

Computing Research Association

Conference at Snowbird 2000



Slides from a workshop

on the topic of

"The Relationship Between Computer
and Computational Science"

presented by

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<http://www.cra.org/Activities/snowbird/00/wk4-1.html>

The Relationship Between Computer Science and Computational Science

CRA Conference, Snowbird 2000

Snowbird, Utah

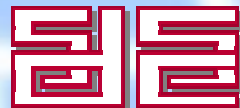
July 11, 2000

*Sid Karin, Director
NPACI and SDSC*



NATIONAL PARTNERSHIP FOR ADVANCED COMPUTATIONAL INFRASTRUCTURE

SAN DIEGO SUPERCOMPUTER CENTER



The Relationship Between Computer Science and Computational Science

- **The object of intellectual curiosity in computer science is the computer**

The Relationship Between Computer Science and Computational Science

- **The object of intellectual curiosity in computational biology is living systems**

The Relationship Between Computer Science and Computational Science

- **The object of intellectual curiosity in computer science is the computer**
- **The object of intellectual curiosity in computational biology is living systems**

The Computational Science Continuum

**Data-intensive computing
(mining)**

Theory

Experiment

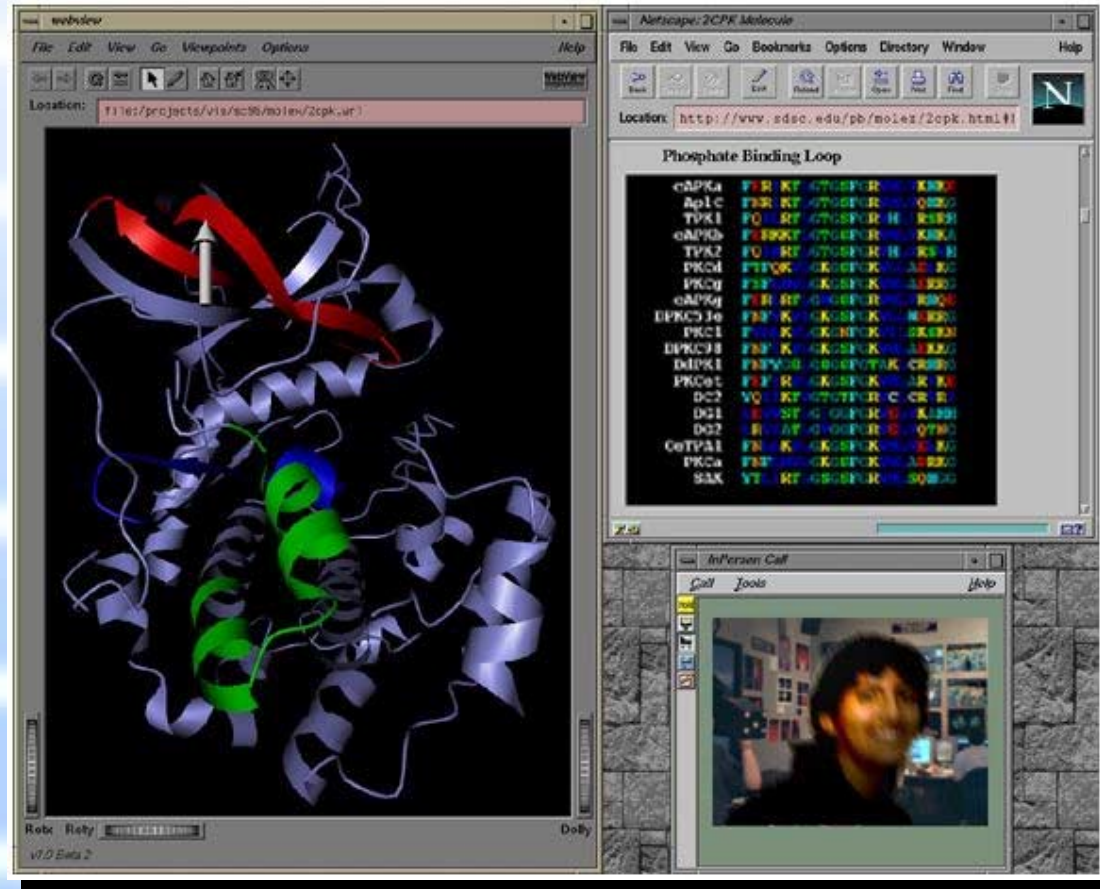
Simulation

**Numerically
intensive
computing**

**Data-
intensive
computing
(assimilation)**

MICE: Transparent Supercomputing

- Molecular Interactive Collaborative Environment
- Gallery allows researchers, students to search for, visualize, and manipulate molecular structures
- Integrates key SDSC technological strengths
 - Biological databases
 - Transparent supercomputing
 - Web-based Virtual Reality Modeling Language



Supercomputers, Networks, and Virtual Reality -- Sharing Science with 80 Million People

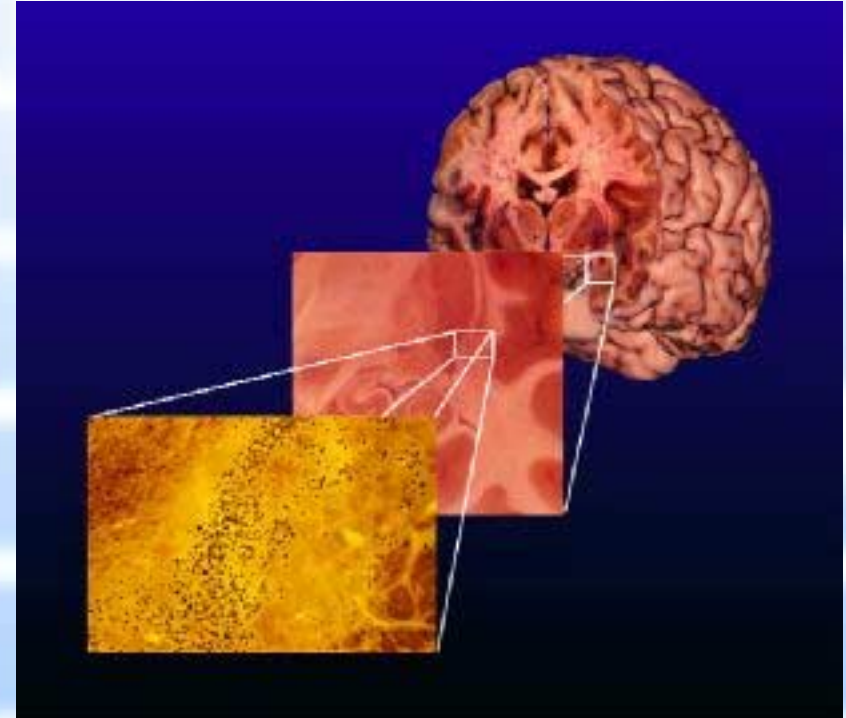


- Virtual Director in CAVE for Choreography of Data
- 1000-Hour SDSC Supercomputer Run to Generate Data
- Tens of Thousands of Hours of NCSA SGI Time to Render Data
- Cross-Country Transfer of 65 GB of data to IMAX Film

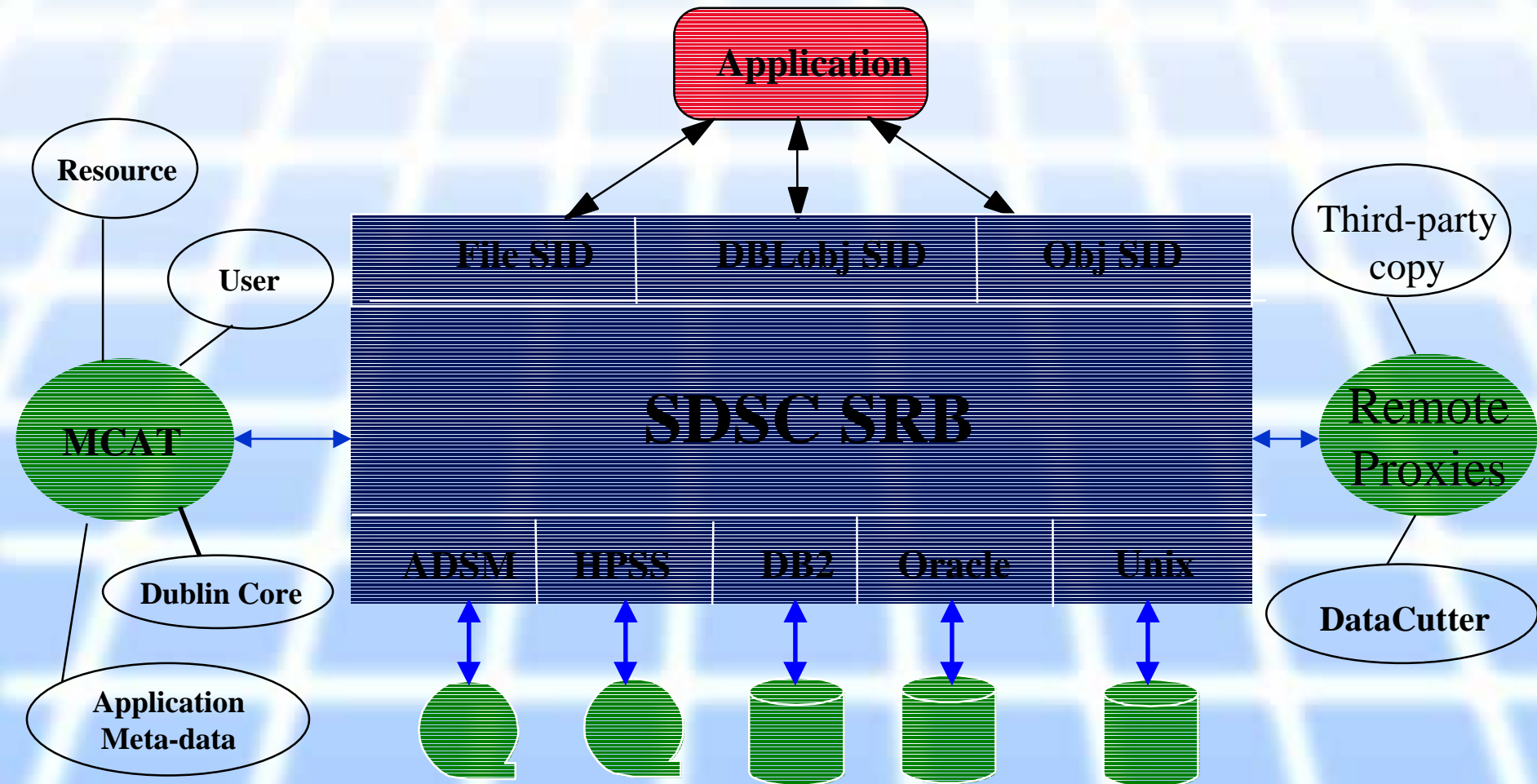
*Visualization by Donna Cox, Bob Patterson, NCSA
From "Cosmic Voyage" (Smithsonian IMAX)*

Brain Mapping

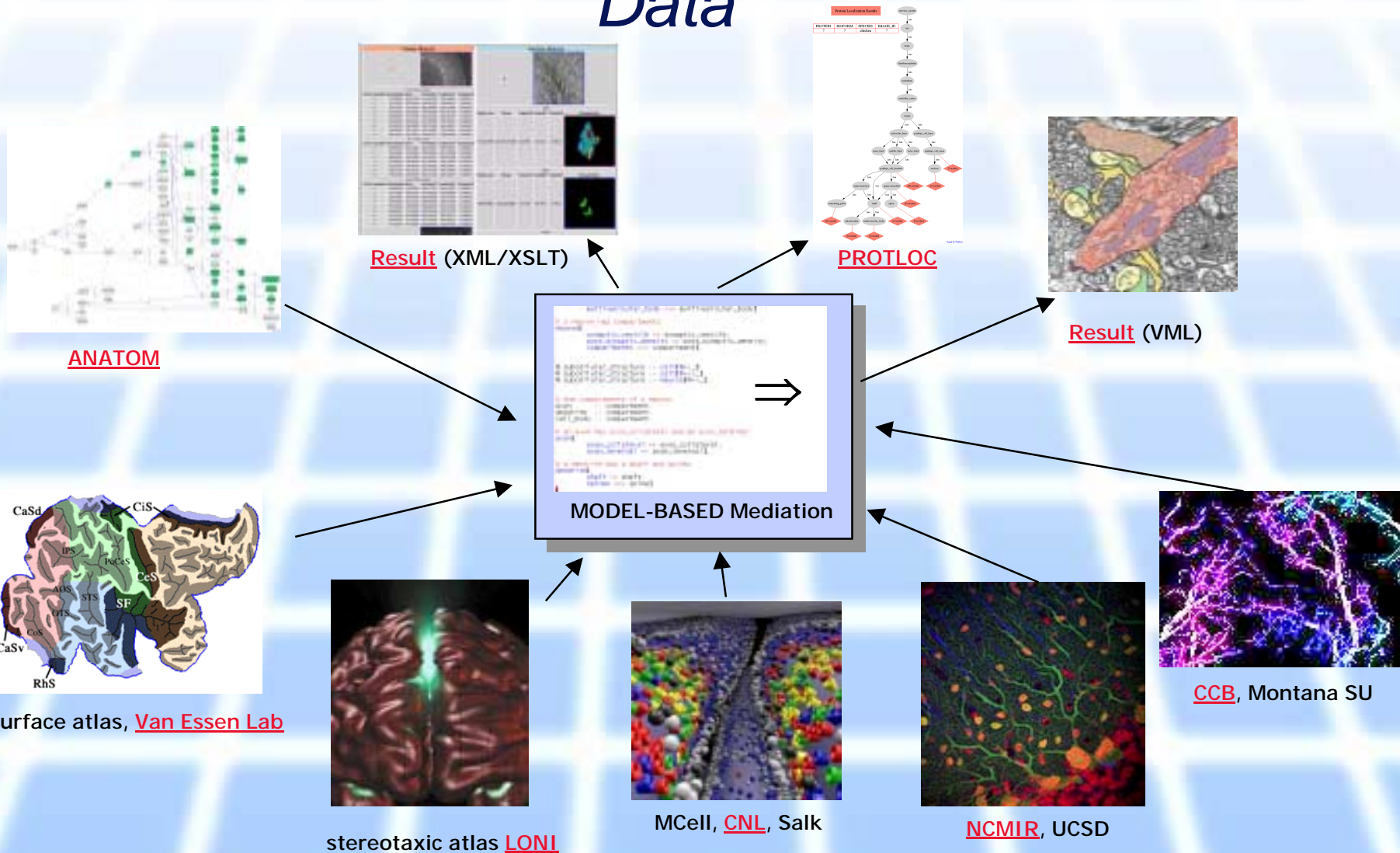
- **One brain = a lot of data**
 - At full-color, micrometer resolution, one brain fills *4.5 petabytes*.
- **Mapping the brain will help understand memory, consciousness, sleep, aging**
 - Insight about brain structure-function relationships in health and disease
 - Federating geographically distributed collections and tools for data exploration, comparison, and simulation
 - Involves all NPACI technology thrusts.



SDSC Storage Resource Broker & Meta-data Catalog



"Collection" Management: Federation of Brain Data





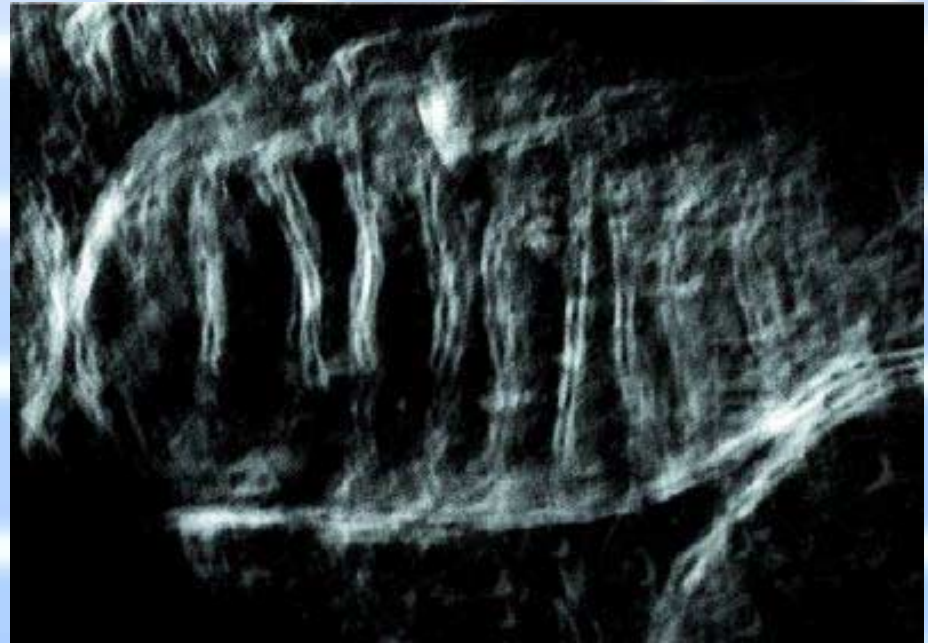
1CD3: The PDB's 10,000th structure.

The Protein Data Bank

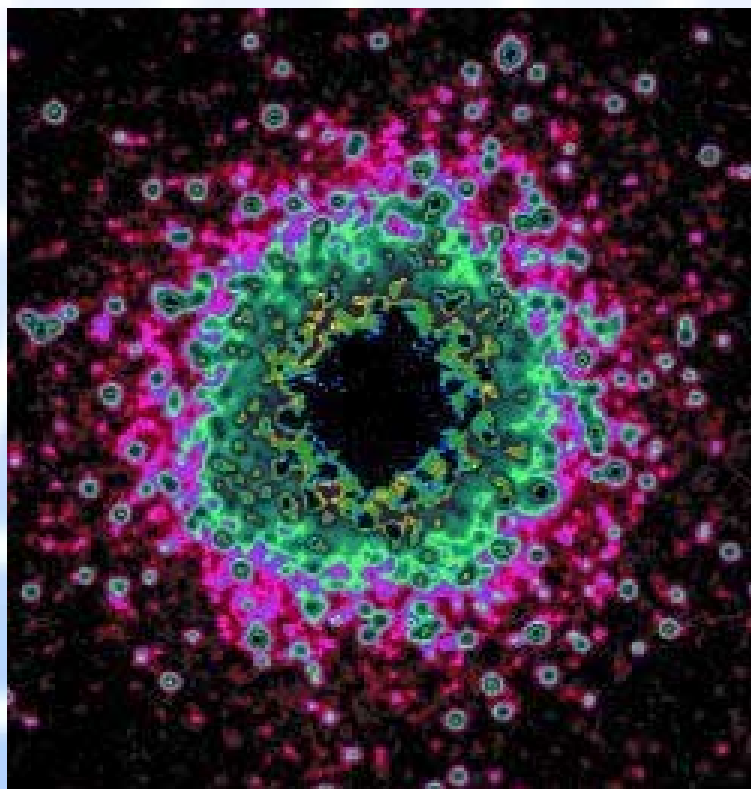
- World's single scientific resource for depositing and searching protein structures
- Protein structure data growing exponentially
 - 10,500 structures in PDB today
 - 20,000 by the year 2001
- Vital to the advancement of biological sciences
- Working towards a digital continuum from primary data to final scientific publication
- Capture of primary data from high-energy synchrotrons (e.g. Stanford Linear Accelerator Center) requires 50Mbps network bandwidth

Telescience for Advanced Tomography Applications

- Integrates remote instrumentation, distributed computing, federated databases, image archives, and visualization tools.
 - Mark Ellisman, UCSD
 - Fran Berman, UCSD
 - Carl Kesselman, USC
- 3-D tomographic reconstruction of biological specimens



The Digital Sky



A globular cluster from the DPOSS archive. Such clusters provide a minimum age for the universe. Image by Thomas Handley, Caltech.

- **Billions of objects can be detected with optical, infrared, and radio telescopes**
 - Tens of terabytes of image and catalog data
- **Digital Sky federating four sky surveys to allow multi-wavelength studies across the data sets**
 - DPOSS, 2MASS, NVSS, FIRST
 - Tom Prince, Caltech, leading federation effort
 - Uses MIX, SDSC SRB, and NPACI mass storage systems