Mantid and SNS software development

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NEUTRON SCIENCES

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Neutron Data Life Cycle

DAS
- Neutron events
- Events from sample environment
- Other triggers

Reduction
- Corrected reduced data (histograms, S(Q,E), ..)
- Merging, reconstruction of data
- Instrument/technique dependent
- Need for 'real' time reduction

Analysis
- Multi dimensional fitting
- Advanced visualization
- Comparison to simulation / feedback
- Field dependent, large variety of approaches

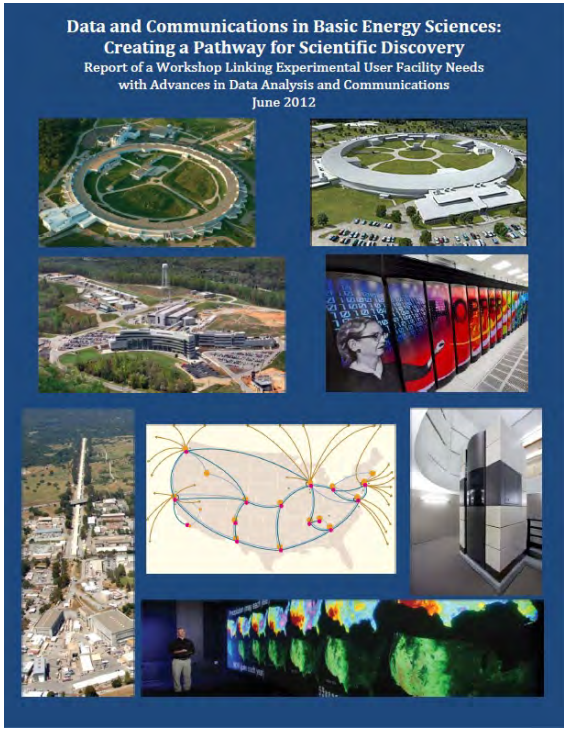
Simulation Modeling
- Multitude of techniques (DFT, MD, ..)
- Advanced simulation of experiments
- 'Refinement' using experimental data
- Multiple experiments / probes

User Facility

- **Variety of experiments, topics, methods and 'computer literacy' of users are significant challenge.**

Creating a Pathway for Scientific Discovery

- **Accelerating discovery in materials science**
- **Enhancing predictive capabilities**



- Theory and analysis components should be integrated seamlessly within experimental workflow.
- Move analysis closer to experiment – future possibility of experiment steering.
- Match data management access and capabilities with advancements in detectors and sources.

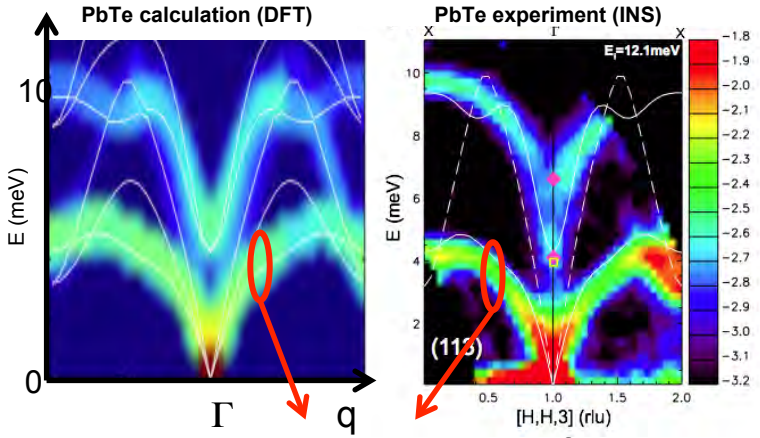
ADARA is enabling real-time feedback from experiment, analysis and computational steering

ADARA

- Leverages our multi-disciplinary capabilities at ORNL coupling Neutron Sciences Directorate with Computing and Computational Sciences Directorate.
- The ADARA Project lets us stream data to computational resources and provide live feedback from experiment in real-time S(Q,E).
- Provides a high performance data backplane for reduction, analysis, and coupling with simulation forming the basis for future work to integrate experiment and simulation.
- Prototype running on HYSPEC instrument. Deployment to other beamlines in 2013/2014.

ORNL has launched the Center for Accelerating Materials Modeling (CAMM)

- The CAMM will integrate materials modeling/simulation (MD/DFT) directly into the chain for neutron scattering data analysis, **offline** and **online** (in near real time)
- Developing workflows for refinement, integration of MD codes, **neutron scattering corrections** ..
- The CAMM is working with ORNL's Materials Science and Technology Division to study coarse grained MD simulations of polymers PEO-AA (CNMS), *ab-initio* MD simulations for ferroelectrics/thermoelectrics



Example: *ab-initio* MD simulations for ferroelectrics/thermoelectrics. Focus on *width* of dispersions

The Center for Accelerating Materials Modeling (CAMM)

- *Partnership between ORNL's Neutron Sciences, Physical Sciences and Computing and Computational Sciences Directorates*
- *ORNL SEED money and DOE funds provided to study force field refinement from quasi-elastic and inelastic neutron scattering data*
- *CAMM formed in response to BES proposal call for* Predictive Theory and Modeling

International Software projects

The Mantid Model

Nick Draper

Tessella

www.mantidproject.org

Tessella
Technology & Consulting

SNS
SPALLATION NEUTRON SOURCE

Science & Technology Facilities Council
ISIS

Project Goals

- Goals
  - Consolidate the data reduction/analysis software for neutron scattering without restricting the needs of the instrument scientists

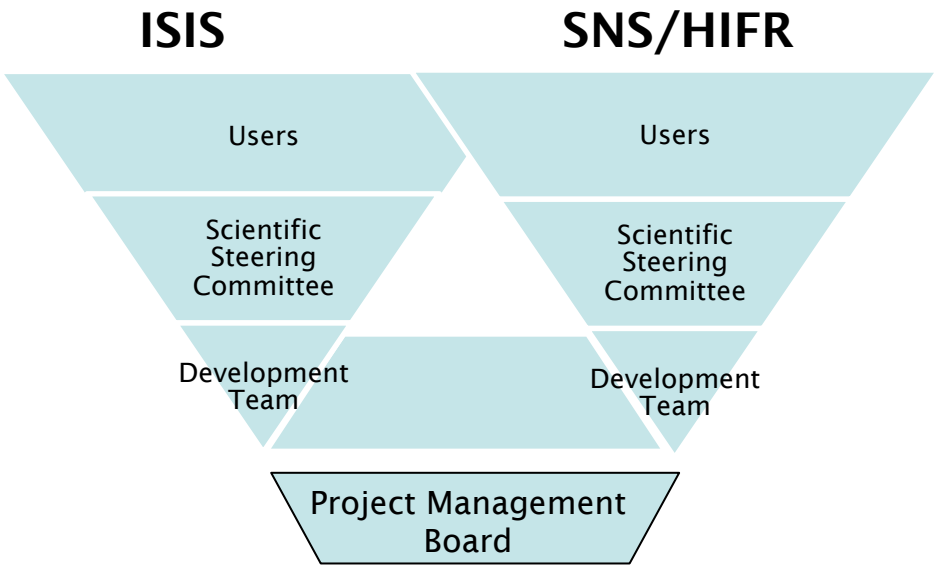
- Key requirement
  - Create a Data Analysis framework
    - not instrument or technique/dependent
  - Cross-platform
    - Windows, Linux, Mac
  - Easily extensible
  - Open source

A Selection of Risks

- Lasting engagement with a large number of stakeholders
- Design needs to support flexibility for future needs
- Technical single point of failure
- Development continuity across the team
- Larger development teams are less efficient
- Testing and deployment takes time & Active development can affect robustness

Lasting engagement with a large number of stakeholders

- Project Organisation
- Active project sponsors
- Frequent releases
- Responsive to change

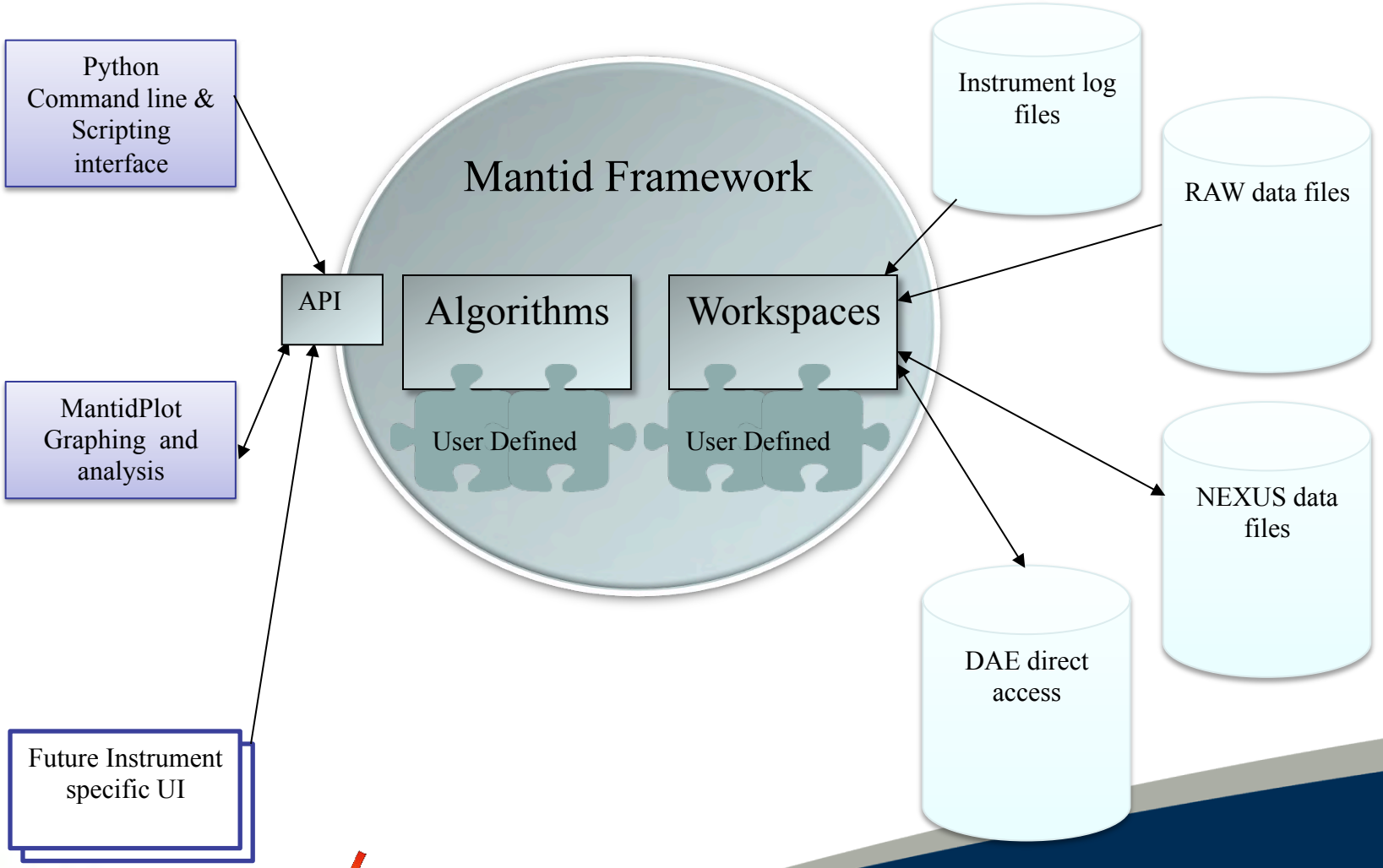


Mantid

SNS SPALLATION NEUTRON SOURCE

Science & Technology Facilities Council ISIS

Architectural Design - Overview

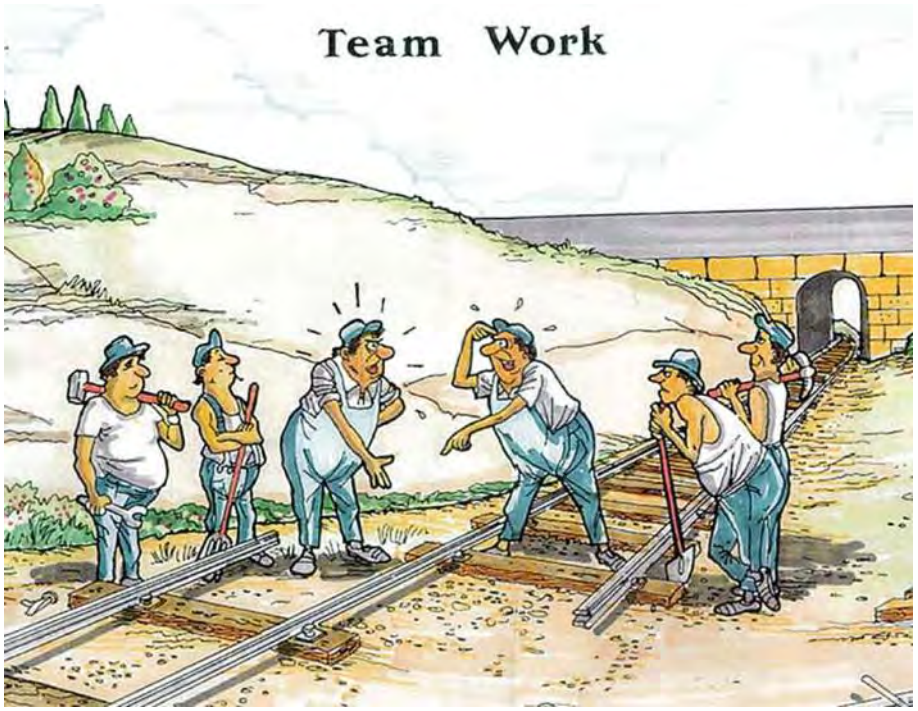


Preventing single points of failure

- No “Code Ownership”
  - Functionality protected via unit tests
- Mobile development talent
- Sub project teams to focus on significant developments
- Knowledge transfer
  - Daily & focused skype meetings
  - Code reviews
  - Architectural and detailed design documentation
  - Developer documentation
  - Annual developer meetings

Development continuity across the team

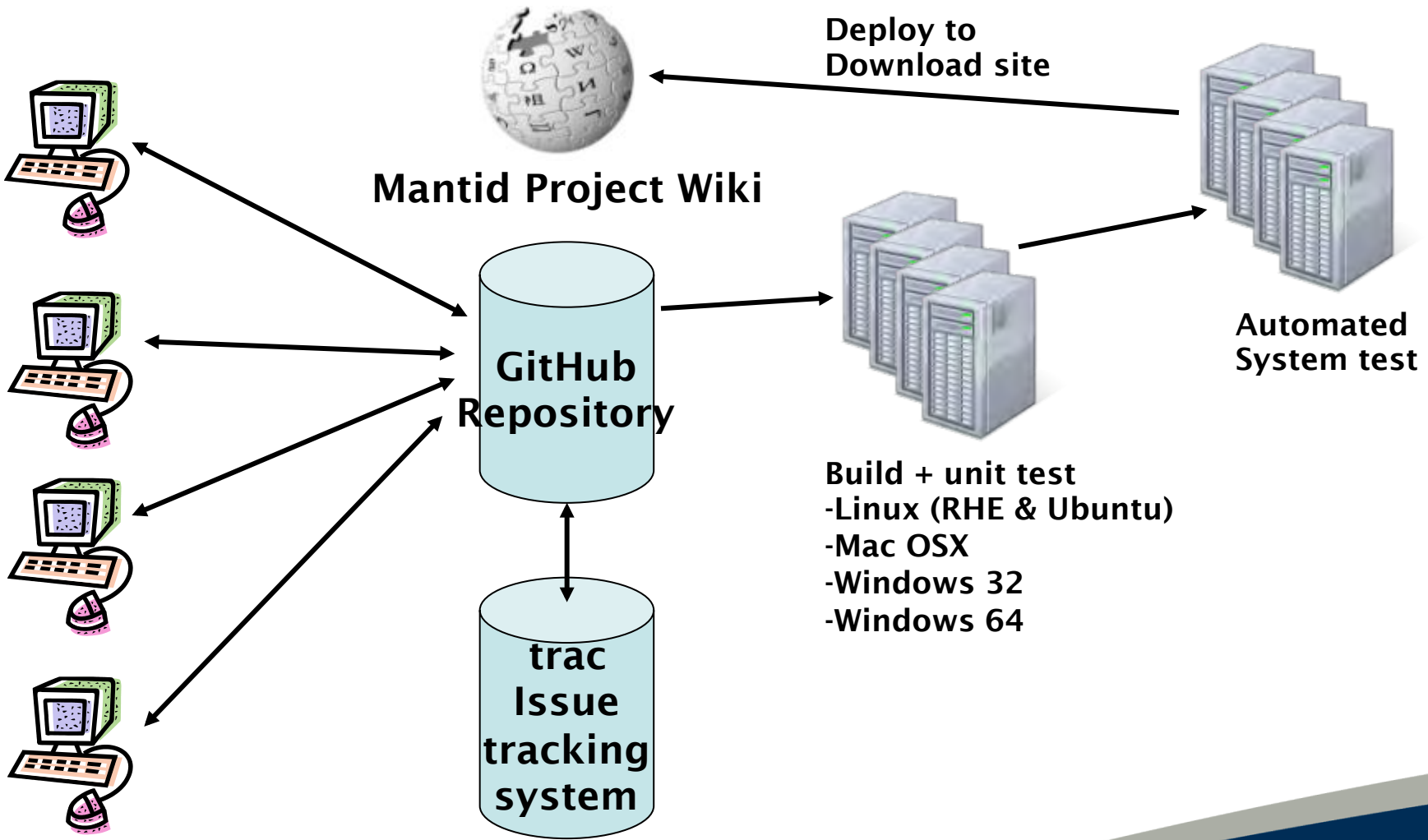
- Coding standards
  - Sensible
  - Agreed
- Shared code ownership
- Support within the team
  - Mentoring
  - Training
- Design and code reviews
- Developer meetings



Larger development teams are less efficient

- Automate repetitive tasks
  - Saves time
  - Ensures they happen
- Optimize meeting time
  - Control attendees at meetings
  - Use the right technology
    - Daily skype chat meetings
  - Ensure the right people talk together
- Use tools to prevent duplicated work and missed tasks
  - Development
  - Testing

Continuous Integration Environment



Thank you ..