1 Introduction

The High-Performance Computing Shared Facility (HPCSF) at provides free computational resources to the Michigan Tech research community. The HPCSF operates and manages two high-performance computing clusters, Superior and Portage.

The HPCSF has served and will continue to serve an important role to attract leading researchers and prospective graduate students to the university, as well as supporting externally funded projects.

2 Facility Leadership

1. Dr. Warren Perger  
   Chair, Research Computing Committee, and ECE and Physics  
   wfp@mtu.edu · 7-2855

2. Research Computing Committee (alphabetical listing of last name)
   (a) Dr. Timothy Havens, ECE and CS (thavens@mtu.edu · 7-3115)  
   (b) Dr. Jinfeng Jiang, BME (jjiang1@mtu.edu · 7-1943)  
   (c) Dr. Adrienne Minerick, Chem. Engg (minerick@mtu.edu · 7-2005)  
   (d) Dr. Gregory Odegard, ME-EM (gmodegar@mtu.edu · 7-2329)  
   (e) Dr. Benjamin Ong, Mathematics (ongbw@mtu.edu · 7-3367)  
   (f) Dr. Ravindra Pandey, Physics (pandey@mtu.edu · 7-2086)  
   (g) Dr. Loredana Valenzano, Chemistry (lvalenza@mtu.edu · 7-1602)  
   (h) Dr. Pengfei Xue, CEE (pexue@mtu.edu · 7-1837)

3. Information Technology
   Includes Dr. Gowtham, Director of Research Computing (g@mtu.edu · 7-4096)

3 Safety Inspection Report

The safety inspection report, including a review of physical facilities and equipment as well as safety requirements in the facility policies and procedures conducted on 2018-02-01 by David Dixon of the Office of Compliance, Integrity, and Safety (OCIS) is available here.
We confirm that the GLRC data center (105A) is clean and safe. However, it is an active data center with components being delivered, staged for installation and removal, etc. But the components - whether staged for installation or removal - are always set away from working/walking areas and we have never had any incident.

4 Conclusion

The HPC Core Facility provides an invaluable resource to the campus research community. An operating budget is needed to maintain reliability and usability of the high-performance computing clusters. The proposed budget will be used to support one student intern for operations support, provide critical software infrastructure for Michigan Tech’s research community, and provide visibility for Michigan Tech’s computational researchers and projects.
1 Introduction

The High-Performance Computing Shared Facility (HPCSF) at provides free computational resources to the Michigan Tech research community. The HPCSF operates and manages two high-performance computing clusters, Superior and Portage. The facility has served and will continue to serve an important role to attract leading researchers and prospective graduate students to the university, as well as supporting externally funded projects.

2 Facility Leadership

1. Dr. Gowtham, Director, HPC Shared Facility (g@mtu.edu · 7-4096)

2. Faculty Advisory Board (alphabetical listing of last name)
   (a) Dr. Timothy Havens, ECE and CS (thavens@mtu.edu · 7-3115)
   (b) Dr. Adrienne Minerick, Chem. Engg. (minerick@mtu.edu · 7-2005)
   (c) Dr. Gregory Odegard, ME-EM (gmodegar@mtu.edu · 7-2329)
   (d) Dr. Ravindra Pandey, Physics (pandey@mtu.edu · 7-2086)

3. Information Technology

3 Infrastructure

Superior is available to all researchers via brief proposal and it has the following computing and storage components:

1. Generation 1.0 (acquired between 2013/06 - 2015/10)
   (a) 92 CPU compute nodes - each having 16 CPU cores (Intel Xeon E5-2670 2.60 GHz) and 64 GB RAM - providing 30 TFLOPS
   (b) 4 CPU compute nodes - each having 24 CPU cores (Intel Xeon E4-2680 2.50 GHz) and 256 GB RAM - providing 2 TFLOPS
   (c) 5 GPU compute nodes - each having 16 CPU cores (Intel Xeon E5-2670 2.60 GHz), 64 GB RAM and 4 NVIDIA Tesla M2090 GPUs - providing 13 TFLOPS
   (d) 3 storage nodes each with 32 TB usable space
2. Generation 2.0 (acquired since 2017/06)

(a) 85 CPU compute nodes - each having 32 CPU cores (Intel Xeon E5-2683 2.10 GHz) and 256 GB RAM - providing 91 TFLOPS

(b) 75 TB enterprise storage solution

*Portage* is a miniature version of *Superior*. Intended primarily for testing, educational (course work and/or senior design projects) and gateway/preliminary research projects involving non-confidential/non-sponsored data, *Portage* has 3 TFLOPS of CPU and 2 TFLOPS of GPU computing capacity with hardware identical to *Superior*’s generation 1.0.

*Superior* and *Portage* have a Gigabit ethernet back-end network that serves the administrative needs, and a 56 Gb/s InfiniBand network that serves the computing needs. They are available for all researchers at Michigan Tech via a brief proposal, very much similar to that of NSF XSEDE.

Dr. Gowtham, serves as the NSF XSEDE Campus Champion. He has access to and trial allocations in several supercomputers around the country and has been helping researchers find an optimal external resource, if/when necessary.

### 3.1 Current Projects

Apart from routine maintenance and collaborative work to help various research groups adopt their workflows to HPC environment, Jen Terlep and Dr. Gowtham have been working on the following major projects:

1. **Front End Upgrade**

   The OS currently installed in *Superior* and *Portage* were installed and customized in 2013. Owing to the nature of *Rocks Cluster Distribution*, frequent updates to critical libraries and packages is nearly impossible without rebuilding the entire HPC infrastructure from scratch. Undertaking such an endeavor frequently, without additional personnel, would have limited the extent of progress our researchers could have achieved.

   However, in the last year or so, a new OS - *OpenHPC* - has made its appearance and established itself as a stable and reliable alternate to *Rocks Cluster Distribution*. Not only it makes frequent updates to system critical libraries relatively easier within a given major release, it includes a vast majority of customizations that Dr. Gowtham had implemented and contributed back to the HPC knowledge base.
In an attempt to be systematic and minimize catastrophic errors (or other issues that could cause long-term delays in research projects), a prototype infrastructure has been set up. Named Portage2, it will transparently replace Portage once the extensive testing of its features as well as migration of our in-house workflows have been successfully completed. This phase is expected to be completed by end of 2019 Summer.

Taking feedback from researches into account through Thanksgiving break, Superior2 built with OpenHPC will transparently replace Superior during 2019 Christmas/Winter break.

In spite of OpenHPC’s stability and reliability, the plan is to keep our infrastructures one minor version/update behind to protect against the bleeding edge of technology.

2. Superior Storage

The new standalone enterprise storage system, with 75 TB of total usable space, will replace the existing 33 TB unit when Superior2 comes into production. The new unit will serve the /research partition and the old unit will be repurposed to serve as an extensive /scratch partition. This will, in turn, provide our researchers an opportunity to tackle more complex problems without the large size of temporary files accounting towards their individual storage quota.
4 User Training

In light of the limited personnel dedicated to supporting HPC endeavors, Dr. Gowtham revamped the HPC website (https://hpc.mtu.edu/) with help from University Marketing and Communications, and designed three courses to provide basic and advanced training. Scenarios that lend themselves to be out of scope for these courses are worked out via one-on-one meetings with individual researchers or research groups.

1. FOSS101: Essentials of Free and Open Source Software

This free, online and learn at your own pace course offers an introduction to command line Linux and Git revision control system, and various aspects of file and data management and processing, and more.

Researchers not yet familiar with aforementioned topics can use it as a formal course and advanced users may use it as reference material.

2. HPC101: Training Camp

Building further upon Michigan Tech’s policy on the Acceptable Use of Information Technology Resources, this free and online course offers step by step training on topics such as remote access, data transfer, generating submission scripts and monitoring simulations. It will also serve as the End User License Agreement (EULA).

Researchers will need to complete this training prior to starting production quality simulations.

3. UN5390: Scientific Computing

Set in a Linux environment, this 3-credit graduate course offers a more formal and an in-depth exposure to using FOSS tools for developing computational and visualization workflows. It is offered in each Fall and Spring semester and cross-listed as BE5390, EE5390, MA5390 and PH5390. Upon successful completion of this course, students will be able to

(a) communicate (oral and written) their thought process, and write usable programs with an emphasis on clarity, readability, understandability and sustainability

(b) translate science and engineering problems into computer programs

(c) compile, debug and profile programs, and understand and resolve sources of error

(d) identify and implement parallel programming techniques

(e) use campus and national high-performance computing (HPC) infrastructures
5 Projects

Sorted by year (descending), college, department and PI. Generic titles are used to protect a researcher’s potential funding and publication interests.

1. Depletion Of Freshwater Lenses On Carbonate Islands Due To Sea Level Rise And Climate Change
   Dr. Alex Mayer (2019, GMES/COE)

2. Computational Investigations In Mechanical Engineering
   Dr. Parisa Abadi (2019, ME-EM/COE)
   Federal agency: 17SDG33660925

3. Structure And Property Relationship Of 2D Materials
   Dr. Ravindra Pandey (2019, Physics/CSA)
   Army Research Office

4. Sub-Sampled Matrix Approximations
   Dr. Benjamin Ong (2018, Mathematics/CSA)

5. Computational Investigations In Mathematical Sciences
   Dr. Cecile Piret (2018, Mathematics/CSA)

6. Computational Investigations In Physics
   Dr. Issei Nakamura (2018, Physics/CSA)

7. Structure And Property Relationship Of 2D Materials
   Dr. Ravindra Pandey (2018, Physics/CSA)
   Army Research Office

8. UN5390: Scientific Computing (Spring 2018)
   Dr. Gowtham (2018, HPC/HPC)

9. Computational Investigations In Forest Resources And Environmental Science
   Dr. Mary Ellen Miller (2018, MTRI/MTRI)
   Federal grant 18-JV-11221634-020

10. Computational Investigations In Biomedical Engineering (Senior Design)
    Dr. Keat Ong (2017, BME/COE)

11. Multiscale Modeling Of Civil And Environmental Engineering Materials I
    Dr. Qingli Dai (2017, CEE/COE)
12. Multiscale Modeling Of Civil And Environmental Engineering Materials II  
   Dr. Qingli Dai (2017, CEE/COE)

13. Computational Investigations In Mechanical Engineering  
   Dr. Chunpei Cai (2017, ME-EM/COE)  
   AFOSR + MTU start-up funds

14. NASA Institute For Ultra-Strong Composites By Computational Design (US-COMP)  
   Dr. Gregory Odegard (2017, ME-EM/COE)  
   NASA

15. Computational Investigations In Mechanical Engineering  
   Dr. Hassan Masoud (2017, ME-EM/COE)  
   MTU start-up funds

16. Control Optimization For Ocean Wave Energy Converters  
   Dr. Ossama Abdelkhalik (2017, ME-EM/COE)

17. Computational Investigations In Mechanical Engineering  
   Dr. Susanta Ghosh (2017, ME-EM/COE)  
   MTU start-up funds

18. Computational Investigations In Mechanical Engineering  
   Dr. Trisha Sain (2017, ME-EM/COE)  
   MTU start-up funds

19. Computational Investigations In Mechanical Engineering  
   Dr. Zequn Wang (2017, ME-EM/COE)  
   MTU start-up funds

    Dr. Bahne Cornilsen (2017, Chemistry/CSA)

21. Multiscale Modeling Studies In Computational Chemistry  
    Dr. Christo Christov (2017, Chemistry/CSA)  
    MTU start-up funds

22. Computational Investigations In Chemistry  
    Dr. Rudy Luck (2017, Chemistry/CSA)

23. Developing Statistical Methods For Genetic Association Studies  
    Dr. Qing Sha (2017, Mathematics/CSA)  
    NIH R15 HG008209
24. Study Of Physical Properties Of Ion-Containing Polymers To Explore High-Performance Electrochemical Energy Storage With Molecular Dynamics And Monte Carlo Simulation Approaches
   Dr. Issaei Nakamura (2017, Physics/CSA)
   MTU start-up funds

25. Computational Investigations In Atmospheric Science
   Dr. Raymond Shaw (2017, Physics/CSA)

26. HOLODEC Participation In The ARM Campaign Aerosol And Cloud Experiments In The Eastern North Atlantic (ACE-ENA)
   Dr. Raymond Shaw (2017, Physics/CSA)
   Pacific Northwest National Laboratory; USD 188,000; USD 11,117 + USD 11,140

27. UN5390: Scientific Computing (Fall 2017)
   Dr. Gowtham (2017, HPC/HPC)

28. Computational Investigations In Machine Learning
   Dr. Joseph Burns (2017, MTRI/MTRI)
   US Army Night Vision Electronic Sensors Directorate via sub-contract to CACI Technologies, Inc. 1608041

29. Computational Modeling Of Mercury Contamination In Lakes
   Dr. Noel Urban (2016, CEE/COE)

30. UHPC Computational Investigations
   Dr. Theresa Ahlborn (2016, CEE/COE)

31. Acoustic Modeling
   Dr. Andrew Barnard (2016, ME-EM/COE)
   Michigan Tech Research Excellence Fund (REF) - Research Seed (RS) grant

32. Computational Investigations In Mechanical Engineering
   Dr. Song-Lin Yang (2016, ME-EM/COE)

33. Microbial Community Dynamics And Response To Environmental Change
   Dr. Stephen Techtmann (2016, Biology/CSA)
   MTU start-up funds

34. Less Is More: Investigating Abbreviated Text Input Via A Game
   Dr. Keith Vertanen (2016, CS/CSA)
   Google Faculty Award

35. Computational Investigations In Mathematical Sciences I
   Dr. Kui Zhang (2016, Mathematics/CSA)
36. Computational Investigations In Mathematical Sciences II  
   Dr. Kui Zhang (2016, Mathematics/CSA)

37. Statistical Methods For Rare Variant Association Studies  
   Dr. Qing Sha (2016, Mathematics/CSA)  
   NIH R15 2016-05-16 – 2019-04-30; USD 436,873; Qing Sha

38. Computational Investigations In Atmospheric Science  
   Dr. Raymond Shaw (2016, Physics/CSA)

39. UN5390: Scientific Computing (Fall 2016)  
   Dr. Gowtham (2016, HPC/HPC)

40. UN5390: Scientific Computing II (Spring 2016)  
   Dr. Gowtham (2016, HPC/HPC)

41. BlueTooth Low Energy As An Implantable Interface (Senior Design)  
   Dr. Orhan Soykan (2015, BME/COE)

42. Development And Application Of A 2-Dimensional Finite Volume Model To Assess  
    Hydrodynamic And Microbial Controls On DNAPL Dissolution And Detoxification  
   Dr. Jennifer Becker (2015, CEE/COE)

43. Ecosystem Modeling In The Great Lakes  
   Dr. Martin Auer (2015, CEE/COE)  
   Contracts with the town of Ajax, Northeast Ohio Regional Sewer District

44. Multiphysics And Multiscale Simulations For Porous Materials  
   Dr. Zhen Liu (2015, CEE/COE)  
   MTU start-up funds

45. Consumer Product Manufacturing (Senior Enterprise)  
   Dr. Tony Rogers (2015, Chem Engg/COE)

46. Porting Legacy Fortran Code To C For MATLAB/Simulink Implementation  
   Dr. Gordon Parker (2015, ME-EM/COE)

47. Development Of Conformable CNG Tanks For Automotive Applications  
   Dr. Gregory Odegard (2015, ME-EM/COE)  
   Southwestern Energy, Inc

48. I/UCRC: Novel High Voltage/Temperature Materials And Structures  
   Dr. Gregory Odegard (2015, ME-EM/COE)  
   National Science Foundation
49. Multiscale Modeling Development And Validation Of Graphene/ULTEM Composites For Structural And Noise Reduction Applications  
Dr. Gregory Odegard (2015, ME-EM/COE)  
National Aeronautics and Space Administration

50. Multiscale Modeling Of Graphite/CNT/Epoxy Hybrid Composites  
Dr. Gregory Odegard (2015, ME-EM/COE)  
Air Force Office of Scientific Research

51. Modeling And Analysis Of Cryogenic Phase Change Experiments  
Dr. Jeffrey Allen (2015, ME-EM/COE)  
NASA Early Stage Innovations (ESI-13) NNX14AB05G

52. Characterization Of The Addition Of Electric Stresses On The Normal Field Instability In Ferrofluids  
Dr. L. Brad King (2015, ME-EM/COE)

53. Modeling Combustion Of Natural Gas RCCI Engines  
Dr. Mahdi Shahbakhti (2015, ME-EM/COE)  
MTU Internal Funds

54. Computational Investigations In Mechanical Engineering  
Dr. Zequn Wang (2015, ME-EM/COE)  
MTU start-up funds

55. Computational Investigations In Computer Science  
Dr. Xiaohua Xu (2015, CS/CSA)

56. Design And Prototype Image-Visualization For A Project In The Humanities In Preparation For An NEH Digital Humanities Proposal  
Dr. Stefka Hristova (2015, Humanities/CSA)

57. Exa-Scale Computing  
Dr. Benjamin Ong (2015, Mathematics/CSA)  
US Air Force Office for Scientific Research FA9550-12-1-0455; MTU start-up funds

58. Bayesian Measures Of Evidence For Hypothesis Testing And Variable Selection In High Dimensional Regression  
Dr. Min Wang (2015, Mathematics/CSA)

59. Bootstrap-Assisted Time Series Analysis  
Dr. Yeonwoo Rho (2015, Mathematics/CSA)

60. Investigations In Computational Physics, Chemistry And Materials Science  
Dr. Maximilian Seel (2015, Physics/CSA)
61. Holodec Data Analysis From The CSET Experiment
   Dr. Raymond Shaw (2015, Physics/CSA)

62. Investigations In Computational Anthropology
   Dr. Kelly Ontl (2015, Social Sciences/CSA)

63. PH4395: Computer Simulations
   Dr. Gowtham (2015, HPC/HPC)

64. UN5395: Scientific Computing II
   Dr. Gowtham (2015, HPC/HPC)

65. Computational Investigations In Animal Ecology And Conservation
   Dr. Joseph Bump (2015, SFRES/SFRES)
   Michigan DNR through the Michigan Tech Grant 751B4300037

66. Investigations In Computational Biomedical Engineering
   Dr. Sean Kirkpatrick (2014, BME/COE)

67. Dielectrophoretic Simulations For Microfluidics
   Dr. Adrienne Minerick (2014, Chem Engg/COE)
   Software costs covered via NSF (PFI) project and collaborative purchase within the department

68. Investigations In Computational Chemical Engineering
   Dr. Adrienne Minerick (2014, Chem Engg/COE)

69. Mapping Multiple Wavelengths Of Separation Distance Between Two Hadamard Matrix Diffusers To Create A Common Optical Path Full Color (RGB) Speckle Reduction Diffuser
   Dr. Christopher Middlebrook (2014, ECE/COE)

70. EE4173: Computer System Engineering And Performance
    Dr. Roger Kieckhafer (2014, ECE/COE)

71. Very Near Ground Wireless Channel Modeling: Theory And Practice
    Dr. Seyed Zekavat (2014, ECE/COE)
    NSF 1101843

72. Sensor-Fused Explosive Hazard Detection
    Dr. Timothy Havens (2014, ECE/COE)
    MTU start-up funds; US Army W909MY-13-C-0029 and W909MY-13-C-0013; (pending) ARiA - ONR BAA 16-001 and SERDP 16 MR01-007
73. Algorithm Design For Underwater Acoustic Signal Processing, Communications, And Networking  
Dr. Zhaohui Wang (2014, ECE/COE)  
MTU ECE

74. Extracting High-Resolution Digital Elevation Models Using Terrestrial And Aerial Structure From Motion Surveys  
Dr. Jason Gulley (2014, GMES/COE)  
MTU GMES

75. High Voltage/Temperature Materials And Structures  
Dr. Gregory Odegard (2014, ME-EM/COE)  
US Air Force Office of Scientific Research FA9550-13-1-0030; REL, Inc.; General Motors; NASA NNX11AO72A; NASA NNX09AM50A

76. Combustion Modeling Of LTC Engines  
Dr. Mahdi Shahbakhti (2014, ME-EM/COE)

77. Large Eddy Simulation (LES) For Turbulence-Chemistry Soot Formation Process Under Diesel Engine Injection Strategy  
Dr. Seong-Young Lee (2014, ME-EM/COE)

78. Phase Field Modeling Of Microstructure Evolution  
Dr. Yongmei Jin (2014, MSE/COE)  
NSF DMR-1409317; NSF CMMI1200038; University of Michigan-Michigan Space Grant Consortium 1211066; MTU Summer Undergraduate Research Fellowship

79. Investigations In Computational Chemistry  
Dr. Cary Chabalowski (2014, Chemistry/CSA)

80. Towards A Reliable Method For Comparing Large Scale Machine Learning Algorithms  
Dr. Laura Brown (2014, CS/CSA)

81. Investigations In Computational Mathematics  
Dr. Allan Struthers (2014, Mathematics/CSA)

82. Numerical Investigation Of Droplet Formation Of Viscoelastic Fluids In A Microfluidic T-Junction  
Dr. Kathleen Feigl (2014, Mathematics/CSA)

83. Investigations In Computational Mathematics  
Dr. Mark Gockenbach (2014, Mathematics/CSA)

84. Investigations In Computational Nano-Electronic Devices  
Dr. John Jaszczak (2014, Physics/CSA)
85. PH4390: Computational Methods  
   Dr. Gowtham (2014, HPC/HPC)

86. PH4395: Computer Simulations  
   Dr. Gowtham (2014, HPC/HPC)

87. UN5390: Scientific Computing I  
   Dr. Gowtham (2014, HPC/HPC)

88. Microbial Community Structure In A Climate Change And Terrestrial Carbon Cycling Context  
   Dr. Evan Kane (2014, SFRES/SFRES)  
   NSF DEB-1146149; Joint Genome Institute CSP 1445

89. A System Biology Approach To Identify Sense And Antisense Genes From High-Throughput Sequences; Construction Of Gene Regulatory Networks For Identifying Genes Controlling Wood Formation  
   Dr. Hairong Wei (2014, SFRES/SFRES)  
   NSF NCSU-550582; USDA 10891240

90. Data Mining And Advanced Simulations From BIG Medical Imaging Data By Employing High Performance Computing Infrastructure  
   Dr. Jinfeng Jiang (2013, BME/COE)  
   MTU start-up funds

91. Rational Design Of Water Treatment And Energy Harvesting Technologies Using Computational Chemistry  
   Dr. Daisuke Minakata (2013, CEE/COE)  
   MTU start-up funds

92. Modeling The Circulation In Lake Michigan -? Lake Huron And The Particle Transport Through The Straits Of Mackinac  
   Dr. Pengfei Xue (2013, CEE/COE)  
   MTU start-up funds; GLRC/MTRI internal funds

93. Computational Investigation Of Nanostructured And Multifunctional Infrastructure Materials By Employing High Performance Computing Infrastructure  
   Dr. Qingli Dai (2013, CEE/COE)  
   NSF CMMI-0900015 and CMMI-1300970; Michigan Tech Research Excellence Fund

94. Multiscale Computer Simulation Of FRRPP Process  
   Dr. Gerard Caneba (2013, Chem Engg/COE)

95. Investigations In Computational Electrical Engineering  
   Dr. Christopher Middlebrook (2013, ECE/COE)
96. Investigations In Computational Electrical Engineering  
Dr. Jeremy Bos (2013, ECE/COE)

97. Optical Identification And Classification  
Dr. Michael Roggeman (2013, ECE/COE)

98. Unsupervised Learning In Big Data And Social Networks  
Dr. Timothy Havens (2013, ECE/COE)  
MTU start-up funds; US Army W909MY-13-C-0029 and W909MY-13-C-0013; (pending) ARIA - ONR BAA 16-001 and SERDP 16 MR01-007

99. Modeling And Simulation Of Integrated Photodetectors For High Speed On-Chip Communication  
Dr. Zhuo Feng (2013, ECE/COE)  
MTU start-up funds

100. Numeric Modeling Of Acoustic Wave Propagation In Lake Superior  
Dr. Roger Turpening (2013, GMES/COE)

101. Implications Of Climate Change For Extreme Air Pollution Meteorology And Air Quality  
Dr. Shiliang Wu (2013, GMES/COE)  
US EPA

102. A Crowd-Sourced Knowledgebase For The Damage Assessment Of Extreme Events  
Dr. Thomas Oommen (2013, GMES/COE)  
NSF 1300720

103. Investigations In Computational Mechanical Engineering  
Dr. Amitabh Narain (2013, ME-EM/COE)

104. Multiscale Modeling Of Advanced Materials And Structures  
Dr. Gregory Odegard (2013, ME-EM/COE)  
US Air Force Office of Scientific Research FA9550-13-1-0030; REL, Inc.; General Motors; NASA NNX11AO72A; NASA NNX09AM50A

105. Trajectory Optimization For Solar Electric Propulsion Satellites  
Dr. Ossama Abdelkhalik (2013, ME-EM/COE)  
NASA SBIR sub-contract

106. Investigations In Computational Materials Science  
Dr. Joshua Pearce (2013, MSE/COE)  
MTU start-up funds; Industrial partnership
107. Investigations In Computational Chemistry  
   Dr. Loredana Valenzano (2013, Chemistry/CSA)  
   MTU start-up funds

108. Computational Synthesis Of Self-Stabilizing Protocols  
   Dr. Ali Ebnenasir (2013, CS/CSA)  
   NSF CCF-1116546

   Dr. Brian Fick (2013, Physics/CSA)  
   DOE (Pierre Auger Observatory)

110. Computational Study Of Charge And Spin Transport In Nanoscale Junctions From First-Principles  
   Dr. Ranjit Pati (2013, Physics/CSA)  
   NSF 1249504

111. Computational Studies Of Nanostructured Materials For Electronics, Biosensing And Human Health Implications  
   Dr. Ravindra Pandey (2013, Physics/CSA)  
   US Army Research Laboratory W911NF-09-2-0026-133417

112. Investigations In Computational Materials Science  
   Dr. Ravindra Pandey (2013, Physics/CSA)

113. PH4390: Computational Methods  
   Dr. Gowtham (2013, HPC/HPC)

114. PH4395: Computer Simulations  
   Dr. Gowtham (2013, HPC/HPC)

115. Lake Erie Circulation Modeling And Particle Tracking Experiments  
   Dr. David Schwab (2013, MTRI/MTRI)  
   MTRI internal funds

116. Isolation With Migration Studies For Two Or More Populations Using A Markov Chain Monte Carlo Method  
   Dr. Oliver Gailing (2013, SFRES/SFRES)
6 Publications

Sorted by year (descending), college, department and PI.

1. Coupling Experimental And Theoretical Investigation Of The Fate Of Photochemical Oxidation Of Nitrosamine And Nitrogen-Containing Species
   D. Minakata, D. Kamath, E. Coscarelli
   257th ACS National Meeting, Orlando, FL, USA (2019)

2. Investigation Of Al-Zn-Zr And Al-Zn-Ni Alloys For High Electrical Conductivity And Strength Application
   O. Fadayomi, R. Clark, V. Thole, P. G. Sanders, G. M. Odegard

3. Multiscale Modeling Of PEEK Using Reactive Molecular Dynamics Modeling And Micromechanics
   Polymer, vol. 163, p. 96 (2019)

4. Conduction Heat Transfer From Oblate Spheroids And Bispheres
   S. J. Kang, E. Dehdashti, H. Masoud

5. A Deep Learning Approach For Deformation Of Multi-Walled Carbon Nanotubes
   U. Yadav, S. Pathrudkar, S. Ghosh
   Society of Engineering Science (SES) 56th Annual Technical Meeting, St. Louis, MO, USA (2019)

6. An Error In Constitutive Equations Approach For Elasticity Imaging Using Ultrasound Data
   Symposium on Computational Modeling and Image Processing of Biomedical Problems, Houghton, MI, USA (2019)

7. Computational And Analytical Modeling For The Fracture Of Micro-Architectured Glass
   S. Ghosh, M. Coldran, P. Bulusu, U. Yadav, T. Sain
   The 16th Pan-American Congress of Applied Mechanics (PACAM XVI), Ann Arbor, MI, USA (2019)
8. Improvement Of Stiffness And Energy Absorption By Harnessing Hierarchical Interlocking In Brittle Polymer Blocks
M. Imam, J. Meaud, S. Ghosh, T. Sain

9. Interface Fracture Of Micro-Architectured Glass: Inverse Identification Of Interface Properties And A Novel Analytical Model
U. Yadav, M. Coldren, P. Bulusu, T. Sain, S. Ghosh
Accepted for publication in Mechanics of Materials, vol. XXX, p. YYY (2019)

10. Investigation Of Wave Trapping And Attenuation Phenomenon For A High Symmetry Interlocking Micro-Structure Composite Metamaterial

11. Modeling Of The Membrane And Their Interaction With Substrate
U. Yadav, S. Ghosh
Symposium on Computational Modeling and Image Processing of Biomedical Problems, Houghton, MI, USA (2019)

12. Detecting Zn(II) Ions In Live Cells With Near-Infrared Fluorescent Probes

13. A FRET-Based Near-Infrared Fluorescent Probe For Ratiometric Detection Of Cysteine In Mitochondria
S. Xia, Y. Zhang, M. Fang, L. Mikesell, T. E. Steenwinkel, S. Wan, T. Phillips, R. L. Luck, T. Werner, K. Liu

14. Near-Infrared Fluorescent Probes Based On TBET And FRET Rhodamine Acceptors With Different PKa Values For Sensitive Ratiometric Visualization Of PH Changes In Live Cells

15. Near-Infrared Fluorescent Probes With BODIPY Donors And Rhodamine And Mero-cyanine Acceptors For Ratiometric Determination Of Lysosomal PH Variance
S. Xia, M. Fang, J. Wang, J. Bi, W. Mazi, Y. Zhang, R. L. Luck, H. Liu
16. A Clustering Linear Combination Approach To Jointly Analyze Multiple Phenotypes For GWAS
   Q. Sha, Z. Wang, X. Zhang, S. Zhang

17. Joint Analysis Of Multiple Phenotypes In Association Studies Based On Cross-Validation Prediction Error
   X. Yang, S. Zhang, Q. Sha
   Scientific Reports, vol. 9, p. 1073 (2019)

18. Bootstrap-Assisted Unit Root Testing With Piecewise Locally Stationary Errors
   Y. Rho, X. Shao

   Y. Jagvaral, Q. Guo, H. He, R. Pandey
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D. Kamath, S. Mezyk, D. Minakata

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D. Minakata, E. Coscarelli

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D. Minakata, M. Zhang, L. Breitner, K. Howe

Mechanical Applications
M. Zhang, K. Howe, D. Minakata

31. Comparing The Mechanical Response Of Di-, Tri-, And Tetra-Functional Resin Epoxies
With Reactive Molecular Dynamics
M. S. Radue, B. D. Jensen, S. Gowtham, D. R. Klimek-McDonald, J. A. King, G. M.
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J. S. Maass, R. K. Wilharm, R. L. Luck, M. Zeller

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X. Liang, Q. Sha, S. Zhang

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Z. Wang, Q. Sham S. Fang, K. Zhang, S. Zhang

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41. Water Dissolution In Ionic Liquids Between Charged Surfaces: Effects Of Electric Polarization And Electrostatic Correlation  
H. Chen, L. An, I. Nakamura  

42. Amino Acids Conjugated Gold Clusters: Interaction Of Alanine And Tryptophan With Au$_8$ And Au$_{20}$  
M. H. Abdalmoneam, K. Waters, N. Saikia, R. Pandey  

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M. L. Larsen, R. A. Shaw, A. B. Kostinski, S. Glienke

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K. Porghasemi, R. K. Saray, E. Ansari, B. K. Irdmousa, M. Shahbakhti, J. D. Naber

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J. R. Murdock, J. C. Ickes, S. L. Yang
77. Amino Acid Analogue-Conjugated BN Nanomaterials In A Solvated Phase: First Principles Study Of Topology-Dependent Interactions With A Monolayer And A (5,0) Nanotube
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78. Amino Acids Conjugated Gold Clusters: Interaction Of Au₈ And Au₂₀ Clusters With Tryptophan And Alanine
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A. Kumar, R. Pandey, P. K. Ahluwalia, K. Tankeshwar  

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139. A Coupled Subsample Displacement Estimation Method For Ultrasound-Based Strain Elastography
   J. Jiang, T. J. Hall

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151. Surface-Dependence Of Interfacial Binding Strength Between Zinc Oxide And Graphene
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Y. Huang, S. Wu, J. C. Kaplan

153. An Apodization Approach For Processing Forward-Looking GPR For Explosive Hazard Detection
A. Webb, T. C. Havens, T. J. Schulz

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A. Pinar, M. Masarik, J. Kelly, T. C. Havens, J. Burns, B. Thelen, J. Becker

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156. Data-Informed Fuzzy Measures For Fuzzy Integration Of Intervals And Fuzzy Numbers
   T. C. Havens, D. T. Anderson, C. Wagner

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   J. Becker, T. C. Havens, A. Pinar, T. J. Schulz

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160. Insights And Characterizations Of L1-Norm Based Sparsity Learning Of A Lexicographically Encoded Capacity Vector For The Choquet Integral
   T. Adeyeba, D. T. Anderson, T. C. Havens

161. A Computational Molecular Dynamic Study On Epoxy-Based Network: Thermo-Mechanical Properties
   O. Aluko, S. Gowtham, S. Chinkanjanarot, M. S. Radue, G. M. Odegard
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B. D. Jensen, K. E. Wise, G. M. Odegard

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A. A. Moiz, S. Som, L. Bravo, S. Y. Lee

171. High-Speed Spray-To-Spray Collision Study On Two-Hole Impinging Jet Nozzles
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174. Effects Of Volumetric Expansion In Molecular Crystals: A Quantum Mechanical Investigation On Aspirin And Paracetamol Most Stable Polymorphs  
K. Adhikari, K. M. Flurchick, L. Valenzano  

175. Viscoelastic Droplet Formation In A Microfluidic T-Junction  
O. Y. Shonibare, K. Feigl, F. X. Tanner  

176. A Graphene-Boron Nitride Lateral Heterostructure - A First-Principles Study Of Its Growth, Electronic Properties, And Chemical Topology  
G. C. Loh, R. Pandey  

177. Atomic Level Understanding Of Site-Specific Interactions In Polyaniline/TiO$_2$ Composite  

G. Wang, R. Pandey, S. P. Karna  

G. Wang, R. Pandey, S. P. Karna  

S. Nigam, S. Gupta, D. Banyai, R. Pandey, C. Majumder  
181. Interaction Of Metallic Clusters With Biologically Active Curcumin Molecules
S. K. Gupta, H. He, C. Liu, R. Dutta, R. Pandey

182. Modulation Of Band Gap By An Applied Electric Field In Silicene-Based Hetero-Bilayers
S. Nigam, S. Gupta, C. Majumder, R. Pandey

183. MoS$_2$ Quantum Dot: Effects Of Passivation, Additional Layer, And h-BN Substrate On Its Stability And Electronic Properties

184. Nature Of Interaction Between Semiconducting Nanostructures And Biomolecules: Chalcogenide QDs And BNNT With DNA Molecules
Z. Wang, H. He, W. Slough, R. Pandey, S. P. Karna

185. Novel Two-Dimensional Silica Monolayers With Tetrahedral And Octahedral Configurations
G. Wang, G. C. Loh, R. Pandey, S. P. Karna

186. Out-Of-Plane Structural Flexibility Of Phosphorene
G. Wang, G. C. Loh, R. Pandey, S. P. Karna

187. Phosphorene Oxide: Stability And Electronic Properties Of A Novel Two-Dimensional Material
G. Wang, R. Pandey, S. P. Karna

188. Pressure And Electric Field-Induced Metallization In The Phase-Engineered ZrX$_2$ (X = S, Se, Te) Bilayers
A. Kumar, H. He, R. Pandey, P. K. Ahluwalia, K. Tankeshwar

189. Robust Magnetic Domains In Fluorinated ReS$_2$ Monolayer
G. C. Loh, R. Pandey
190. Semiconductor-To-Metal Phase Transition In Monolayer ZrS$_2$: GGA+U Study  
A. Kumar, H. He, R. Pandey, P. K. Ahluwalia, K. Tankeshwar  

191. Size And Edge Roughness Effects On Thermal Conductivity Of Pristine Antimonene Allotropes  
S. K. Gupta, Y. Sonvane, G. Wang, R. Pandey  

192. Versatile Electronic Properties Of Atomically Layered ScO$_2$  
G. C. Loh, R. Pandey  

193. A Merit Based Priority Scheme To Optimize The Use Of Shared Computing Infrastructure  
Gowtham  
HPC Advisory Council Conference, Stanford University, Stanford, CA (2015)

194. Can We Predict Intermediate-Radicals And Stable-Byproducts In The Aqueous Phase Advanced Oxidation Processes Using Computational Chemistry?  
D. Minakata, S. Mezyk, J. C. Crittenden  
Borchardt Conference, University of Michigan, Ann Arbor, MI, February 25-26, 2014

195. Coupling Experimental And Theoretical Molecular-Level Investigations To Visualize And Predict The Fate Of Degradation Of Organic Compounds In Aqueous Phase Advanced Oxidation Systems  
D. Minakata, M. Rouleau  
ACS National Meeting, San Francisco, CA, August 10-14, 2014

196. Development Of Linear Free Energy Relationships For Aqueous Phase Radical-Involved Chemical Reactions  
Environmental Science and Technology, vol. 48, p. 13925 (2014)

197. New Reaction Pathway Discovery For Fate Of Transformation Products In Aqueous Phase Advanced Oxidation Processes  
D. Minakata, S. P. Mezyk  
IWA World Congress, Lisbon, Portugal, September 21-26, 2014

P. Xue, E. A. B. Eltahir  
Ocean Sciences Meeting, Honolulu, HI (2014)
199. Local Feedback Mechanisms Of The Shallow Water Region Around The Maritime Continent
P. Xue, E. A. B. Eltahir, P. Malanotte-Rizzoli, J. Wei

200. 2D Cohesive Zone Modeling Of Crack Development In Cementitious Digital Samples With Microstructure Characterization
Q. Dai, K. Ng

201. Computational Investigation Of Pore Permeability And Connectivity From Transmission X-Ray Microscope Images Of A Cement Paste Specimen
X. Sun, Q. Dai, K. Ng


203. Investigation Of Internal Frost Damage In Cementitious Materials With Micromechanics Analysis, SEM Imaging And Ultrasonic Wave Scattering Techniques
K. Ng, Y. Sun, Q. Dai, X. Yu

204. Numerical Investigation Of Internal Frost Damage Of Digital Cement Paste Samples With Cohesive Zone Modeling And SEM Microstructure Characterization
K. Ng, Q. Dai

205. Side-Groove Influenced Parameters For Determining Fracture Toughness Of Self-Healing Composites Using A Tapered Double Cantilever Beam Specimen
R. J. Lemmens, Q. Dai, D. D. Meng

206. A Generalized Fuzzy T-Norm Formulation Of Fuzzy Modularity For Community Detection In Social Networks
J. Su, T. C. Havens
207. Fuzzy Community Detection In Social Networks Using A Genetic Algorithm  
J. Su, T. C. Havens  

208. Multi-Band Sensor-Fused Explosive Hazard Detection In Forward-Looking Ground-Penetrating Radar  
T. C. Havens, J. Becker, A. Pinar, T. J. Schulz  

209. Quadratic Program-Based Modularity Maximization For Fuzzy Community Detection In Social Networks  
J. Su, T. C. Havens  

210. Real Time Fuzzy Controller For Quadrotor Stability Control  
P. Bhatkhande, T. C. Havens  
IEEE International Conference on Fuzzy Systems (in press)

211. Predicting Mechanical Response Of Crosslinked Epoxy Using ReaxFF  
G. M. Odegard, B. D. Jensen, S. Gowtham, J. Y. Wu, J. Y. He, Z. L. Zhang  

212. Predicting Thermo-Mechanical Response Of Crosslinked Epoxy Using ReaxFF  
G. M. Odegard, B. D. Jensen, S. Gowtham, J. Y. Wu, J. Y. He, Z. L. Zhang  
AIAA SciTech, National Harbor, MD, USA (2014)

213. Advanced Combustion Model Of LTC Engines  
M. Nazemi, S. Polat, M. Shahbakthi  
2014 CONVERGE User Group Meeting, Madison, WI, September 23-25, 2014

214. Solar Electric-Powered Low-Thrust Trajectory Optimization Using Genetic Algorithm  
E. Taheri and O. Abdelkhalik  
AIAA Space and Astronautics Forum and Exposition, AIAA-2014-4464, San Diego, CA, August 4-7, 2014

215. Acetylcholinesterase Inhibition By Aricept And Analogs To Decrease Memory Loss In Alzheimer’s Patients  
K. Weinand, K. Adhikari, L. Valenzano  
ACS Student Research Symposium, Marquette, MI. March 2014

216. Action Of A Broad Spectrum Antiviral Drug Against Human Herpes: A Quantum Chemical Investigation  
M. Szatkowski, A. Perla, K. Adhikari, L. Valenzano  
ACS Student Research Symposium, Marquette, MI. March 2014
217. Assembling The Bacterial Cell Wall Of E. Coli: A Stepwise Quantum Chemical Approach
   D. Beegle, K. Adhikari, L. Valenzano
   ACS Student Research Symposium, Marquette, MI. March 2014

218. Computational Quantum Chemical Study Of The Adsorption Of Light Hydrocarbons In Metal-Organic Frameworks
   G. Degaga, K. Adhikari, L. Valenzano
   Michigan Tech GRC, Houghton, MI. February 2014

219. Encapsulation Of Atmospheric Gases In A Fullerene Cage: A Quantum Chemical Investigation
   C. Stewart, K. Adhikari, L. Valenzano
   ACS Student Research Symposium, Marquette, MI. March 2014

   M. Pirkola, K. Adhikari, L. Valenzano
   ACS Student Research Symposium, Marquette, MI. March 2014

221. A Novel Statistical Method For Rare Variants Association Studies In General Pedigrees
   H. Zhu, Z. Wang, X. Wang, Q. Sha
   The 19th Genetic Analysis Workshop, Vienna, Austria. August 2014

222. Simulation Of Charge Transport In Disordered Assemblies Of Metallic Nano-Islands: Application To Boron Nitride Nanotubes Functionalized With Gold Quantum Dots (QDs-BNNTs)
   MRS Symposium, Spring 2014

223. A Theoretical Study Of Structural And Electronic Properties Of Alkaline-Earth Fluoride Clusters

   G. C. Loh, S. Nigam, G. Mallick, R. Pandey
225. Decoding The Mechanism Of The Mechanical Transfer Of A GaN-Based Heterostructure Via An h-BN Release Layer In A Device Configuration
G. Wang, D. Z. Yang, Z. Y. Zhang, M. S. Si, D. Xue, H. He, R. Pandey

226. Effect Of Si Doping On The Electronic Properties Of BN Monolayer
S. K. Gupta, H. He, D. Banyai, M. Si, R. Pandey, S. Karna
Nanoscale, vol. 6, p. 5526 (2014)

A. Kumar, D. Banyai, P. K. Ahluwalia, R. Pandey, S. P. Karna
Physical Chemistry Chemical Physics, vol. 16, p. 20157 (2014)

228. Strain Engineering Of Dirac Cones In Graphyne
G. Wang, M. Si, A. Kumar, R. Pandey

229. Boron Nitride Nanotubes For Spintronics
K. B. Dhungana, R. Pati

230. Electrical Tuning Of Spin Current In A Boron Nitride Nanotube Quantum Dot
K. B. Dhungana, R. Pati
Physical Chemistry Chemical Physics, vol. 16, p. 7996 (2014)

231. Fluorinated Boron Nitride Nanotube Quantum Dots: A Spin Filter
K. B. Dhungana, R. Pati

232. Giant Amplification Of Tunnel Magnetoresistance In A Molecular Junction: Molecular Spin-Valve Transistor
K. B. Dhungana, R. Pati

233. Revision Control System (RCS) In Computational Sciences And Engineering Curriculum
S. Gowtham
XSEDE’14 Proceedings; ACM 978-1-4503-2893-7, 2014

234. Streamlining Research Computing Infrastructure: A Small School’s Perspective
Gowtham
HPC Advisory Council Conference, Stanford University, Stanford, CA (2014)
P. Xue, E. A. B. Eltahir, P. Malanotte-Rizzoli, J. Wei
13th International Conference on Estuaring and Coastal Modeling (ECM13), San Diego, CA, 2013

236. Investigation Of Internal Frost Damage In Concrete With Thermodynamic Analysis, Micro-Damage Modeling And Time-Domain Reflectometry Sensor Measurements
Q. Dai, K. Ng, Y. Liu, X. Yu

D. Kumar, M. Palaniswami, S. Rajasegarar, C. Leckie, J. C. Bezdek, T. C Havens

238. Extension Of The Fuzzy Integral For General Fuzzy Set-Valued Information
D. T. Anderson, T. C. Havens, C. Wagner, J. M. Keller, M. F. Anderson, D. J. Wescott

239. Scalable Approximation Of Kernel Fuzzy C-Means
Z. Zhang, T. C. Havens

240. Revealing The Performance Barrier: First Principles Prediction Of The Physical-Chemical Properties Of New Co-Crystals For Rocket Propulsion
M. P. Pirkola, K. Adhikari, L. Valenzano
MSGC-NASA Annual Meeting, Ann Arbor, MI.

241. Room-Temperature Tunneling Behavior Of Boron Nitride Nanotubes Functionalized With Gold Quantum Dots

242. Simulation Of Charge Transport In Multi-Island Tunneling Devices: Application To Disordered One-Dimensional Systems At Low And High Biases
M. A. Savaikar, D. R. Banyai, P. L. Bergstrom, J. A. Jaszczak

243. Electron Tunneling Characteristics Of A Cubic Quantum Dot, (PbS)32
244. First-Principles Computation Of Structural, Elastic And Magnetic Properties Of Ni$_2$FeGa
Across The Martensitic Transformation
M. B. Sahariah, S. Ghosh, C. S. Singh, S. Gowtham, R. Pandey
7 Degrees

Sorted by year (descending), college, department, PI and student.

1. Statistical Methods For Mixed Frequency Data Sampling Models
   Yun Liu, PhD
   Advisor: Dr. Yeonwoo Rho (2019, Mathematics/CSA)

2. Atmospheric Physics
   Ashfiqur Rahman, MS
   Advisor: Dr. Raymond Shaw (2019, Physics/CSA)

3. Aircraft-Borne In-Situ Measurements Of Microphysical Properties Of Marine Stratocumulus Clouds
   Susanne Glienke, PhD
   Advisor: Dr. Raymond Shaw (2019, Physics/CSA)

4. Effects Of The Dielectric Response Of Single-Component Liquids And Liquid Mixtures On Electrochemical Properties Between Charged Plates
   Hongbo Chen, PhD
   Advisor: Dr. Issei Nakamura (2018, Physics/CSA)

5. First-Principles Investigation Of The Interfacial Properties Of Boron Nitride
   Kevin Waters, PhD
   Advisor: Dr. Ravindra Pandey (2018, Physics/CSA)

6. Probing Quantum Transport In Three-Terminal Nanojunctions
   Meghnath Jaishi, PhD
   Advisor: Dr. Ranjit Pati (2018, Physics/CSA)

7. Investigation Of Microphysical Properties Of Laboratory And Atmospheric Clouds Using Digital In-Line Holography
   Neel Desai, PhD
   Advisor: Dr. Raymond Shaw (2018, Physics/CSA)

8. Computational Ultrasound Elastography: A Feasibility Study
   Yu Wang, PhD
   Advisor: Dr. Jingfeng Jiang (2017, BME/COE)

9. Predicting RO Removal Of Toxicologically Relevant Unique Organics
   Muxue Zhang, MS
   Advisor: Dr. Daisuke Minakata (2017, CEE/COE)

Michigan Technological University
10. Toward A New Modeling Approach For Management Of Nuisance Cladophora Growth In The Great Lakes
   Anika Kuczynski, PhD
   Advisor: Dr. Martin Auer (2017, CEE/COE)

11. Understanding Soil-Water Interaction Mechanisms Via Molecular Simulations
    Chao Zhang, PhD
    Advisor: Dr. Qingli Dai (2017, CEE/COE)

12. Feature And Decision Level Fusion Using Multiple Kernel Learning And Fuzzy Integrals
    Anthony Pinar, PhD
    Advisor: Dr. Timothy Havens (2017, ECE/COE)

    Matthew Radue, PhD
    Advisor: Dr. Gregory Odegard (2017, ME-EM/COE)

    Sorayot Chinkanjanarot, PhD
    Advisor: Dr. Gregory Odegard (2017, ME-EM/COE)

    Olabanji Shonibare, PhD
    Advisor: Dr. Kathleen Feigl (2017, Mathematics/CSA)

16. Laboratory, Computational And Theoretical Investigations Of Ice Nucleation And Its Implications For Mixed Phase Clouds
    Fan Yang, PhD
    Advisor: Dr. Raymond Shaw (2017, Physics/CSA)

17. The Spatial Ecology Of Gray Wolves In The Upper Peninsula Of Michigan, 1994-2013
    Shawn O’Neil, PhD
    Advisor: Dr. Joseph Bump (2017, SFRES/SFRES)

18. Property Analysis Of The Asphalt Materials Using Molecular Dynamics (MD) Method
    Hui Yao, PhD
    Advisor: Dr. Qingli Dai (2016, CEE/COE)
19. Smart Aerodynamic Control Devices Design And Vibration Reduction Analysis For Wind Turbine Blades  
Xiao Sun, PhD  
Advisor: Dr. Qingli Dai (2016, CEE/COE)

20. Integrated Computational And Experimental Evaluation Of Electromagnetic Energy-Induced Self-Healing Performance Of Asphalt Composites  
Zigeng Wang, PhD  
Advisor: Dr. Qingli Dai (2016, CEE/COE)

21. Impacts Of Global Change On Tropospheric Ozone And Mercury  
Huanxin Zhang, PhD  
Advisor: Dr. Shiliang Wu (2016, CEE/COE)

22. Computational Investigations In Chemical Engineering  
Jeana Collins, MS  
Advisor: Dr. Adrienne Minerick (2016, Chem Engg/COE)

23. Representation And Analysis Of Multi-Modal, Nonuniform Time Series Data: An Application To Survival Prognosis Of Oncology Patients In An Outpatient Setting  
Jennifer Winikus, PhD  
Advisor: Dr. Laura Brown and Timothy Havens (2016, ECE/COE)

24. Low Temperature Split Injection Spray Combustion: Ignition, Flame Stabilization And Soot Formation Characteristics In Diesel Engine Conditions  
Ahmed Moiz, PhD  
Advisor: Dr. Seong-Young Lee (2016, ME-EM/COE)

25. A Self-Normalizing Approach To The Specification Test Of Mixed-Frequency Models  
Henriette. Gronvik, MS  
Advisor: Dr. Yeonwoo Rho (2016, Mathematics/CSA)

26. First Principles Studies Of Group IV And Group V Related Two Dimensional Materials  
Gaoxue Wang, PhD  
Advisor: Dr. Ravindra Pandey (2016, Physics/CSA)

27. Global Modeling Of Atmospheric Ozone And Aerosols: Model Improvement And Applications  
Yaoxian Huang, PhD  
Advisor: Dr. Shiliang Wu (2015, CEE/COE)

28. Pose Estimation And 3D Reconstruction Using Sensor Fusion  
Anuj Potnis, MS  
Advisor: Dr. Timothy Havens (2015, ECE/COE)
29. Molecular Modeling Of Epon 862-DETDA/Carbon Composites
   Cameron Hadden, PhD
   Advisor: Dr. Gregory Odegard (2015, ME-EM/COE)

30. Visiting PhD Student From Sahand University Of Technology, Iran
   Kamran Poorghasemi, PhD
   Advisor: Dr. Mahdi Shahbakhti (2015, ME-EM/COE)

31. Modeling And Analysis Of Reactivity Controlled Compression Ignition (RCCI) Engine Combustion
   Mohammadreza Nazemi, MS
   Advisor: Dr. Mahdi Shahbakhti (2015, ME-EM/COE)

32. Visiting PhD Student From Gazi University, Turkey
   Seyfi Polat, PhD
   Advisor: Dr. Mahdi Shahbakhti (2015, ME-EM/COE)

33. Understanding Electronic Structure And Transport Properties In Nanoscale Junctions
   Kamal Dhungana, PhD
   Advisor: Dr. Ranjit Pati (2015, Physics/CSA)

34. Integrated Computation And Experimental Characterization For Alkali-Silica Reaction Damage In Concrete
   Shuaicheng Guo, PhD
   Advisor: Dr. Qingli Dai (2014, CEE/COE)

35. Active Material Actuator Design And Computation For Smart Turbine Blade
   Xiaowei Sun, MS
   Advisor: Dr. Qingli Dai (2014, CEE/COE)

36. Modularity Based Fuzzy Community Detection In Social Networks
   Jianhai Su, MS
   Advisor: Dr. Timothy Havens (2014, ECE/COE)

   John Becker, MS
   Advisor: Dr. Timothy Havens (2014, ECE/COE)

38. Real Time Fuzzy Controller For Quadrotor Stability Control
   Pranav Bhatkhande, MS
   Advisor: Dr. Timothy Havens (2014, ECE/COE)
39. Scalable Approximation Of Kernel Fuzzy C-Means  
Zijian Zhang, MS  
Advisor: Dr. Timothy Havens (2014, ECE/COE)

40. Predicting The Mechanical Properties Of Carbon-Based Materials Using Molecular Dynamics  
Benjamin Jensen, PhD  
Advisor: Dr. Gregory Odegard (2014, ME-EM/COE)

41. Density Of Amorphous Carbon By Using Density Functional Theory  
Sorayot Chinkanjanarot, MS  
Advisor: Dr. Gregory Odegard (2014, ME-EM/COE)

42. Fuzzy Logic Controller For Energy Management Of Power Split Hybrid Electrical Vehicle Transmission  
Varun Navale, MS  
Advisor: Dr. Timothy Havens (2013, ECE/COE)

43. Molecular Modeling Of PMR-15 Polyimide  
Pruthul Ravindranath, MS  
Advisor: Dr. Gregory Odegard (2013, ME-EM/COE)
8 Usage Spectrum

Usage spectrum for different queues (i.e., logical grouping of a set of compute nodes for a specific purpose or to identify a source of funding) as well as hierarchies of user population for FY 2018-19 are presented in the following tables.

Table 1: By queue

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<thead>
<tr>
<th>#</th>
<th>Queue</th>
<th>Sims</th>
<th>Time (hh:mm:ss)</th>
<th>Wall</th>
<th>CPU</th>
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<td>Grand total</td>
<td>697623</td>
<td>1538249:19:31</td>
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## Table 2: By college/institute

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<th>#</th>
<th>College/Institute</th>
<th>Sims</th>
<th>Time (hh:mm:ss)</th>
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<th>CPU</th>
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<td>Grand total</td>
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<td>1538249:19:31</td>
<td>10155132:36:44</td>
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</table>

## Table 3: By department (grouped by college)

<table>
<thead>
<tr>
<th>#</th>
<th>Department</th>
<th>Sims</th>
<th>Time (hh:mm:ss)</th>
<th>Wall</th>
<th>CPU</th>
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<tbody>
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<td>GMES</td>
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<td>Mathematics</td>
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### Table 4: By research group (grouped by department and college)

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9 Media Coverage

Dr. Gowtham attended the annual Supercomputing (SC18) - The International Conference for High Performance Computing, Networking, Storage and Analysis - in Dallas, TX, and the Spring meeting of Coalition for Academic and Scientific Computation (CASC) in Alexandria, VA.

At SC18, he was part of the organizing committee for the Fifth SC Workshop on Best Practices for HPC Training and was interviewed by the conference organizers featuring highlights of Michigan Tech’s research projects. Listed below are some of the key media coverage entities.

1. [Interview: HPC at Michigan Tech](https://www.facebook.com/SCconferences/videos/112984306323786)
   SC18, Dallas, 2018

   SC17, Denver, 2017

3. [A Merit Based Priority Scheme to Optimize the Use of Computing Infrastructure](https://insidehpc.com/2015/02/a-merit-based-priority-scheme-to-optimize-the-use-of-computing-infrastructure)
   HPC Advisory Council, Stanford University, 2015

   Interview with HPC Advisory Council, 2014

5. [Streamlining Computing Infrastructure: A Small School's Experience](https://insidehpc.com/2014/02/streamlining-computing-infrastructure-small-schools-experience)
   HPC Advisory Council, Stanford University, 2014

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10 Safety Inspection Report

The safety inspection report, including a review of physical facilities and equipment as well as safety requirements in the facility policies and procedures conducted on 2018-02-07 by David Dixon of the Office of Compliance, Integrity, and Safety (OCIS) is available at http://labcliq.com/summary/report.cfm?insp_id=427

The GLRC data center (105A) is confirmed to be clean and safe. However, it is an active data center with components being delivered, staged for installation and removal, etc. But the components - whether staged for installation or removal - are always set away from working/walking areas and there has never been any injury or accident and authorized staff rarely ever work in isolation. The HPCSF will strive and do its best to keep it a clean and safe working environment.