I2S2

Infrastructure for Integration in Structural Sciences

Manjula Patel

Scaling-up to Integrated Research Data Management Workshop

6th International Digital Curation Conference

Holiday Inn, Mart Plaza

Chicago, Illinois

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Outline

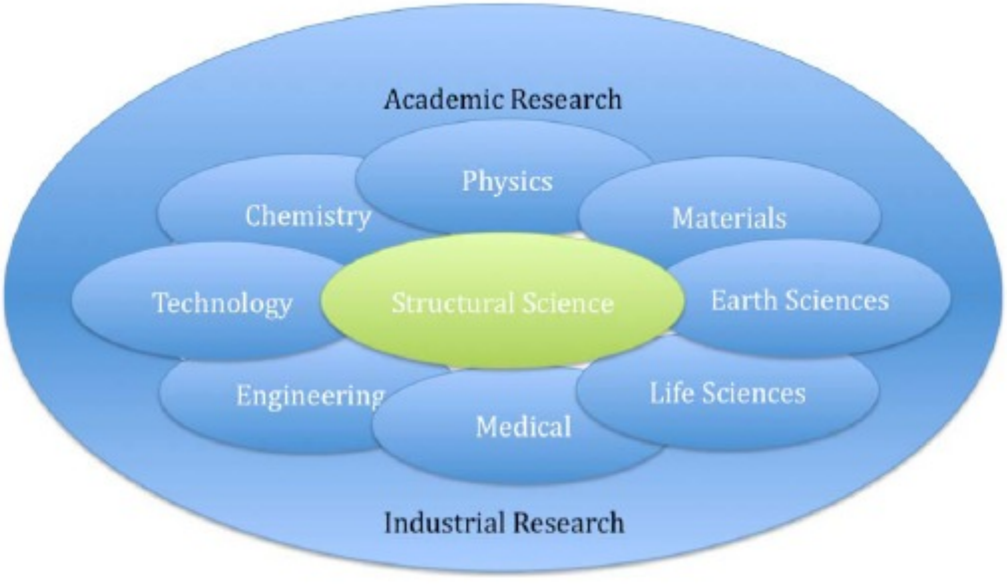
- I2S2 Project overview and objectives
- Research Data & Infrastructure
- Requirements analysis
- A Scientific Research Activity Lifecycle Model
- An integrated information model
- Use cases
- Cost-Benefits Analysis

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

I2S2 Project Overview

Infrastructure for Integration in Structural Sciences

- 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



Objectives

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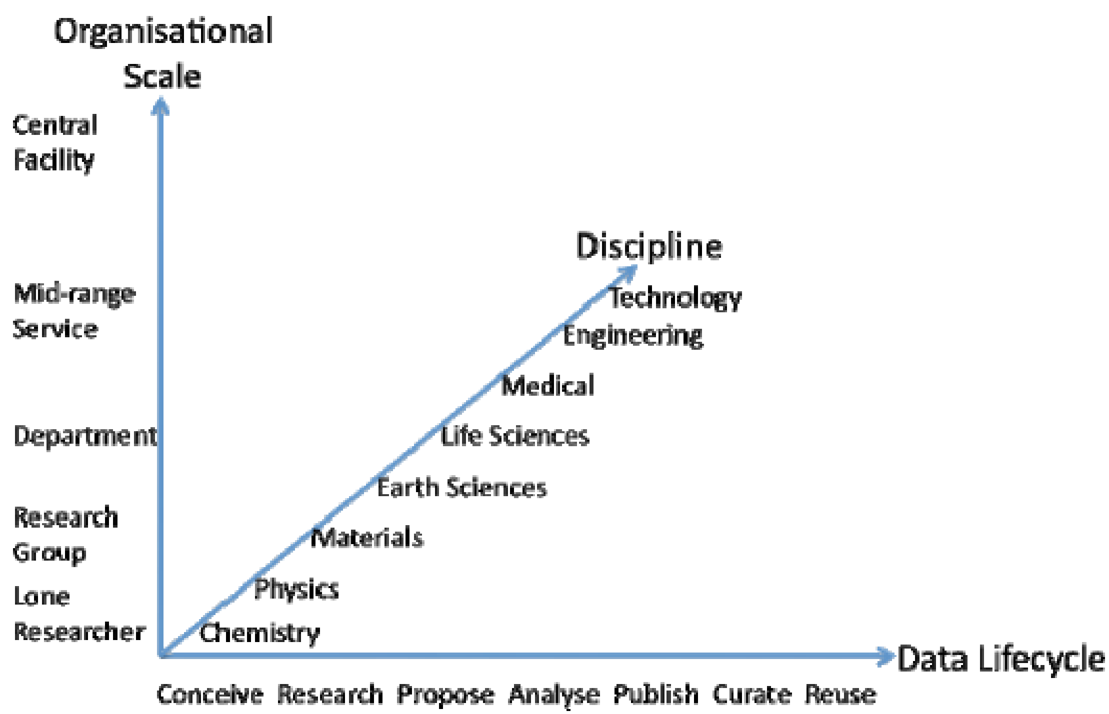
Scale and complexity: small laboratory to institutional installation to large scale facilities e.g. DLS & ISIS, STFC
Interdisciplinary issues: research across domain boundaries
Data lifecycle: data flows and data transformations over time

DLS & ISIS, STFC

EPSRC National Crystallography Service

University of Cambridge (Chemistry)

University of Cambridge (Earth Sciences)



Research Data & Infrastructure

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- Research Data includes (all information relating to an 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

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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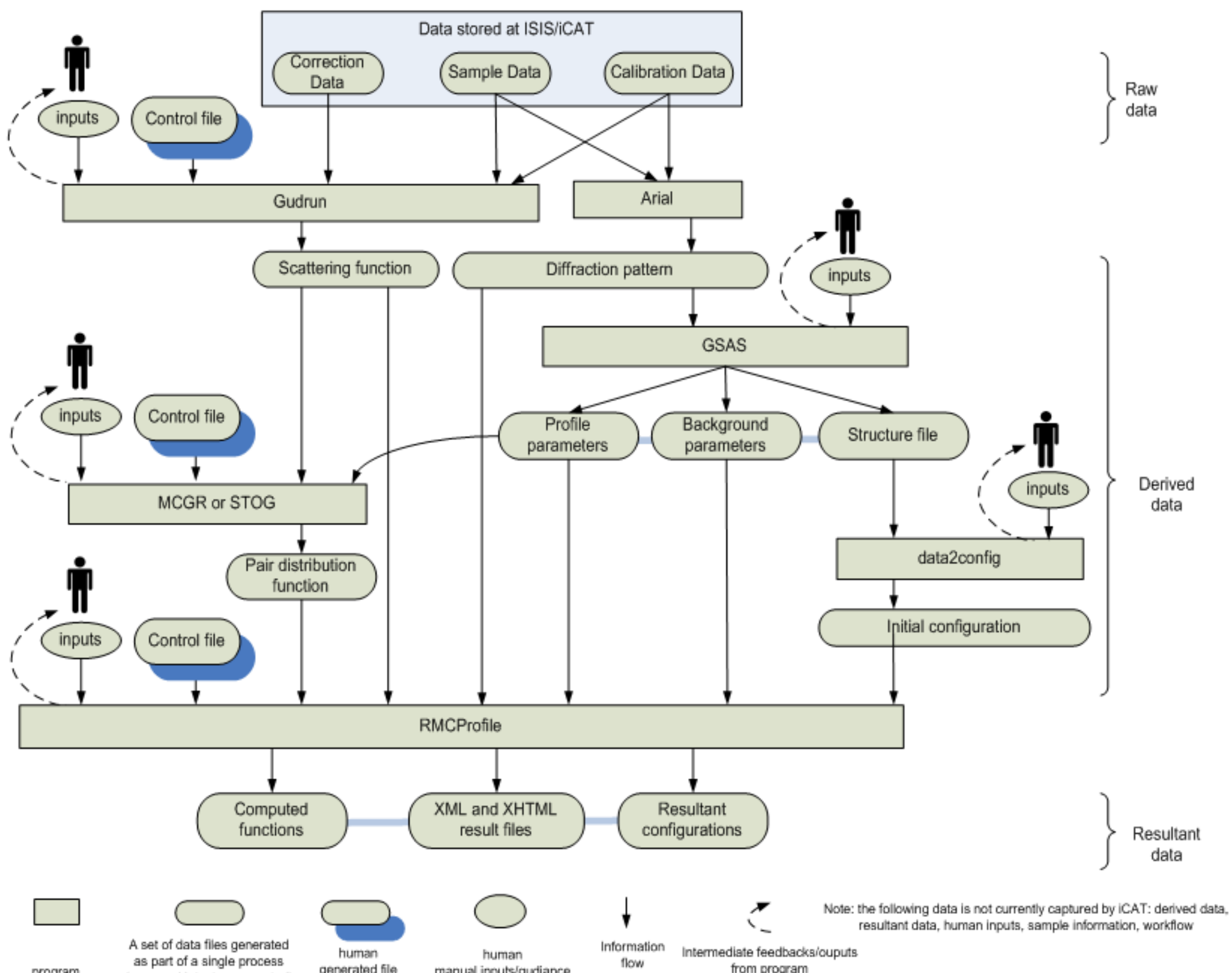
Earth Sciences, Cambridge: Typical workflow



Martin Dove & Erica Yang, July 2010

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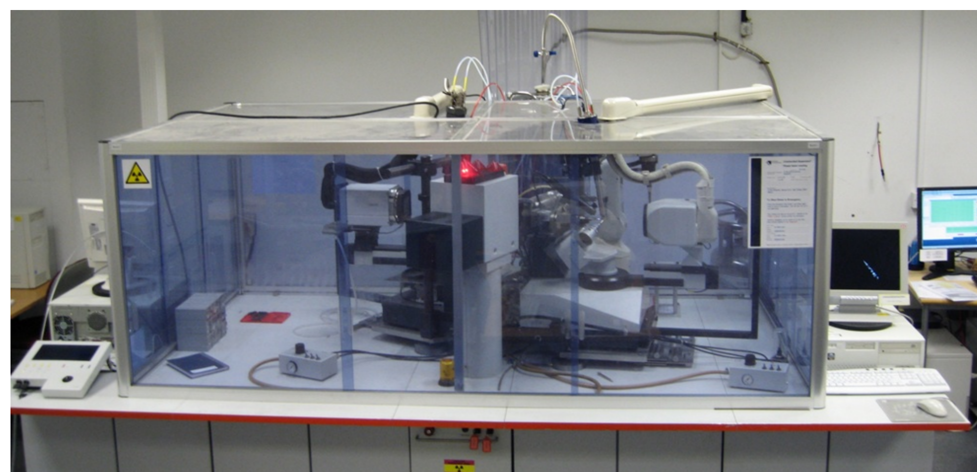
Chemistry, Cambridge

- 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

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

EPSRC NCS: typical workflow

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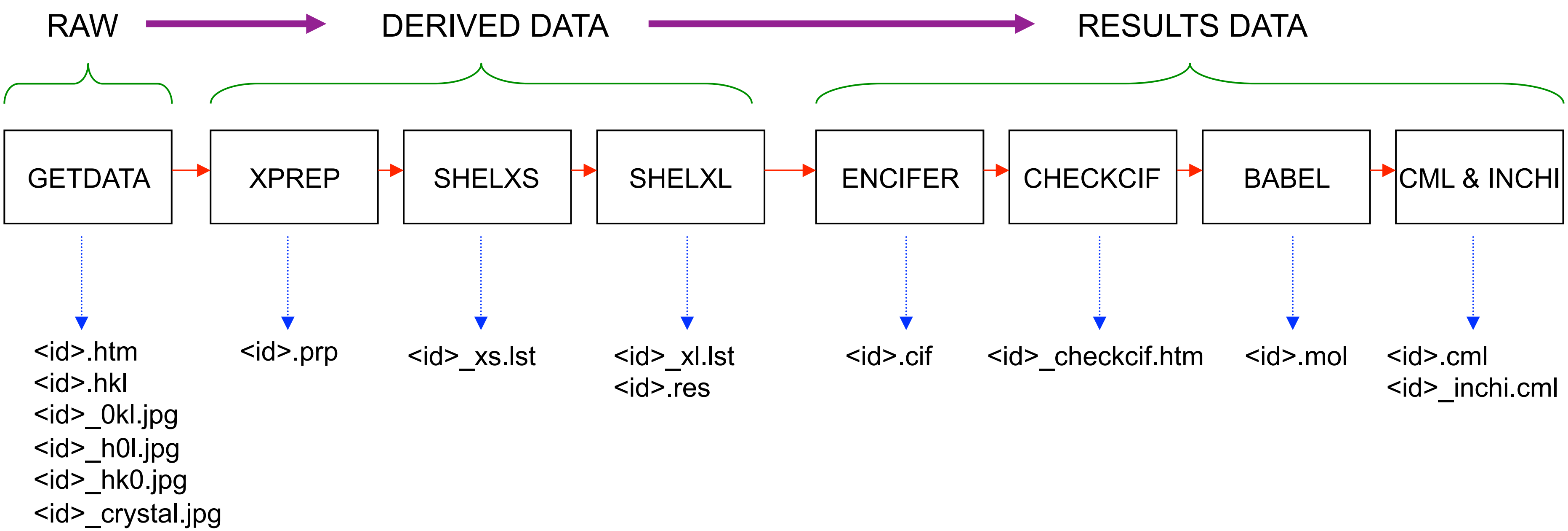

- Initialisation: mount new sample
- Collection: collect data
- Processing: process and correct images
- Solution: solve structures
- Refinement: refine structure

- CIF: produce Crystallographic Information File
- Validation: chemical & crystallographic checks
- Report: generate Crystal Structure Report
- CML, INChI

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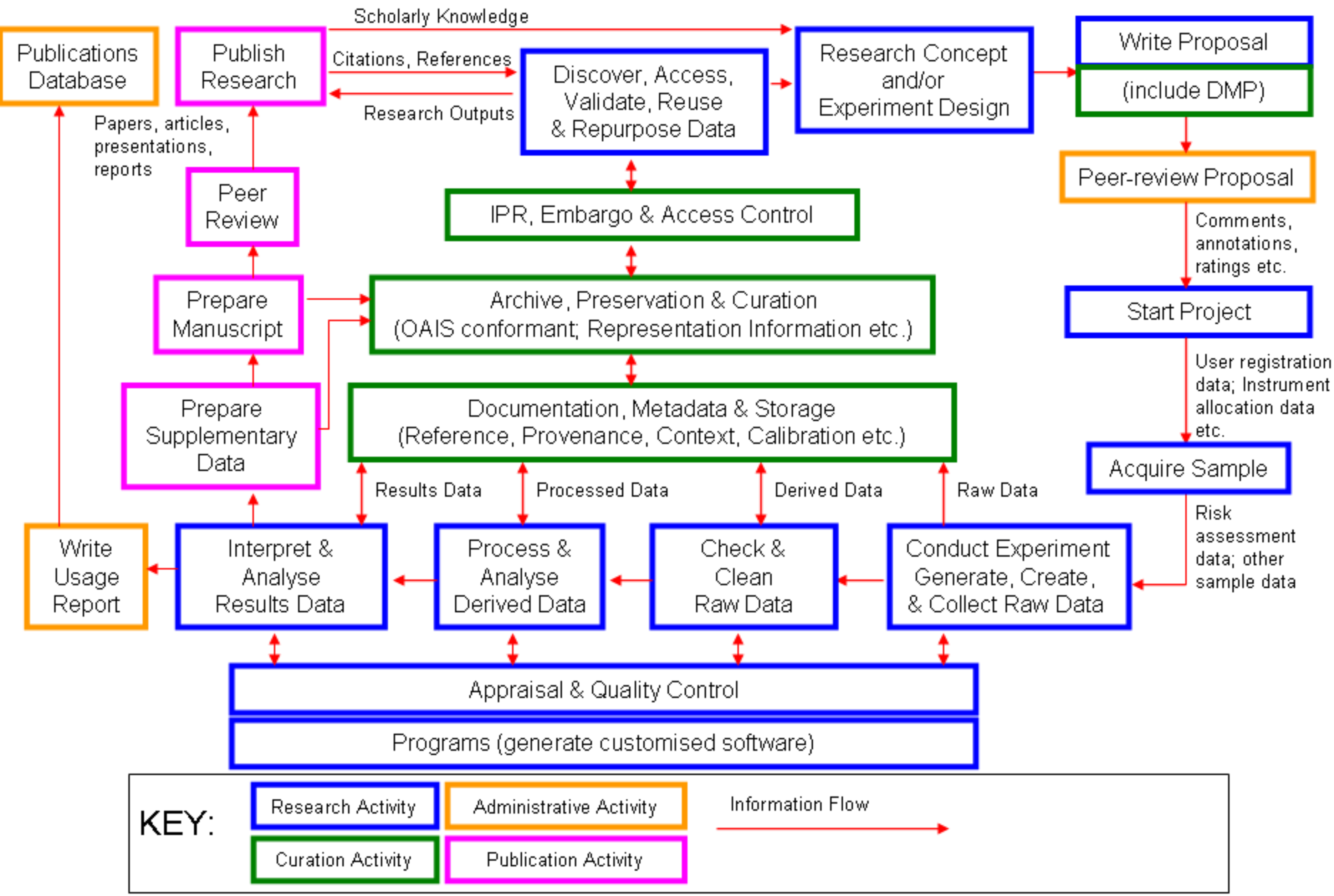
DLS & ISIS, STFC

- 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

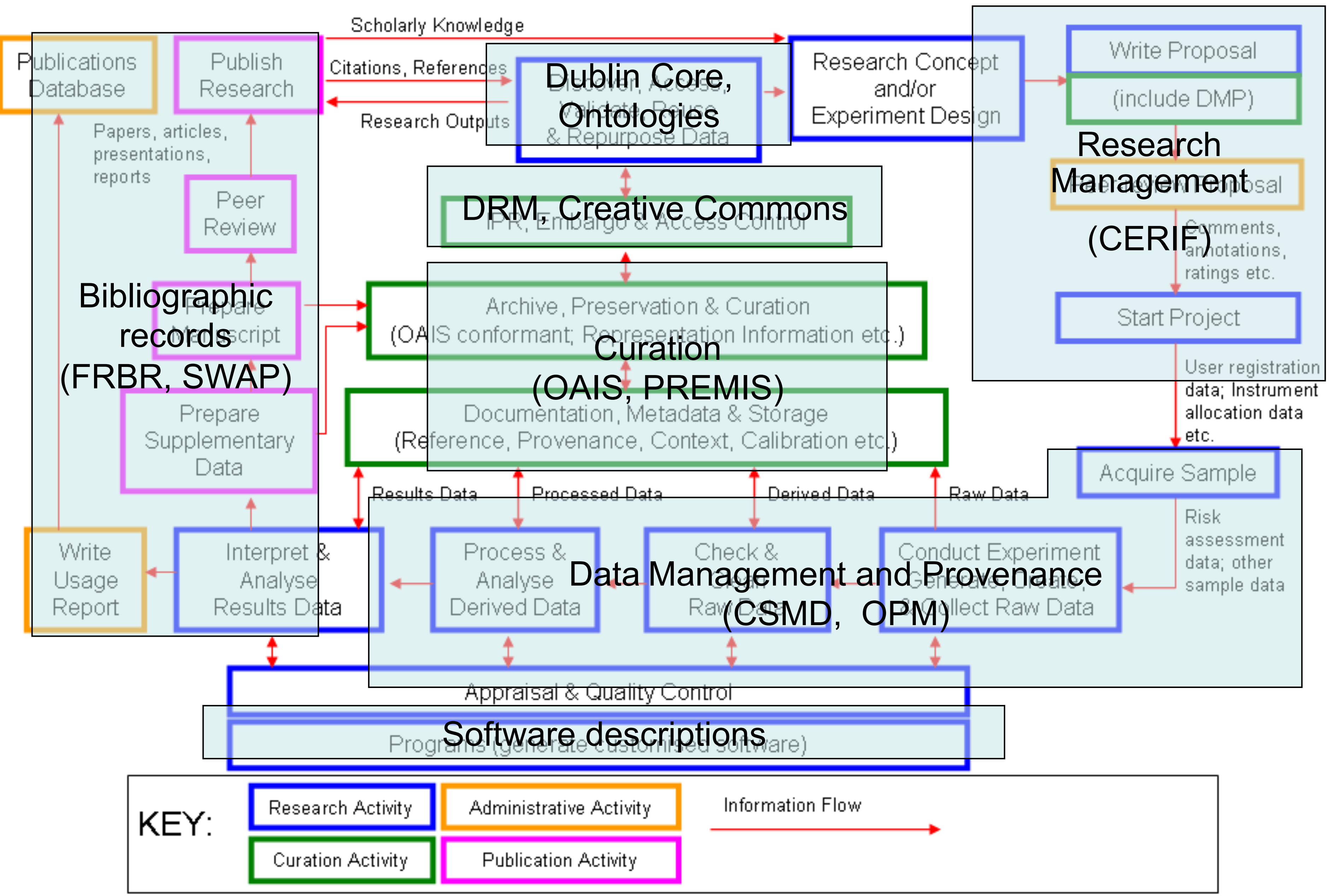
Generalised Requirements

- Basic requirement for data storage and backup facilities to sophisticated needs such as structuring and linking together of data
- Contextual information is not routinely captured
- The actual workflow or processing pipeline is not recorded
- Processing pipeline is dependent on a suite of software
- 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
  - Standardised ERA forms
  - Unique persistent identifiers
- Solutions should be as non-intrusive as possible

An Idealised Scientific Research Activity Lifecycle Model

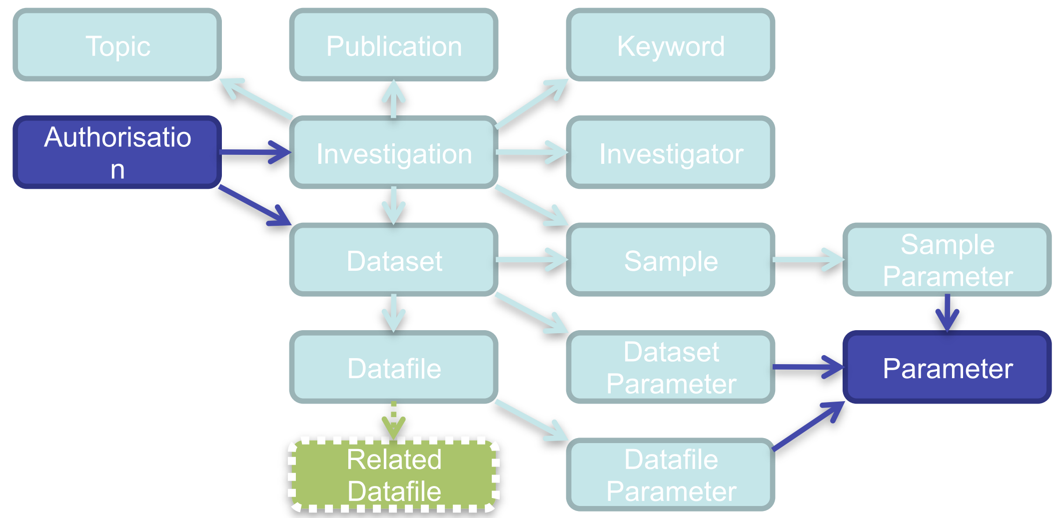


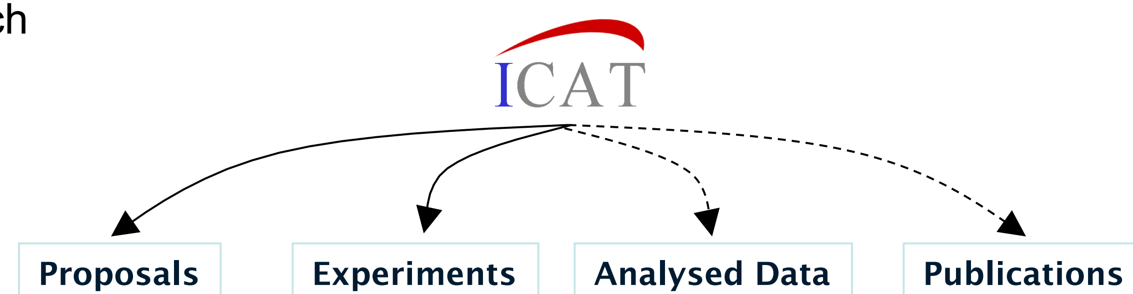
An Idealised Scientific Research Activity Lifecycle Model



Core Scientific Metadata Model

- Designed to describe facilities based experiments in Structural Science
- CSMD is the basis of I2S2 integrated information model
- Forms a basis for extension to:
  - Laboratory based science
  - Derived data
  - Secondary analysis data
  - Preservation information
  - Publication data
- Aim to cover the scientist's research lifecycle as well as facilities data





http://code.google.com/p/icatproject/

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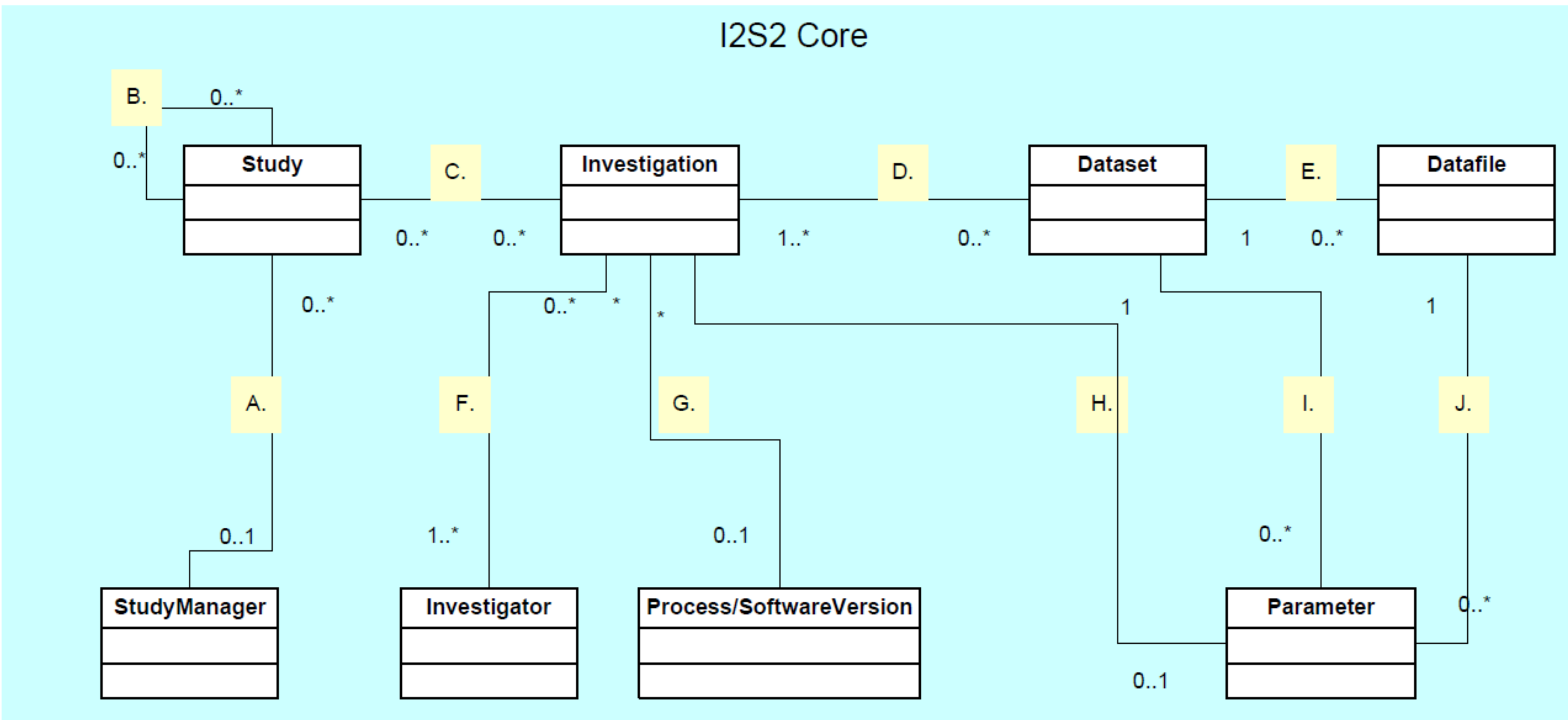
CSMD-Core

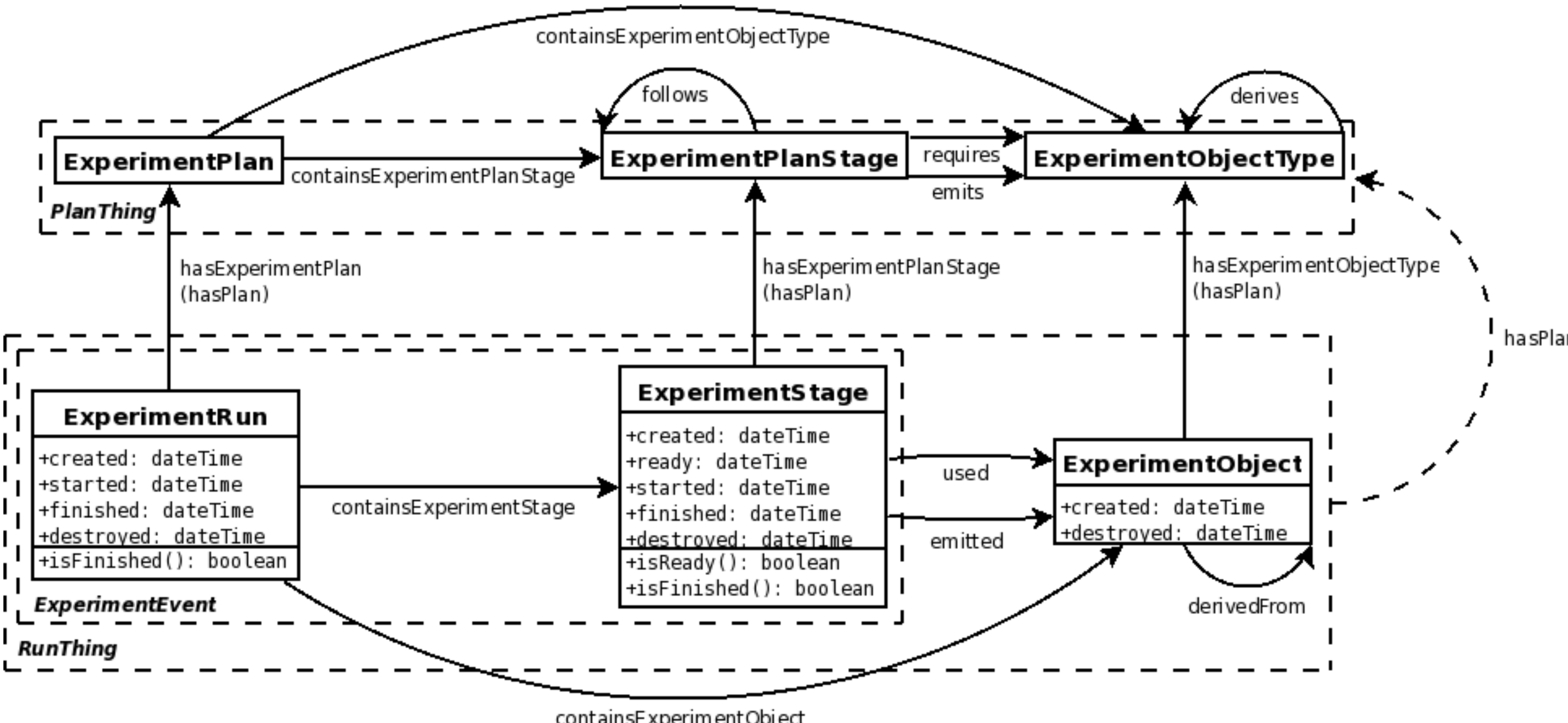
- Removal of facility specific information
- A simple model to describe datasets



Erica Yang, STFC, 2010

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



Mark Borkum, Soton, Feb 2010

I2S2 Integrated Information Model

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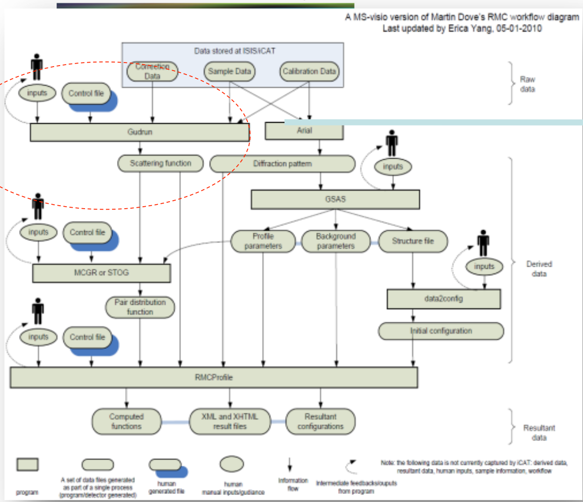
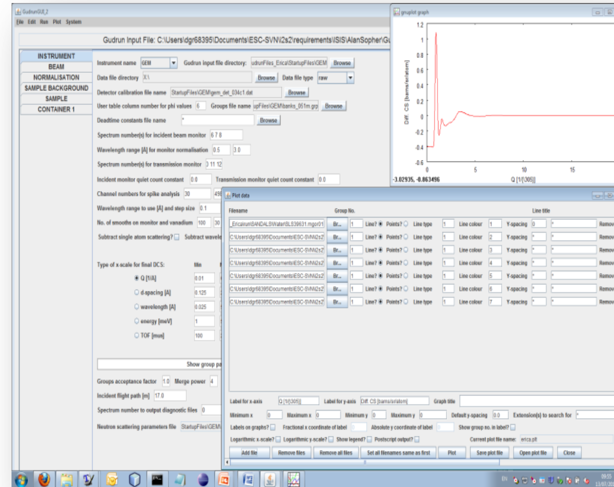
- I2S2-IM = CSMD-Core + oreChem Model
- Use oreChem to describe planning and enactment of scientific process
- Use CSMD to describe the data-sets from the experiment
- I2S2-IM being implemented at STFC in the form of ICAT-Lite
  - A personal workbench for managing data flows
  - Allows the user to commit data
  - Enables capture of provenance information

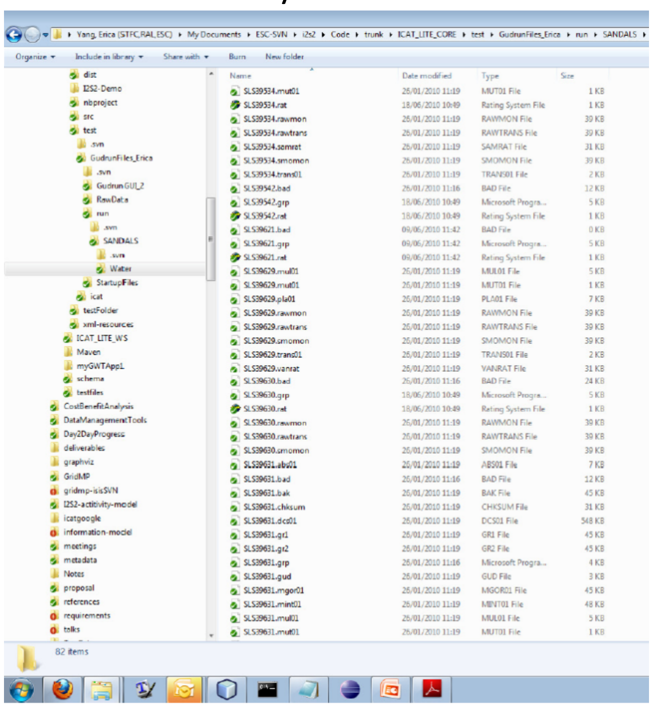
Data analysis workflow

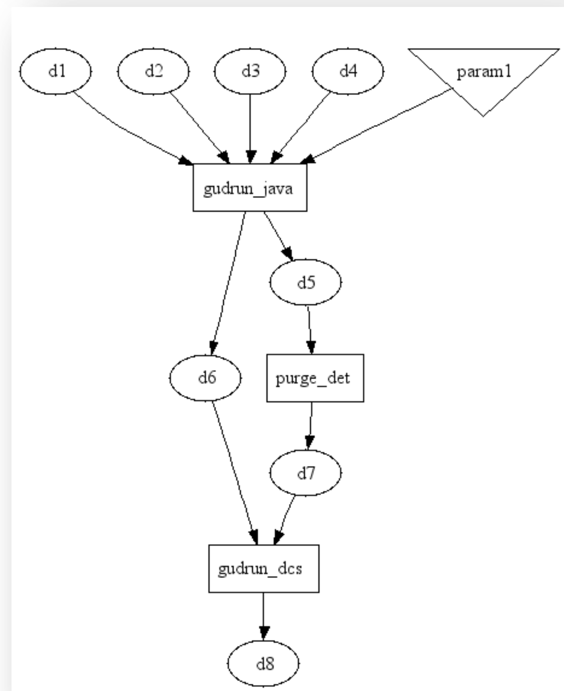


Scientific software: Gudrun



Data analysis folders





Archive
Browse
Restore

Derived Data

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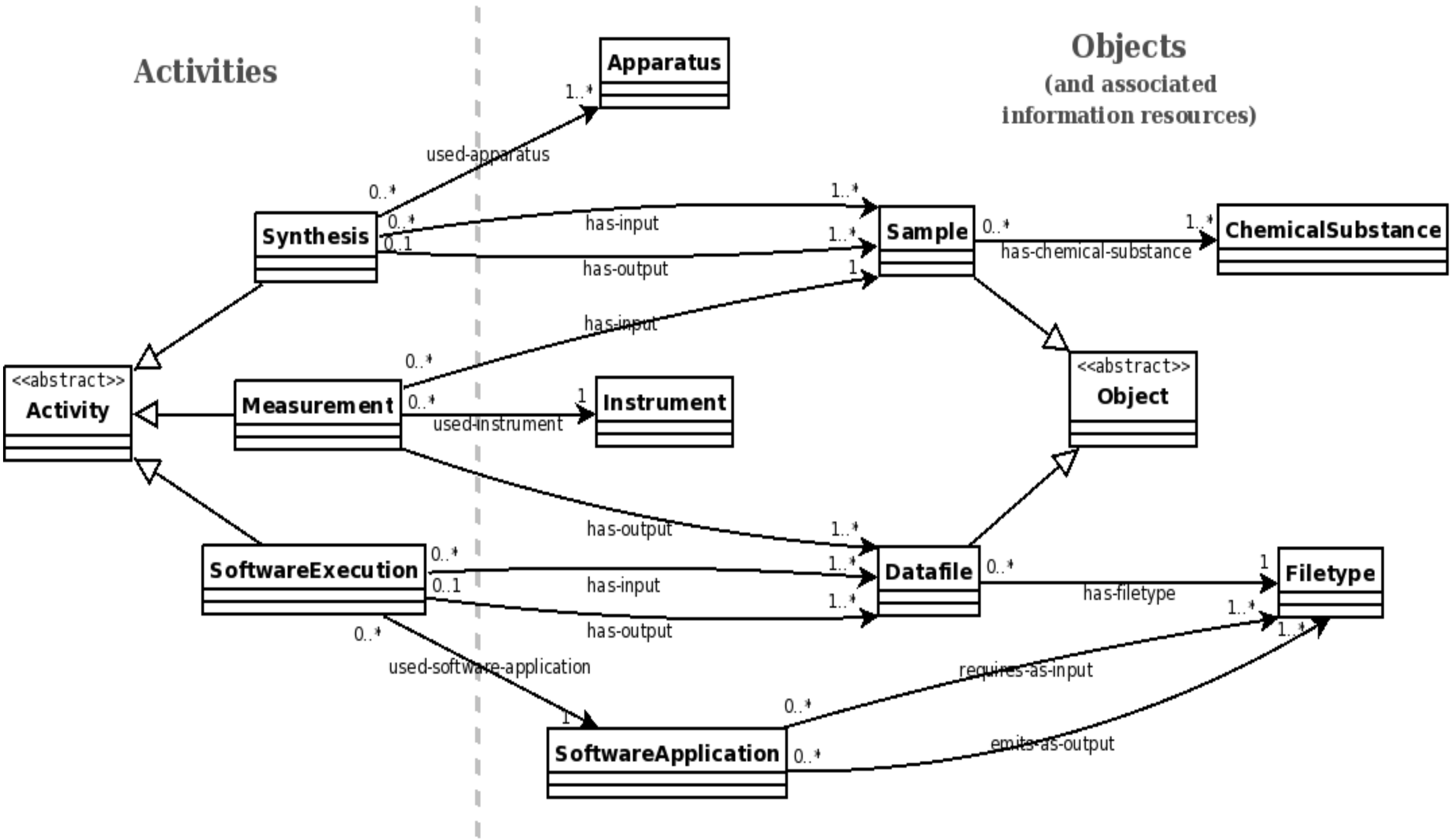
I2S2-IM



Testing the I2S2-IM

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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: Inter-disciplinary issues

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

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Cost-Benefits Analysis

- A before and after cost-benefit analysis using the Keeping Research Data Safe model
- Extending the KRDS Model
  - Focus has been on extensions and elaboration of activities in the research (KRDS "pre-Archive") phase
- Metrics and assigning costs
  - Identification of activities in research activity lifecycle model that will represent significant cost savings or benefits
  - Work to identify 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)

Conclusions

- Considerable variation in requirements between differing scales of science
- At present individual researcher, group, department, institution, facilities all working within their own frameworks
- Merit in adopting an integrated approach which caters for all scales of science:
  - Aggregation and/or cross-searching of related datasets
  - Efficient exchange, reuse and repurposing of data across disciplinary boundaries
  - Data mining to identify patterns or trends
- I2S2 Integrated information model aims to:
  - Support the scientific research activity lifecycle model
  - Capture processes and provenance information
  - Interoperate with and complement existing models and frameworks
- Before and after cost-benefits analysis to assess impact

I2S2
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Project Team

- Liz Lyon (UKOLN, University of Bath & Digital Curation Centre)
- Manjula Patel (UKOLN, University of Bath & Digital Curation Centre)
- Simon Coles (EPSRC National Crystallography Centre, University of Southampton)
- Brian Matthews (Science & Technology Facilities Council)
- Erica Yang (Science & Technology Facilities Council)
- Martin Dove (Earth Sciences, University of Cambridge)
- Peter Murray-Rust (Chemistry, University of Cambridge)
- Neil Beagrie (Charles Beagrie Ltd.)

m.patel@ukoln.ac.uk
http://www.ukoln.ac.uk/projects/I2S2/