



Xport Collaboratory for X-ray Crystallography

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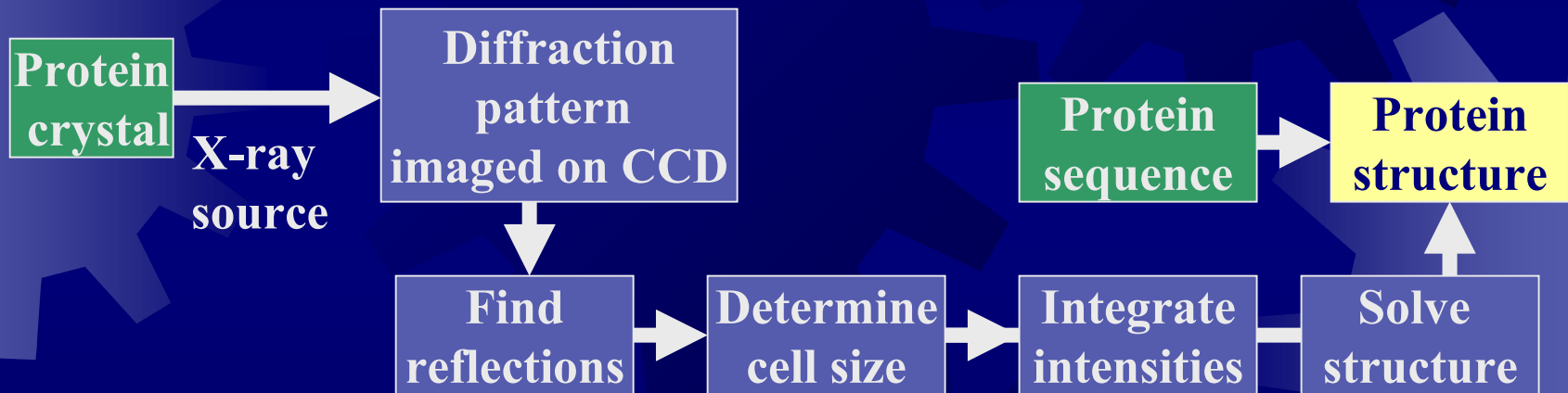
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Macromolecular Crystallography

- ✦ Mission critical tool in biochemistry
 - ✦ Structure of large biological molecules
 - ✦ Function from structure
- ✦ Crystallographic experiment
 - ✦ Crystals diffract X-ray wavelength light
 - ✦ Diffraction pattern can be used to determine size of the unit cell of the crystal and location of atoms
 - ✦ For large molecules diffraction pattern is spatially compact requiring high image resolution
 - ✦ Requires high-brilliance X-ray source
 - Advanced Light Source (LBL)
 - Advanced Photon Source (ANL)

The Crystallographic Experiment



Problems

✦ Travel/presence

- ✦ Beam time is hard to come by and expensive
- ✦ Researcher must be at beam line for effective use of beam time

✦ Data management

- ✦ Typical experiment generates 200-400 images at 5-20MB per image
- ✦ Different researchers use different packages for analysis and visualization
- ✦ File formats

Xport Architectural Goals

- ✦ Framework for
 - ✦ experiment setup and monitoring
 - ✦ Data storage and management
 - ✦ Data reduction and analysis
 - ✦ Collaboration
- ✦ Leverage existing middleware and services
- ✦ Use existing hardware and infrastructure
- ✦ “Minimally invasive”
- ✦ Allow remote users to use the tools they are familiar with

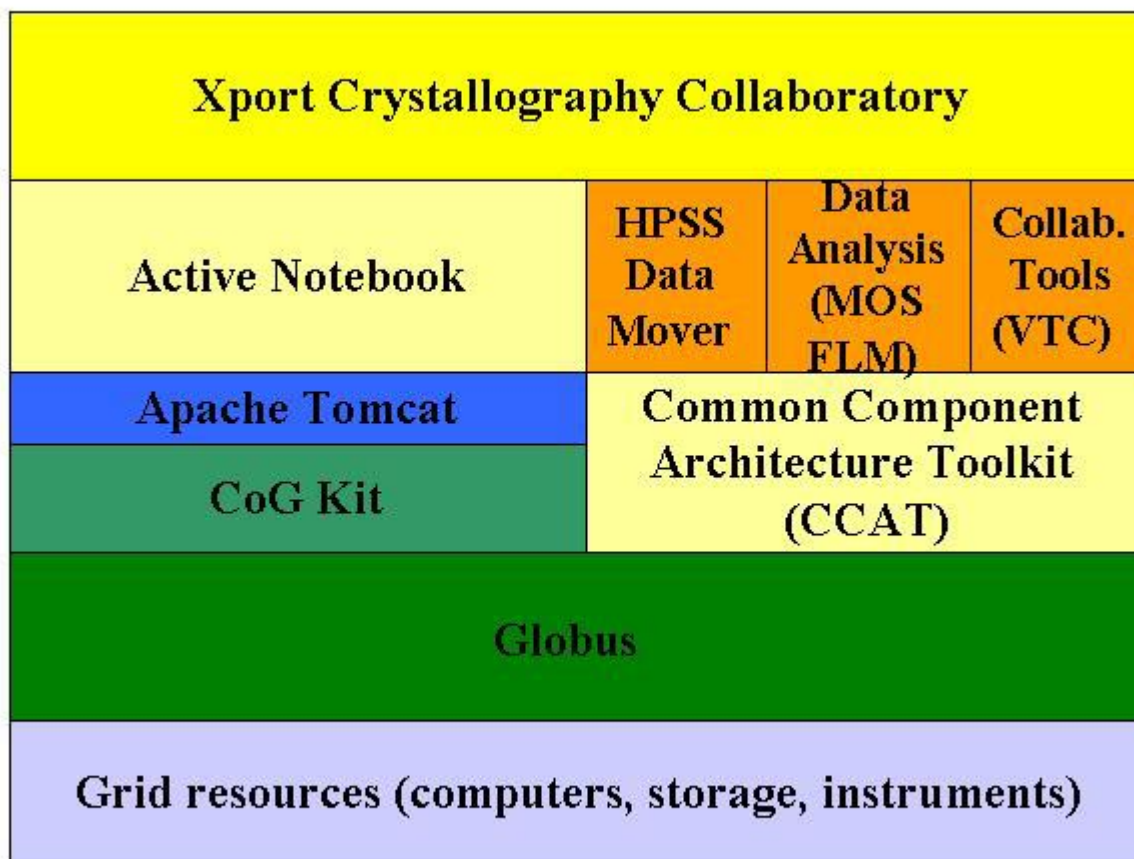
Xport Architecture Goals (2)

- ★ Leverage existing middleware and services
 - ★ Globus for authentication and job execution
 - ★ Common Component Architecture Toolkit (CCAT) for modularization and reuse
 - ★ CCAT Active Notebook as focal point for data and process management
 - ★ GARA for bandwidth management
 - ★ HPSS for storage

Xport Architecture Goals (3)

- ✦ Use existing hardware and infrastructure
 - ✦ Add “Proxy-cache” to beamline data collection system – consistent interface
 - ✦ Grid computing facilities
 - ✦ ESNNet and Abilene/I2 QoS testbeds
 - ✦ Support multiple sites and users with different data collection systems and analysis software

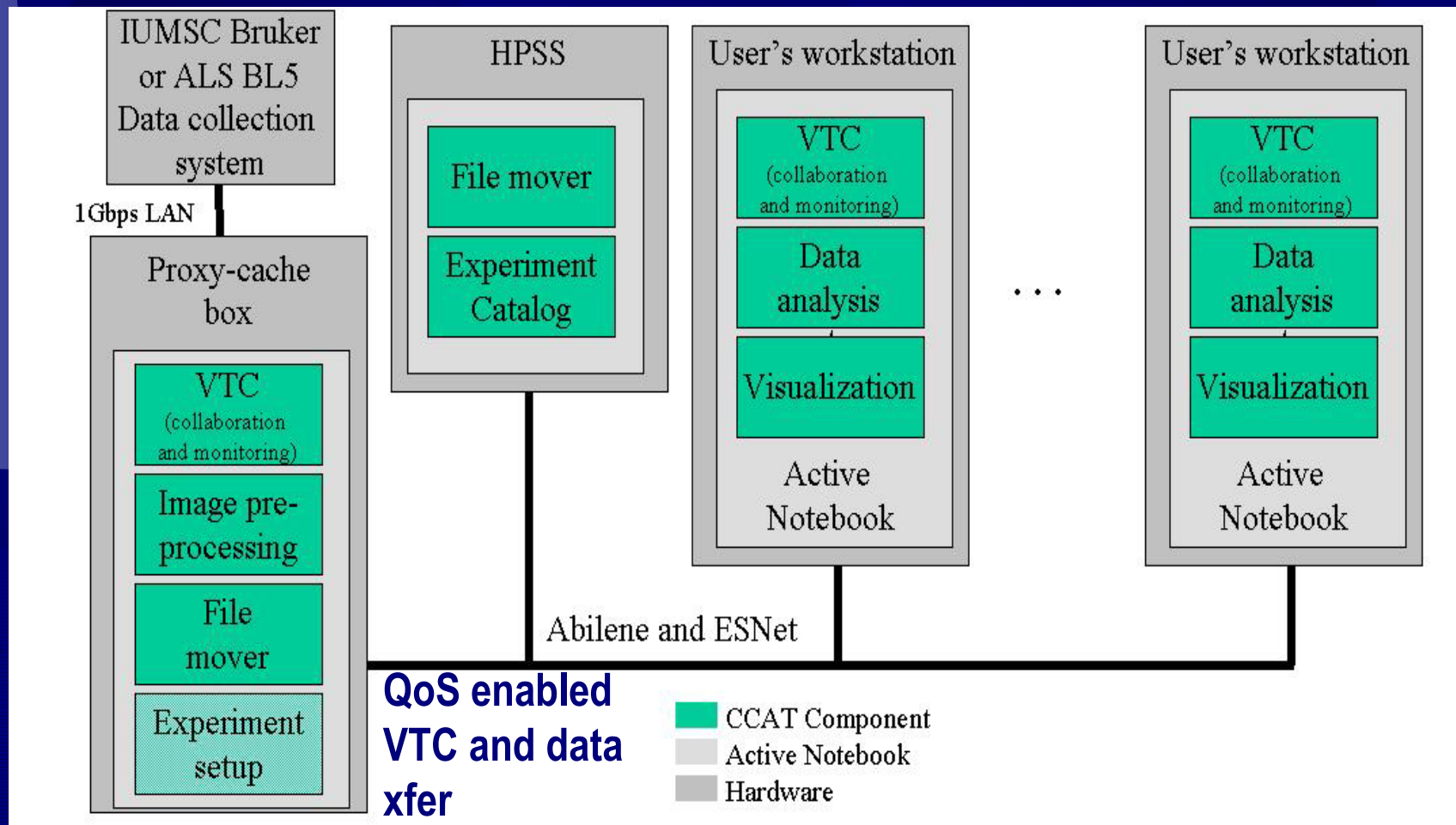
Xport Architecture



The SC2000 Xport Testbed



Xport Testbed Components



Demonstration

- ✦ With crystallographers Dr. John Bollinger at the IU-MSU and Kia Huffman
- ✦ Source is diffractometer at IU
- ✦ Remote user at sc2000

