Towards Lensfield: data management, processing and semantic publication for vernacular e-science

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Linked Data



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Selling Linked Data

Make it transparent Make it easy



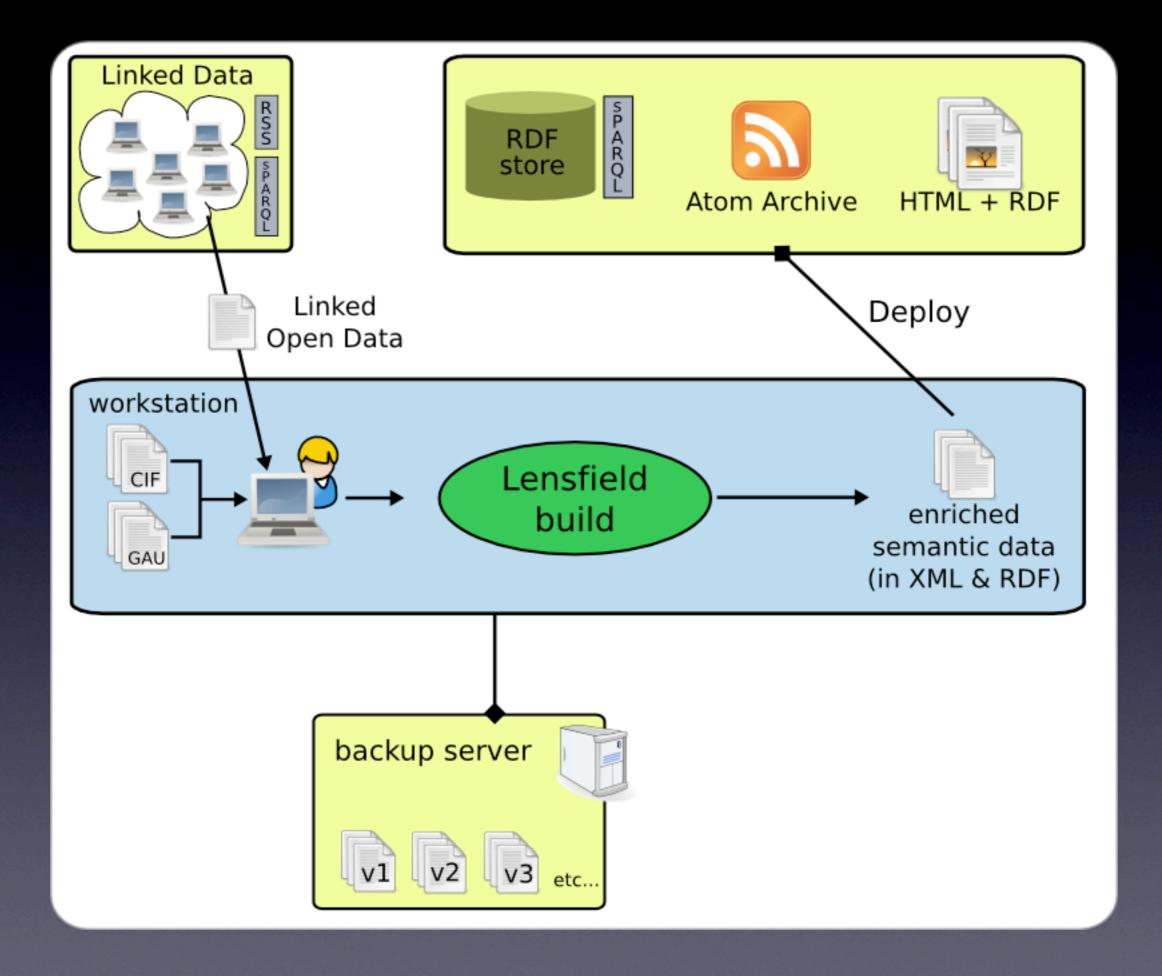
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Selling Linked Data



Selling Linked Data

- Visualizations
- Data management
- Automation





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

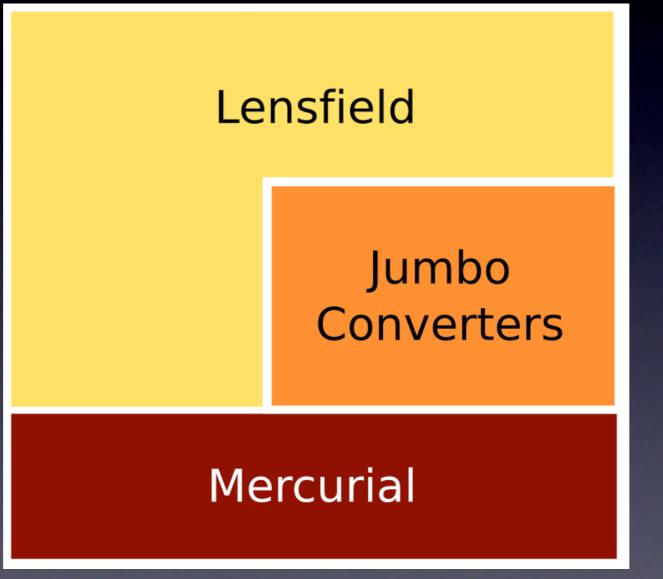
Lensfield Principles

- Make it easier to do the right thing
- Vernacular
- KISS and Embrace constraints

Constraints

- Work on the desktop without infrastructure installation
- Processing tasks could be anything and aren't predictable

Re-use



Jumbo-Converters

- Library of chemistry file format converters, semantifiers and enhancers
- Part of the CML Java libraries
- http://sourceforge.net/projects/cml/

Version Control

Mercurial

- Excellent support for experimentation
- Backup to remote machine
- P2P sharing

- Track script changes with data
- Automatically ignore deterministic intermediates

Build metaphor

- Describing state transitions rather than process better for provenance tracking
- Alternative to graphical programming languages / workflow packages
 - hard problems are re-use and comprehension



Strong on concurrency

- Functional
- Software Transactional Memory
- Lisp
 - Snapshots, pause and resume, continuations

Future Development

- Templated Parameter Sweeps & sensitivity analysis
- Design of Experiments
- Multicore performance testing
- Grid processing



http://fascinator.usq.edu.au/

Users

CLARION project

- Embargo management and publication of Electronic Lab Notebook data.
- OREChem
 - Distributed chemistry eScience using Linked Data.
- Computational Chemical engineering

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Users

You?

Thanks

Colleagues Nick Day John Aspden Lezan Hawizy Peter Murray-Rust

Funds





Collaboration and Inspiration Nico Adams (Dept of Genetics, Cambridge) Jerry Winter (Unilever) Noel Ruddock (Unilever) Markus Kraft, Weerapong Phadungsukanan (Chemical Engineering, Cambridge)