The Facility Perspective

## Tim Snow

Diamond Light Source

Introduction

- Diamond Light Source
  - Synchrotron x-ray radiation source

- ISIS Neutron and Muon Source
  - Spallation radiation source

- Scientific Computing Application Resource for Facilities (SCARF)
  - Joint computing resource on the RAL site

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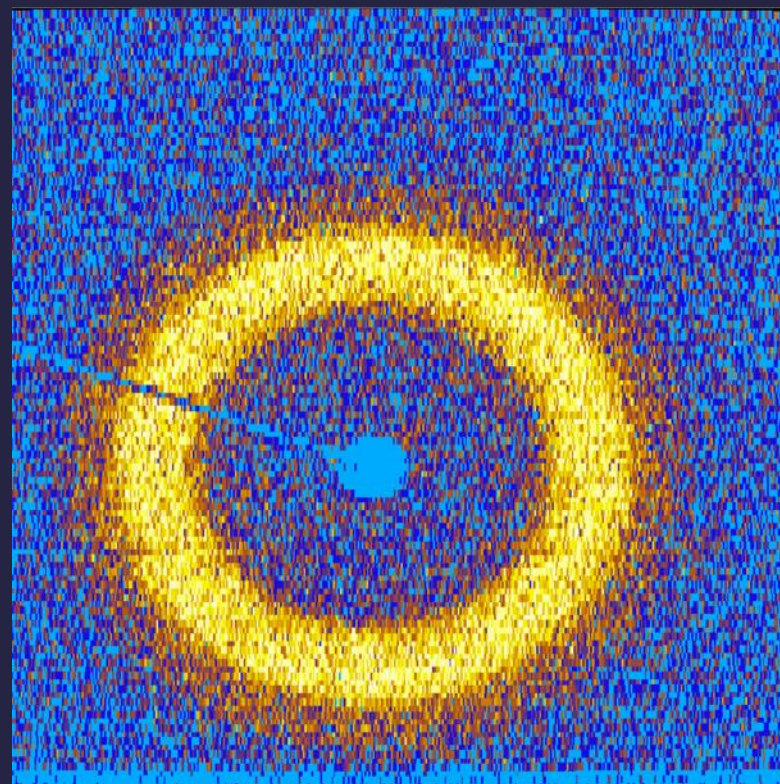ISIS Neutron and Muon Source

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Small angle scattering

*X-ray data*
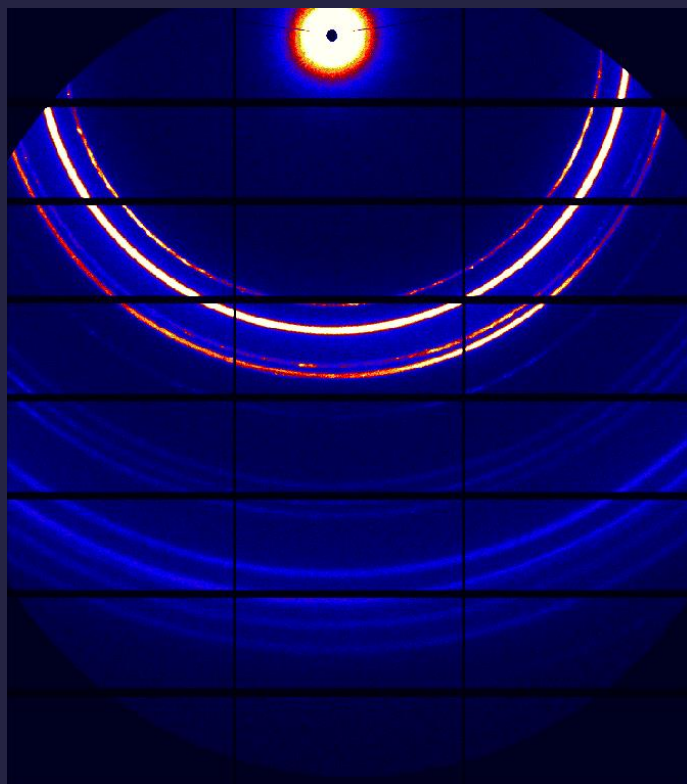
Neutron data

Image integration

- Advantages
  - Averaging data points mitigates scattering variation at a given q or χ value
  - Yields smaller datasets which can be compared by eye and analysed relatively quickly by computer

- Disadvantages
  - Image integration results in information loss
  - Mutual exclusivity between orientation and structural information
  - Obscures the true nature of the sample scanned

Small angle scattering
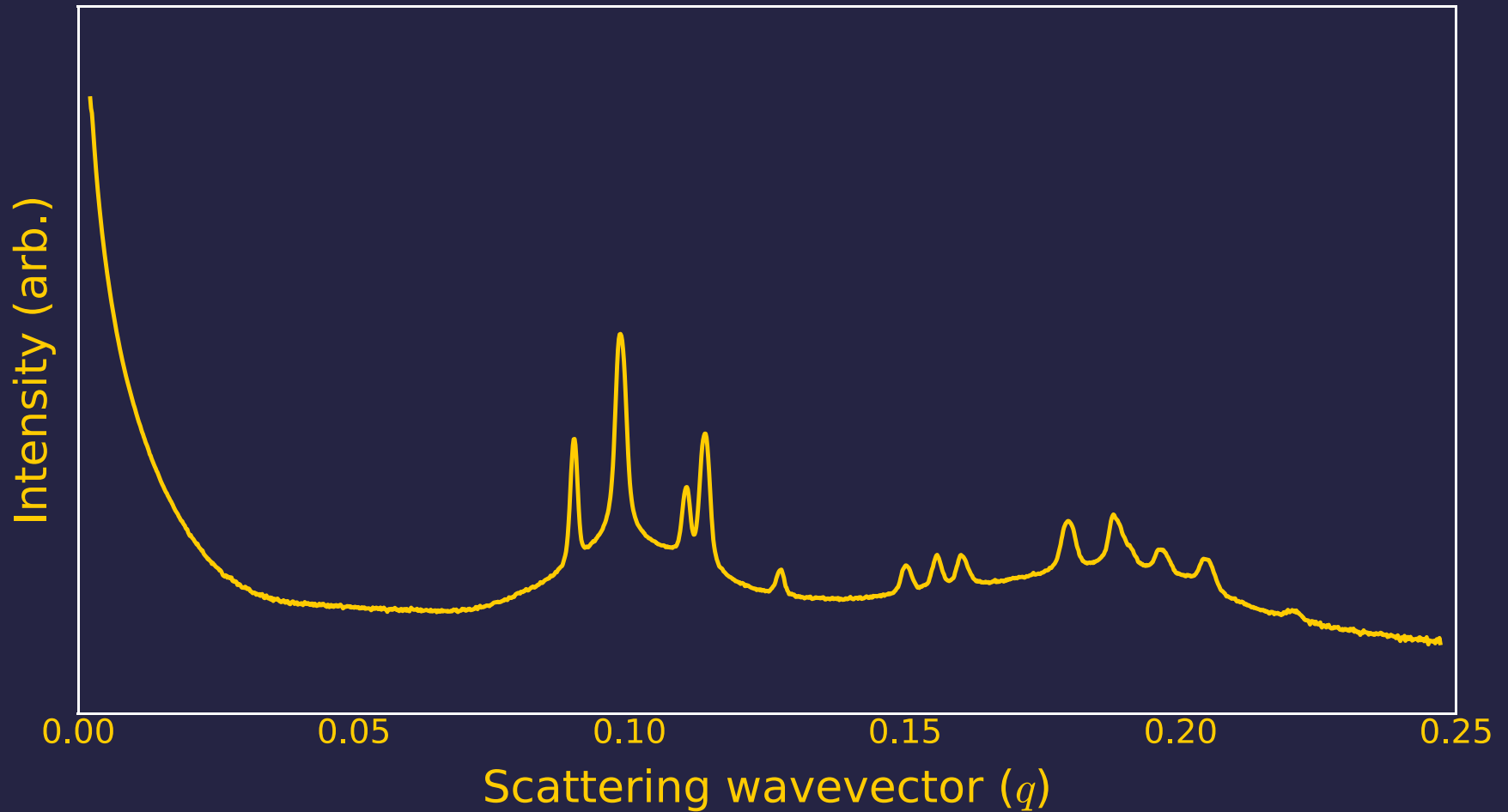
Small angle scattering

Azimuthal (I vs. q) analysis

- SasView
  - Shape and size fitting to SAS data

- Scåtter
  - P(r) and R_g values from solution scattering

- SAS Portal
  - List of small angle scattering software
    - www.smallangle.org

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How far should facilities go?

- Scattering is a tool and part of providing the tool should be analysis tools
  - The job of the facilities

- Analysis is where the science is to be found
  - The job of the user

Data on disk is useless to everybody

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Analysing complex datasets

- Currently

  - Biological users

    - Advantage from protein databank
    - Creation of simulation trajectory files catered for

  - Groups with simulation expertise

- Future

  - Polymer systems

  - Soft matter systems

  - Bio-mimetic systems

HPC at RAL

- SCARF resources available
  - 420 nodes, 6,176 CPU cores, 32.5 TB RAM
  - Access, *via* FED ID, to all Diamond and ISIS users

- SASSIE is being installed on SCARF
  - Most dependencies installed
  - Collaboration with J. Curtis
    - www.github.com/zazzie_1.5

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First steps

- Trajectory files and simulation constraints
  - Simplify process of creation
  - Some form of 'intelligence' required
  - Prevent users from analysing unphysical systems

- Commitment to SASSIE
  - Installation and setup of SASSIE on SCARF
  - Provision of HPC time by Diamond and ISIS
  - Initial user training

Future steps

- Building on biological roots
  - Suite of tools for trajectory files
    - Colloidal systems
    - Polymer systems
    - Soft matter systems

- Develop simulation expertise at facilities
  - First point of contact

- Integrating SASSIE with RAL data analysis

Final thoughts

- Scattering is a tool and part of providing the tool should be analysis tools
  - Pooling of resources and collaborations facilitating better resources for users

- Analysis is where the science is to be found
  - We must help users but, ultimately, they must work with their data to make discoveries

Data on disk is useless to everybody

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Acknowledgements

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