HPC/CFD Clusters in MABE at UT





Reza Abedi (rabedi@utsi.edu), http://rezaabedi.com/

Research: Applied mathematics, computational mechanics, and fracture modeling. Multiphysics applications in solid, fluid, and thermal mechanics, electromagnetics, and acoustics, particularly for highly multiscale and parallel simulations and problems with nonsmooth features such as shocks and singular features.

Computational Resource: 2 stand-alone HPC servers (Euler, Gauss) and a 256-core HPC cluster (UTSI SIRC cluster)



James G. Coder (jcoder@utk.edu)

Research: Computational aerodynamics, Unsteady aerodynamics, Rotorcraft aeromechanics, Turbulence and transition modeling, Hybrid RANS/LES methods, Aerodynamic design and optimization

Computational Resources: Newton HPC





Sudarsanam Suresh Babu (sbabu@utk.edu)

Research: Advanced manufacturing including Additive and Transient field processing, Materials Joining and Welding, Hybrid Materials, Structural Metals and Alloys, Phase Transformations, in-situ and ex-situ Characterization, Atom Probe Tomography, Integrated Process Modeling, Material Constitutive Properties during Extreme processing

Computational Resource: ORNL



Jay I. Frankel (jfranke1@utk.edu)

Research: Calibration mathematics, methodologies and experimental design, Heat transfer in hypersonics (TPS's and combustors) Aerospace temperature and heat flux measurements and sensors Integral and integro-differential equations of mathematical physics, heat transfer, fluid mechanics, and vibrations Weighted-residual methods: spectral and radial basis functions





Kivanc Ekici (<u>ekici@utk.edu</u>)

Research: Unsteady Aerodynamics and Aeroelasticity, CFD, Wind Turbine Aeroelasticity, Turbomachinery, Fluid-Structure Interactions in Nuclear Reactors, Flapping Flight, Rotorcraft Aerodynamics, Aerodynamic Design, Lattice-Boltzmann Methods, Parallel and High Performance Computation

Computational Resource: 3 stand-alone HPC servers (Euler, Blasius and D'Alembert) and a HPC cluster (Ohain). Newton HPC



Matthew M. Mench (<u>mmench@utk.edu</u>), <u>http://ecpower.utk.edu/</u>

Research: Multiphase Heat and Mass Transport and Visualization, Computational and Experimental Studies of Electrochemical Energy Conversion and Storage Systems including Polymer Electrolyte Fuel Cells, Microbial Fuel Cells, Flow Batteries, and Sensors. Simulation of multi-phase flow in porous media





Trevor M. Moeller (tmoeller@utsi.edu), http://cear.utsi.edu/

Research: Computational and Experimental Plasmadynamics, High-Temperature Gases, Radiation Transport, Chemically-Reacting Flows, Plasma diagnostics, Advanced Space Propulsion, and In-Orbit Space Environment Ground Testing



Kwai L. Wong (<u>kwong@utk.edu</u>)

Research: computational science and engineering on HPC platforms, parallel numerical linear algebra, finite element method, and Inter-disciplinary large-scale simulation workflow framework

Computational Resource: NICS/JICS/XSEDE





John Schmisseur (jschmiss@utsi.edu)

Research: Computational Fluid Dynamics focusing on high-speed viscous flows, turbulent and transitional shock interactions. Integration of empirical and numerical simulations within a comprehensive framework.



Seungha Shin (<u>sshin@utk.edu</u>), <u>http://nanoheat.utk.edu</u>

Research: Energy, momentum, mass, and charge transport and energy conversion using multiscale, multiphysics simulations (*ab initio*, molecular dynamics, and meso or Boltzmann, Quantum to Classical Mechanics)

Computational Resource: Newton HPC, XSEDE, NICS, Group server





Stephanie TerMaath (stermaat@utk.edu)

Research: Multi-scale structural mechanics problems using a physics-based approach implemented on high performance computing systems. Structural analysis performed by integrating and automating disparate methods. Hybrid structures, variability in additive manufacturing, and ventricular catheter modeling.

Computational Resource: JICS and DoD HPCMP

1) Computational fluid mechanics

Faculty members: Reza Abedi, Phuriwat Anusonti-Inthra, Jim Coder, Kivanc Ekici, Trevor M. Moeller, John Schmisseur, Kwai Wong

2) Computational heat transfers

Faculty members: Jay Frankel, Matthew M. Mench, Seungha Shin, Kwai Wong

3) Computational structural mechanics

Faculty members: Reza Abedi, Phuriwat Anusonti-Inthra, Sudarsanam Suresh Babu, Stephanie TerMaath

4) Micro-/Nanoscale modelling

Faculty members: Seungha Shin



Computational Resource - Hardware

1. Newton HPC at UT (<u>https://newton.utk.edu/</u>)



The Newton HPC Program is a joint effort between the <u>Office of Research</u>, the<u>Office of Information Technology (OIT</u>), and the departments of the University of Tennessee to establish a campus research computing environment in support of HPC and data-intensive computing applications. OIT operates <u>a variety of computing systems</u> which are accessed by researchers through a unified software environment. <u>Newton membership</u> is available to University of Tennessee researchers from all UT System campuses and institutes.

2. JICS (<u>http://www.jics.utk.edu/centers</u>)/NICS (<u>https://www.nics.tennessee.edu/</u>)



The *National Institute for Computational Sciences (NICS)* at the University of Tennessee, Knoxville is one of the leading high performance computing centers for excellence in the United States. NICS is co-located on the University of Tennessee, Knoxville campus as well as in the Secret City of Oak Ridge, on the Oak Ridge National Laboratory Campus (ORNL), the nation's most powerful computing complex. The center's missions is to expand the boundaries of human understanding while ensuring the United States' continued leadership in science, technology, engineering, and mathematics



Computational Resource - Hardware



3. XSEDE (https://www.xsede.org/overview)

The Extreme Science and Engineering Discovery Environment (XSEDE) is the most advanced, powerful, and robust collection of integrated advanced digital resources and services in the world. XSEDE is a single virtual system that scientists can use to interactively share computing resources, data and expertise. People around the world use these resources and services - things like supercomputers, collections of data and new tools - to improve our planet.

4. Group servers

Some research groups in MABE hold their own group servers.







Computational Science for Undergraduate Research Experiences

HPC Compute and data intensive Sciences, cfdlab.utk.edu/csure-reu



COMSOL, Fluent, Openfoam, DEALII, SimVascular, WRF, FEM, DG, Agent Based, LAMMPS, NAMD, DFTB, GROMAC, PETSC, TRILINOS,DAKOTA, PSUADE, SCALAPACK, MAGMA, OPENMP, CUDA, MPICUBIT, VISIT, PARAVIEW









TENNESSEE KNOXVILLE

Computational Aerodynamics (Coder)



Current Research Areas

- High-speed flows
- Rotorcraft aerodynamics
- Hybrid RANS/LES methods
- Aerodynamic shape optimization
- Transition modeling
- Natural-laminar-flow technologies

CFD Codes

- OVERFLOW
- SU2
- OpenFOAM











Spacetime Discontinuous Galerkin (SDG) method











Dynamic and probabilistic Contact/fracture mechanics







Dynamic PDEs: Electromagnetics, heat conduction, advectiondiffusion equation, etc.

