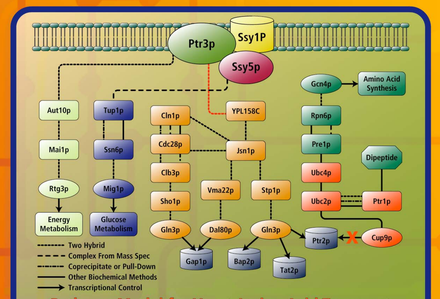
Genomes to Life Center for Molecular and Cellular Systems: A Research Program for Identification and Characterization of Protein Complexes.

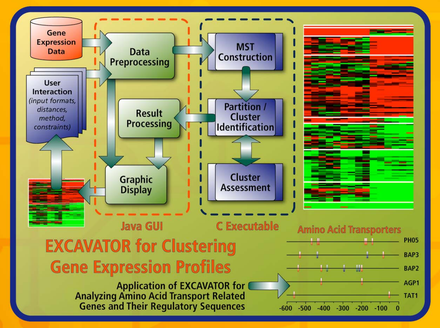
Bioinformatics and Computing in the Genomes to Life Center for Molecular and Cellular Systems

Deborah Payne, *Pacific Northwest National Laboratory*

A Joint Project of Oak Ridge National Laboratory and Pacific Northwest National Laboratory

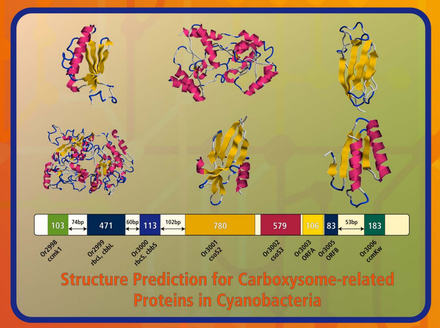


Pathway Model for Yeast Amino Acid Transport



EXCAVATOR for Clustering Gene Expression Profiles

Application of EXCAVATOR for Analyzing Amino Acid Transport Related Genes and Their Regulatory Sequences



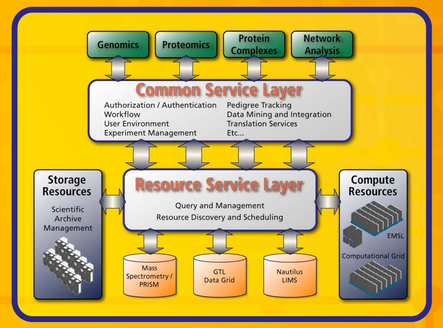
Structure Prediction for Carboxysome-related Proteins in Cyanobacteria

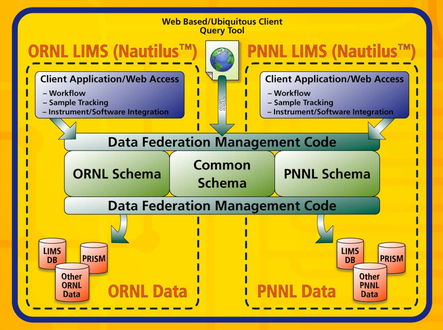
Oak Ridge National Laboratory

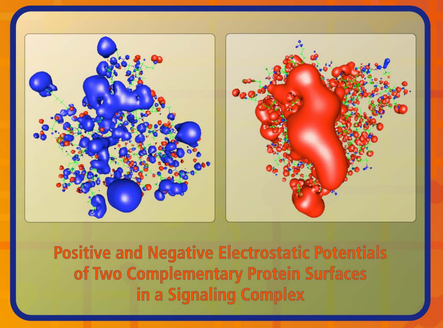
Project Lead: Ying Xu

Manesh B. Shah, Dong Xu, Denise D. Schmoyer, Serguei Passovets, Inna E. Vokler, Jane Razumovskaya, Tema Fridman, Victor N. Olman, Andrey A. Gorin Edward C. Uberbacher, Frank W. Larimer

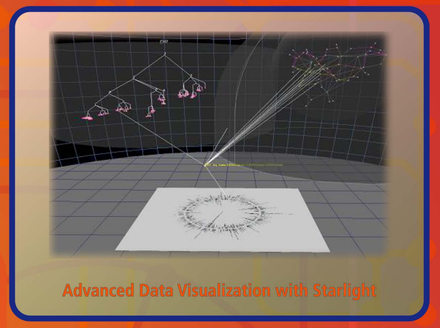
Problem Solving Environment







Positive and Negative Electrostatic Potentials of Two Complementary Protein Surfaces in a Signaling Complex

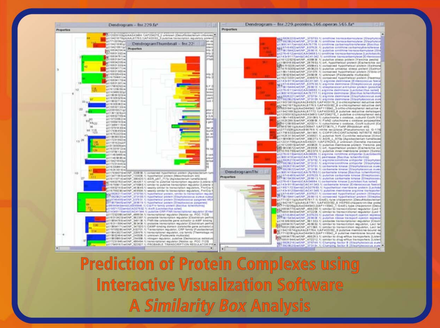


Advanced Data Visualization with Starlight

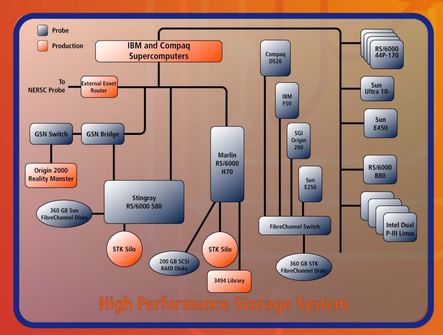
Pacific Northwest National Laboratory

Project Lead: David A. Dixon

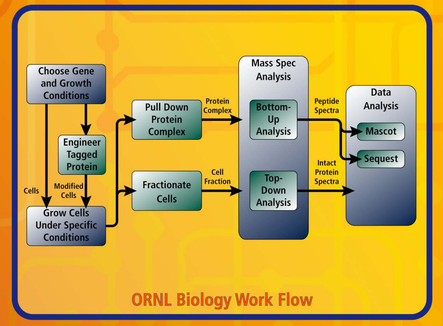
Deborah A. Payne, Heidi J. Sofia, T. P. Straatsma, Elena S. Mendoza, Gordon A. Anderson, Deborah K. Gracio, William R. Cannon, Haluk Resat



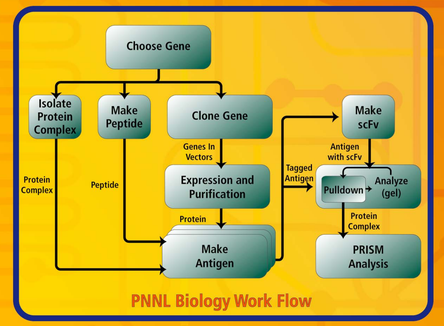
Prediction of Protein Complexes using Interactive Visualization Software
A *Similarity Box* Analysis



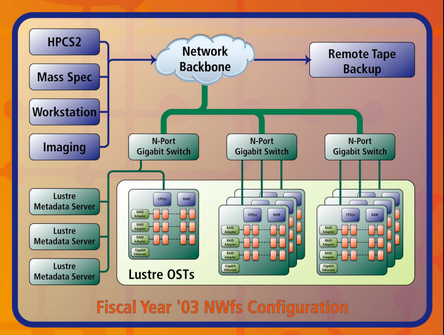
High Performance Storage System



ORNL Biology Work Flow



PNNL Biology Work Flow

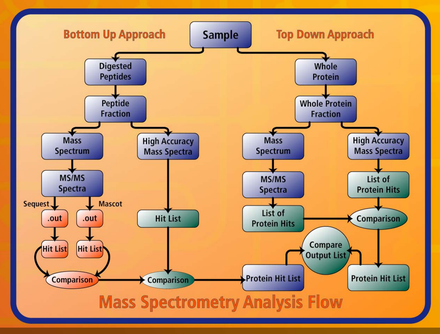


Fiscal Year '03 NWfs Configuration

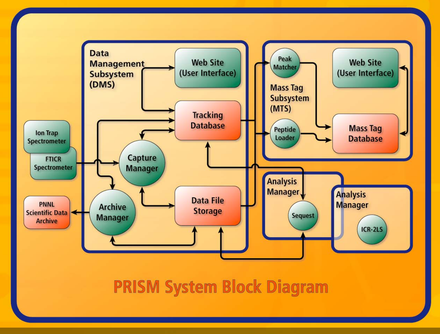
Mass Spectrometric Analysis of Proteome Data

Cheetah
27 Node IBM pSeries System
864 1.3 GHz Power4 processors
4.5 TeraFLOP/s

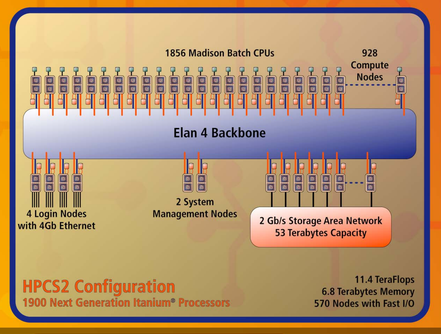
High Performance Computing at ORNL



Mass Spectrometry Analysis Flow



PRISM System Block Diagram



HPCS2 Configuration
1900 Next Generation Itanium® Processors

GENOMES to LIFE
BIOLOGICAL SOLUTIONS FOR ENERGY CHALLENGES
U.S. DEPARTMENT OF ENERGY
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