

Facilities, Equipment, and Other Resources

Facilities: The key personnel can support all of the proposed modeling and computational work with dedicated high-performance facilities. August 2014 saw the opening of The Science Building (SCI), a \$147 million, 248,000 square foot, state-of-the-art structure. In addition, SCI features areas set aside for formal instruction, server rooms, classrooms, offices, and areas that promote conversation and cooperation. Similar to the Science Building, the refurbished Davis /Wiser Patten Science Complex opened in the spring of 2017 and houses additional offices and equipment. Additionally, Walker Library has a few specialized high-performance server rooms.

Computational facilities: A 2500-core cluster is currently located in MTSU Walker Library server room. It includes 41× 16-core 2.3GHz Opteron-based nodes, each with 64GB of RAM and 2TB of local SATA disk space, 1 × 48-core 2.2GHz Opteron-based "supernode" with 16TB of local RAID0 SATA disk space and 256 GB of RAM, and 2 × 48 TB RAID systems. This cluster is maintained by the Computational Science Ph.D. program. A 256-cpu-core / 41,984-GPU-core Computational Chemistry cluster is currently located in the Telecommunications Building Data Center that includes 10 × 8-core 3.0 GHz Xeon nodes (48 GB of RAM and 750 GB of local SATA disk space per node) and 11 × 24-core 2.8GHz Piledriver/K10-based Opteron 6348 nodes (128 or 256 GB of RAM and 32 TB of RAID0 disk space per node). Each Opteron-based node is also equipped with 2 × Radeon HD 7980 GHz edition video cards (each includes 2048 processing cores and 3 GB of RAM). This cluster is maintained by Dr. Volkov. Available parallel computing software includes GROMACS, Gaussian, Molpro, GAMESS-US, GAMESS-UK, NW Chem, Spartan, CRYSTAL, and Amber.

Proposed HPC Cluster Environment: The equipment costs have been approximated based on estimations and detailed specifications. This includes 10 Dell Compute Nodes, priced at \$40,405.81 per unit, resulting in a total of \$458,000. Additionally, there are 2 Nvidia Mellanox SN2010 units with rack hardware and support contracts, estimated at \$10,000.00 per unit, totaling \$20,000.00, and 1 Nvidia Mellanox SN2201 with a support contract, estimated at \$4,000.00. The power infrastructure comprises 6 APC Smart-UPS 3000VA 2700 Watt 2U Units, each estimated at \$3,000.00, summing up to \$18,000.00.

The tentative total for the core equipment is \$500,000. To complement and ensure the efficiency of this infrastructure, additional costs for supporting accessories, cables, software, and hardware are expected to exceed \$20,000, along with an allocation of \$30,000 or more for supporting construction and facilities. Consequently, the estimated total for the project stands at \$550,000. To facilitate budgeting, a rounded estimation of \$550,000.00 has been established. These figures provide a comprehensive overview of the anticipated equipment costs, enabling effective planning for the successful execution of the project.

Technical and Administrative Staff

Technical Personnel: The proposed research will be supported by departmental staff. Senior staff members Bryan Schuder, a full-time computer science administrator, and Thomas Golf, a full-time computational science administrator, train users and maintain the high-performance cluster. This covers the HPC instruments that have been requested. The High-Performance Computational Biology and Cognitive Science Lab is maintained by Dr. Joshua Phillips, who will also provide support for the research in this proposal. Additionally, Dr. Jaishree Ranganathan will collaborate on research on text classification and cloud computing. A full-time stockroom and safety manager places orders for materials and supplies, and a systems administrator oversees the computer facilities. To free up faculty time for research activities, most introductory laboratories are taught by Graduate Teaching Assistants and Laboratory Coordinators.

Administrative Staff: Departmental staff are available to do accounting, hiring, and routine grant paperwork for funded projects. The departmental system admin orders all, supplies, and equipment. Dissemination Forum. To prepare for presentation opportunities at the regional (usually the Southeastern Meeting of the American Computer Machinery, ACM-Midsouth East) or national level (usually IEEE/ACM).