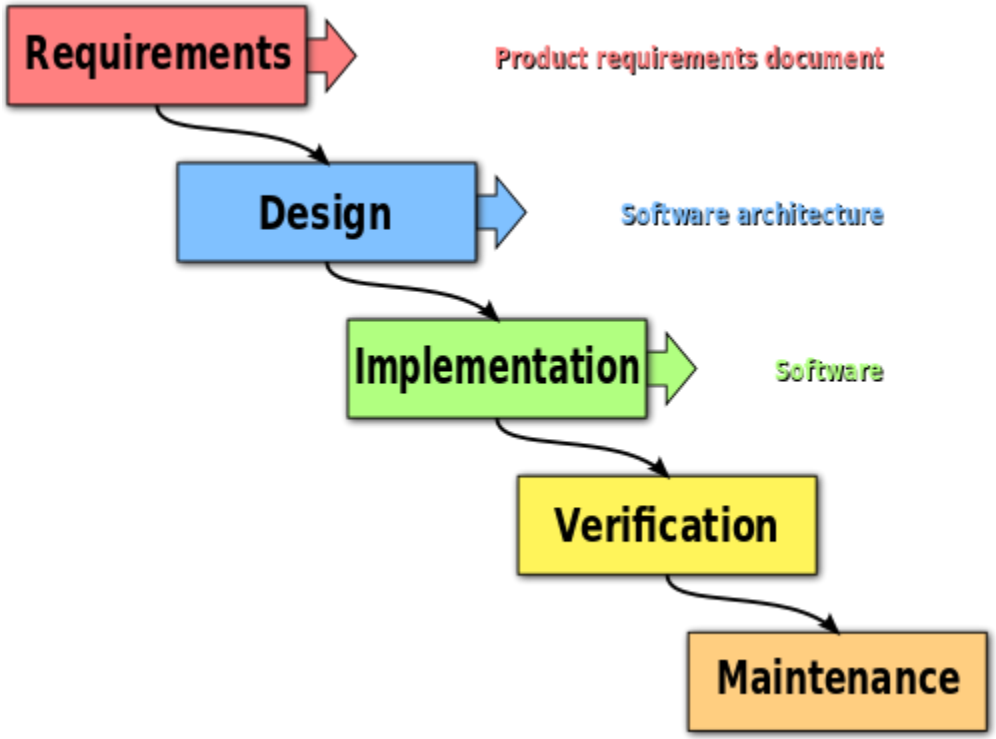

Diagram copied from http://en.wikipedia.org/wiki/Waterfall_model

Modern Software Engineering – eg Rapid Application Development

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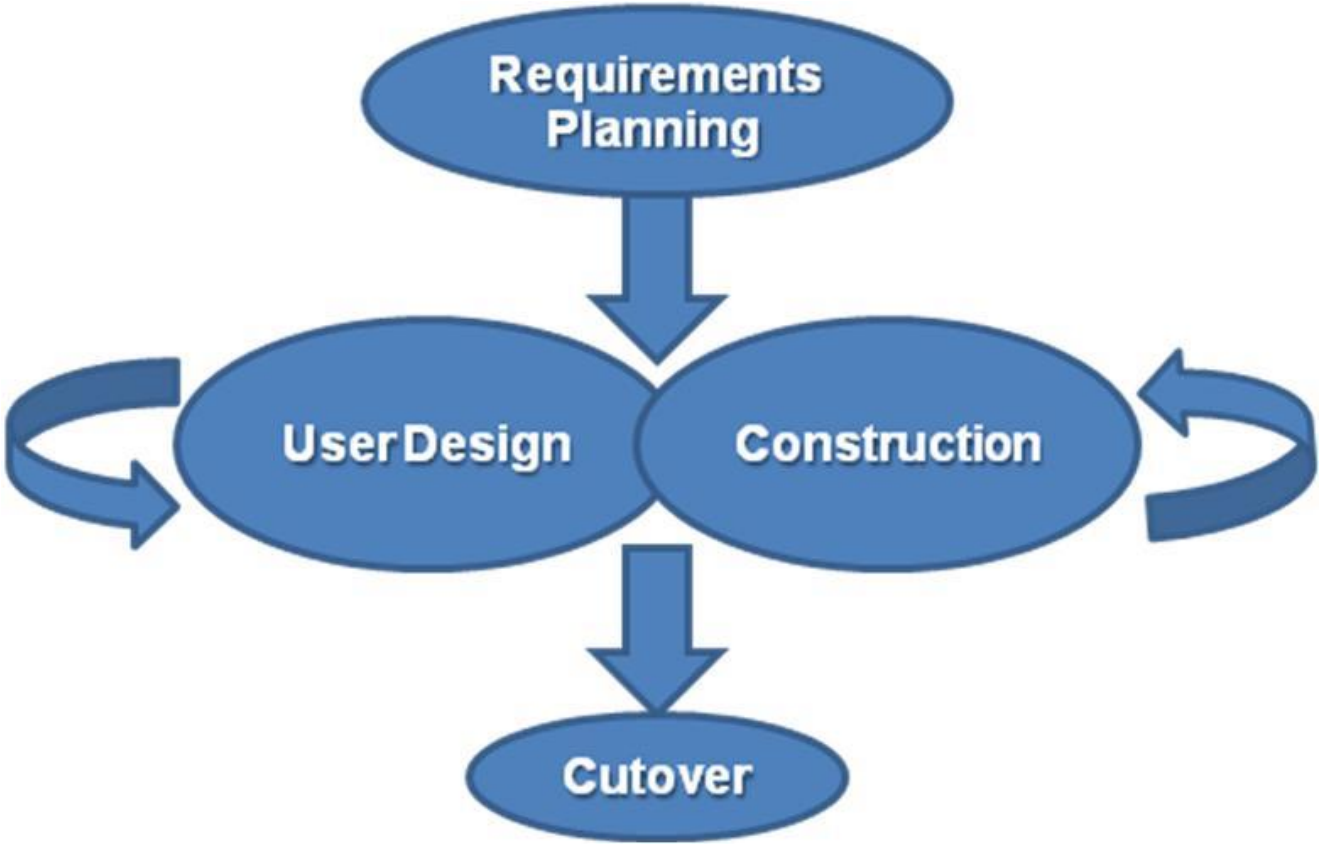

Diagram taken from http://en.wikipedia.org/wiki/Software_development_process

Rapid Methods Need Craftsmanship

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- Practice makes perfect
- Skills are application area specific
- Skills are programming language specific
- Methods and processes are adaptive so they can respond to client and the market
- Communication between programmers and clients are important so less administration is needed

Academia – Scientific Visualization

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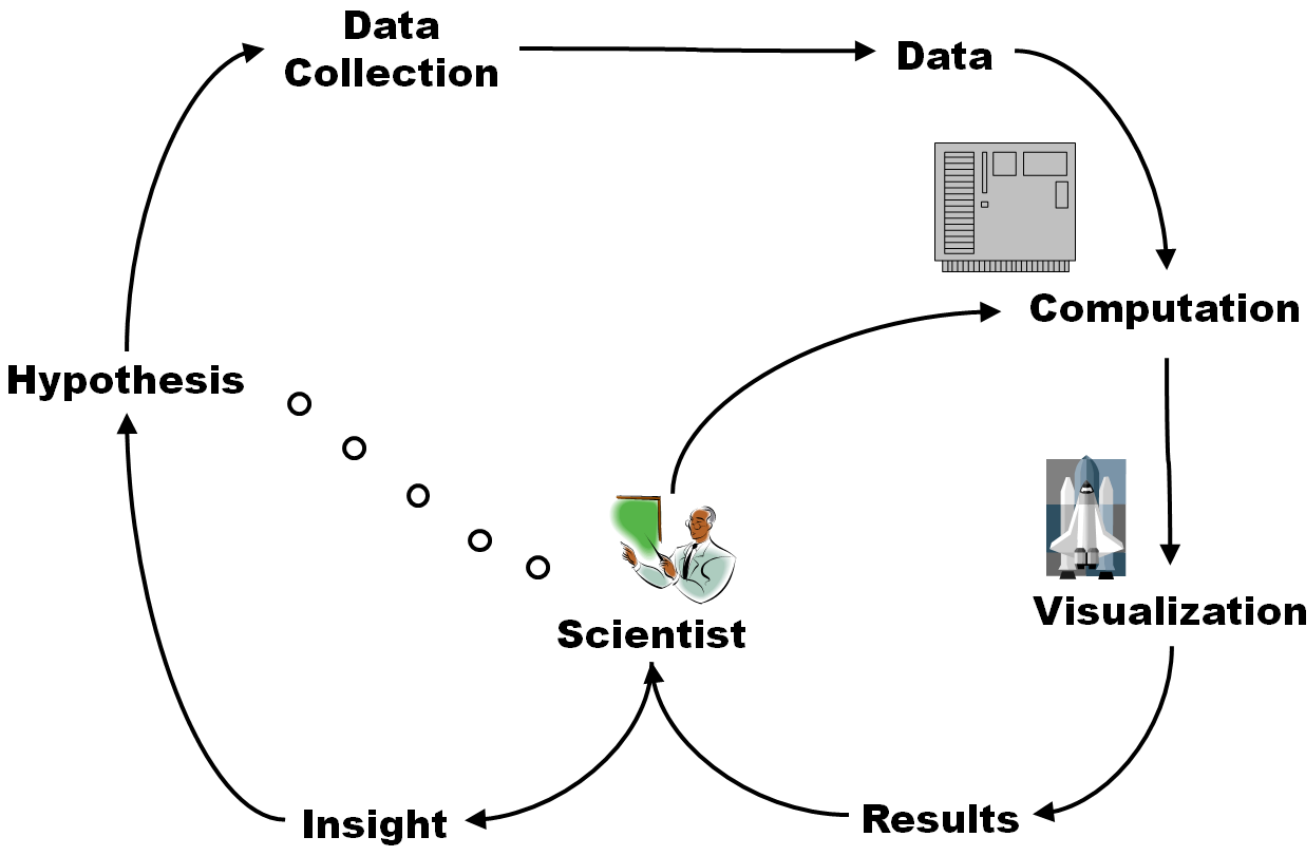

Watson's model of scientific investigation was used by the visualization community to design software frameworks. It can be adapted to cover data science. Diagram from "Collaborative Practices In Computer Aided Research" by Leng and Sharrock

Academia – Scientific Visualization

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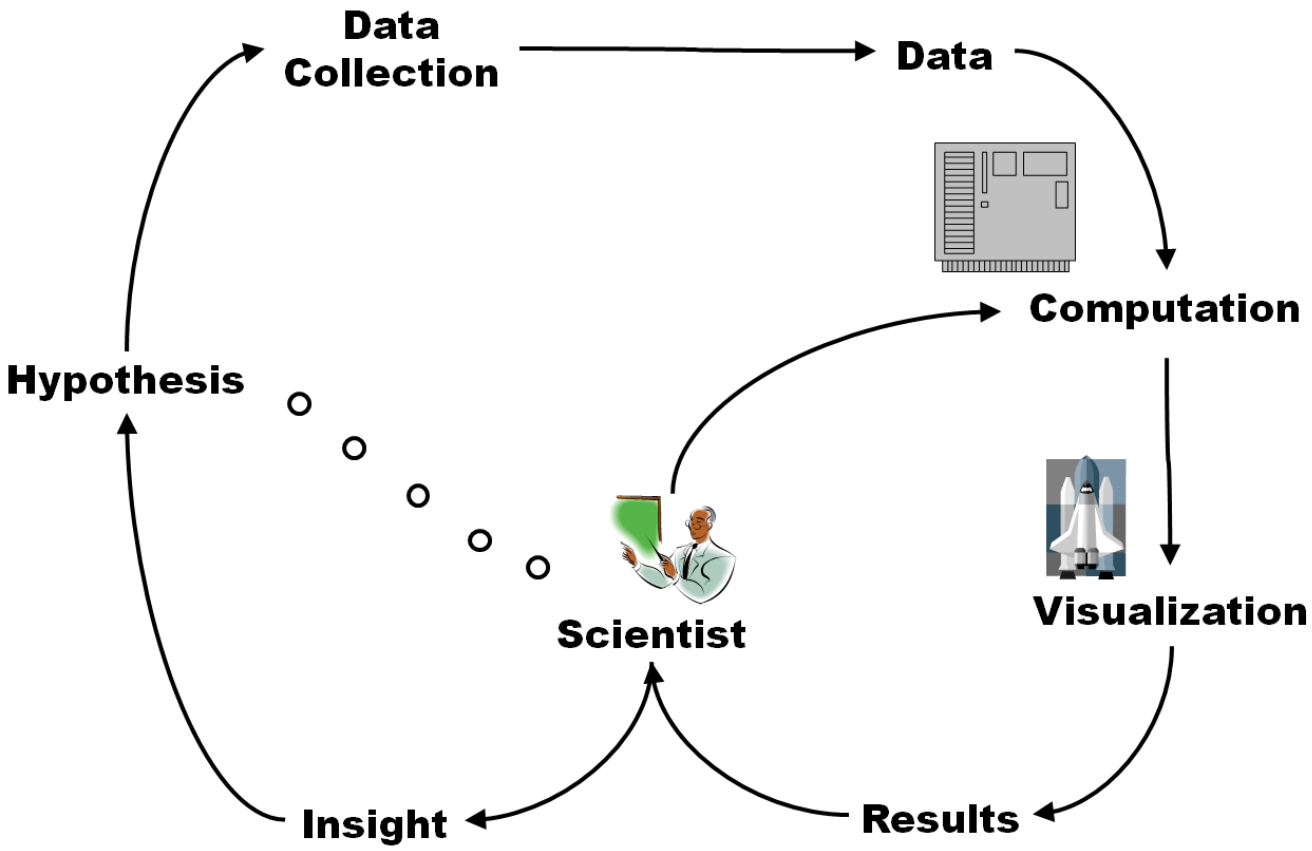

Designed for **Interactivity** and **exploration** in the **visualization** brings **new insights** because **research is a fluid process!!!**

Watson's model of scientific investigation was used by the visualization community to design software frameworks. It can be adapted to cover data science. Diagram from "Collaborative Practices In Computer Aided Research" by Leng and Sharrock

Evolution of Research Software, Based on the Abernathy-Utterback Curve (1)

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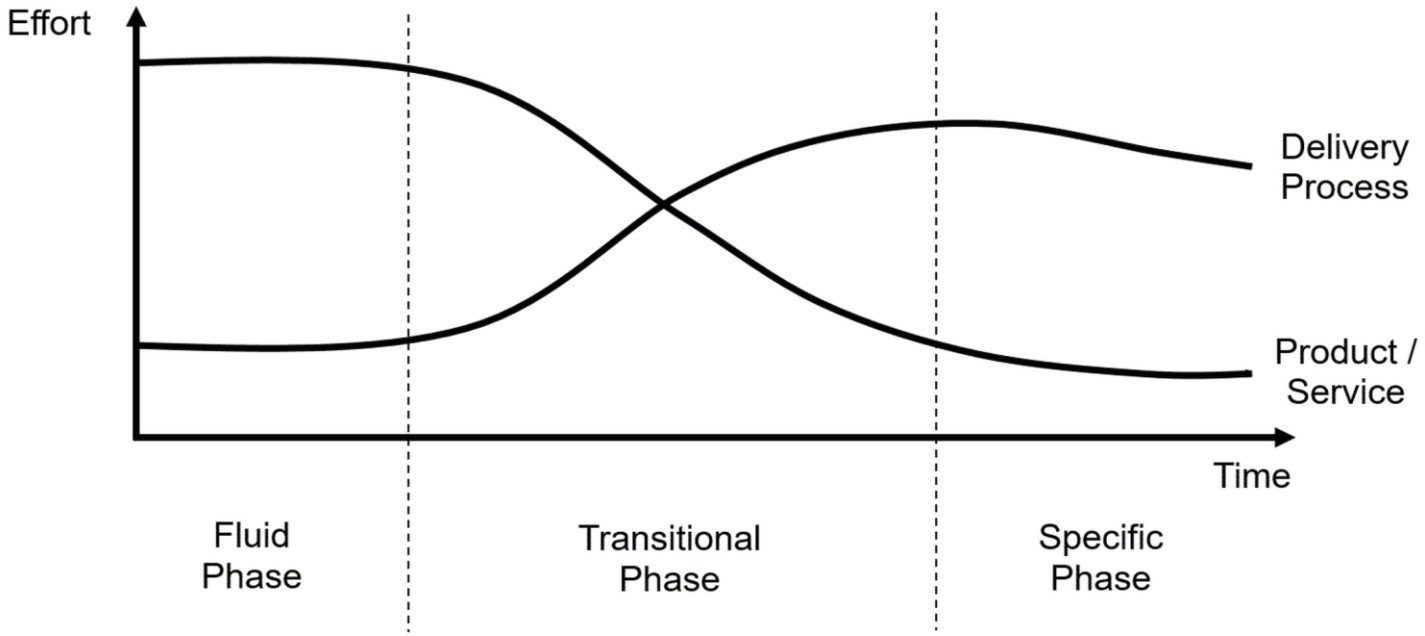

- Innovations in the fluid phase undergo churn, eventually yielding a dominant design.
- In the transitional phase, delivery processes become more important than feature sets.
- In the specific phase, the innovation is well established, and effort is mainly devoted to efficient operation.

Evolution of Research Software, Based on the Abernathy-Utterback Curve (2)

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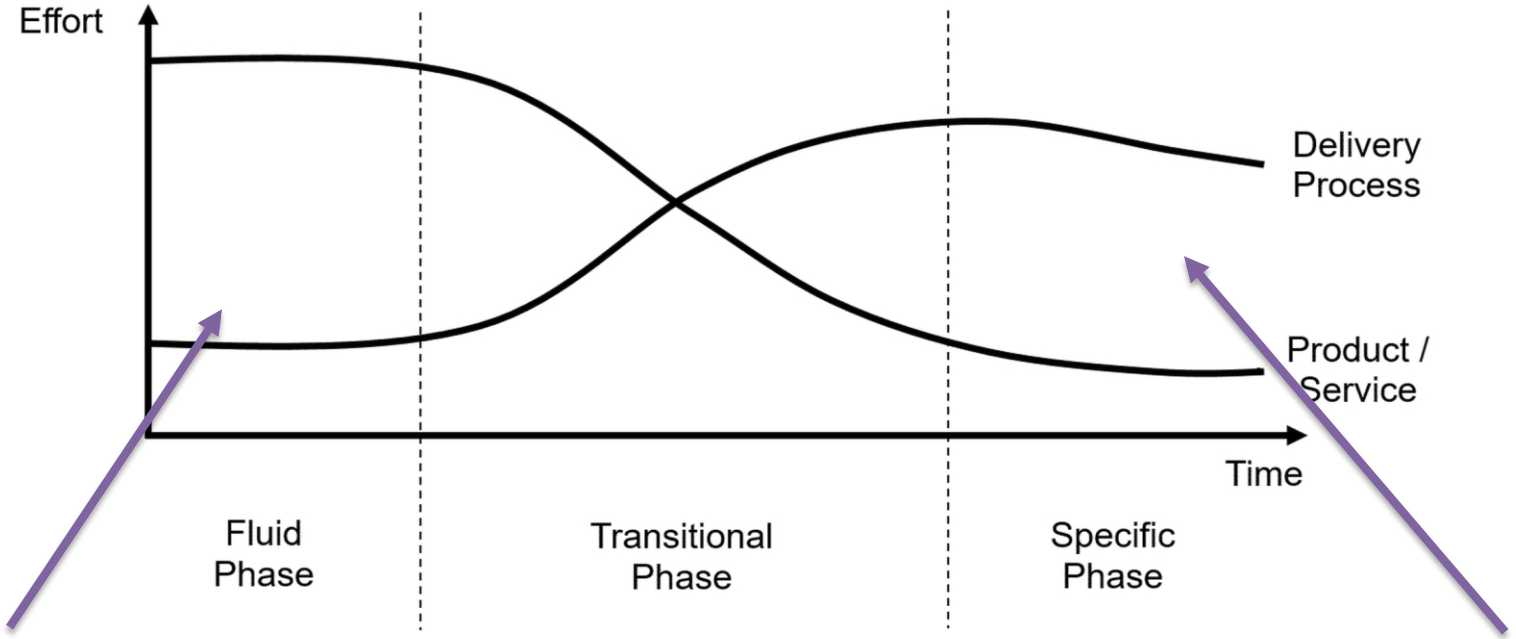

Fluid development methods

Waterfall development methods

Evolution of Research Software, Based on the Abernathy-Utterback Curve (3)

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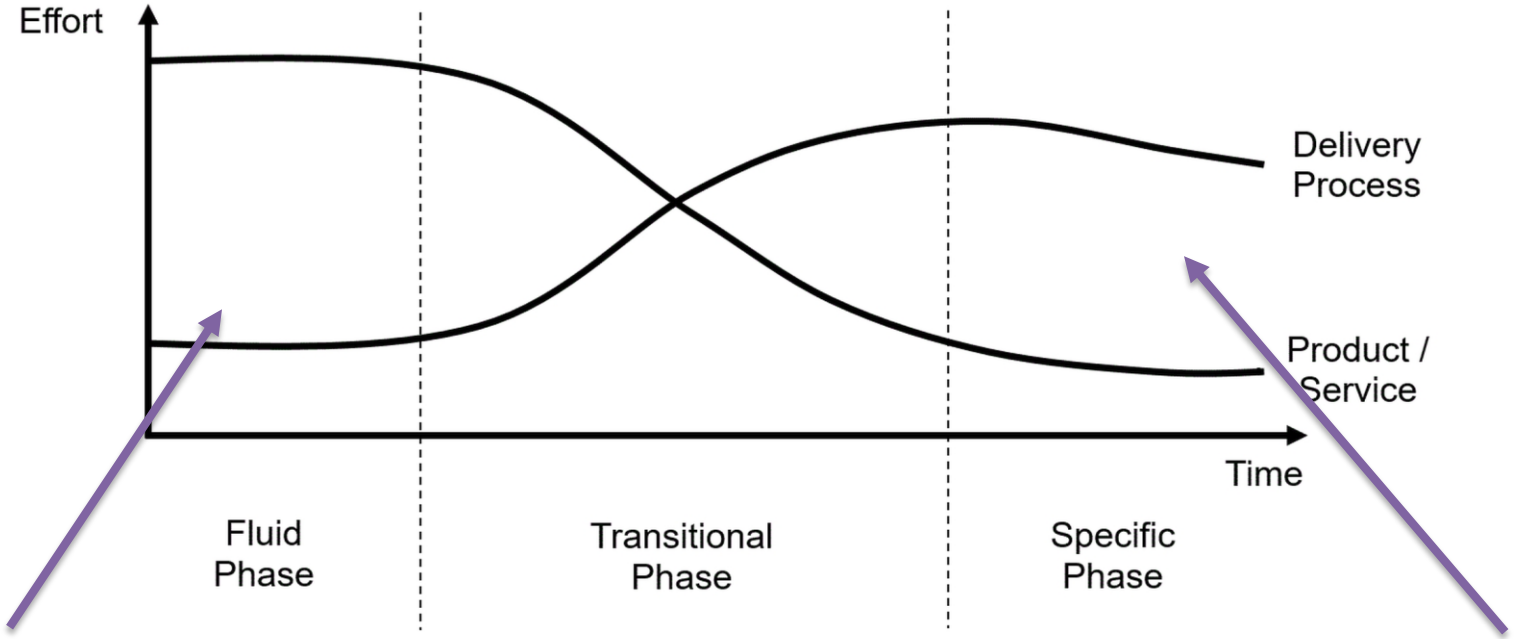

Fluid development methods

Waterfall development methods

Seeing the waterfall as traditional and fluid as modern is WRONG! They are suited to different parts of the innovation pathway.

Python

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- Is an increasingly popular programming language in academia.
- Is an interpreted programming language so you can test syntax on the command line.
  - More interactive and exploratory than complied languages:
  - Ipython and Jupyter note books have been ground breaking offering new types of interactivity and sharing but are not always easy to convert into software run in batch mode.
  - The Spyder IDE as has interactive shell; good for interaction bad for secure software
- Major differences between version 2 and 3 inhibit the adoption of version 3 in academia

Command Line Interfaces (CLI) vs Graphical User Interfaces (GUI)

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- There are large debates about which is better CLI or GUI. They can be very heated.
- Generally as software becomes more complex it is easier to use a GUI however this reduces the options available and means it will not run in batch mode so…..
- While some people prefer to use software via the command line (CLI) for some tasks others prefer to use a Graphical User Interface (GUI)
- It is **much harder to develop software** that executes through a GUI than through the command line.

Consider the Visualization Pipeline

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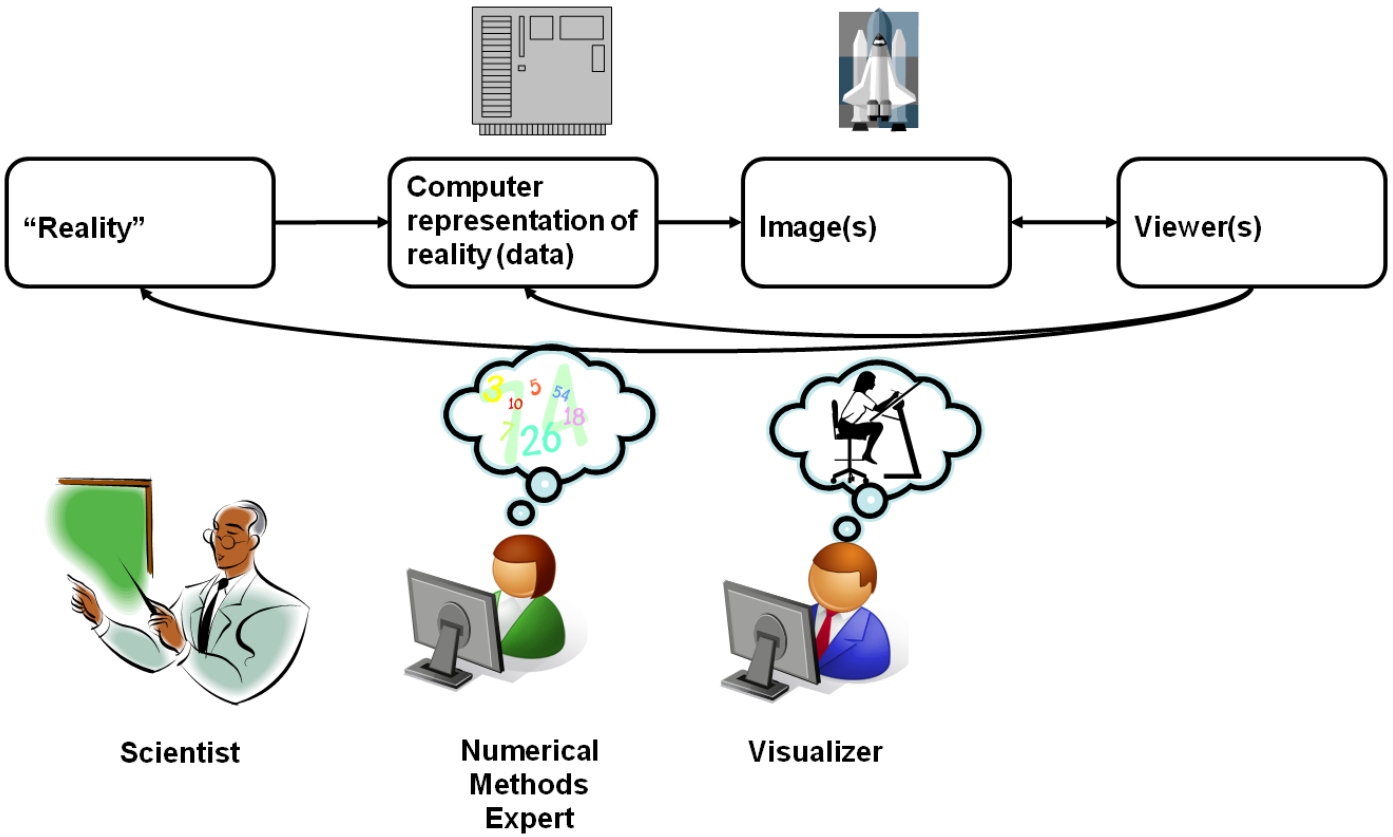

Hardware in the Visualization Pipeline

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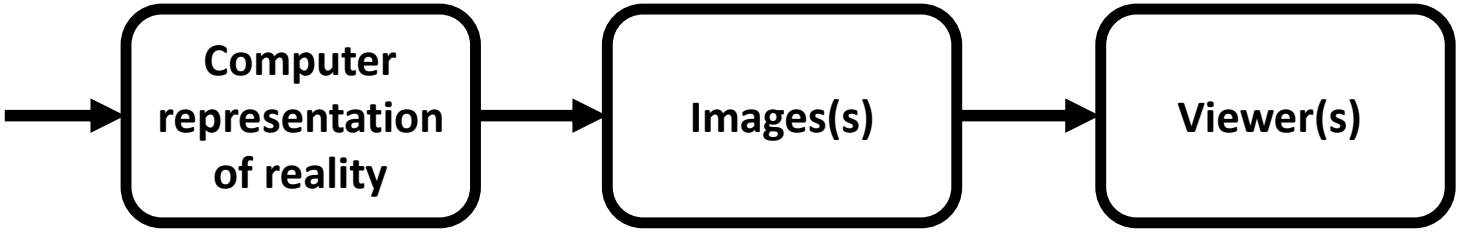
HARDWARE

CPU (nodes and cores)

Graphics card

Screen



PROCESSES

simulation or analysis

Rendering

More complex as for Example you need to create and manage canvases and scenes not good for CLI

Evolution of Research Software, Based on the Abernathy-Utterback Curve (4)

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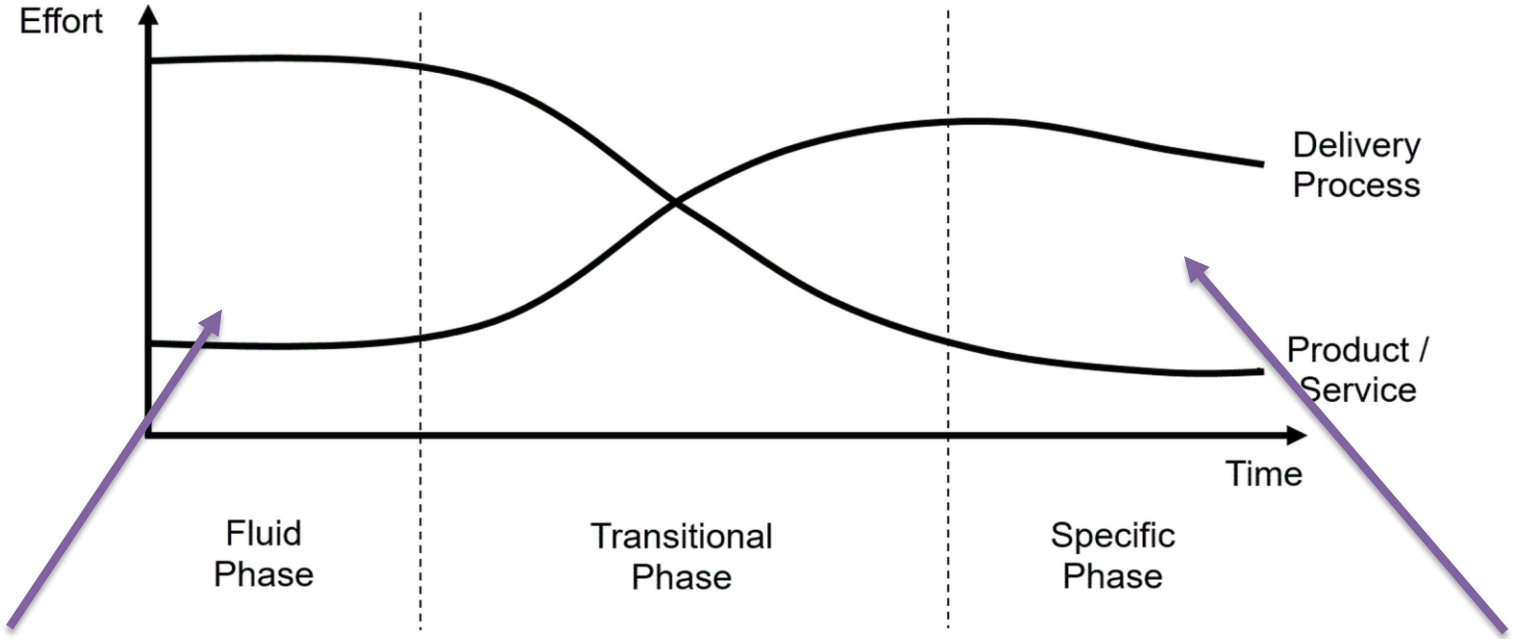

Command Line Interface

Less skills needed

perpl

Graphical User Interface

More skills needed

Interactive visualization software needs extra skills to develop and needs to be stable for a good user experience

Perpl

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- Developed in python 2
- The original developer is skilled in developing algorithms for dSTORM but is not a software engineer
- His skills are suited to a Command Line Interface but wants to develop a GUI for ease-of-use
- This is at odds with his skills, career path and this being a new area of innovation that requires flexability.

Perpl – from the Command Line

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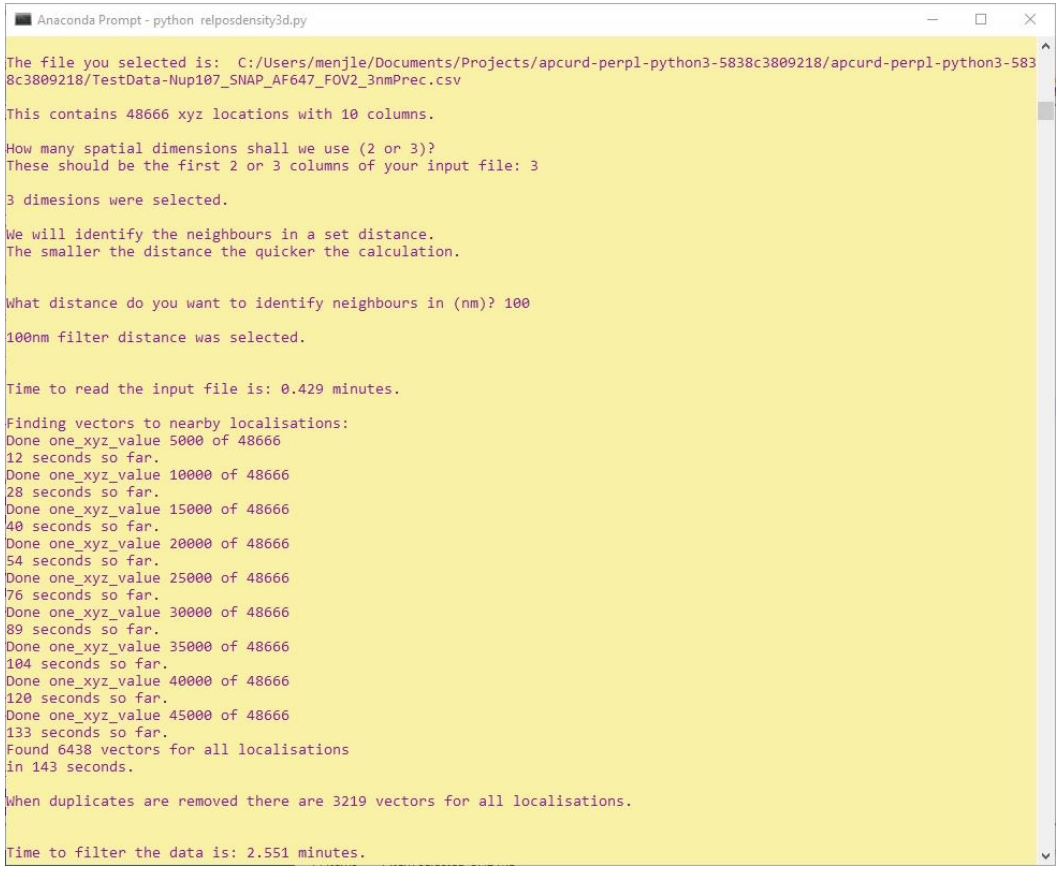
- Mainly a command line utility but with a a GUI for file browsing and reading



Perpl – Data in an interactive Visualization System, GlueVis

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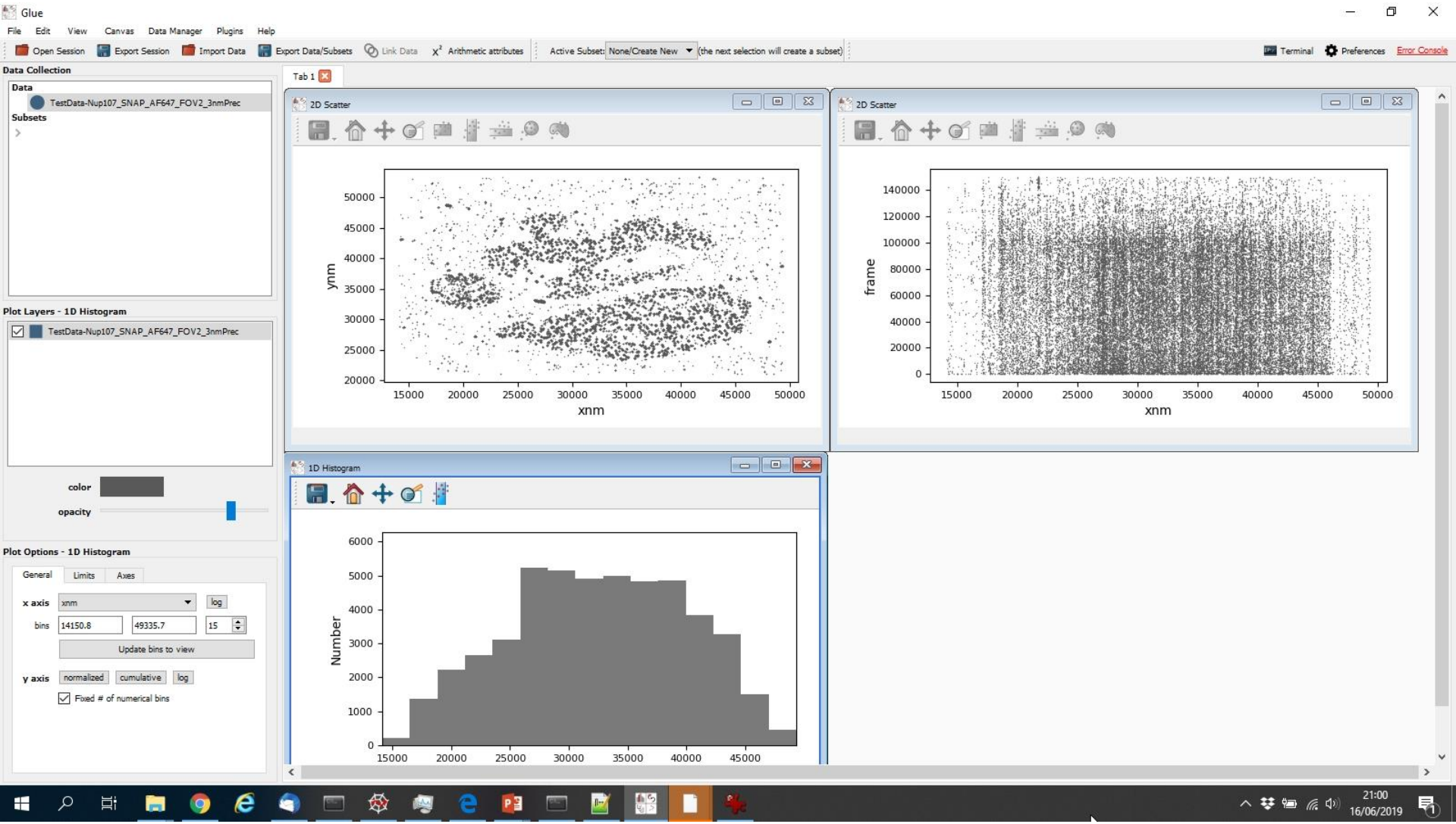

Perpl – Data in an interactive Visualization System, GlueVis

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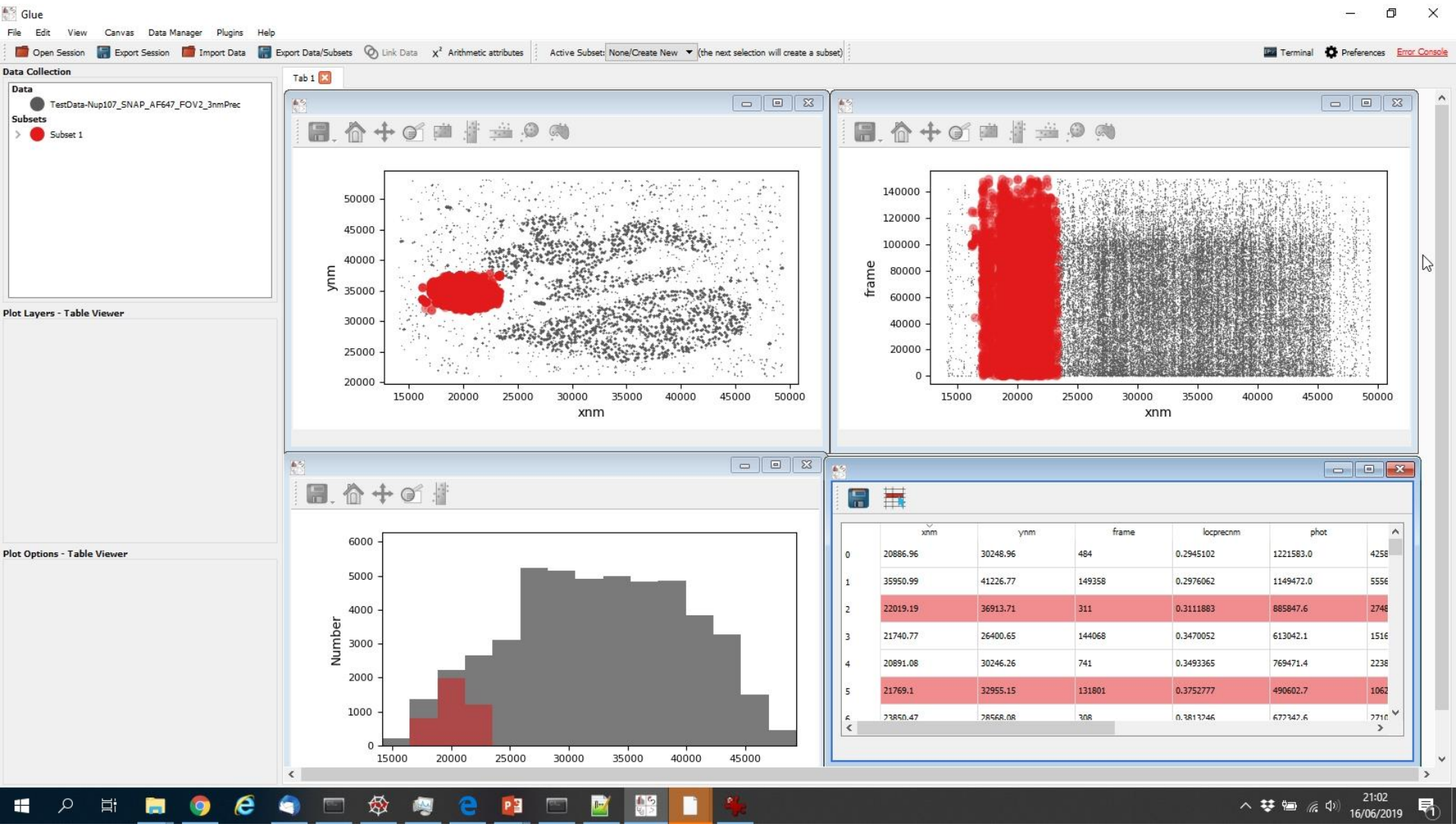

Perpl – Redesigned

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- GlueVis allows interactive visualization to a point but does not have the everything needed.
- ImageJ is the standard application in this area but the python stack and the workflow does not easily translate into it. ImageJ uses Java and is designed for image array data but we have point data.
- Reasonable effort is needed to get this working in either ImageJ or GlueVis
- Now when the script runs a html report is created with graphs that we identified in GlueVis

Perpl – 3 Orthogonal Views

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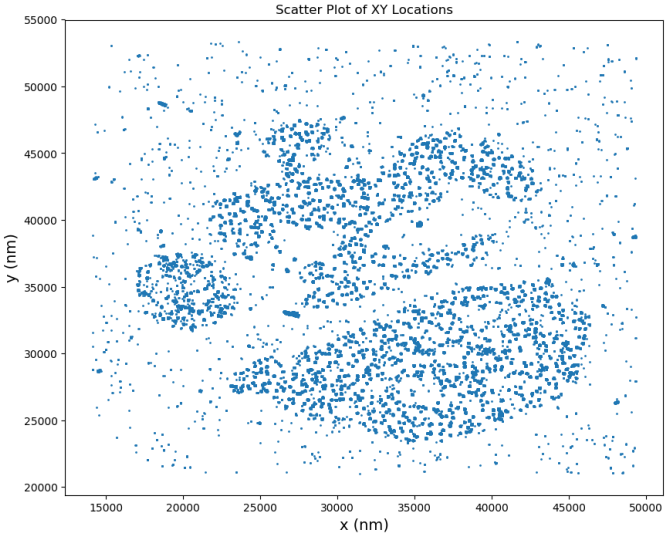

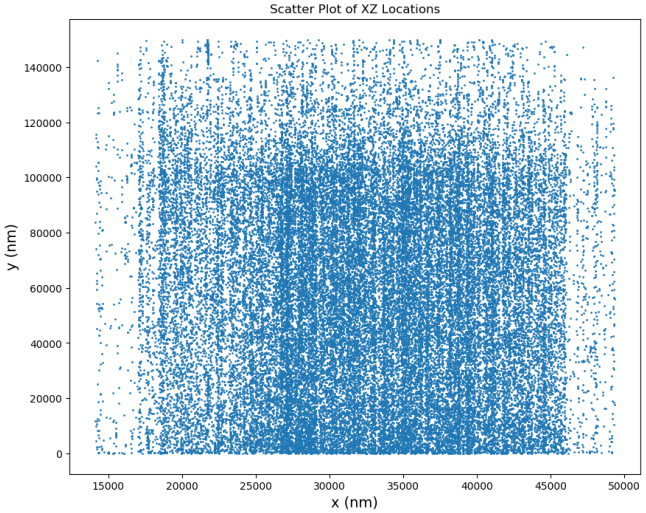

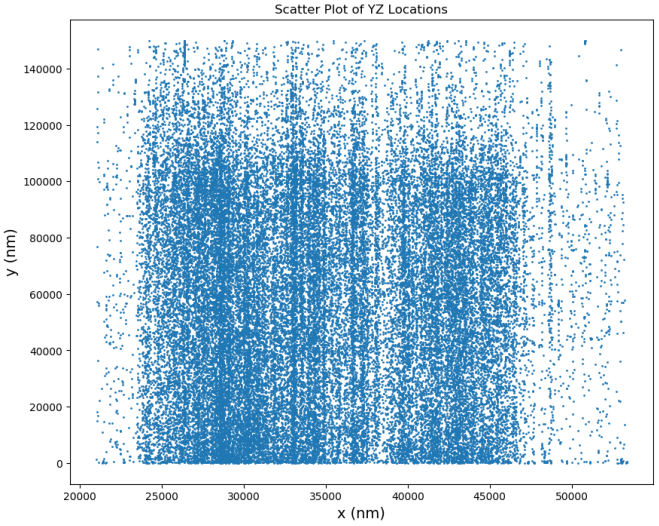

Perpl – 3 Orthogonal Zoom Views

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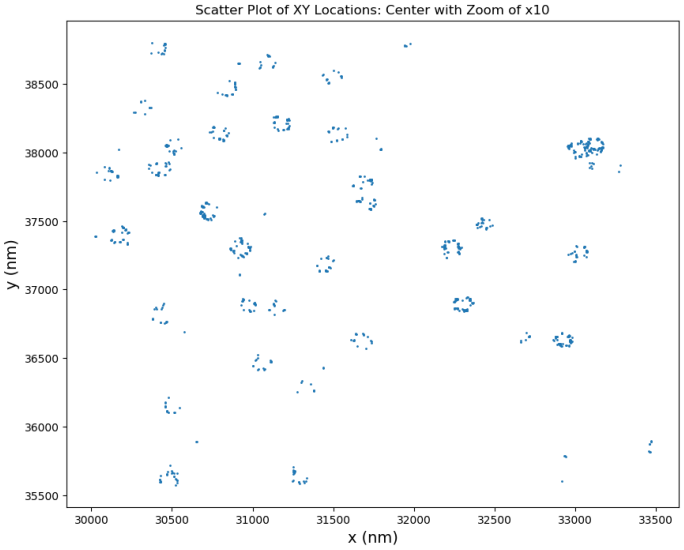

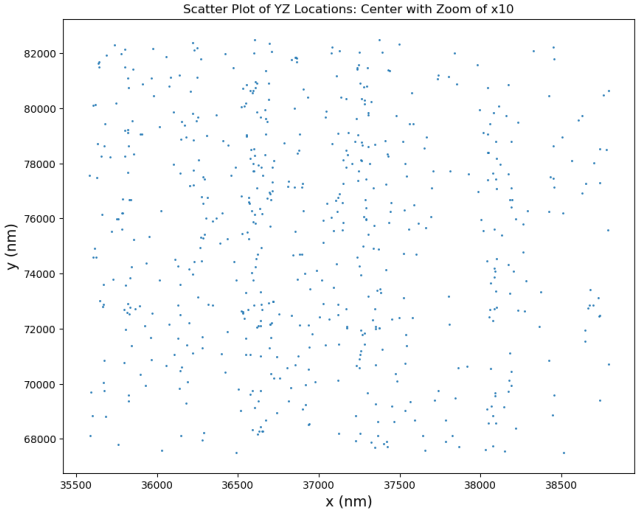

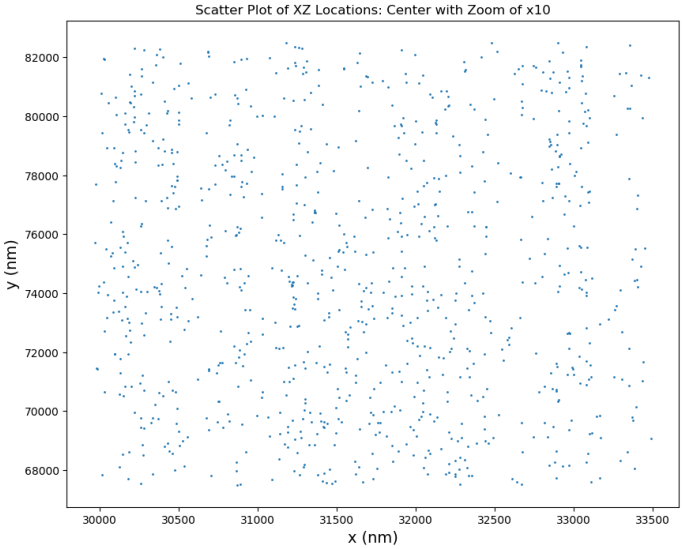

Perpl – Histograms

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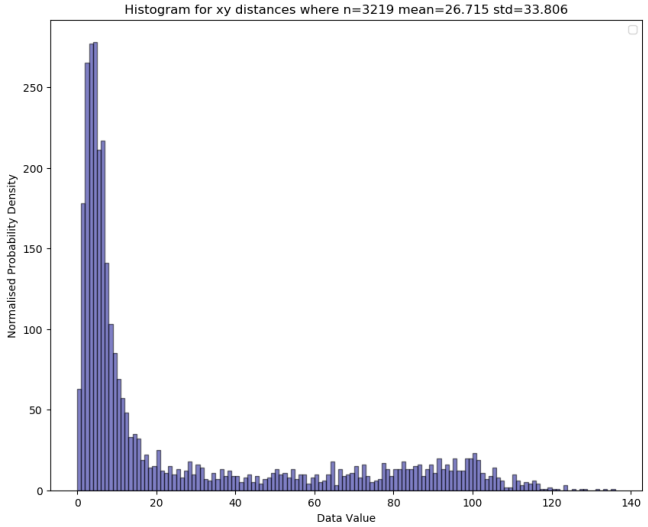

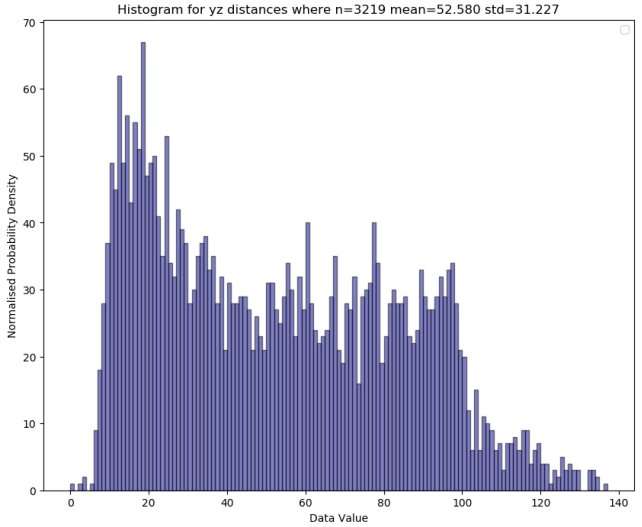

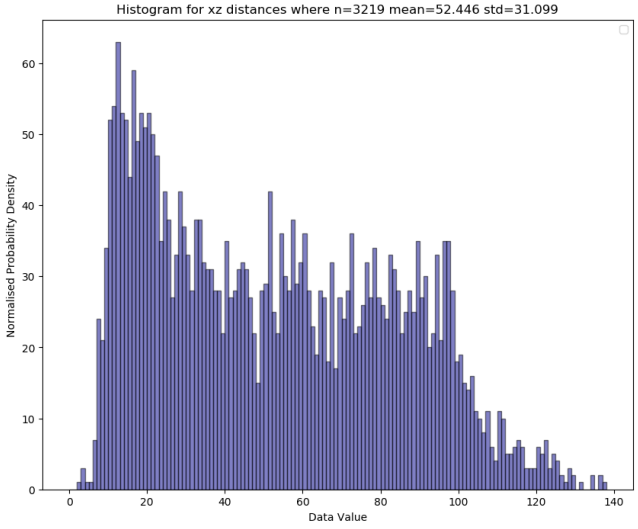

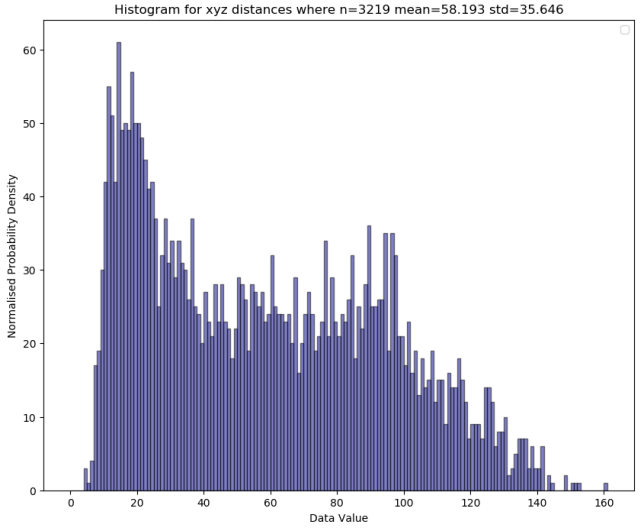

Perpl – The Future

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- Need a new function where we compare the image data to simulated data.
- The visualization and user interface design of this function will depend on the scientific needs and we will have to keep the design and development flexible until we have fully explored the scientific correctness of what is needed.

General Purpose Interactive Visualization Systems in Research Software Development

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- Allows the data to be **explored** without specialist knowledge of graphics or visualization.
- Opens up a conversation with the research team to **design** the visualizations and the software architecture.
- If the interactive visualization system does not have all the required functions you may be able to add modules and **prototype** within that system.
- Once there is a prototype the research team can **develop** and **optimize** the final research software and workflow to their research problem inside or outside the interactive visualization package.

RSE Leeds Network

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- Mailing List has 61 members: http://lists.leeds.ac.uk/mailman/listinfo/rse-network
- Twitter: @RSELeeds
- Committee has 6 people
- Next meeting is “The Benefits of Having an RSE Team” by Alun Ashton a senior RSE from Diamond Light Source

Other RSE resources

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- The RSE Association
- http://rse.ac.uk/join-us/
    - Mailing list, slack channel
    - RSE conference
- Software Sustainability Institute
- https://www.software.ac.uk/
    - Mailing list
    - Collaborations Workshop
- Software Carpentry Foundation
- https://software-carpentry.org/
    - Mailing list and git repositories

Women in HPC

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- http://womeninhpc.org/
  - The is a newsletter and mailing list
- Raising Awareness of Women in HPC through Research; Raising the Profile of Women in HPC by Networking; Increasing the Visibility of Women in HPC through Events
- They run a variety of events at the main HPC conferences eg ISC and Supercomputing