HPCC
High Performance Computing Center

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https://hpc.mst.edu/
Google group: hpcc-grp@mst.edu
HPCC factsheet

• Formally established in the spring of 2019 (spearheaded by Richard Dawes), after a preparation period of several years

• Initial discussions with former Provost Marley and former VPR involved Richard Dawes, Steve Gao, Tom Vojta etc.

• Currently HPCC has 35 members, including 32 faculty from 10 different academic departments, and 3 ITRSS staff members

• In FY2020, HPCC has a direct cost split of $2,185,406 (a 1065% increase over FY19) which ranks 4th among the 9 centers.

• Indirect cost share $173,507 (a 99% increase over FY19)
A Major HPCC Success

Funding of an ~$2 M NSF MRI proposal (submitted by Richard Dawes, Thomas Vojta, Steve Gao, Julia Medvedeva, and Serhat Hosder).

The new system (named Foundry) has 9152 cores running at 2.3 Ghz across 143 compute nodes; 6 GPU nodes with 4 Nvidia V100 GPUs a piece.

A 10-fold increase in computing power over the previous system!

Photo and information courtesy of Buddy Scharfenberg, ITRSS
HPCC objectives

1. Promoting continued growth and ongoing investment in locally hosted hardware infrastructure
2. Expanding the capacity, capabilities and role of high-performance computing related research support staff (one example is hiring an associate director for HPCC using the NSF MRI matching fund)
HPCC objectives

3. Coordinating and promoting high-performance computing related research collaborations, both on and off campus

NSF MRI project partner schools
HPCC objectives

• 4. Participating in mentoring junior faculty and postdocs
• 5. Training activities, both on campus and for outside users
HPCC activities

• Offering regularly scheduled seminar talks by center members and outside speakers (starting from next spring)

• Actively searching for funding opportunities and sharing the info with the HPCC community

• Organizing collaborative research and instrumentation proposals

• Establishing a “Common Codes Depository” (CCD) where common purpose codes can be shared among the members (and perhaps non-members on campus or the outside world – need to figure out copyright issues)

• Organizing workshops with various themes
Example Theme 1: Computational Geophysics: Locating millions of earthquakes and analyzing elastic waves from the quakes for imaging the Earth’s internal structure
Example theme 2: Study and design of materials by large scale computational simulations (Diagram from Dr. Julia Medvedeva, Physics)
Example theme 3: Molecular potential energy surface construction (from Dr. Richard Dawes, Chemistry)
Example Theme 4: Hypersonic flows simulation (diagram from Dr. Serhat Hosder, MAE)
Example theme 5: Novel states of matter in superconductors, superfluids, and magnetic materials (diagram from Dr. Thomas Vojta, Physics)

Figure 4: Illustration of an electronic wave function in a topologically disordered material.
Why joining HPCC?

• Get connected with other computing-intensive researchers on campus (through seminars, meetings, workshops etc.)
• Receive information regarding funding opportunities
• Write joint proposals with other similar-minded S&T faculty
• HPCC can provide (a small amount of) funds or matching funds for essential soft/hardware purchases for its members. ~6.5% of the returned indirect cost goes to the research centers (and to HPCC only if it is included in the proposal PSRS form).
• Help shape the newly established HPCC and high-performance computing at Missouri S&T