

## General Computing Resources

The following computing resources are available for the research and business needs of the Edward A. Doisy, Department of Biochemistry and Molecular Biology.

General resources available from the University include centralized email and calendaring, authentication services, high-speed data routing, gigabit ethernet and authenticated, as well as guest, wireless internet access and SMB file services to a centralized Storage Area Network. Additionally, the University provides connections to Internet2 for high-speed data transfer, as well as a direct pipeline to other nearby institutions, including The Washington University School of Medicine.

Within the Department additional resources are provided to administrative personnel and research laboratories; These include:

16 TB Active Storage high performance storage arrays in a redundant RAID 5 configuration, with redundant power, redundant 4 Gb/s fibre file server connections and hot swappable drive modules.

16 TB of direct to disk data storage is provided for authenticated disk-encrypted user initiated system backups via Apple's Time Machine system service.

Tandberg 224L LTO-3 tape drive unit for daily backups of central department servers and data storage units. Aggregate in-system tape storage is approximately 18.4 TB (compressed) operating at 490 GB/hr disk to tape transfer rate over optical fibre. Backups are performed using Retrospect.

4x Intel Nehalem 8-core Apple Xserve's operating between 2.2 and 3.0 GHz, each configured with software enabled RAID 1 hot swappable primary disk drives at 7200 rpm, 8-12 GB RAM, 4 Gb/s fibre to storage interconnects, redundant power supplies and 1 Gb/s ethernet and 1 TB scratch disk. Running OS X Server version 10.7 and providing AFP, SMB and NFS file services.

1x Intel Core i7 4-core Mac Mini operating at 2.0 GHz, 8 GB RAM, 2x 500 GB internal storage.

2x APC Smart 2200 UPS battery backup units.

## High Performance Computing Resources

The hardware specifications are 1x Dell PowerEdge R720 headnode, 5x Dell PowerEdge C6220 compute chassis each with 4 nodes (20 nodes total). Each node has 2x Intel Xeon E5-2650 8-core CPUs, 20 M L2 Cache with 8 GT/s via Quick Path Interconnects on each core, 64 GB RAM, Mellanox ConnectX-2 Quad Data Rate Infiniband at 40 Gb/s. Each node is connected to a Dell C410x PCIe expansion chassis, 8 HIC inputs and quantity 16, x16 channel PCIe sleds, with each containing an NVIDIA M2075 Fermi GPU, 6 GB GDDR5 RAM at 150 GB/s. 1x 36-port Quad Data Rate Infiniband switch. 1x Dell PowerConnect 6224, 24-port 10 GbE managed switch. 2x PV MD1200 storage units each with 12x 2TB 7200 rpm SAS hotplug disk drives (48 TB aggregate).

The equipment is located in the DRC main data room providing through floor, front facing cooling and redundant power on emergency generator backup. The cluster is housed in a 42 U enclosure with redundant 100 A PDUs and an additional front facing cooling blower at the bottom of the rack.

The systems software stack runs CentOS 7 with the Bright Computing Cluster Manager, the full suite of SBGrid software tools for macromolecular structure determination and Intel compilers are available. Additional software for specific research applications will be installed and managed on an as needed basis