Xport Collaboratory for X-ray Crystallography

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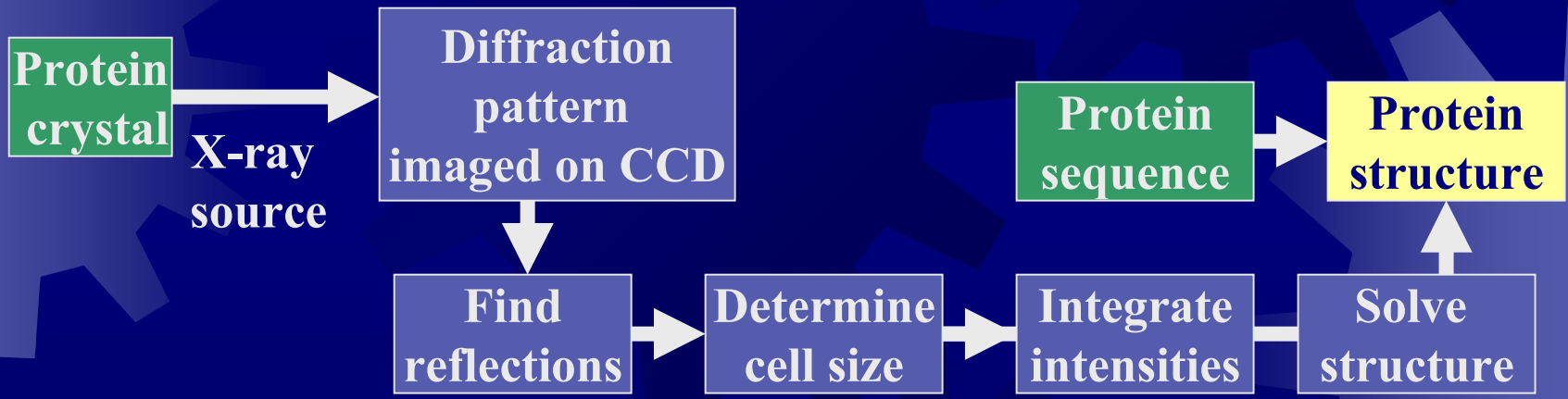
Macromolecular Crystallography

- 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 expen$ive
  - 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

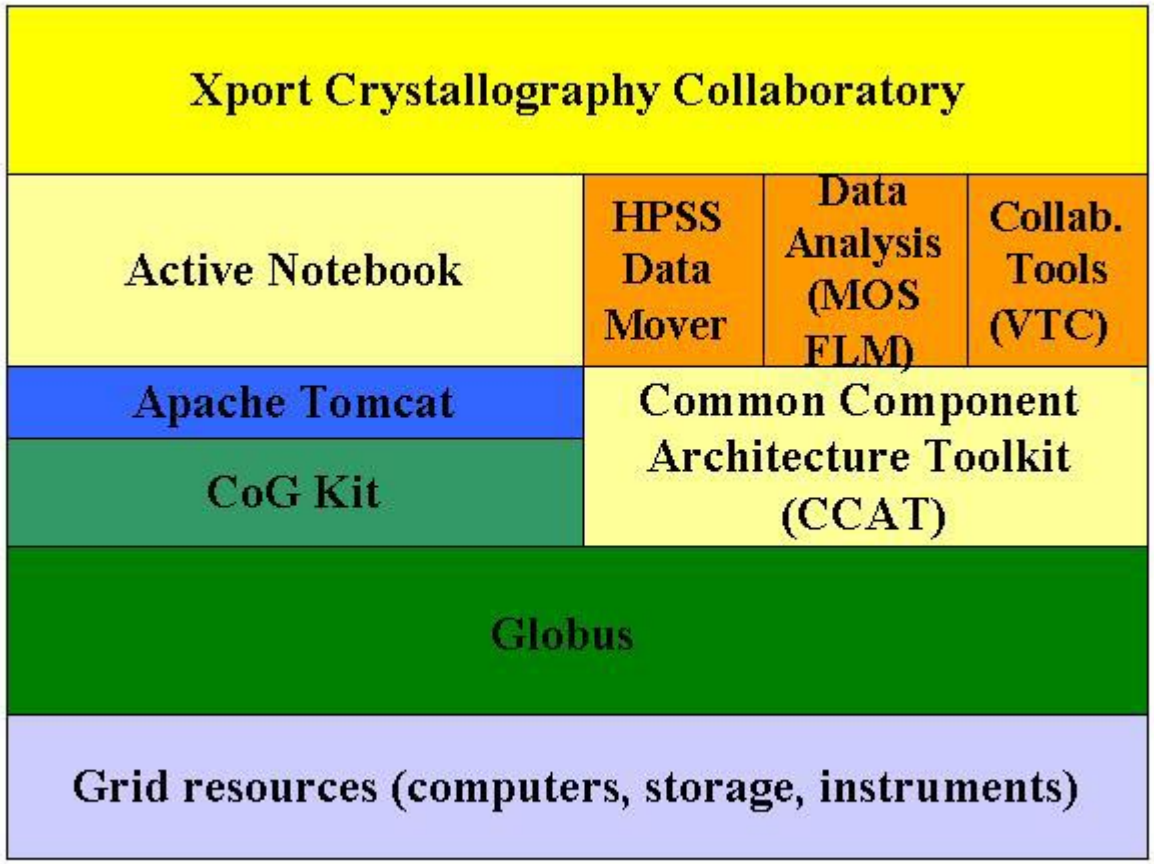
Xport Architecture Goals (2)

- 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

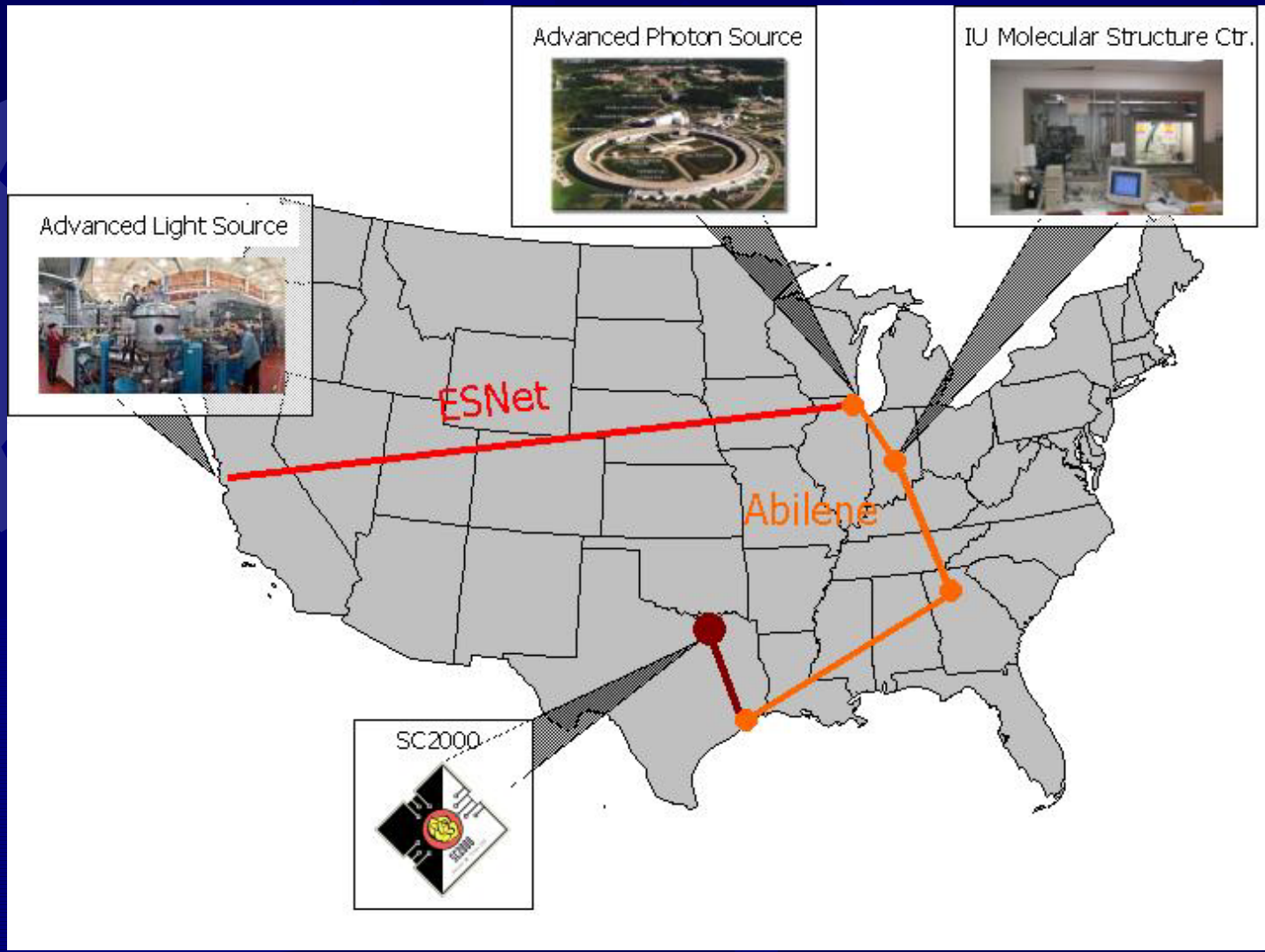
Xport Architecture Goals (3)

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

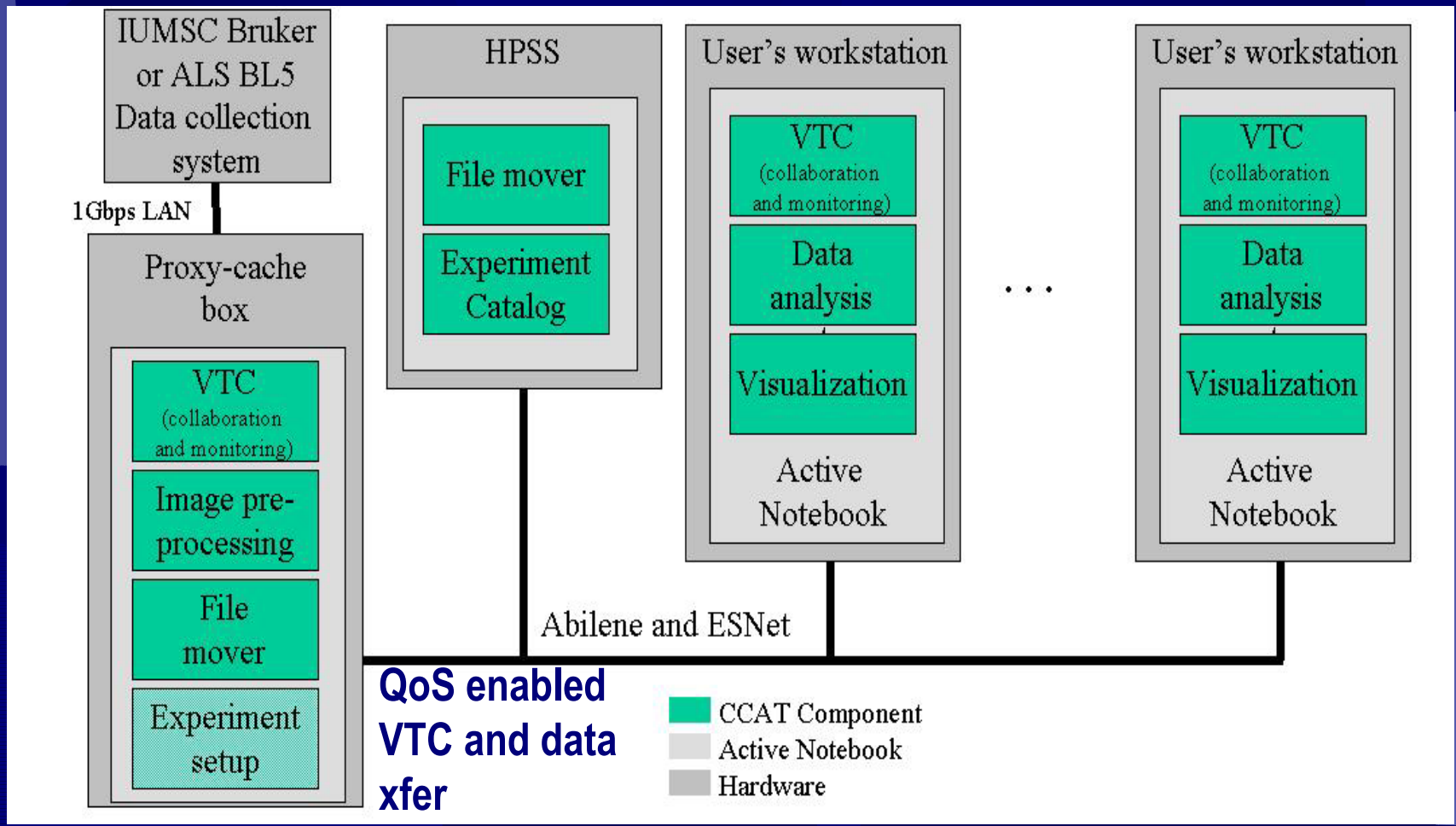
Xport Architecture

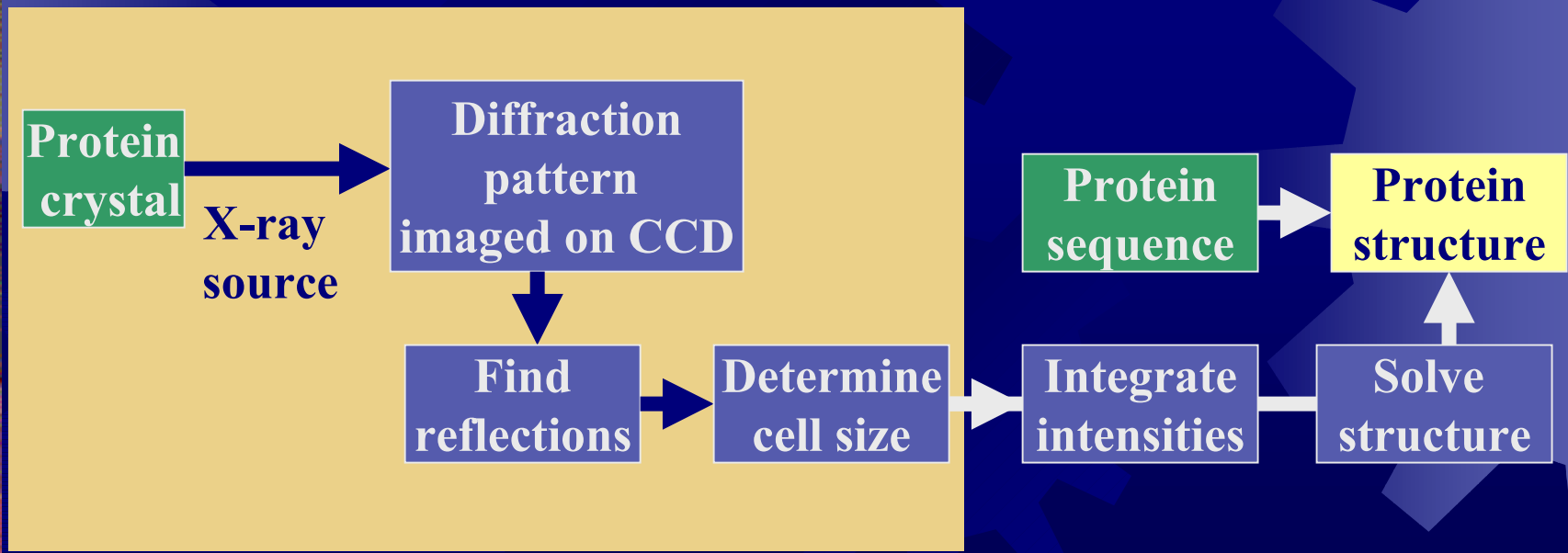


The SC2000 Xport Testbed



Xport Testbed Components



Demonstration

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