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# Real Time Analysis of Advanced Photon Source Data


Dan Fraser (ANL)

Director, Community Driven Improvement of Globus Software

Brian Tieman (APS)

And a host of others ….


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Exploiting the GRID for Synchrotron Radiation Data Analysis

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# Special Thanks

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# Outline

- Experiments we are working with at APS that require HPC/Grid Access
- Leveraging Grid & Workflow Technology
  - Databases
  - Workflow
  - Cluster Computing
  - Experiment Integration
  - Security
- High Level Architectures
- Areas for Collaboration

# Tomography Characteristics

- High Throughput—A Data Factory
  - ~100 samples per day
  - Processes >1 TB/day
  - Requires local (APS) processing power
    - ~16 cores process one “Standard” sample in < 1 hour
    - ~64 cores to keep up with peak demand
- Well Automated
  - Well defined dashboard
    - GUI for control/acquisition
    - GUI for reconstruction/experimental feedback
  - Mail in samples possible
    - Not enough beamline support to be practical
    - Possible to use remote access through services
- Runs at multiple beamlines

# 3D X-Ray Diffraction Microscopy Characteristics

- Modest data rates
  - 100GB/day acquired reduces to <10MB
  - Local APS processing power for data reduction step
    - 8 cores(?) to keep up with demand
- Reconstruction step is CPU intensive
  - Requires large (non-APS) clusters
    - Single plane of sample takes ~24 hours on 68 processors (APS cluster Orthros)
      - 300 planes per day
    - Happily parallelizable to > 1000 cores
  - Requires tight integration of remote resources into operations of experiment
- Not well automated (yet)
  - Users required to be here (setup, sample changes)
    - Setup
    - Sample Changes

# X-Ray Photon Correlation Spectroscopy

- High data rates
  - >1TB/day acquisition possible
  - Online acquisition compression can reduce by 80%
  - Requires local APS processing power
    - Online data reduction with very low latency
      - < 16 cores
    - Further reduces data to <1GB
- Partially automated
  - Acquisition well automated with SPEC
  - Data reduction not automated
- Real Time analysis could really benefit XPCS
  - Unsure when enough statistics have been acquired

# Microdiffraction Characteristics

- High Throughput—Potential Data Factory
  - New hardware purchase
    - 3 detectors capable of 15 FPS at 4MPixel
    - 32 cores to add to Orthros
    - 10Gb ethernet to connect beamline to cluster
  - More data to come…

# HPC/Grid Topics

- Databases (sample tracking)
- Workflow
- Cluster Computing
- Experiment Integration
- Security (including access & auditing)

# Sample Databases

- In development
  - Tomography
    - PostgreSQL—database server
    - Sample Crawler—parses directory trees and recognizes tomography samples
      - Java/JDBC
      - Cron job
      - User initiated
    - TomoMPIController—database front end
      - Java
      - ImageJ plugin
  - 3DXDM (Dr Robert Suter's group at CMU)
    - Developed in house at CMU

# Sample Database Principles

- Catalog all samples
  - Automated/nonintrusive updates of “live” data
  - User driven cataloging of “archived” data
- Specific schema per technique
  - Contain technique specific information of user interest
- Information common to all experiments
  - Contain URL of current data location
  - ESAFs, GUPs, user information, etc…
  - Relate sample to data acquired by different techniques
- Database openly available
  - Query from anywhere
  - Users can only see data they are authorized to see (security)
- Security

# Workflow Integration

- In development
  - Tomography
    - TomoScript—Dashboard for experiment control
      - EPICS—Control system
      - Sample Changer—Automated sample changer (Chris Rhoerig)
      - Image Server—2D detector acquisition program
    - Sample Crawler—Catalogs samples
    - TomoMPIController—ImageJ plugin for sample browsing/reconstruction control
      - TomoMPI—Parallel reconstruction code
  - 3DXDM
    - SPEC
      - EPICS—Control system
      - Image Server—2D detector acquisition program
  - XPCS
    - SPEC
      - EPICS—Control system
      - Image Server—2D detector acquisition program

# Workflow Integration

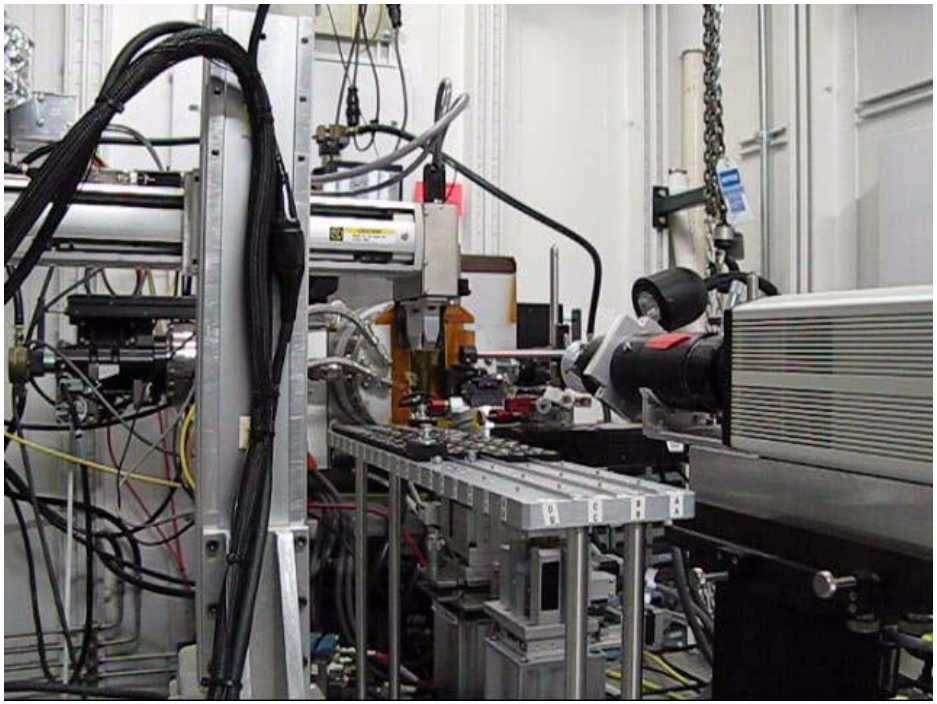
- Principles
  - Hide details of system—users want simplicity!
    - EPICS on multiple platforms
    - Image Server on Windows
    - Data processing code on Linux
    - Data reconstruction code on cluster
  - Automation
    - Data flows out of one step into another
  - Interaction
    - Peek at any step
    - Cancel/reprioritize/redirect any step

# Cluster Computing

- In development
  - General Use
    - Sun Grid Engine
      - Not generally used as a priority scheduler for different applications
      - Batch submission
      - Node partitioning
    - Globus
      - GSI (Grid Security Infrastructure)—Credentialing subsystem (audit based on identity)
      - GridFTP—High performance ftp protocol
      - RFT (Reliable File Transfer)—Service interface to GridFTP
      - Globus Resource Allocation Manager—Abstraction layer to job scheduler
      - Tools for creating and orchestrating services (Globus Core, gRAVI)
  - Tomography
    - TomoMPI—Parallel reconstruction application
  - 3DXDM
    - XdmMPI—Parallel reconstruction application
  - XPCS
    - XPCSMPI—Parallel data reduction application
  - Microdiffraction
    - Hundreds of instances of non-parallel applications

# Experiment Commonality

- Basic Workflows are Similar
  - Sample Database
  - Automation
    - Sample changing
    - Data analysis
  - High Throughput
- Different Implementation
  - Redundant database development
  - Redundant Sample Changer code
  - Redundant Workflow Infrastructure



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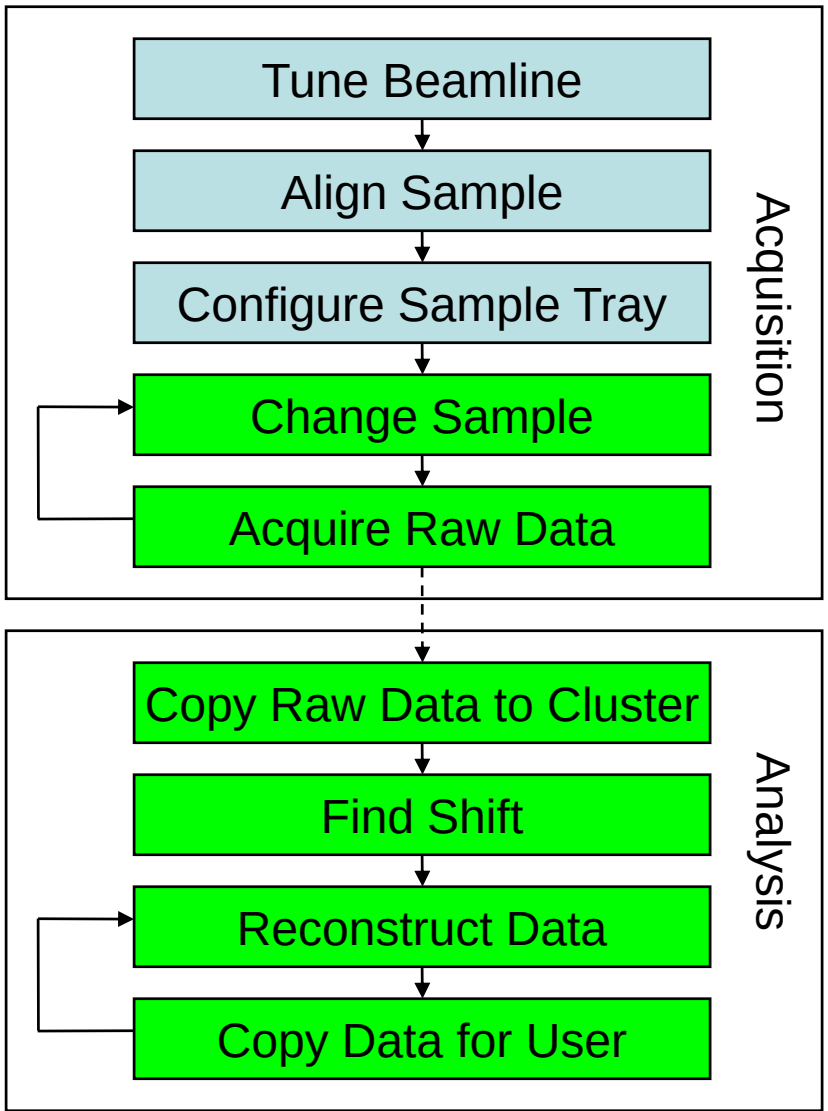
# Sample Workflow— (Tomography at 2BM) Simplified




Currently Done Through Human Intervention

Easily Automated for Similar Samples

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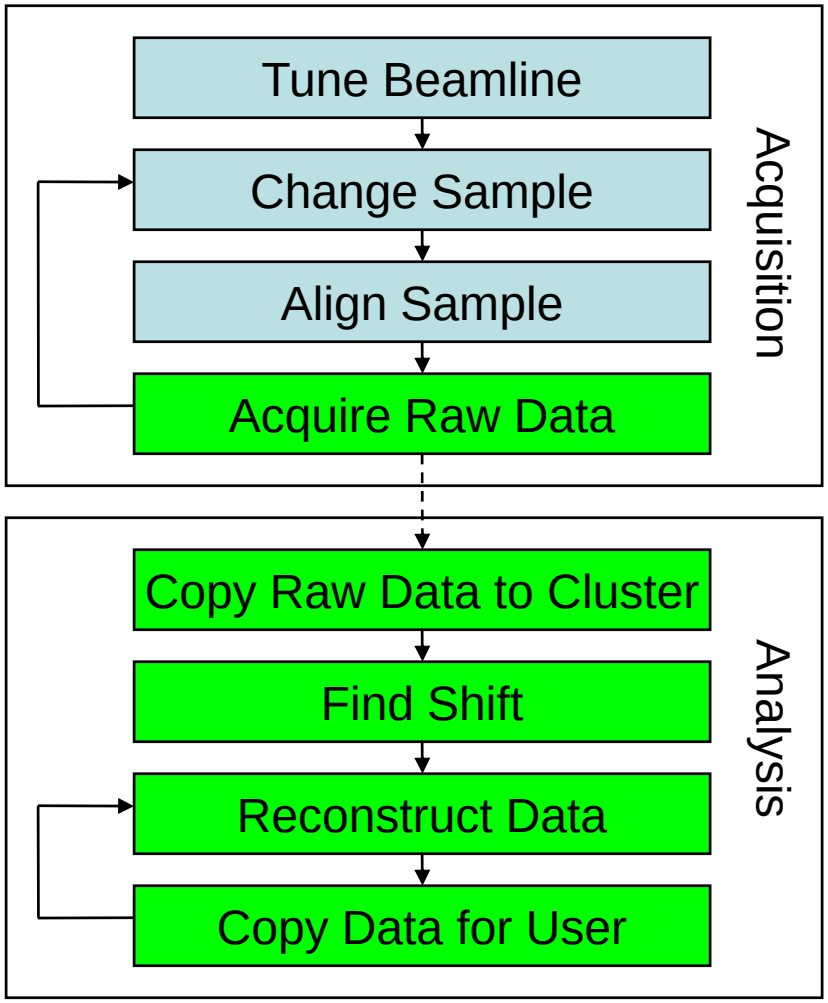
# Sample Workflow—Tomography at 1 & 32ID Simplified

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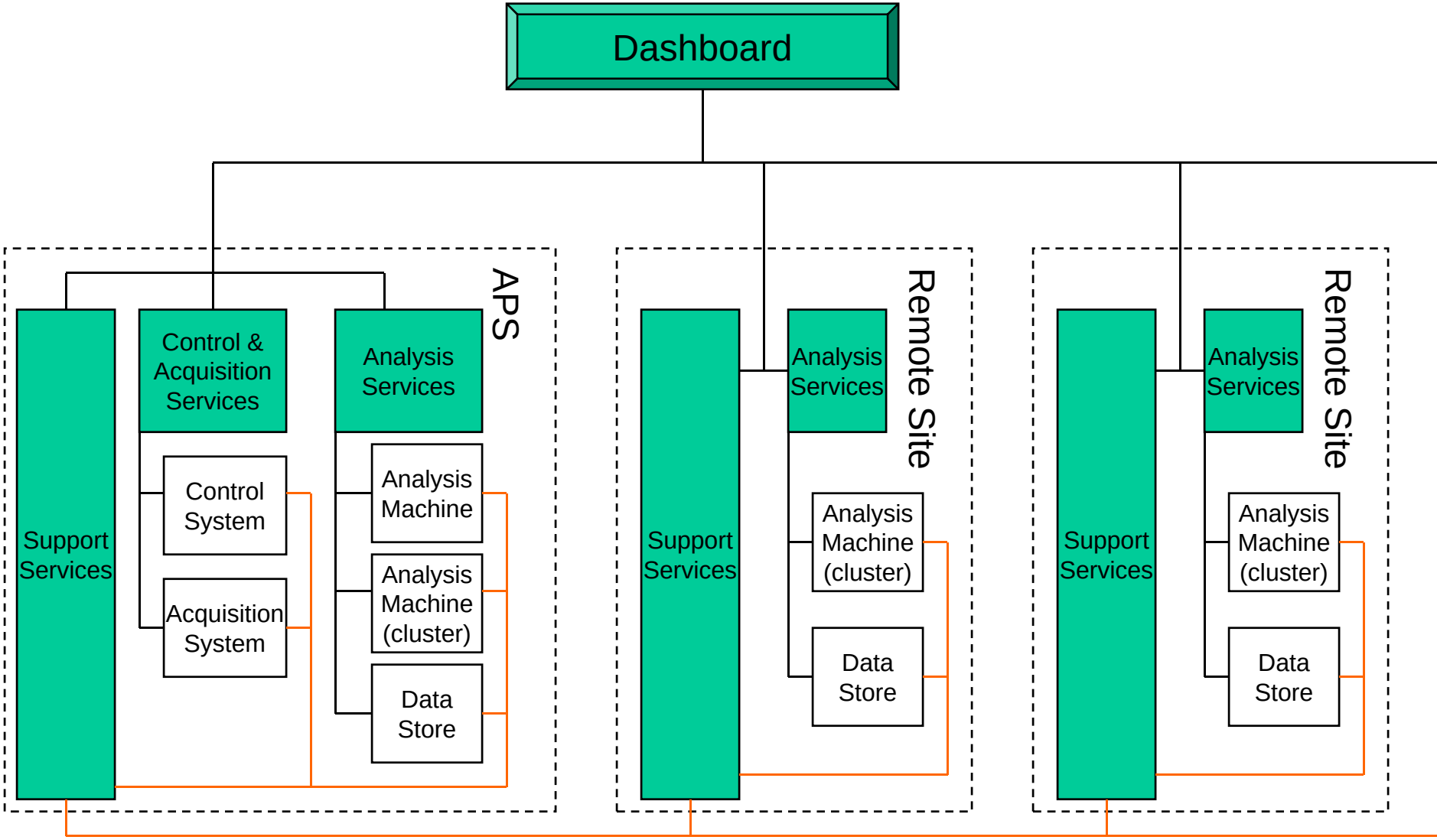
# Experiment Integration



# Dashboard Pictures

# Sample Workflow Services From Tomography Dashboard

- Support Services
  - Globus Security Infrastructure (GSI)
  - GridFTP
  - Reliable File Transfer (RFT)
  - Sample Database
  - Globus Resource Allocation Management (GRAM)
  - Many more!
- Control and Acquisition Services
  - Focus
  - Cross Correlation
  - Configure Samples
  - Change Sample
  - Sample Acquisition
- Analysis Services
  - Find Shift
  - Reconstruct Sample
  - Crop Sample
  - Scale Sample
  - Convert Data Format

# Principles

- Sophisticated Programmers set up workflows
- Users should not need to learn “the grid”
  - Provide a simple user interface (Dashboard)
    - Built on top of the CoG Kit
- Users run workflows (easy push button)
  - Control the experiment
  - Manage data acquisition
  - Select samples for processing
  - View Intermediate Results…
- We’re proceeding cautiously on integration of Experiment Control w/data acquisition

# A Data Problem

- The APS generates massive amounts of data
  - Many experiments can create a TB or more
- There is no long term storage at the APS
  - Data can usually be stored short term (mos.)
- Users take home their data any way they can:
  - Memory sticks, hard drives, CD, Fed-ex
  - Sometimes problems occur and users get home without their data

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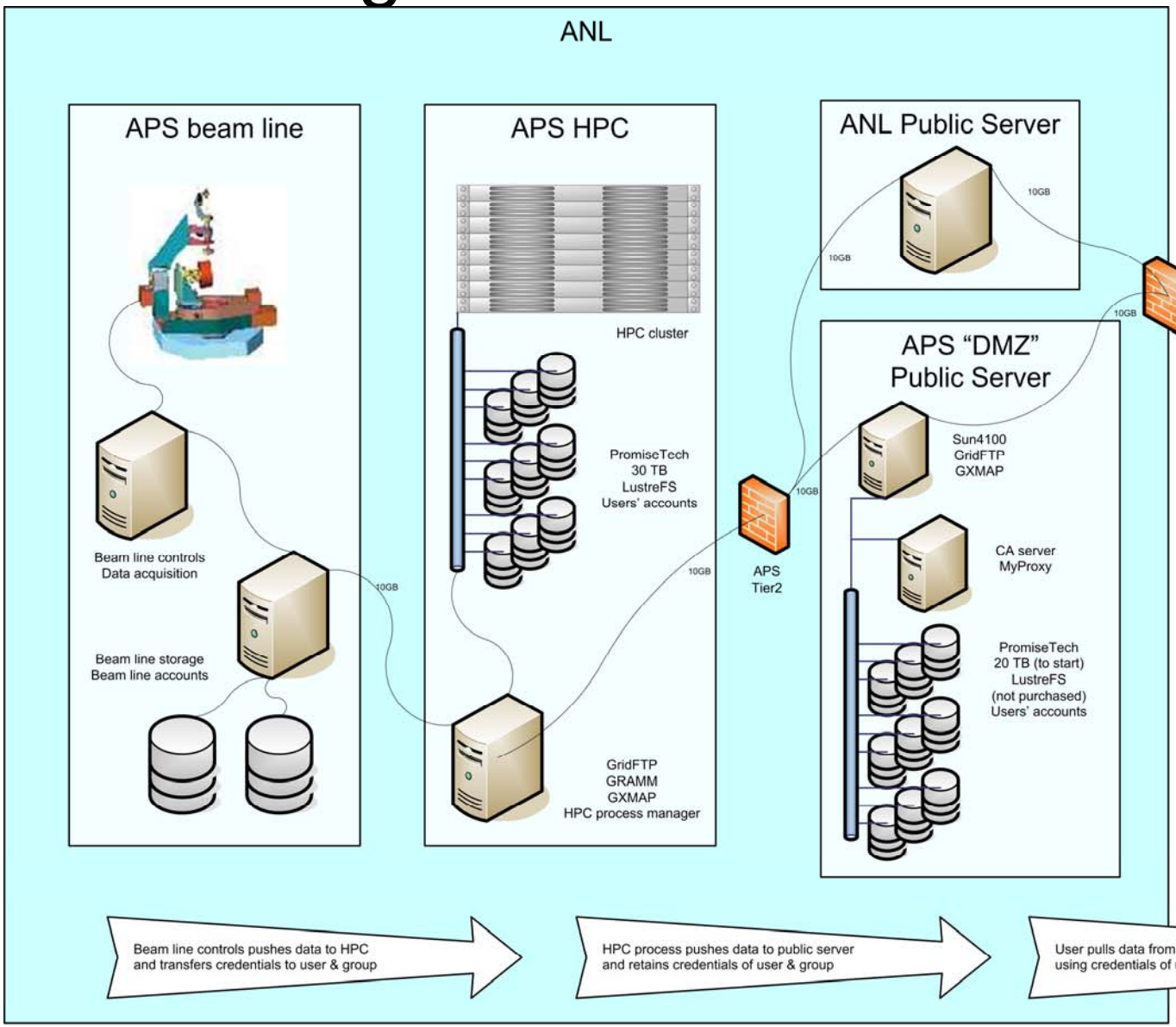
# Proposed High Level Architecture




draft: 2008-11-12

# Areas for Collaboration

- Andy Götz
  - Collaboration w/Ulrich Lienert
    - High Energy Diffraction Microscope
  - FABLE can find grains associated w/peaks
  - Ken Evans (ANL) would like to install & use
- Cloud Computing Collaboration (~years)
  - Share applications via VMs
- Data Sharing Between Sites (~soon?)
  - Both sites provide external high performance file transfer (GridFTP?)

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# Thank You

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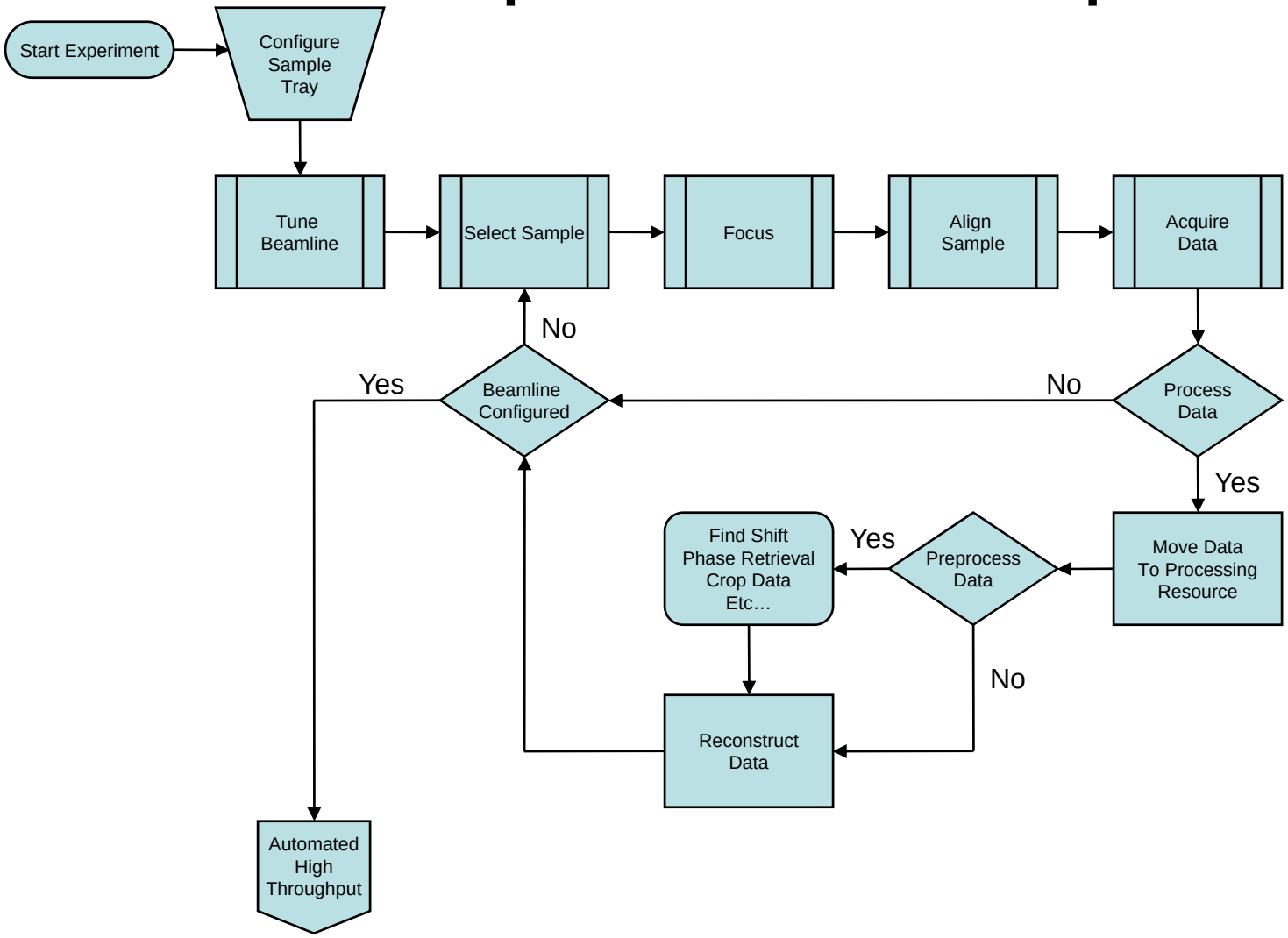
# Sample Experiment Setup



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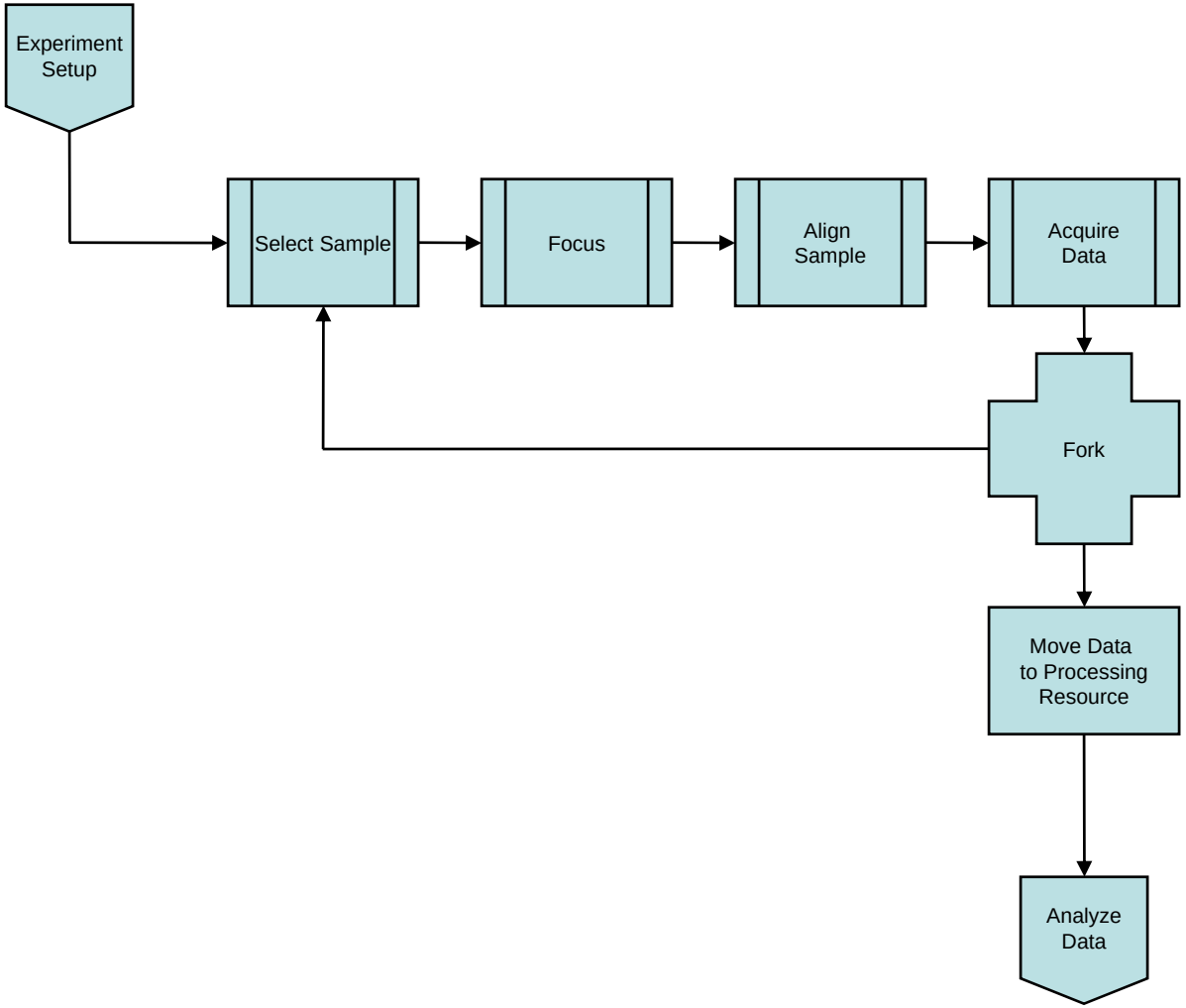
# Sample
# High Throughput



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# Sample Data Reduction