Center for Predictive Materials Modeling and Simulation (PMMS)

**Center Focus**
The Center for Predictive Materials Modeling and Simulation focuses on the potential for prediction of damage (irreversible and cumulative deformation) in polymer composites due to mechanical and environmental loading. These predictions are now feasible by utilizing a hierarchy of advanced modeling techniques including atomistic and molecular simulation, polymer mechanics, mesoscale micromechanical modeling and composite mechanics validated via nanometrology and macroscopic measurements.

**A Broader Impact**
Cyber-enabled, predictive tools for the simulation of polymer nanocomposites have the potential to help develop next generation high strength polymer based materials that will impact well established industries including aerospace and automobile as well as emerging applications like MEMS. We foresee that the developments in modeling and experimental characterization techniques for nanostructured materials, being generally applicable, will impact the broader soft materials community. Our goal is to develop the first, freely and widely available, experimentally validated, simulation framework for nano-structured materials. We expect these resources will be used by a large number of scientists and engineers in industry and national labs thus facilitating the technology transfer from academia to the end users of our technology who can transform it into products that benefit society.
Facilities / Equipment

Computational Resources

- **Compute nodes** - Access to 400 processors in the Steele cluster at RCAC:
  - 30 Dell PowerEdge 1950 nodes (dual Intel processor, quad core nodes - 8 cores, 160 GB of local disk, 16 GB of memory) and a Gigabit Ethernet interconnect
  - 32 node (each node has a dual 3.2GHz (2MB Cache), Xeon 800MHz processors and 4 Gigabyte of memory) and
  - 24 node Opteron cluster (each node has a dual processor, dual core (4 processors per node) 2.6 GHz and 8 GB of memory).

Visualization
- An active stereographic projection system (Christie’s Mirage HD3K)

Institutional resources
- Access to institutional resources such as the nanohub (nanohub.org) part of the NSF-funded Network for Computational Nanotechnology (NCN)

Experimental Facilities

**Birck Nanotechnology Center** - Capabilities for (a) nanoscale sample fabrication, cantilever modification and (b) characterization include:
- 20,000 Sq. ft. Scifres Nanofabrication Lab
- XPS, Scanning Electron microscopy, Transmission Electron Microscopy facilities
- Dedicated micromanipulation stages and dark field microscope
- Agilent 5500 AFM system
- Laser Scanning Doppler Interferometer

**Polyimide Nanocomposite Laboratory (PNCL):**
- Branson 1510 ultrasonic cleaner
- Hielscher UP200S Ultrasonic Processor
- VWR 1415M vacuum oven
- Olympus ZX-12 stereomicroscope
- Digital Instruments SPOT digital camera
- INSTEC heating stage
- Q100 TA instruments MDSC / DSC
- Q500 TA instruments TGAQ800 TA instruments DMA