NCNR Raw Data Archive System

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- Facility Overview
- Data Management Considerations
- Evolution of the archive
- Archive Construction and Operation
- Lessons learned

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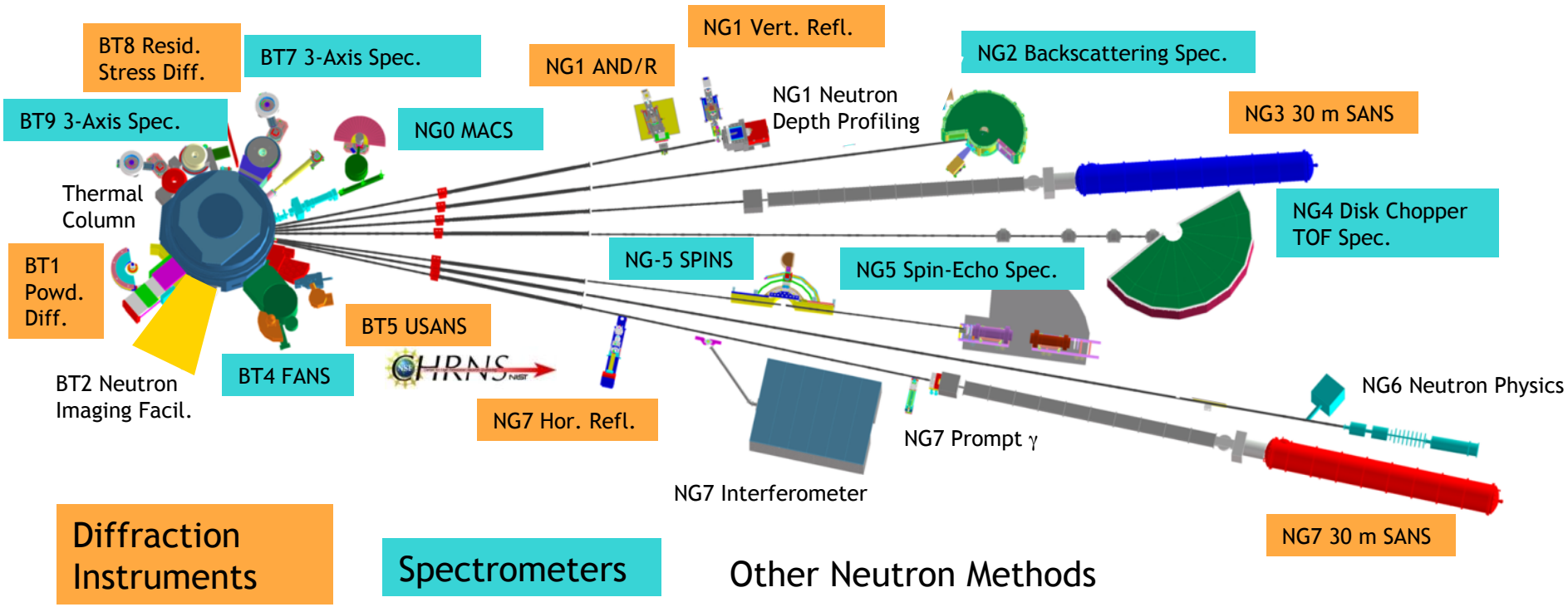

Diffraction Instruments

Spectrometers

Other Neutron Methods

20 MW Reactor in service since 1967
21 instruments

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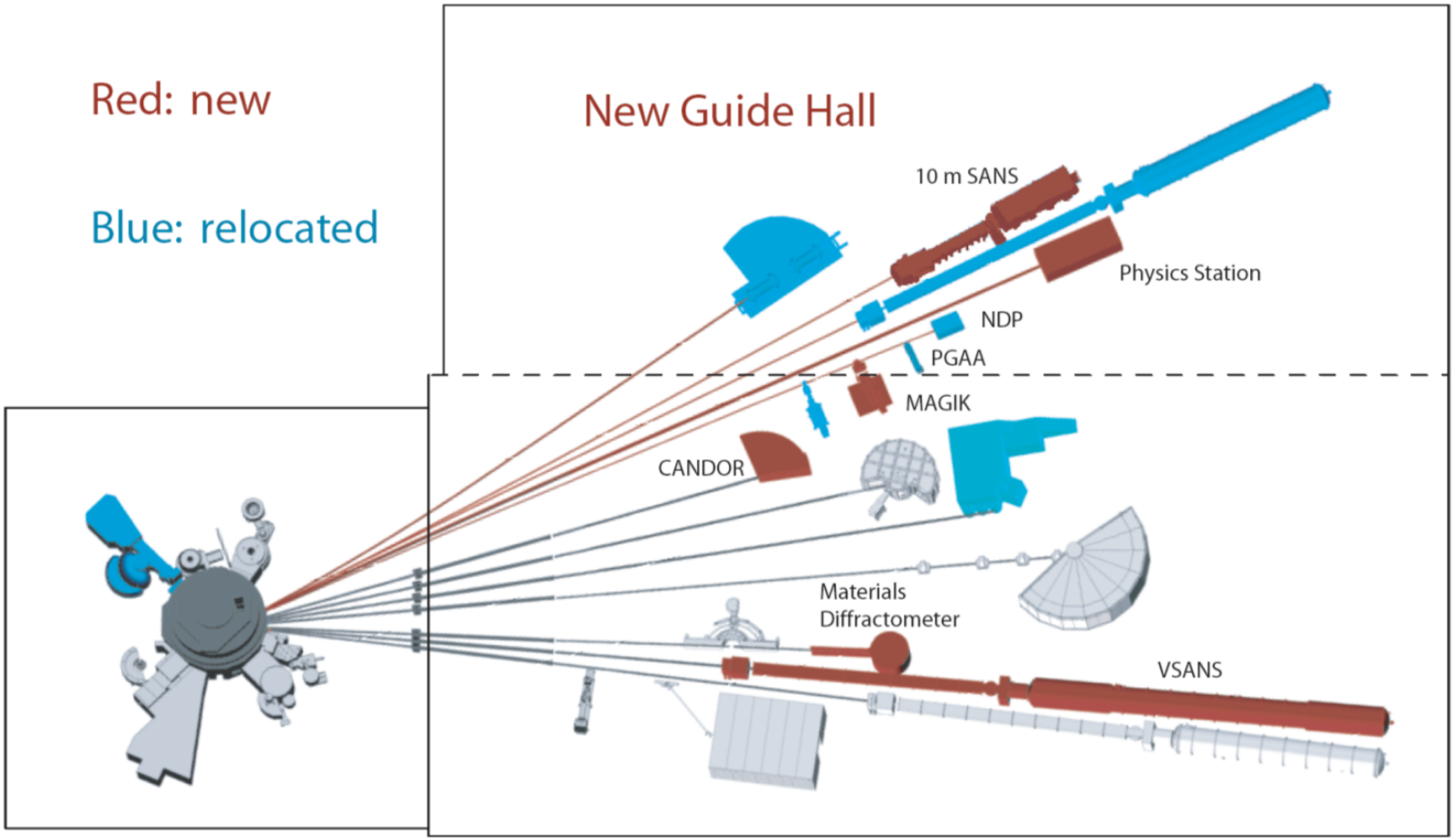
NCNR Expansion



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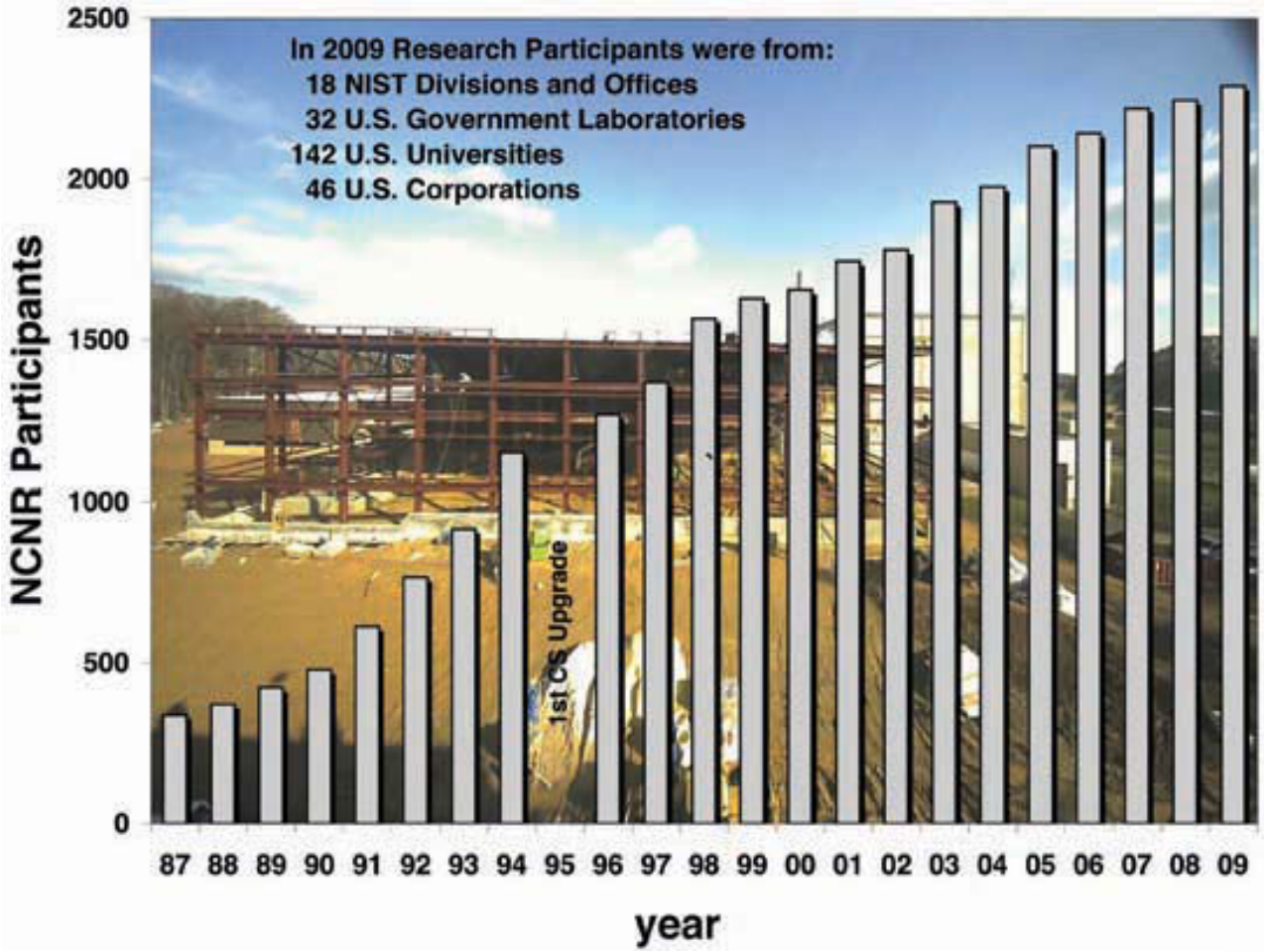
NCNR User Program



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Data Management Considerations

- Policy
- Culture
- Technology
- Resources

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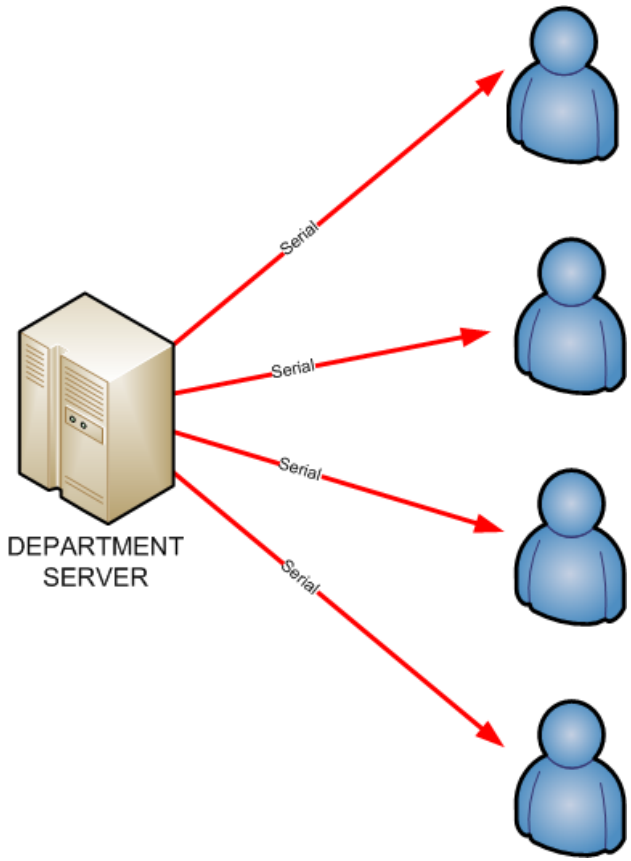
The Early Years (1970s – 1980s)



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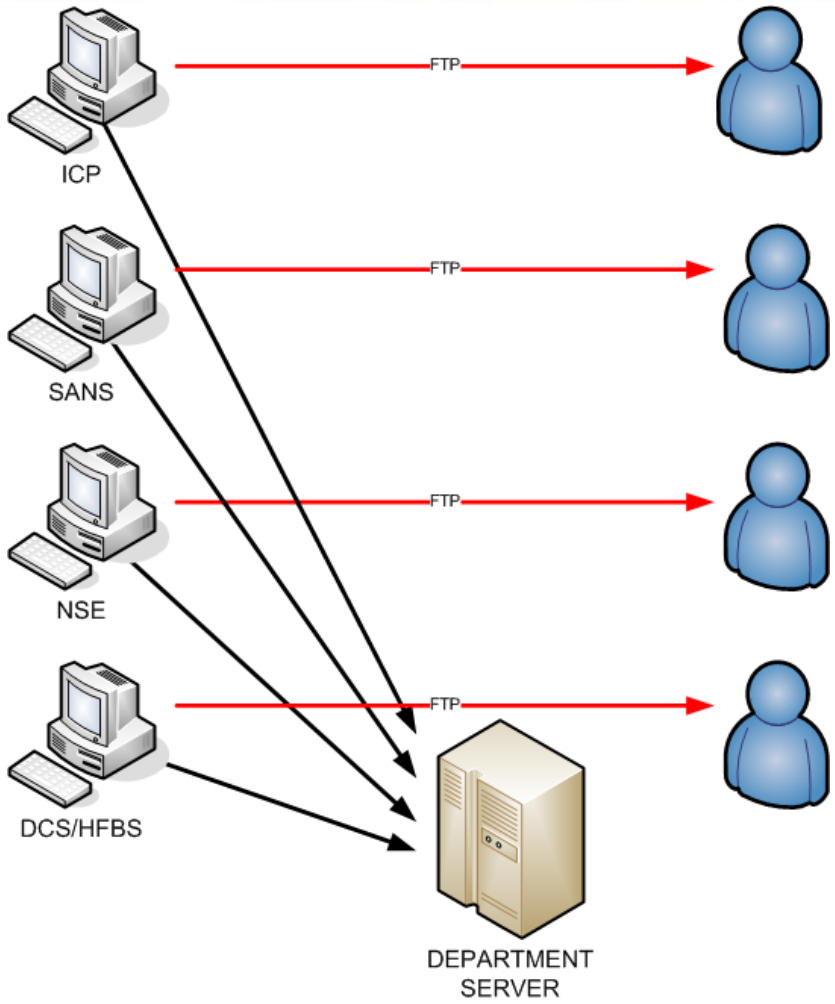
The Recent Past (1990)



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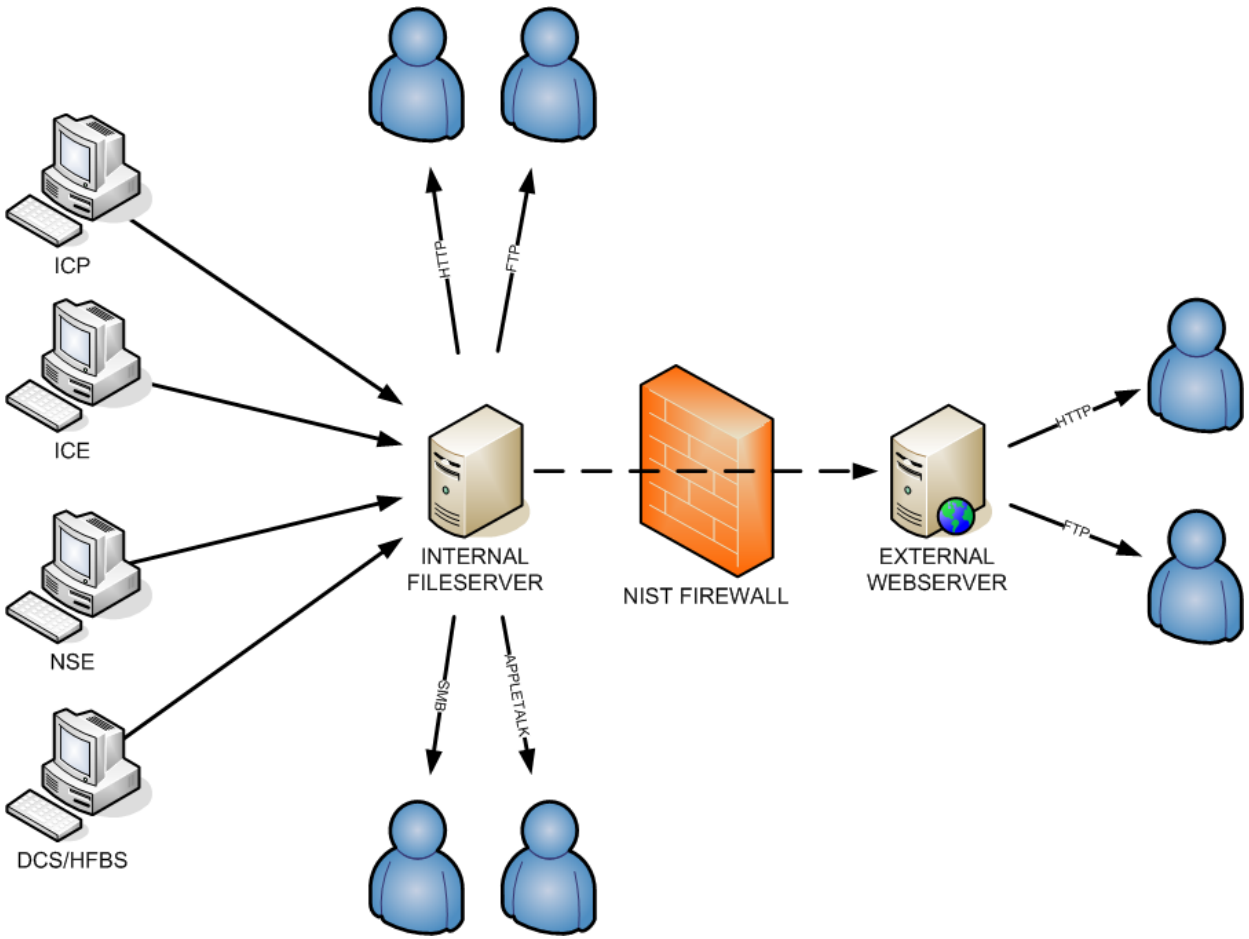
The Present (2010)



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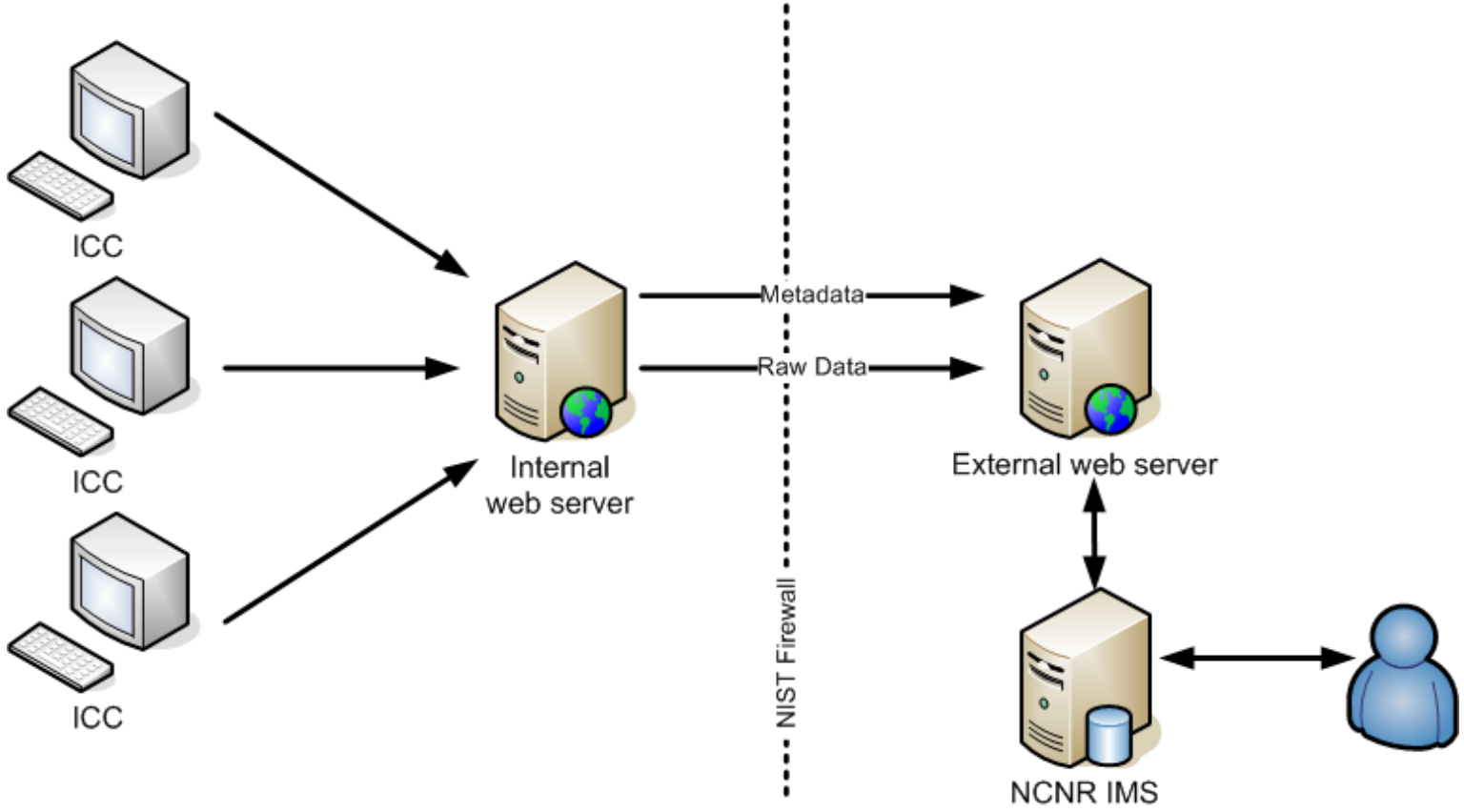
The Vision



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Tools

- Linux (Fedora variants) – Platform
- MySQL – Metadata RDBMS
- Perl/Net::SFTP, DBI, DBD/MySQL – Scripts
- PHP – Search pages
- Apache, VsFTP, Samba, Appletalk – Content delivery

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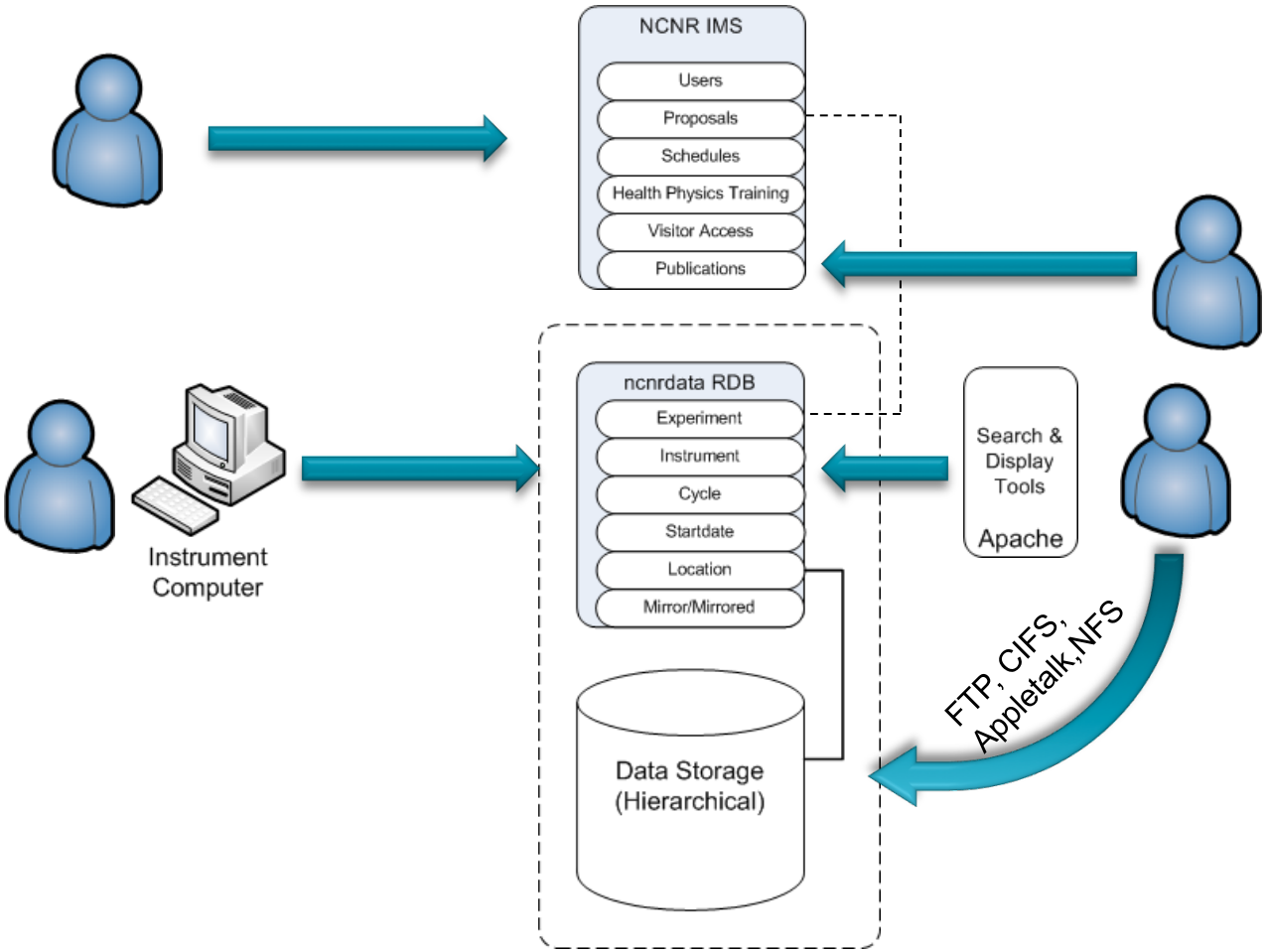
Experiment Lifecycle



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Archive process

- Instrument Control Software (all suites)
  - Writes a manifest of data files written
- Archive Script (per instrument control suite)
  - Retrieves manifest file from instrument computer
  - Retrieves all files on the manifest; skipping those already present in repository (or which haven't changed)
    - Files organized in repository by instrument, reactor cycle, and working directory
  - Harvests metadata from manifest and raw data
  - Assigns experiment number based on instrument schedule
  - Writes metadata to database
- Mirror Script
  - Periodically copies raw data to external fileserver and mirrors metadata to external database

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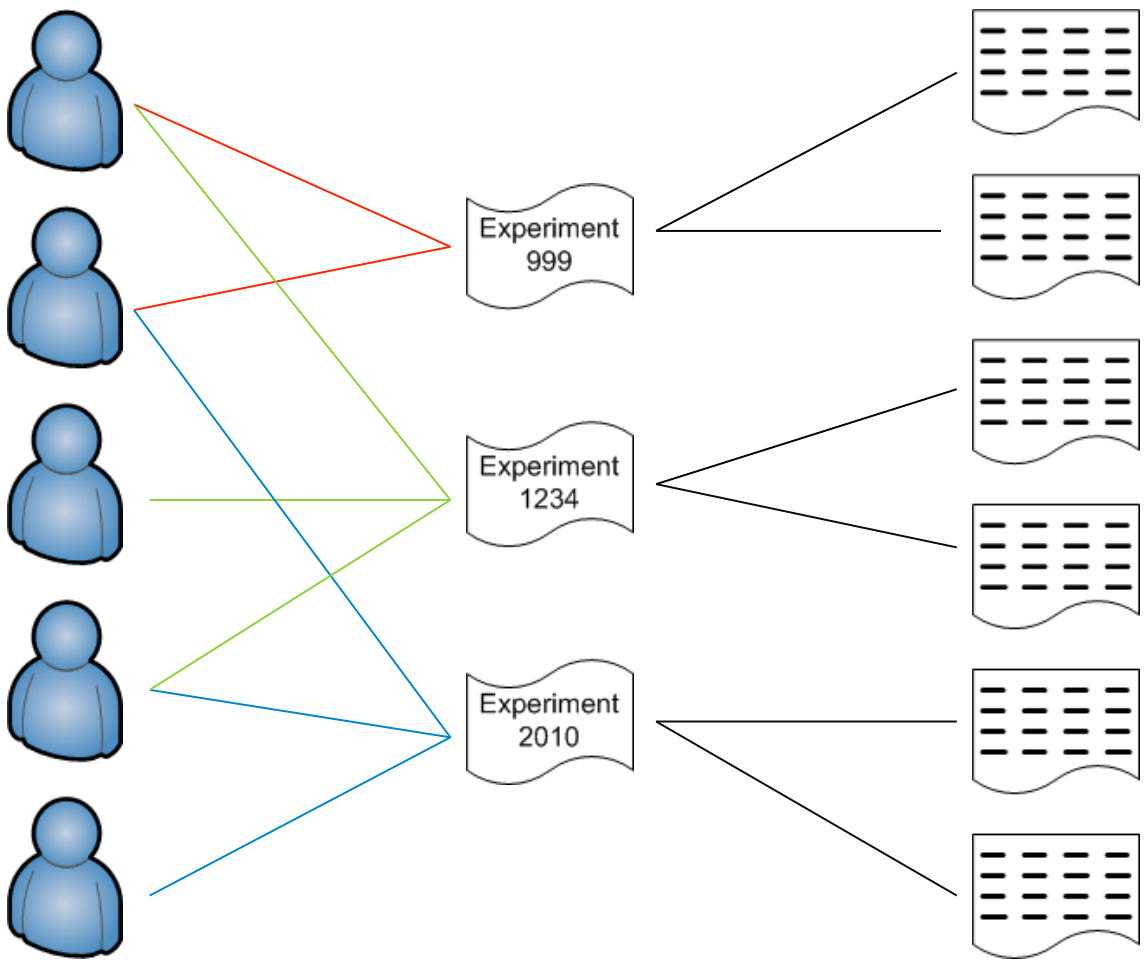
Establishing File Ownership



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Exporting data to public

- No access controls
  - Determined to be useful, but potentially a logistical nightmare for the benefit obtained
- A mirror script checks database for files marked to be mirrored
  - Those files and associated metadata are written to a server in public webspace
  - Those files are marked as having been mirrored in database
- By default, all datasets are marked to be mirrored.
  - NCNR Policy announced August 2010
  - Obama Administration Open Government Directive (Dec 2009)
- Users may opt out of the mirror process for a period of up to 18 months

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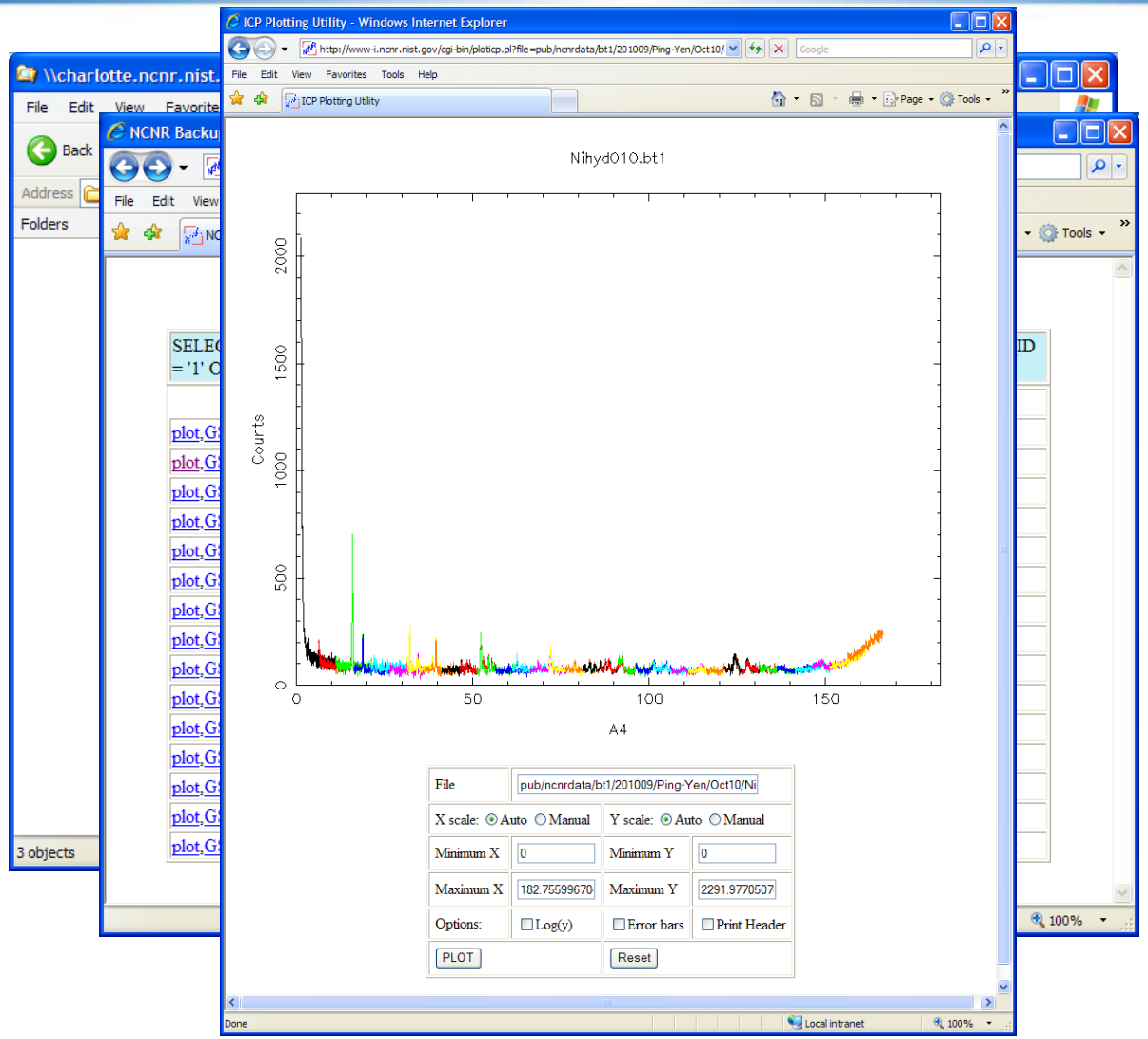
Accessing the repository



- File exploration tools
- Searchable catalog
- Web based tools

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Capturing Metadata

- In theory –
  - End users provide context for the measurement before the measurement starts
  - Experiment metadata can be harvested from other systems (proposal/ scheduling)
  - The published schedule is authoritative information
- In practice –
  - Most end users skip past dialogs requesting metadata and instead keep their own notes or generate comments meaningful to them
  - Metadata required by the proposal process is the most complete, but you may not be able to fully interoperate with that or other systems
  - The as-run schedule can differ from the published schedule by hours or days

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Delivering content

- In theory
  - Access controls are important and prevent unauthorized access to data
  - Serving raw data from central location is easier
  - Archived raw data are immutable

- In practice
  - Convenience trumps access controls
  - Many old hands don't adapt easily to new schemes for sharing
  - If data served centrally, archival copies are expected to be "hot off the presses"

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Role of Data Format

- In Theory
  - Self describing, extensible formats will encapsulate all necessary information required to reduce and analyze the raw data
  - The entire instrument suite at a facility should write the same data format
- In Practice
  - That information is only as good as our means of obtaining it
  - Changing data formats on “production” instruments requires a great deal of coordination between producers and consumers of data

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What's next

- Better integration with other business systems
  - NCNR User Portal?
- Unified data format
  - Foothold established following 2011 outage?
- Whatever is needed as it is needed

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