

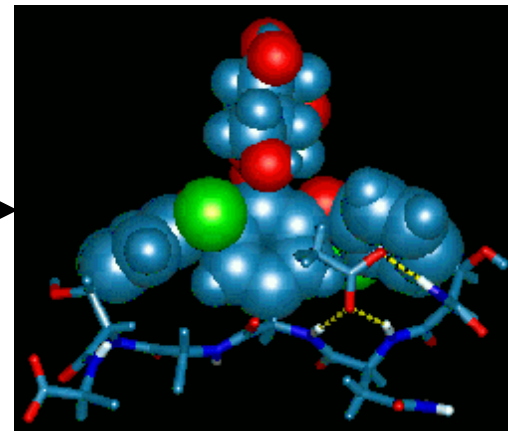
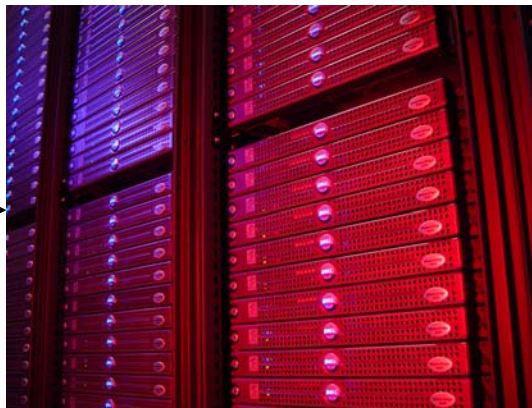
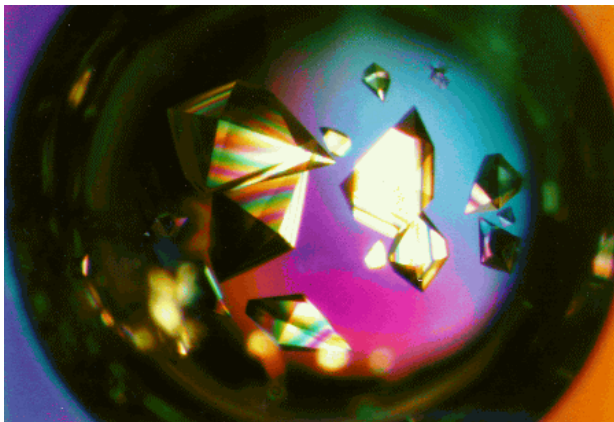
SC2003 Panel: The Simplification of Supercomputing: Clustering, Appliances and Grid Computing

The WNY Bioinformatics Grid Russ Miller

Director, Center for Computational Research

UB Distinguished Professor, Computer Science & Engineering

Senior Research Scientist, Hauptman-Woodward Medical Inst



Biomedical Advances

■ PSA Test (screen for Prostate Cancer)

■ Avonex: Interferon Treatment for Multiple Sclerosis

■ Artificial Blood

■ Nicorette Gum

■ Fetal Viability Test

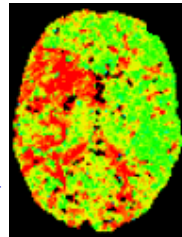
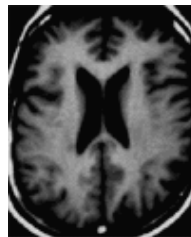
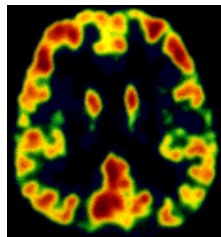
■ Implantable Pacemaker

■ Edible Vaccine for Hepatitis C

■ Timed-Release Insulin Therapy

■ Anti-Arrhythmia Therapy

□ Tarantula venom



■ Direct Methods Structure Determination

□ Listed on “Top Ten Algorithms of the 20th Century”

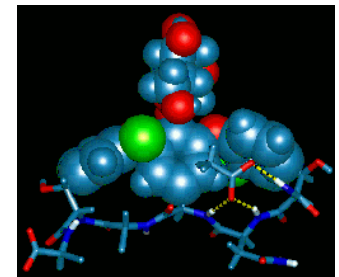
□ Vancomycin

□ Gramacidin A

■ High Throughput Crystallization Method: Patented

■ NIH National Genomics Center: Northeast Consortium

■ Howard Hughes Medical Institute: Center for Genomics & Proteomics



Center for Computational Research (10TF/20TF & 90TB)

■ Dell Linux Cluster

- ❑ 600 P4 Processors (2.4 GHz)
- ❑ 600 GB RAM; 40 TB Disk; Myrinet

■ Dell Linux Cluster

- ❑ 4036 Processors (PIII 1.2 GHz)
- ❑ 2TB RAM; 160TB Disk; 16TB SN



■ SGI Origin3800

- ❑ 64 Processors (400 MHz)
- ❑ 32 GB RAM; 400 GB Disk

■ IBM RS/6000 SP

- ❑ 78 Processors
- ❑ 26 GB RAM; 640 GB Disk

■ Sun Microsystems Cluster

- ❑ 48 Sun Ultra 5s (333MHz)
- ❑ 16 Dual Sunblades (750MHz)
- ❑ 30 GB RAM, Myrinet

■ SGI Intel Linux Cluster

- ❑ 150 PIII Processors (1 GHz)
- ❑ 75 GB RAM, 2.5 TB Disk Storage

■ Apex Bioinformatics System

- ❑ Sun V880 (3), 6800, 280R (2), PIIIs
- ❑ Sun 3960: 7 TB Disk Storage

■ HP/Compaq SAN (4Q03)

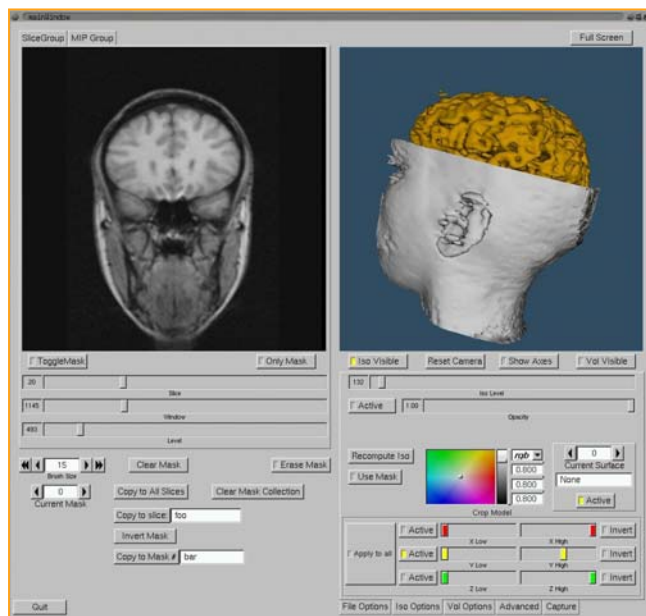
- ❑ 75 TB Disk; 200 TB Tape



Bioinformatics in Buffalo

A \$360M Initiative

- New York State: \$121M
- Federal Appropriations: \$13M
- Corporate: \$146
- Foundation: \$15M
- Grants & Contracts: \$64M



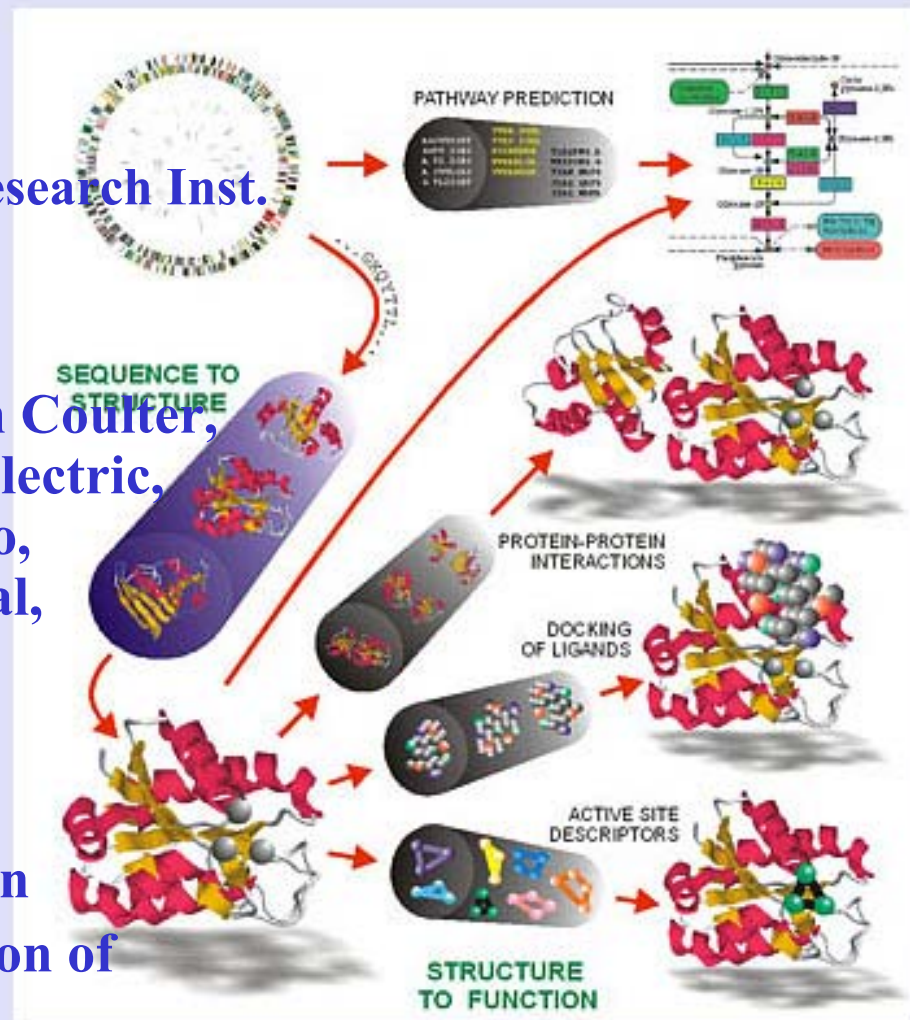
Bioinformatics Partners

■ Lead Institutions

- ❑ SUNY-Buffalo
- ❑ Hauptman-Woodward Medical Research Inst.
- ❑ Roswell Park Cancer Institute

■ Corporate Partners

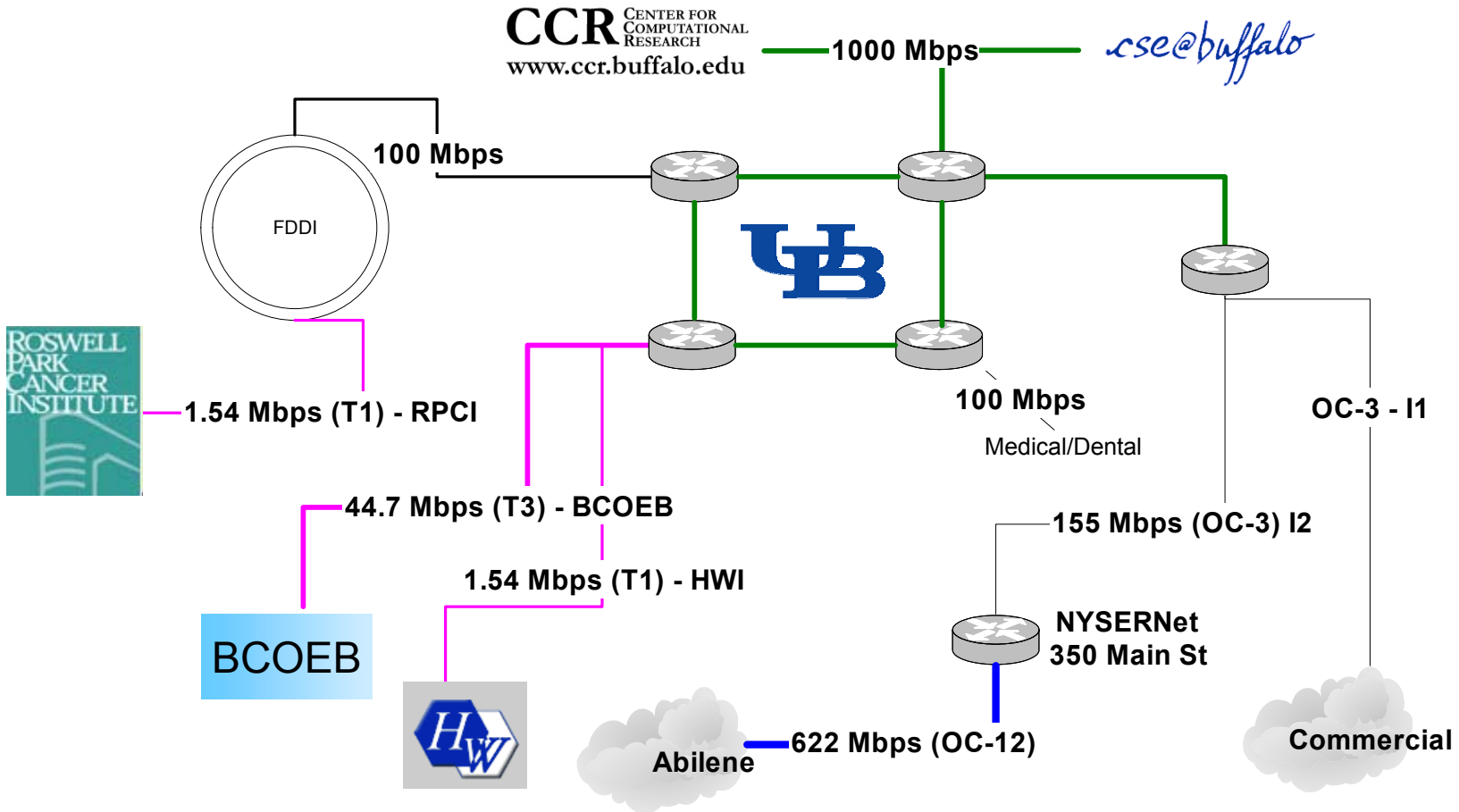
- ❑ Amersham Pharmacia, Beckman Coulter, Bristol Myers Squibb, General Electric, Human Genome Sciences, Immco, Invitrogen, Pfizer Pharmaceutical, Wyeth Lederle, Zeptomatrix
- ❑ Dell, HP, SGI, Stryker, Sun
- ❑ AT&T, Sloan Foundation
- ❑ InforMax, Q-Chem, 3M, Veridian
- ❑ BioPharma Ireland, Confederation of Indian Industries



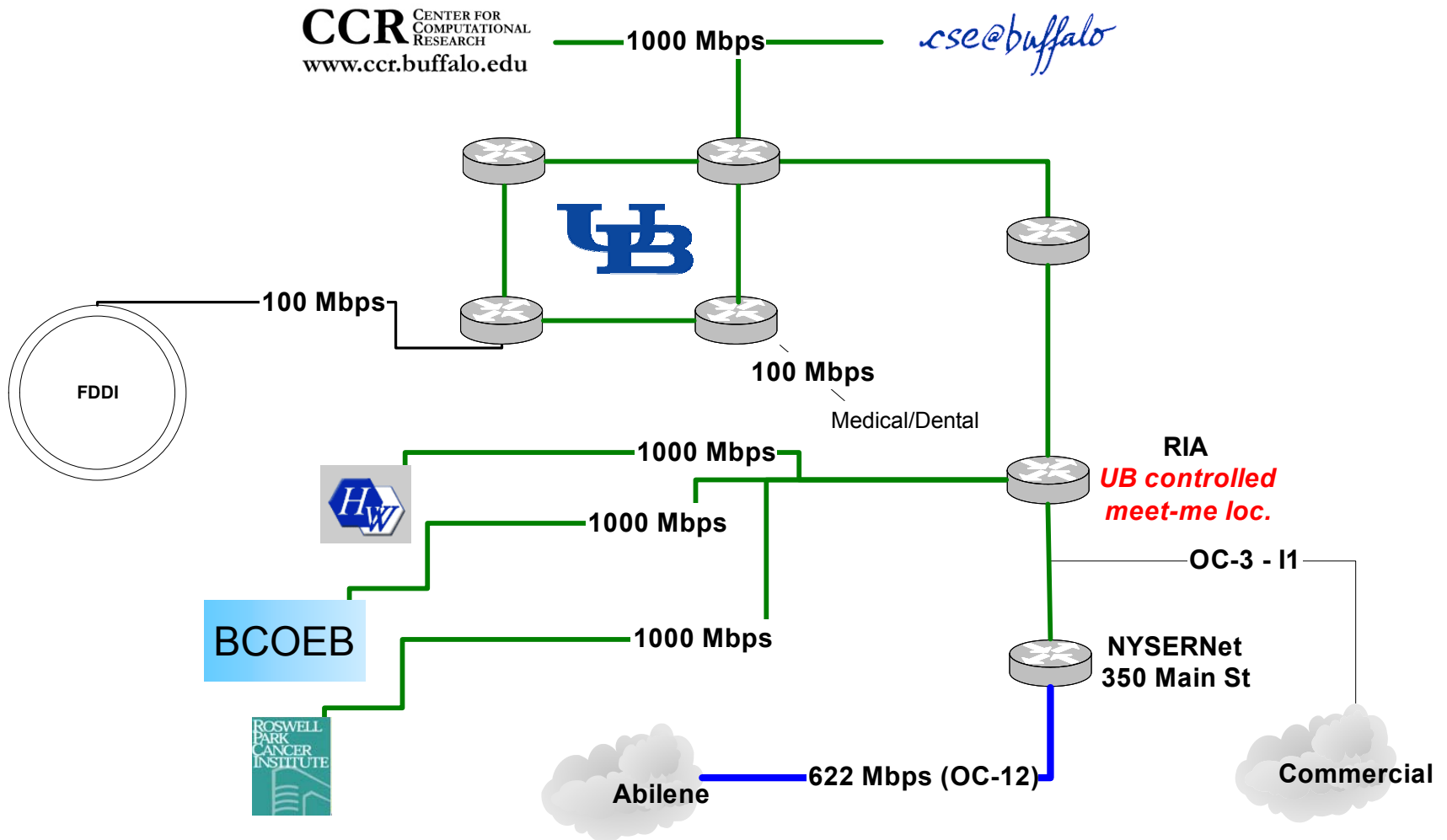
Critical Resources

- **Computational Resources (CCR)**
 - 10TF Computing & 75TB Storage
- **Instruments (HWI, RPCI)**
 - Microarray; Diffractometer; NMR
 - High-Throughput Crystallization Laboratory
- **Data Generation (HWI)**
 - 7TB per year
- **Databases (UB-N, UB-S, BGH, CoE)**
 - *SnB*; Multiple Sclerosis; Protein/Genomic

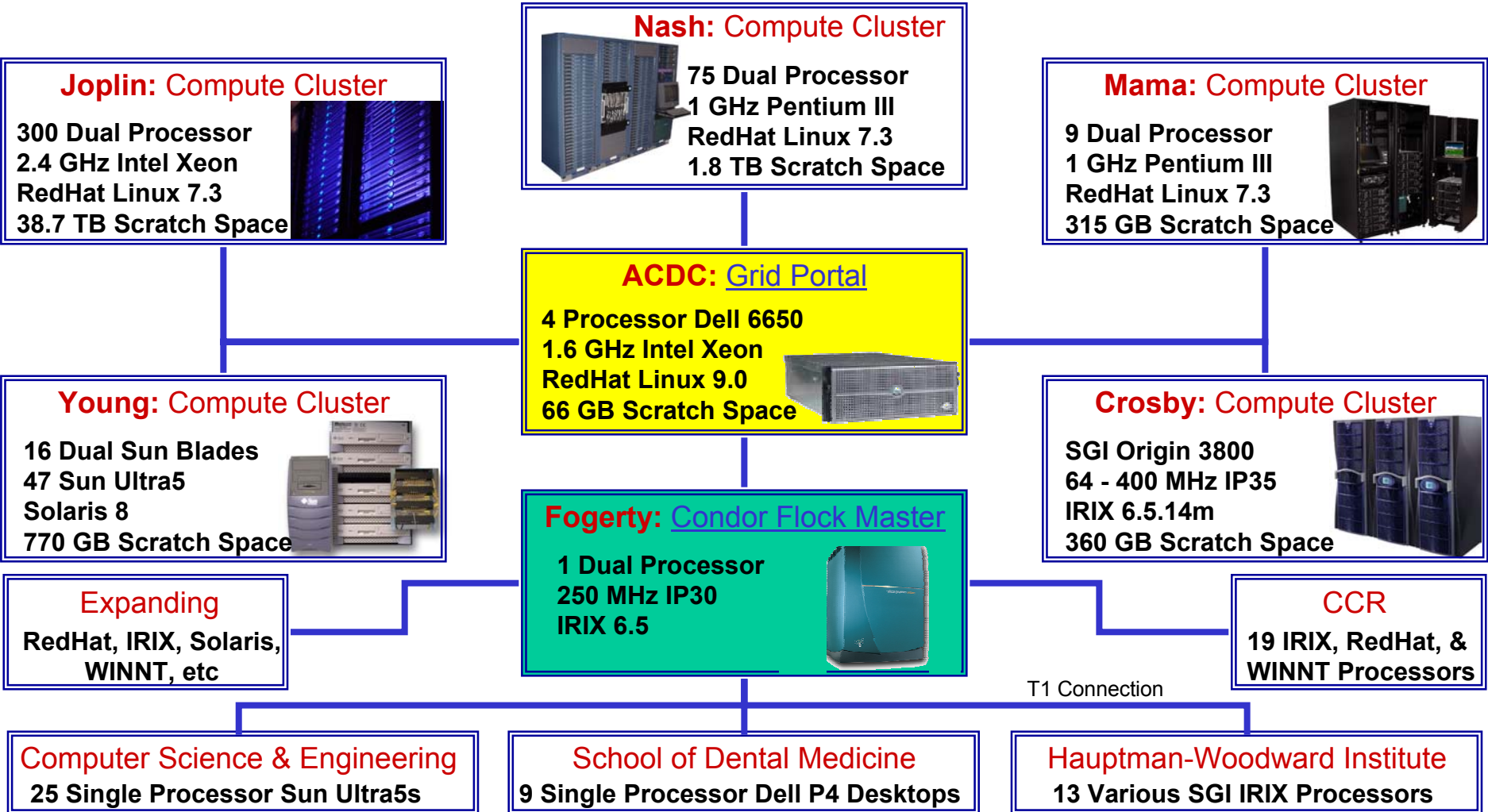
Network Connections



Network Connections (New)

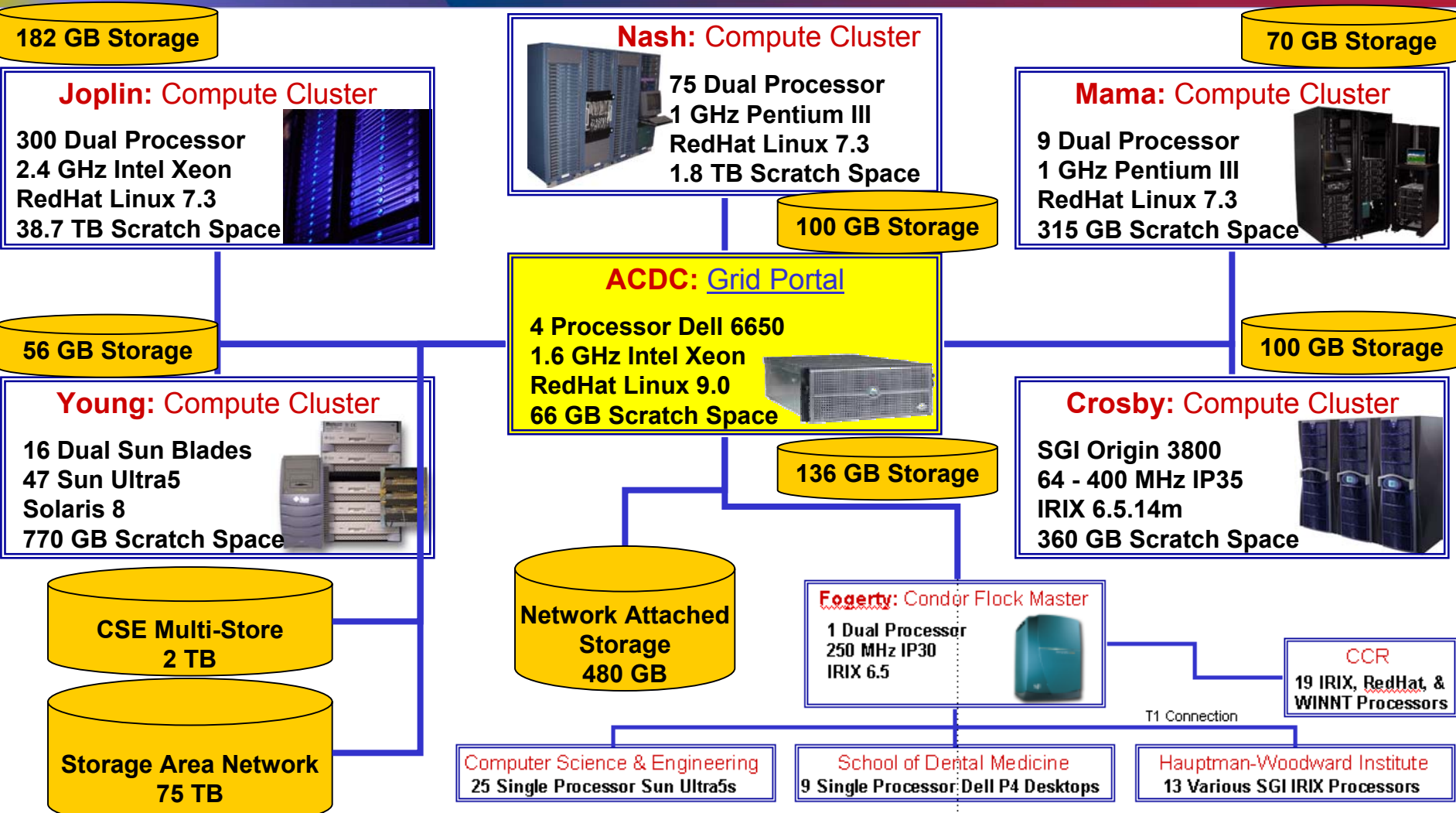


Advanced CCR Data Center (ACDC) Computational Grid Overview



Note: Network connections are 100 Mbps unless otherwise noted.

ACDC Data Grid Overview



Note: Network connections are 100 Mbps unless otherwise noted.



Grid Overview

- **Heterogeneous Computational & Data Grid**
- **Currently in Beta with *Shake-and-Bake***
- **WNY Release in March**
- **Bottom-Up General Purpose Implementation**
 - **Ease-of-Use User Tools**
 - **Administrative Tools**
- **Back-End Intelligence**
 - **Backfill Operations**
 - **Prediction and Analysis of Resources to Run Jobs (Compute Nodes + Requisite Data)**

Conclusion

■ Mission

□ *Enable Science!!*

■ Short-Term Goals

□ Limited Scope

□ Cooperative Organizations

□ Production Quality (hands off)

□ User Centric

