Infrastructure for Integration in Structural Sciences

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Data Infrastructure Challenges: working across scale, disciplinary and institutional boundaries

University of Leicester
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I2S2
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Integration in Structural Sciences

Outline

- I2S2 Project overview & aims
- Project Team
- Research data & infrastructure
- Requirements analysis
- A Scientific Research Activity Lifecycle Model
- An integrated services approach
- Testing the I2S2 information model
- Cost-Benefits analysis

Diamond Light Source (DLS),
Science & Technology Facilities Council, UK

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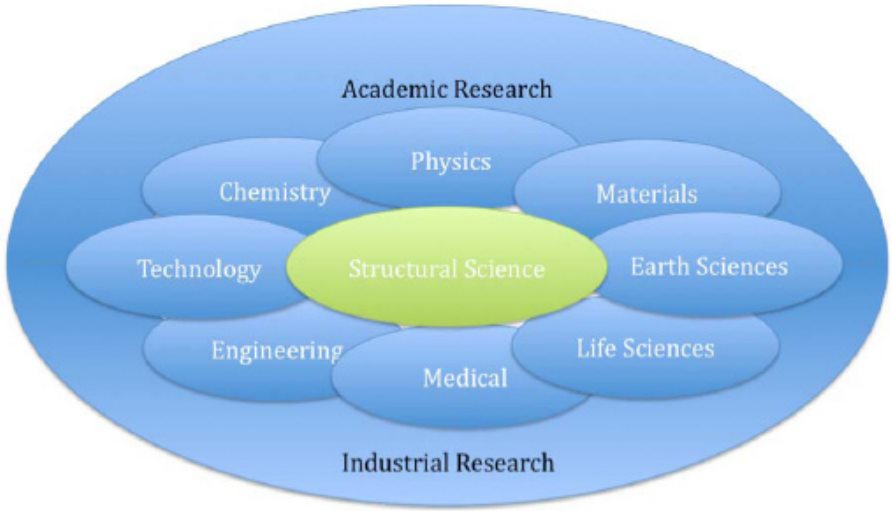
Overview & Aims

- Research Data Management Infrastructure strand of the JISC's Managing Research Data Programme (18 month project, Oct 2009 - March 2011)
- Understand and identify requirements for a data-driven research infrastructure in the Structural Sciences
  - Examine localised data management practices
  - Investigate data management infrastructure in large centralised facilities
- Show how effective cross-institutional research data management can increase efficiency and improve the quality of research



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Project Team

- Liz Lyon (Project Director, UKOLN (University of Bath) & Digital Curation Centre)
- Manjula Patel (Project Manager, UKOLN (University of Bath) & Digital Curation Centre)
- Sarah Hext (Financial Administrator, UKOLN (University of Bath))
- Simon Coles (EPSRC National Crystallography Centre, University of Southampton)
- Neil Beagrie (Charles Beagrie Ltd.)
- Brian Matthews (Science & Technology Facilities Council)
- Erica Yang (Science & Technology Facilities Council – now at Bodleian libraries, University of Oxford)
- Martin Dove (Earth Sciences, University of Cambridge)
- Peter Murray-Rust (Chemistry, University of Cambridge)

- Simon Hodson (JISC Managing Research Data Programme Manager)

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http://www.ukoln.ac.uk/projects/I2S2/

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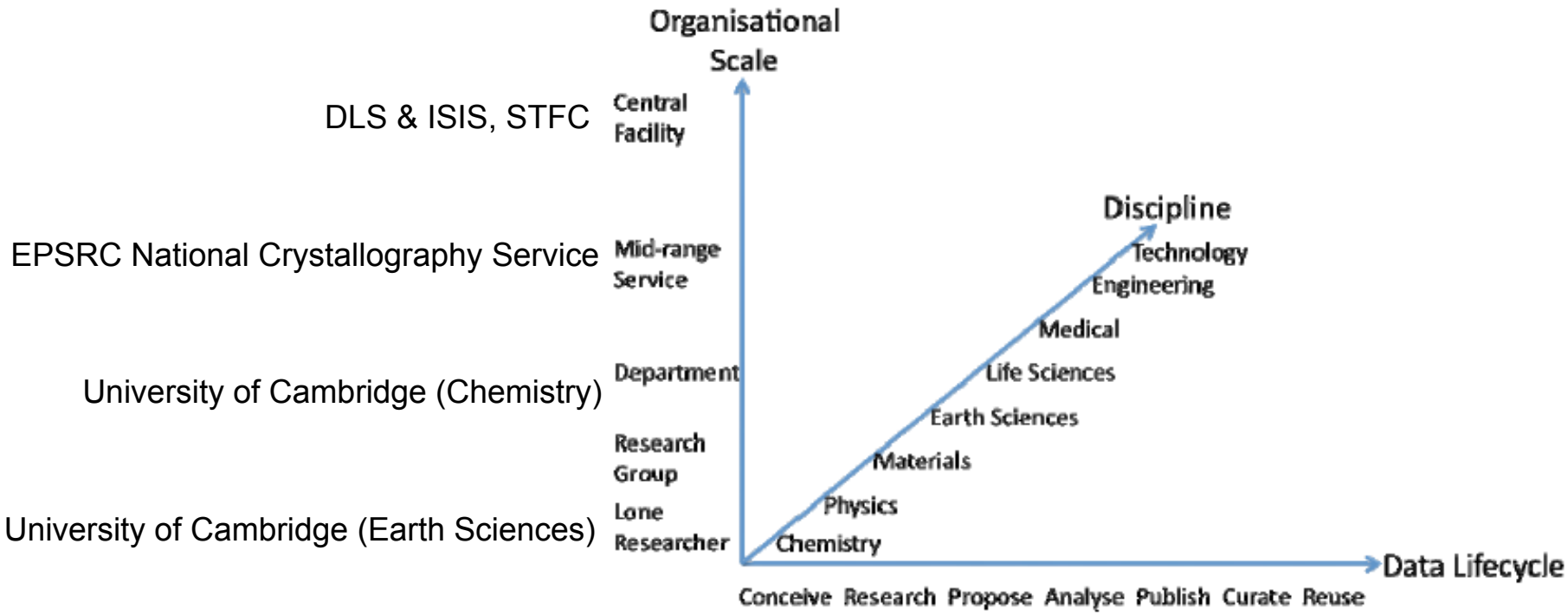
Overall Methodology

Scale and complexity: small laboratory to institutional installation to large scale facilities e.g. DLS & ISIS, STFC

Interdisciplinary issues: research across domain boundaries

Data lifecycle: data flows and data transformations over time



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Research Data & Infrastructure

- Research Data includes (all information relating to a physical experiment):
  - raw, reduced, derived and results data
  - research and experiment proposals
  - results of the peer-review process
  - laboratory notebooks
  - equipment configuration and calibration data
  - wikis and blogs
  - metadata (context, provenance etc.)
  - documentation for interpretation and understanding (semantics)
  - administrative and safety data
  - processing software and control parameters
- Infrastructure includes physical, technical, informational and human resources essential for researchers to undertake high-quality research:
  - Tools, Instrumentation, Computer systems and platforms, Software, Communication networks
  - Documentation and metadata
  - Technical support (both human and automated)
- Effective validation, reuse and repurposing of data requires
  - Trust and a thorough understanding of the data
  - Transparent contextual and provenance information detailing how the data were generated, processed, analysed and managed

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Earth Sciences, Cambridge

- Construct large scale atomic models of matter that best match experimental data; using Reverse Monte-Carlo Simulation techniques
- Experiment and data collection conducted at ISIS Neutron Source (GEM)
- Little or no shared infrastructure
  - Data sharing with colleagues via email, ftp, memory stick etc.
  - Data received from ISIS is currently stored on laptops or WebDAV server
- Management of intermediate, derived and results data a major issue
  - Data managed by individual researcher on own laptop
  - No departmental or central institutional facility
- Data management needs largely so that
  - Data can be shared internally
  - A researcher (or another team member) can return to and validate results in the future
  - External collaborators can access and use the data
- Any changes should be embedded into scientist's workflow and be non-intrusive

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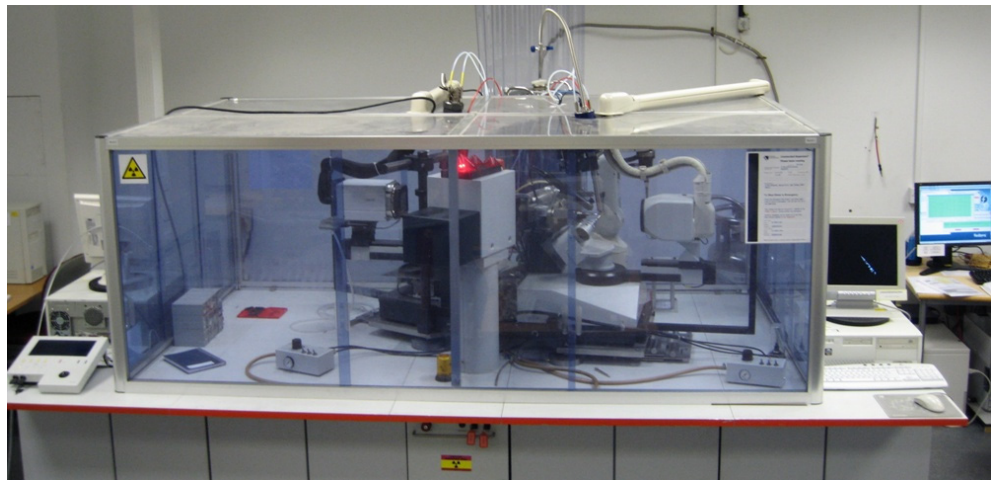
Chemistry, Cambridge

- Implementation and enhancement of a pilot repository for crystallography data underway (CLARION Project)
- Need for IPR, embargo and access control to facilitate the controlled release of scientific research data
- Information in laboratory notebooks need to be shared (ELN)
- Importance of data formats and encodings (RDF, CML) to maximise potential for data reuse and repurposing



EPSRC National Crystallography Service,
University of Southampton, UK

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EPSRC NCS, Southampton

- Service provision function (operates nationally across institutions)
  - Local x-ray diffraction instruments + use of DLS (beamline I19)
  - Retain experiment data
  - Maintain administrative data
- Raw data generated in-house is stored at ATLAS Data Store (STFC)
- Local institutional repository (eCrystals) for intermediate, derived and results data
  - Metadata application profile
  - Public and private parts (embargo system)
  - Digital Object Identifier, InChi
- Experiments conducted and data collected by NCS scientists either in-house or at DLS
- Labour-intensive paper-based administration and records-keeping
  - Paper-based system for scheduling experiments
  - Paper copies of Experiment Risk Assessment (ERA) get annotated by scientist and photocopied several times
  - Several identifiers per sample
- Administrative functions require streamlining between NCS and DLS
  - e.g. standardisation of ERA forms, identifiers

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DLS & ISIS, STFC

- Operate on behalf of multiple institutions and communities
- Scientific (peer) and technical review of proposals for beam time allocation
- User offices manage administrative and safety information
- Service function implies an obligation to retain raw data
- Large infrastructure, engineered to manage raw data
  - Designed to describe facilities based experiments in Structural Science
    e.g. ISIS Neutron Source, Diamond Light Source.
  - ICAT implementation of Core Scientific Metadata Model (CSMD)
- No storage or management of derived and results data
  - Derived data taken off site on laptops, removable drives etc.
  - Results data independently worked up by individual researchers
- Experiment/Sample identifiers based on beam line number

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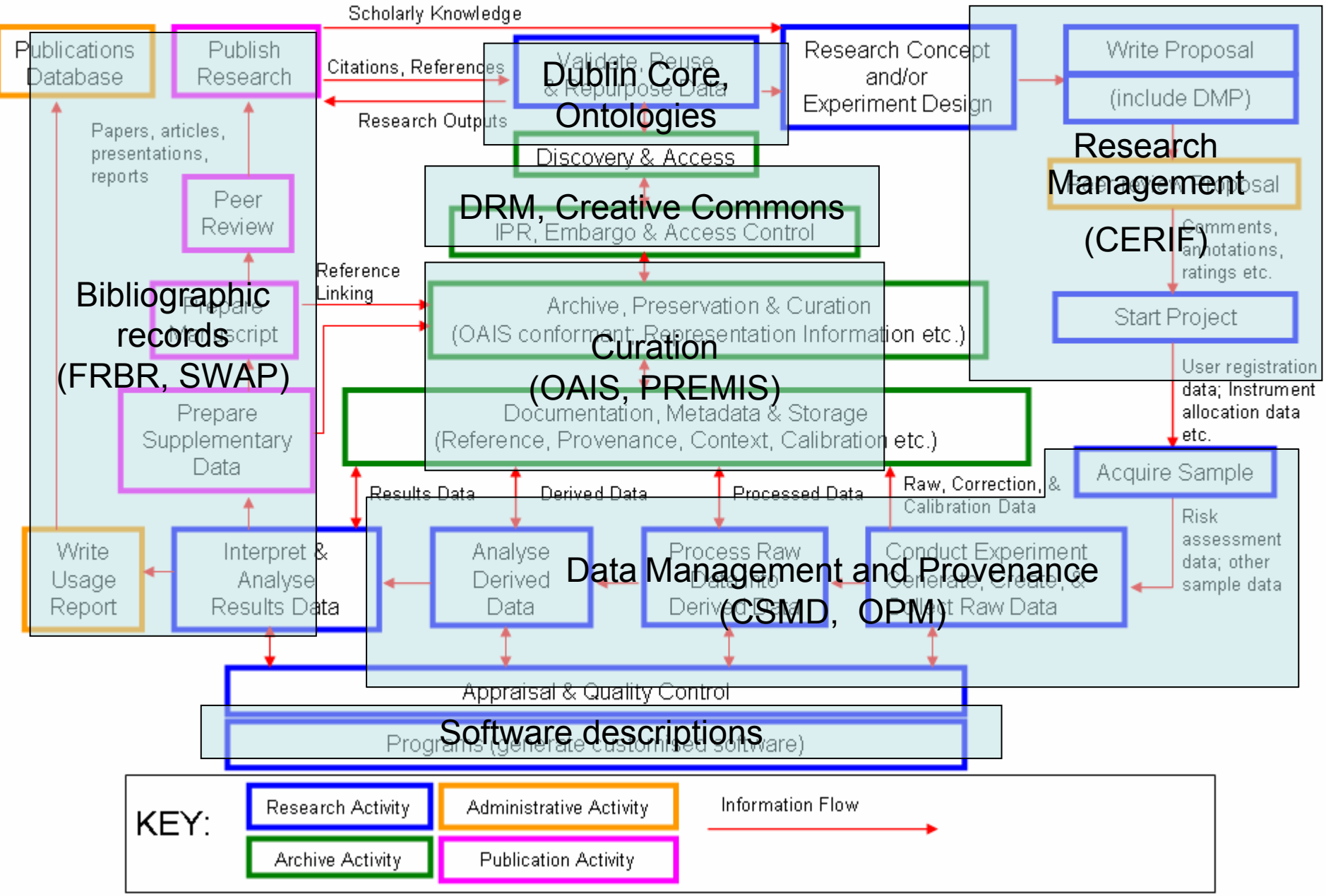
Generalised Issues

- Basic requirement for robust data storage and backup facilities to sophisticated needs such as structuring and linking together of data
- Management of intermediate, derived and results data a major issue
- Contextual information is not routinely captured
- Processing pipeline is dependent on a suite of software
- The actual workflow or processing pipeline is not routinely recorded
- Need for adequate metadata and contextual information to support:
  - Maintenance and management; Linking together of all data associated with an experiment; Referencing and citation; Authenticity; Integrity; Provenance; Discovery, Search and retrieval; Curation and preservation; IPR, embargo and access management; Interoperability and data exchange
- Simplification of inter-organisational communications and tracking, referencing and citation of datasets
  - Unique persistent identifiers
  - Standardised Experiment Risk Assessment forms
- Solutions should be as non-intrusive as possible

An Idealised Scientific Research Activity Lifecycle Model



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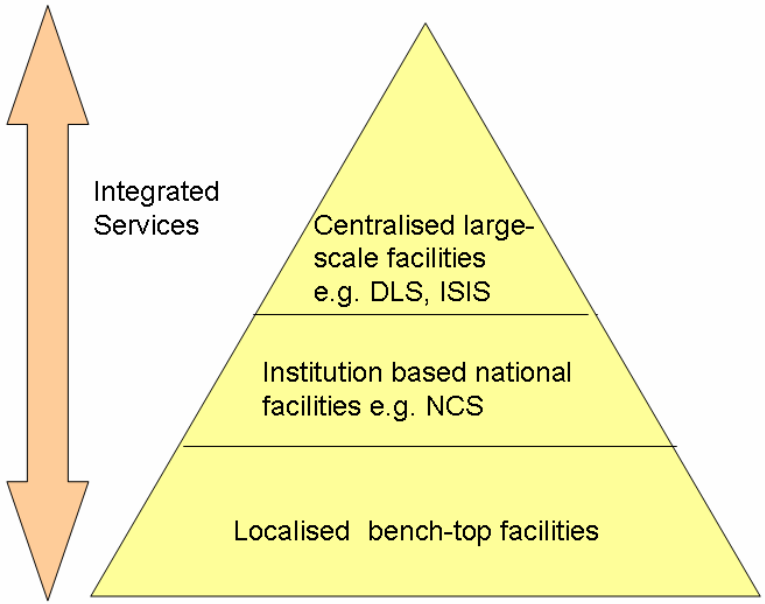
An Integrated Service Approach

- Individual researcher, group, department, institution, facilities all working within their own frameworks
- Merit in adopting an integrated framework which caters for all scales of scientific research
- Researchers need to be able to manage their data across institutional and domain boundaries in a seamless manner



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I2S2 Integrated Information Model

- Core Scientific Metadata Model (CSMD)
  - Designed to describe facilities based experiments in Structural Sciences
  - Forms a basis for extension to: Laboratory based science; Derived data; Secondary analysis data; Preservation information; Publication data
  - Aim to cater for the scientist's research lifecycle as well as facilities data
- oreChem Model
  - An abstract model for planning and enacting chemistry experiments
  - Enables exact replication of methodology in a machine-readable form
  - Allows rigorous verification of reported results
- I2S2-IM = CSMD-Core + oreChem Model
  - Underpins distributed data management
  - Effective inter-disciplinary data sharing
- I2S2-IM being implemented at STFC in the form of ICAT-Lite
  - A personal workbench for managing data flows
  - Allows the user to "commit data" for long-term storage
  - Enables capture of provenance information

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Testing the I2S2-IM

Case study 1: Scale and Complexity

- Data management issues spanning organisational boundaries in Chemistry
- Interactions between a lone worker or research group, the EPSRC NCS and DLS
- Traversing administrative boundaries between institutions and experiment service facilities
- Aim to probe both cross-institutional and scale issues

Case Study 2: Disciplinary issues

- Collaborative group of scientists (university and central facility researchers) in Earth Sciences
- Use of ISIS neutron facility and subsequent modelling of structures based on raw data
- Identification of infrastructure components and workflow modelling
- Aim to explore the role of XML for data representation to support easier sharing of information content and derived data

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Cost-Benefits Analysis

- A cost-benefit analysis using the Keeping Research Data Safe (KRDS) model
- Extending the KRDS Model
  - Focus has been on extensions and elaboration of activities in the research phase (KRDS “pre-Archive” stage)
- Metrics and assigning costs
  - Identification of activities in research activity lifecycle model that will represent significant cost savings or benefits
  - Identification of non-cost benefits and possible metrics
- 2 use case studies
  - Quantitative - cost-benefits in terms of service efficiencies (NCS)
  - Qualitative - researcher benefits (improvement in tools; ease of making data accessible etc.)

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Conclusions

- Considerable variation in data management requirements across differing scales of science
- I2S2 Integrated framework aims to:
  - Support the scientific research activity lifecycle model
  - Capture processes and provenance information
  - Streamline flow of metadata, administrative information and experiment data across organisations
  - Interoperate with and complement existing models and frameworks
- Cost-benefits analysis to assess impact of interventions

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