Resources and Facilities

Facility: The MCCF is located on the 4th floor of the Skaggs Building (SB), and consists of a suite that includes a workstation lab (SB 482, 5 work areas, each with a Linux or iMac workstation). Most electrical power is conditioned and surge suppressed, with 10-minute, uninterruptable power backup supply system for MCCF-hosted Linux workstations. Network connectivity provided by Cisco devices allowing up to 48 ports of routine 100 MB – 1 GB switched data access and data flow.

MCCF Equipment and Software:

GPU Linux cluster with 20 CUDA enabled NVIDIA GeForce GTX 1080 GPUs and 15 TB storage (newton.umt.edu). The newton.umt.edu cluster is co-administered with Dr. Travis Hughes (BMED).

Linux Workstations all with GPU acceleration: 5 GPU-accelerated workstation for molecular dynamics and other CUDA-enabled software, each with either 4 CUDA enabled NVIDIA GeForce GTX A5500 GPUs, 4 NVIDIA GeForce GTX 1080 ti GPUs, or 4 NVIDIA GeForce GTX 2080 ti GPUs.

Other Workstations: 3 iMac workstations, each with 96 GB memory and 4 TB storage. These iMac workstations are available to lend out to users with specific projects.

Software: Spark and Flare (cresset-group.com); Amber22 and AmberTools23; YASARA; Gaussian16/GaussView6; AutoDock v. 4.2.6 and Autodock Vina (Scripps); Avagadro; VMD v2 (www.ks.uiuc.edu/Research/vmd/); NAMD v. 2.11; MODELLER (UCSF); R; PyMol incentive v.2.5; Relion software (www3.mrc-lmb.cam.ac.uk/relion); amongst others.

Software description:

- **Drug discovery platforms**
  - **Spark** (cresset-group.com/software/spark/) for small molecules and peptide design using algorithms and pipelines for moiety similarity searching, toxicity analysis, R group exploration, electrostatic mapping and to grow and link small molecule and peptides ligands.
  - **Flare** (cresset-group.com/software/spark/) for structure based design of small molecules and peptides. Flare combines quantum mechanics, molecular dynamics, and electrostatic mapping to calculate relative affinities between ligands and receptors.
  - **Spark and Flare** are designed for intuitive, structured drug discovery and are meant to be used together iteratively for drug design and optimization.
- **Small molecule docking**
  - **YASARA Autodock and Vina** (yasara.org/docking.htm). YASARA provides a simple-to-use and versatile graphical interface for the time-tested docking algorithms used in Autodock (autodock.scripps.edu/) and Vina (autodock.scripps.edu/) docking programs.
  - **GOLD** (ccdc.cam.ac.uk/solutions/csd-discovery/components/gold/) for small molecule docking and virtual screening of compounds. GOLD is fast, accurate, and relatively simple to use to quickly identify probable binding modes using a variety of genetic algorithms.
  - **Flare** (cresset-group.com/software/flare/) for small molecule docking and design optimization using multiple receptor conformations.
- **Molecular dynamics (MD**)
  - **Amber22 and AmberTools23** (ambermd.org) for GPU-accelerated molecular dynamics. We use Amber to calculate micro- and even low millisecond trajectories. The Amber force field has been well tested and found to be robust at calculating the dynamical movements of proteins and small molecules. Currently we offer training and fee-for-service accelerated MD techniques such as two-dimensional umbrella sampling and replica exchange, as well as code development for implementation of techniques.
  - **YASARA** for graphical interface to implement multiple MD force fields, including Amber force fields) to calculate GPU-accelerated MD trajectories. YASARA provides an intuitive interface for shorter, traditional MD calculations and can be used for affinity calculations and to help with drug discovery.
  - **Visual Molecular Dynamics** (ks.uiuc.edu/Research/vmd/) is used for MD trajectory analysis.

- **Molecular mechanics**
  - **Amber, Flare, and YASARA** can be used to evaluate quantum properties to inform MD calculations.
- **Quantum mechanics calculations**
  - **Gaussian16 and GausView6** (gaussian.com) for density functional theory (DFT) calculations, Semi-empirical calculations, Hartree-Fock approximations, etc.
  - **Flare** (cresset-group.com/software/flare/) uses the Extended Electron Distribution force field that draws on a library of small molecule quantum derivatives to simulate dynamical nature of partial charges, allowing for rapid, accurate charge estimations. This aids in small molecule and peptide structure-based design.
- **Protein and small molecule modeling and visualization**
  - **YASARA**, **Chimera** (cgl.ucsf.edu/chimera/), **VMD**, **PyMol incentive** (pymol.org), **Avogadro** (avogadro.cc/) and **Modeller** (salilab.org/modeller/) are all available at the MCCF for molecular modeling, energy minimization and short MD of small molecules and proteins, and sequence alignment optimization and structural refinement for homology and comparative modeling.

Resources

The University of Montana provides a combination of centralized and unit-based support for high performance computing, including the following facilities:

- A Campus Grid Framework that provides access to computational resources centrally supported on the campus.
- Unit-based Compute Facilities and Support which support specialized computation facilities, software, and staff support for various discipline-specific computing needs.

Advanced Networking

- On-Campus Networks: The University of Montana is served by a campus core network based on multi-10 Gb links. On-campus buildings are connected to the core at a minimum of 1 GB, ranging up to 10 GB as needed. Internally, buildings support a minimum 100 Mb switched connectivity to desktops and servers, ranging up to 1 GB or higher as needed.
- State Network Connectivity: The University of Montana participates in the Montana State network, which is in the process of being upgraded to a network with a multi-GB core and minimum of 45 MB connections to the endpoints, which connects the multiple campuses of each university and connects the universities to the State and University System Office.

Network Infrastructure: The MCCF network is composed of a single vendor (Cisco) network solution that links campus edge devices to ensure the ability of UM to participate fully in the Internet2 initiative. Specifically the Cisco solution enhances end-to-end management of the network, in particular Quality of Service (i.e., priority based routing) and allows for deployment of a campus-wide multicast network, which is a key consideration for the future deployment of Access Grid Node technologies. The MCCF is composed of Category-5 and -6 cabling, and also single and multi-mode fiber capabilities to servers and workstations, with dedicated gigabit links to the campus backbone.