The Molecular Computational Core Facility (MCCF) at the University of Montana provides state-of-the-art computational infrastructure to support research in molecular modeling, drug discovery, and structural biology. The facility supports a comprehensive suite of software tools, including Amber24/AmberTools25, YASARA, Gaussian16 and GaussView6, AutoDock, MODELLER, and Cresset's Spark and Flare, enabling capabilities for structure-based drug design, pharmacophore modeling, small molecule docking, molecular dynamics, quantum and molecular mechanics, DFT calculations, and protein-ligand interaction analysis. These tools are leveraged for advanced simulation techniques such as replica exchange, umbrella sampling, and advanced free energy calculation methods such as free energy perturbation calculations using Cresset's Flare platform. The facility is backed by the University's high-performance computing infrastructure, including multi-gigabit connectivity and Cisco-based network management optimized for high-throughput data flow.

MCCF hardware includes four high-performance GPU-accelerated workstations, each equipped with either four CUDA-enabled NVIDIA GeForce GTX A5500 GPUs or four NVIDIA GeForce GTX 2080 Ti GPUs. These workstations support computationally intensive, long running tasks such as molecular dynamics simulations and analysis and DFT-based quantum mechanics calculations, providing researchers with local computing power for precision-driven modeling and analysis.

In addition to MCCF's in-house resources, Dr. Holley, the MCCF manager, provides support for UM users accessing the University of Montana's Griz Shared Computing Cluster (GSCC). The GSCC comprises 32 nodes with a total of 1,056 computing cores and approximately 15 TB of memory. Notably, it includes 12 GPU nodes, each equipped with four NVIDIA RTX 2080 Ti GPUs, facilitating high-performance parallel processing for computationally intensive tasks.