The Mantid Project: Notes from an international software collaboration

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Overview

- Mantid Introduction
- Why collaborate?
- Collaboration Models
- ISIS - SNS & HFIR collaboration
  - Organisation
  - Benefits
  - Lessons Learned

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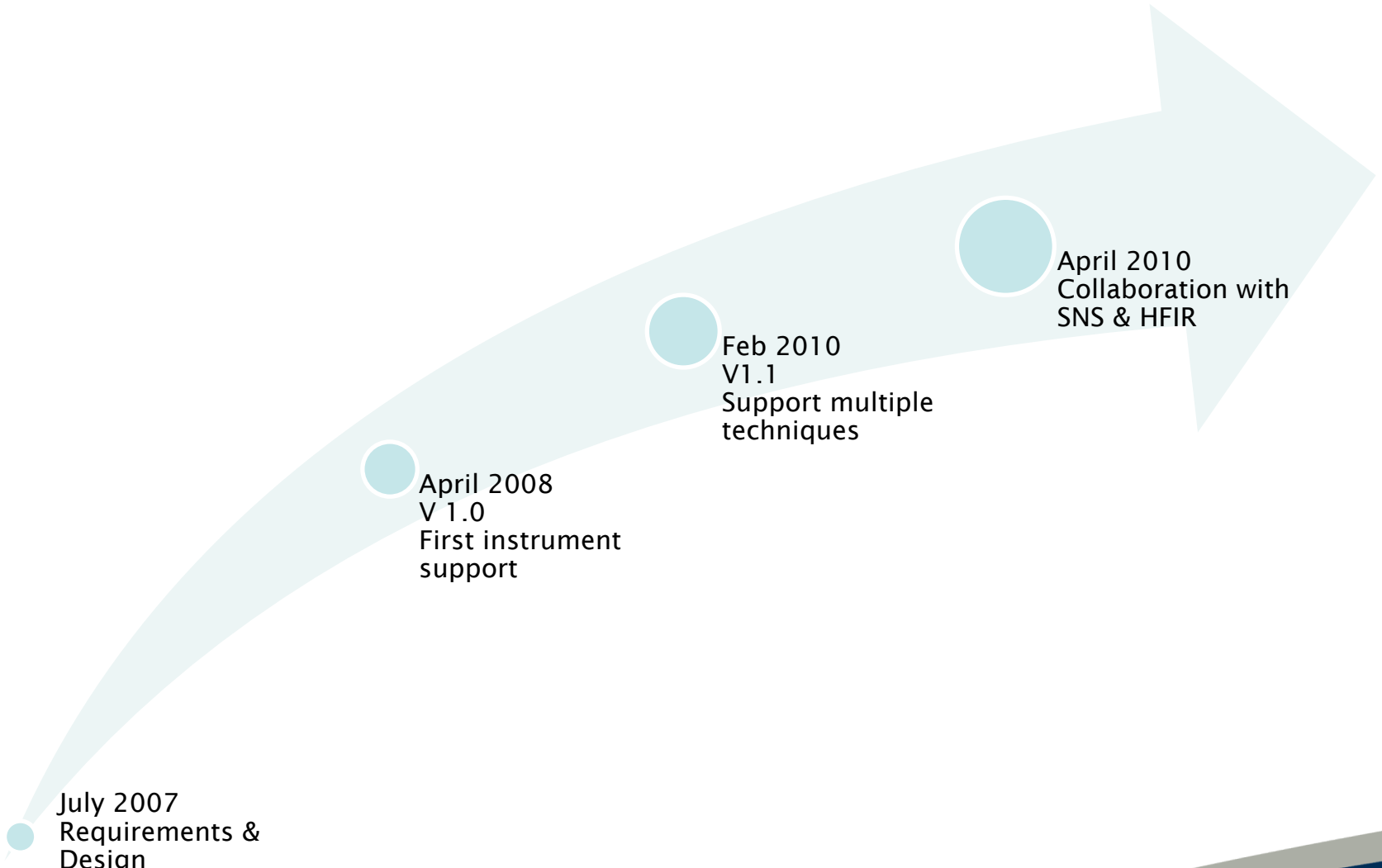
Project History



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Project Goals

- Goals
  - Consolidate the data 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
  - Freely redistributable

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Framework vs individual applications

- Less time spent developing input and output routines
- More time on scientific algorithms
- Cross benefits from other groups
- Lower support requirements
- Better documentation and training
- Fewer single points of failure
- Structure for further developments

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Framework flexibilty

- Instrument independence
  - Virtual instrument defined
    - Loaded from xml definition
      - Location, rotation and shape of every pixel
      - Sample
      - Source
- Technique independence
  - Algorithms
    - Unit Reduction and analysis steps
  - Workflow scripts
    - Chain algorithms to perform a reduction workflow

Framework flexibilty

- Plug in extensions
  - Common
    - Algorithms – C++ or Python
    - Instruments
    - Workflow scripts
    - Custom user interfaces
    - Custom algorithm dialogs
  - Less frequent
    - Workspaces
    - Units
    - Optimisation
      - Functions & models
      - Optimisers & cost functions
      - Constraints

Open Source

- GPL v3
  - Free to use
  - Source code openly available
  - Results cannot be sold
    - Unless you own the copyright
- Good basis for collaboration
- Sharing benefits to wider community
- Why not LGPL, BSD etc?

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Future Development Scope

- Reduction
- Analysis
- Spallation & Reactor
- Technique support
  - Inelastic
    - Direct
    - Indirect
  - Diffraction
    - Powder
    - Engineering
    - Single Crystal
    - Diffuse scattering
  - Disordered Materials
  - Large Scale Structures
    - Small angle
    - Reflectometry
  - Muons

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Collaboration Benefits

- Why Collaborate?
  - Solve big problems
  - Cover a wide scope
  - ↑ access to skills and talents
  - Reduce costs
  - Access to existing code
  - Improved support
- All parties should benefit

Collaboration Challenges

- Why Collaborate?
  - Larger development team
  - ↑ induction
  - ↑ communication
  - ↑ project structure
  - Generic solutions take time
  - ↑ documentation

- It is important to minimise these effects

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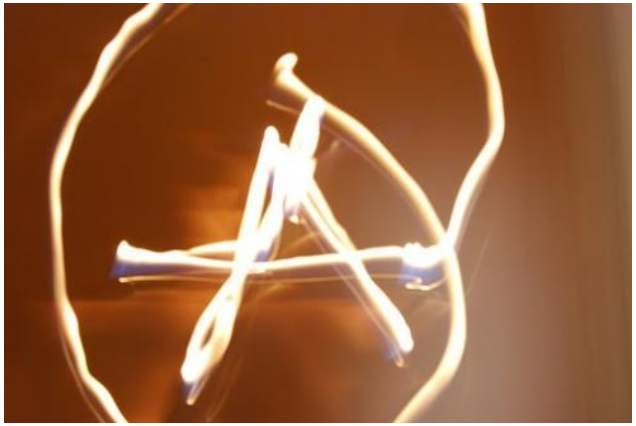
Collaboration Models

- Many possible models
- Several used within Mantid
  - Open contributions - Informal Anarchy
  - User donated code
  - Joint distributed team
  - Application integration
- Important to pick the right model for the situation

Open Contributions - Informal Anarchy



- Key Features
  - People choose their own priorities
  - Anyone can submit code
  - Immediately available to all
- Advantages
  - Very lightweight
- Drawbacks
  - Negative effect on quality
  - Likely to repeat work
- Use in Mantid
  - User script library

User donated code

- Key Features
  - Users submit code to the dev team
  - Dev team adopt the code
    - Review & Refactor
    - Test
    - Document
- Advantages
  - High quality additions to functionality
- Drawbacks
  - Significant dev team involvement
- Use in Mantid
  - User supplied algorithms and key scripts

Joint distributed team

- Key Features
  - Single project management lead
  - Geographically separated, but joint dev teams
- Advantages
  - Consistent, planned development
  - Increased support hours
- Drawbacks
  - Increased communication
  - Initially introduction of a whole dev team
- Use in Mantid
  - ISIS – SNS Development

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Application integration

- Key Features
  - Integration with well known tools
  - Smooth transfer to/from Mantid
  - Rapid increase in functionality
- Advantages
  - Can be simple file format support
  - Avoids reinventing the wheel
- Drawbacks
  - Imperfect user experience
  - Lack of direct control
- Use in Mantid
  - GSAS, Fullprof & other tools

ISIS - SNS & HFIR collaboration

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SNS Collaboration Timeline

- March 2009 - ICNS 2009
  - Initial meeting & discussions
- Oct 2009 - Due Diligence visit
  - Week with the development team
  - Discussions with several scientist users
  - Future plans
  - Areas of common interest
- Jan 2010 - Go / No Go decision
- Apr 2010 - Memorandum of Understanding
- May 2010 - Joint development begins
- Aug 2010 – Initial SNS & HFIR support

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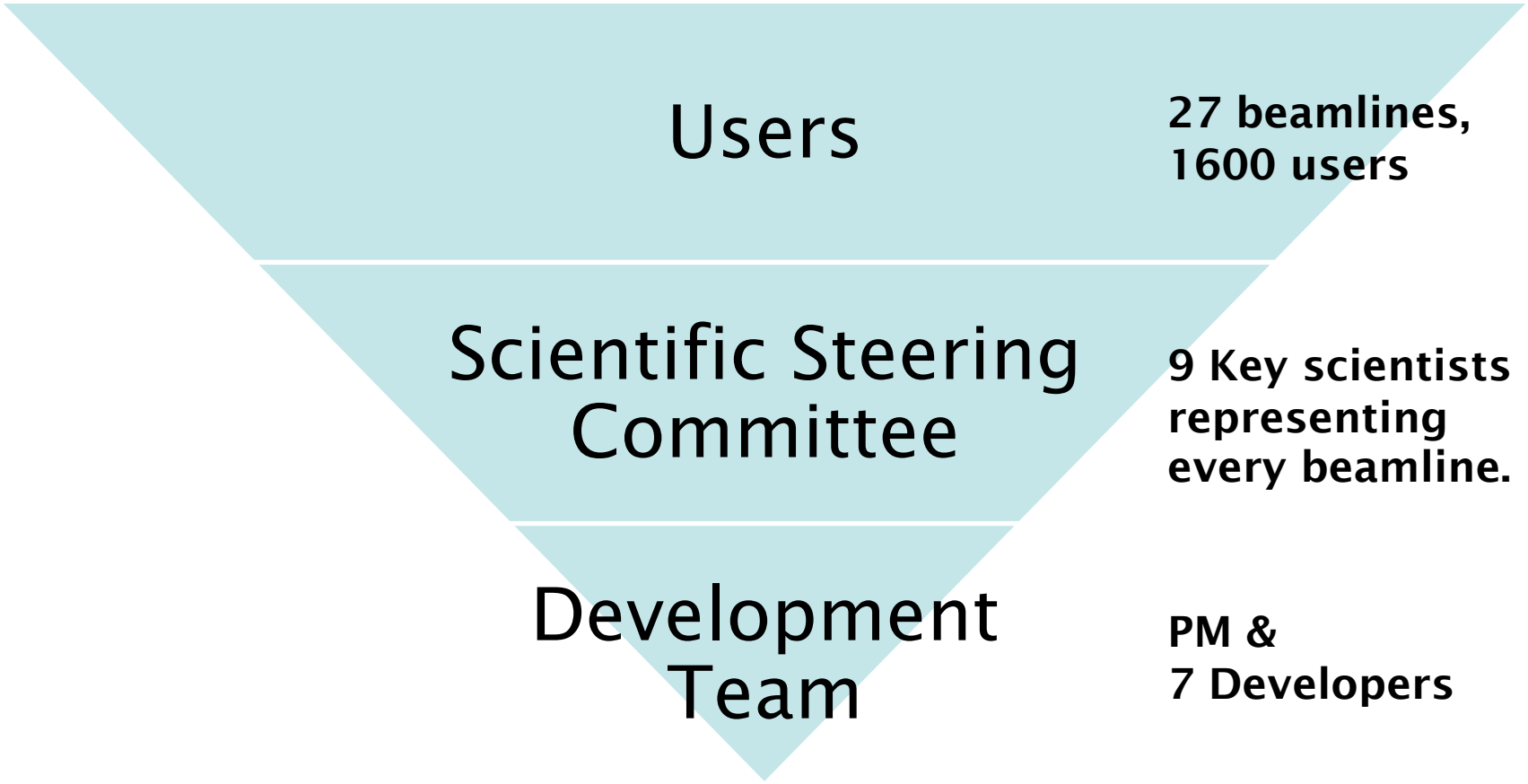
Previous Project Organisation



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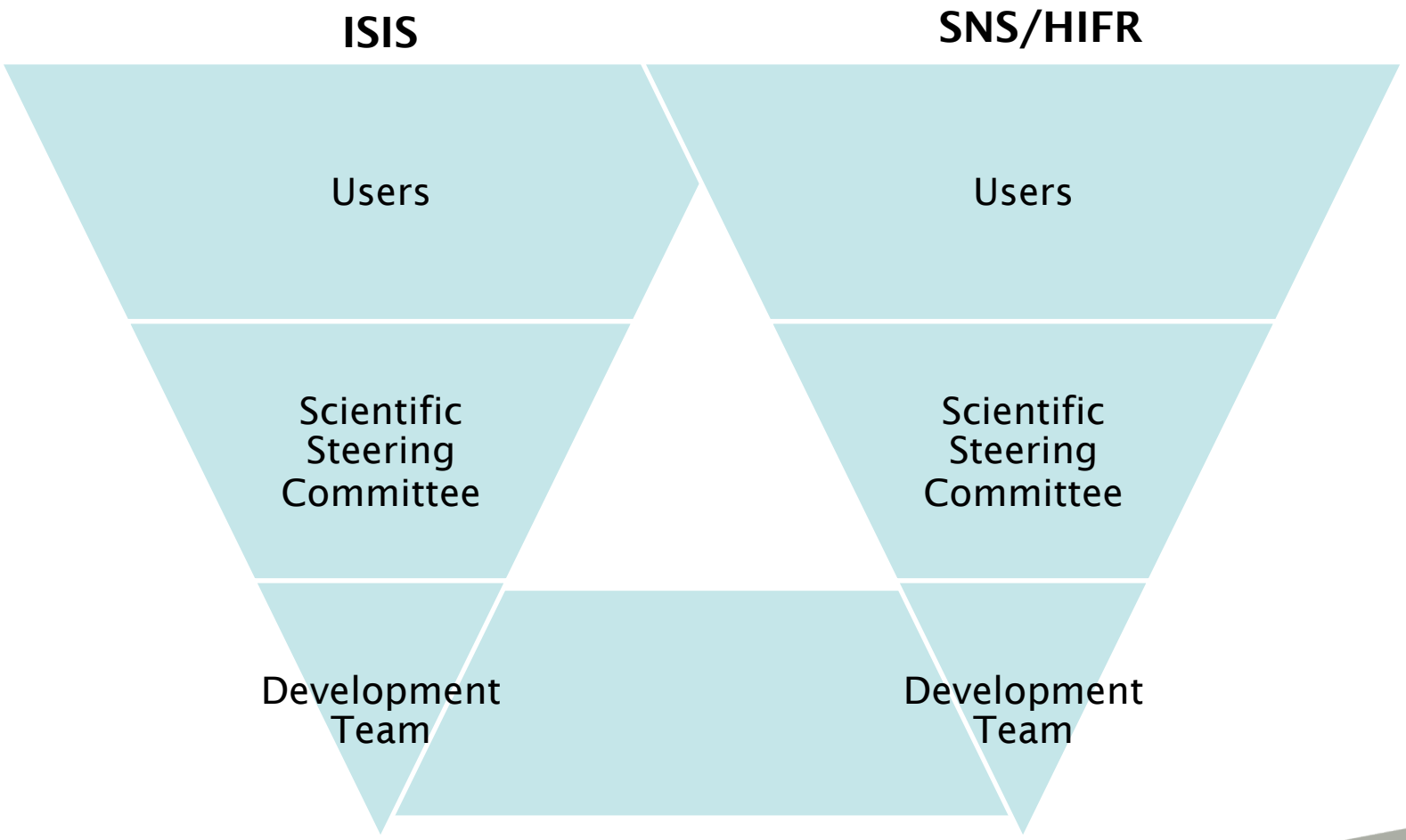
Project Organisation



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Team Structure

- Joint project management board
- Two scientific steering committees
- One project manager
  - Control overall project direction
  - Final point of decision making
- Local Development Team Leaders
- One Development Team
  - 7 FTE staff at ISIS
  - 9+ FTE staff at SNS and still growing

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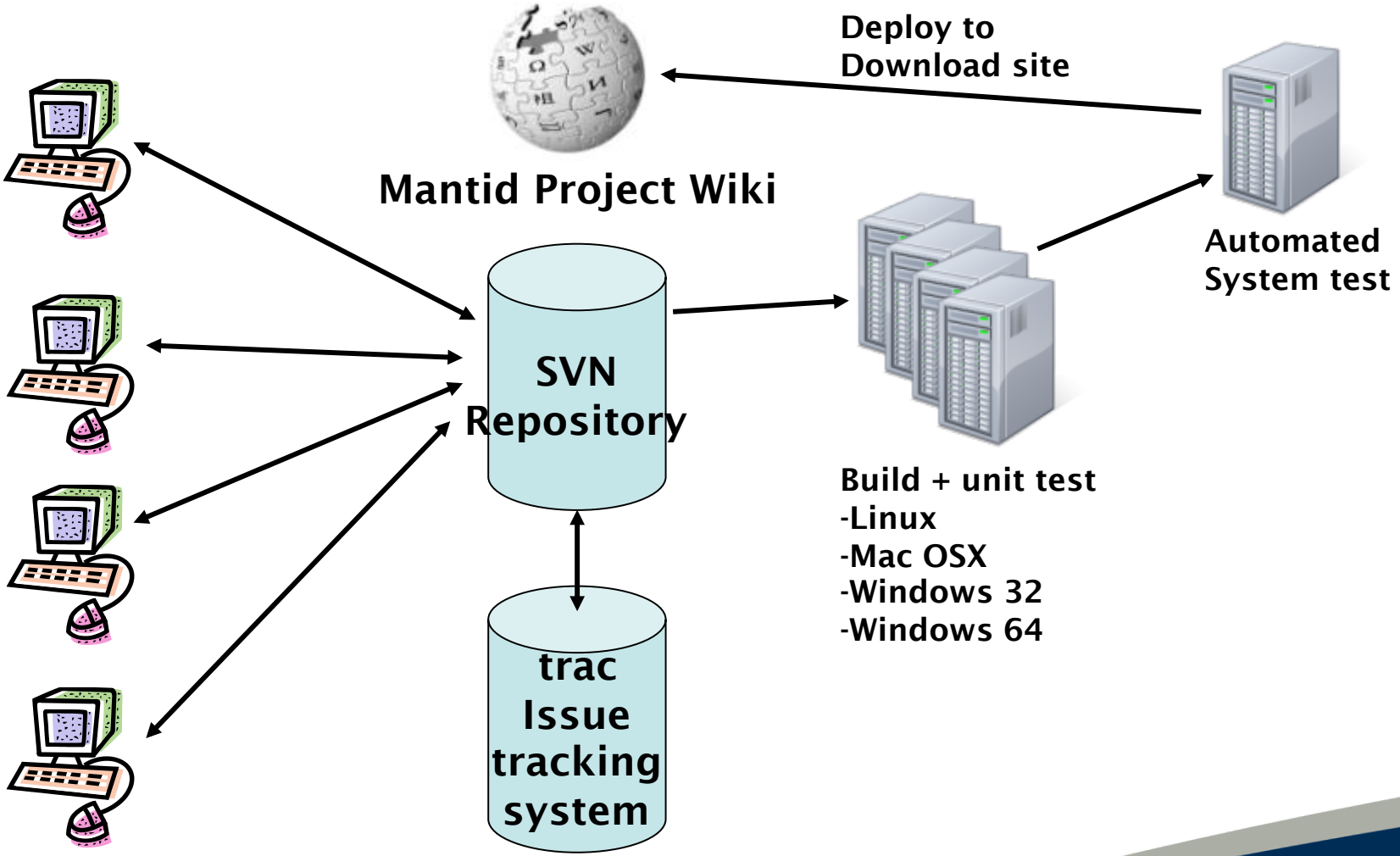
Continuous Integration Environment



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Communication

- Face to face meetings
  - PM 3-4yr
  - Developer visit program
  - Developer workshops
- Developer Transfer
  - ISIS lead developer transferred to US
- Easy communication channels
  - Developer email list
  - Skype
  - Phone
  - Screen sharing
  - Video conferencing

ISIS -> SNS wins

- Robust framework
  - Common development structure
  - Multithreaded performance
  - Documentation and training
  - Automated build, test and deployment
- Algorithms
  - Over 100 algorithms already developed
- Development support

SNS -> ISIS wins

- Improvements to build process
  - Cmake, Hudson
- Event Workspaces
- Event Filtering
  - Currently by time
  - Will expand
- Improved python code framework
- New file format support
  - NxSPE
  - Event Nexus

Lessons Learned

- Developer documentation
  - Need to rapidly induct several new developers
  - Will not be good enough
- Communication
  - Has to be encouraged
  - Will take some time
- Personal relationships
  - Are key to working together in a team
- High level support is essential
- No two facilities are the same
  - Archive structure
  - Information catalog

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Lessons Learned

- Minor irritations
  - You may have learned to live with them
  - Will be much more irritating to new developers
    - Make use of this enthusiasm
- Development Environments
  - Will differ across facilities
  - Set up can be painful
  - Don't let issues linger
- Design
  - Consider implications
  - Design for flexibility

Further Information

- Project Web Page
  - www.mantidproject.org

- Project Introduction Document
  - http://svn.mantidproject.org/mantid/trunk/Documents/Requirements/Project%20Introduction%20Document.doc
- User Requirements Document
  - http://svn.mantidproject.org/mantid/trunk/Documents/Requirements/URD.doc
- Architectural Design Document
  - http://svn.mantidproject.org/mantid/trunk/Documents/Design/Architecture%20Design%20Document.doc

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Questions, Comments, Opinions?

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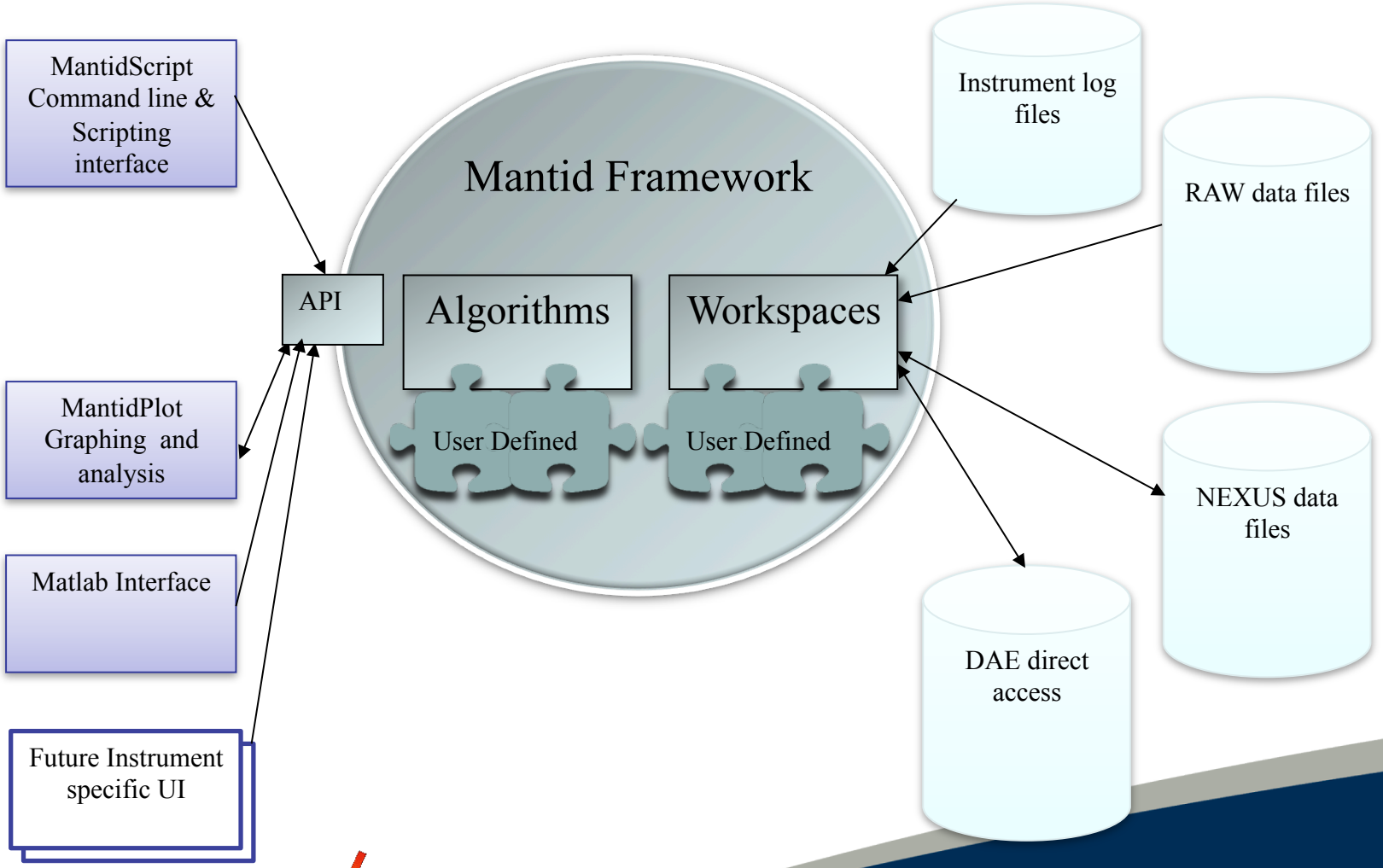
Architectural Design - Overview



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