Scientific Data Management at the Environmental Molecular Sciences Laboratory

Daniel R. Adams, David M. Hansen, Kevin G. Walker

Pacific Northwest National Laboratory

John D. Gash

Lawrence Livermore National Laboratory

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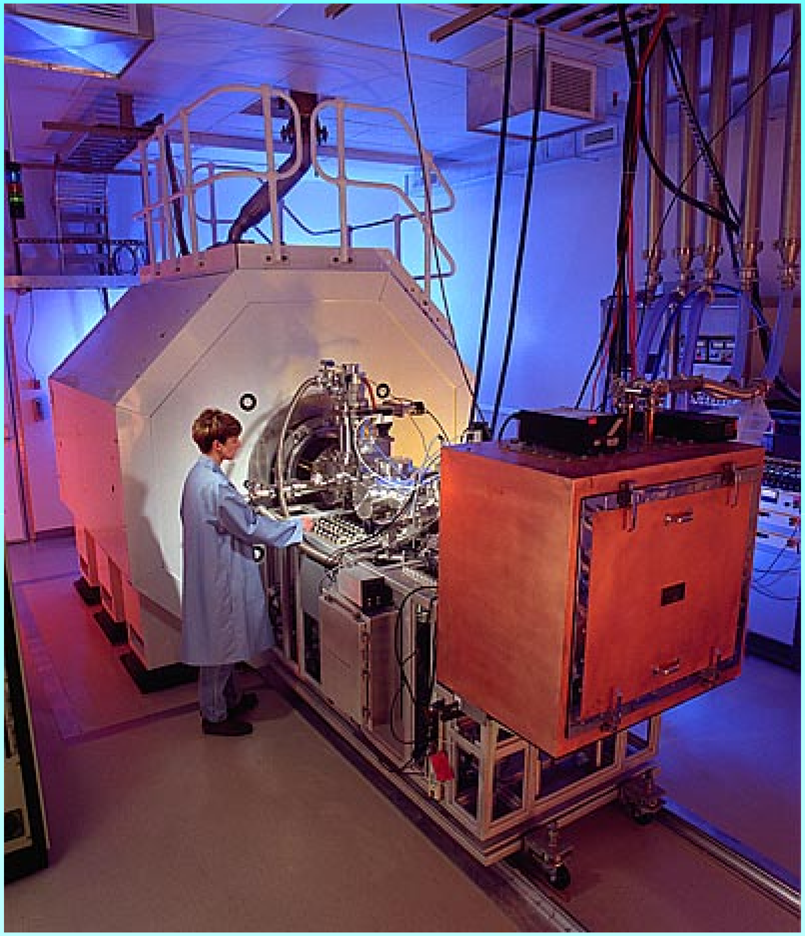
Environmental Molecular Sciences Laboratory

As a research organization, the EMSL seeks to

- **attain an understanding of the physical, chemical, and biological processes needed to solve critical environmental problems**
- advance molecular science in support of the DOE's long-term environmental mission.

- As a national scientific user facility, the mission of the EMSL is to
  - **provide advanced and unique resources to scientists engaged in research on critical problems in the environmental molecular sciences**
  - educate young scientists in the molecular sciences to meet the demanding environmental challenges of the future.

Environmental Molecular Sciences Laboratory



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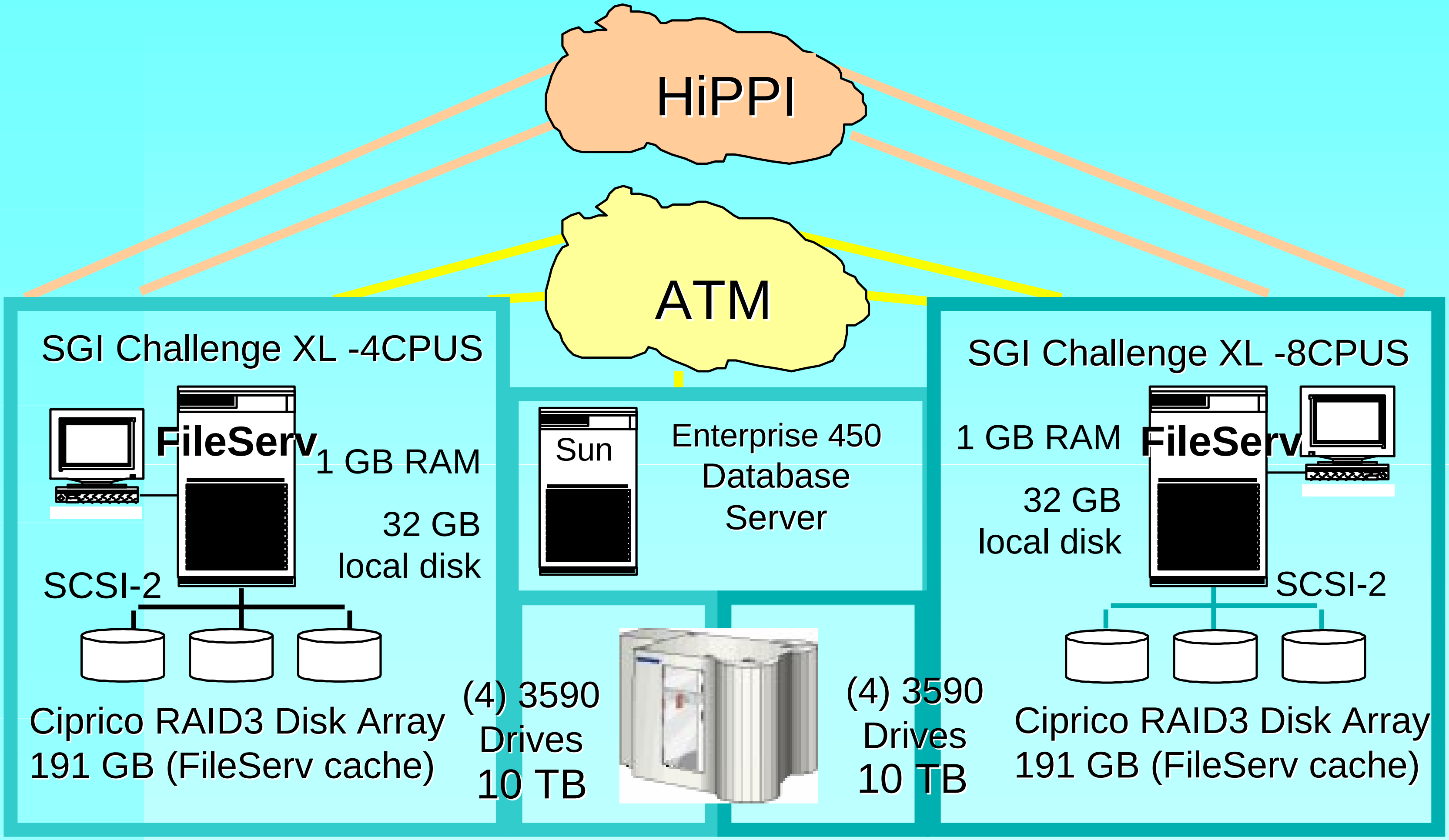
NWArchive Hardware Configuration



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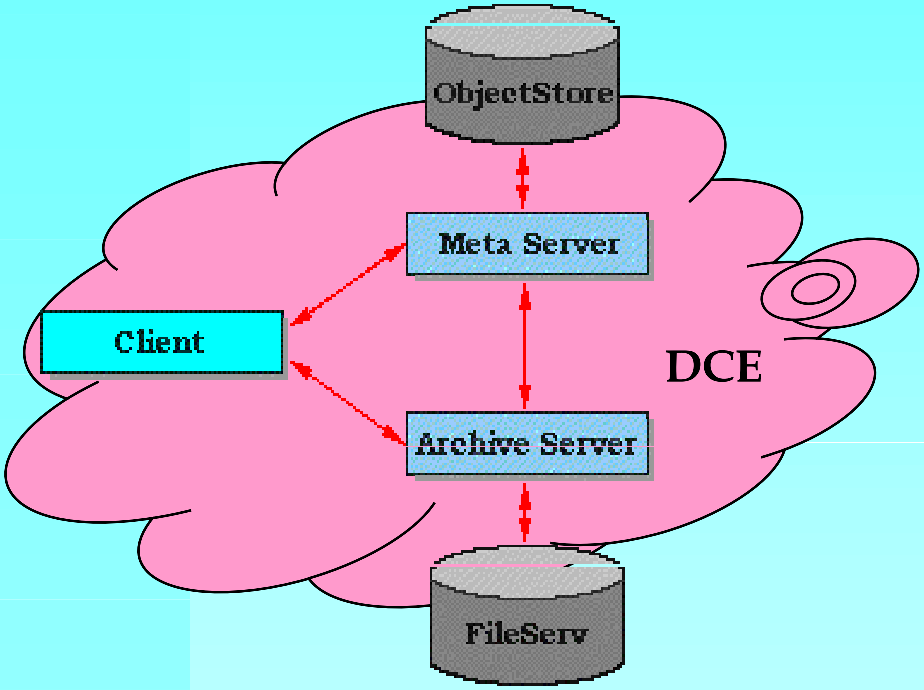
Scientific Data Management - Context

- Wide variety of data types produced
  - Computational chemistry
  - Experimental data
- Some data irreplaceable
- Must be accessible for 20+ years
- Must be able to find data
  - in spite of staff changes
  - without *a priori* knowledge of directory and naming conventions (and without grep)

Scientific Data Management - Design

- File oriented access
- Distributed, heterogeneous clients
- Distributed, homogeneous storage
  - but users see single file system
- Built using DCE
- Conservatively dependable
- Metadata Required
  - do not use predefined ontology
  - keep the metadata separate from the data

Scientific Data Management - Architecture



- Metaserver and database are key
  - maintain all metadata
  - maintain state of distributed transactions
  - balance storage distribution
- Archive Server
  - honors contracts
  - interacts with file system and transfers files

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Scientific Data Management - Metaserver

- Distributed transactions implemented with “contracts”
- Metaserver and associated database
  - maintain state of contracts
  - implement unified file system view
  - maintain all metadata
  - implements access control
    - uses DCE groups
- Makes it possible to “hide” the file system

Scientific Data Management - Metadata

- Extensible, searchable metadata is key to making terabytes of data accessible for decades
- Three classes of metadata
  - File oriented
    - includes access notifications
  - Content oriented
    - Free text
    - Attribute=Value pairs (no predefined ontology)
  - Context oriented
- “Documentize” our metadata for searching

Scientific Data Management - Implementation

- Multiple threads x multiple vendors = multiple headaches
  - 2 stage delete
  - Solaris server added to mitigate DCE/ODI problems
- Clients
  - Command Line Interface
  - X interface (based on LLNL's xdir)
  - Web Interface (using Transarc's DFSWeb)

Scientific Data Management - Summary

- Client-Server architecture built on DCE
  - distributed transactions
  - authentication and authorization
- Metadata is key to long-term utility of system
  - extensible
  - file, content, and context
  - contemporaneous and *a posteriori* metadata
  - searchable
- “Just say ‘no’ to file systems”