

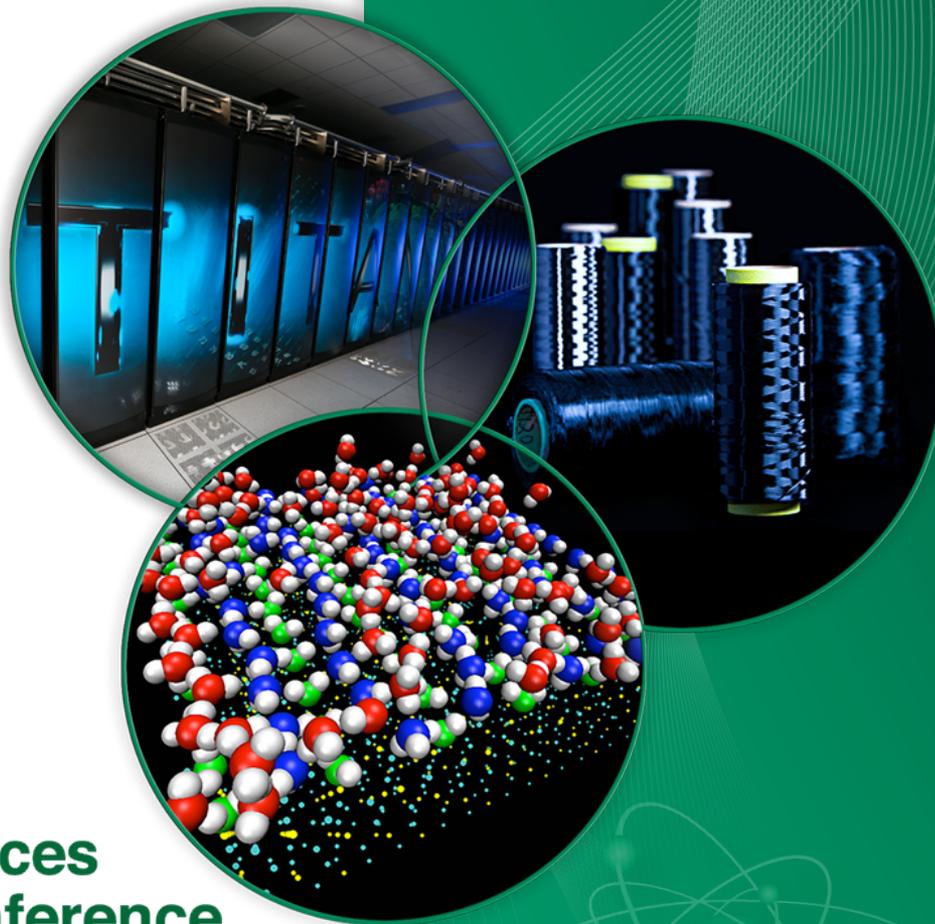
# Session 3: Delivering Breakthrough Science

Jack Wells



**Smoky Mountains  
Computational Sciences  
and Engineering Conference**

Gatlinburg, TN September 5, 2013



# Using integrated computing and data to achieve science breakthroughs

- How are individuals and programs using this instrumentation to deliver science and engineering breakthroughs?
- What science achievements are being made?
- What are the requirements for greater integration of compute and data that will drive future science and engineering achievement?

## The Talks

High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome

Delivering Breakthrough Science through High-Performance Computing: Relevance to Additive Manufacturing Computational End-Station (ACE)

Big Data in the Geosciences: Data Mining Methods for Characterizing Ecoregions, Designing Sampling Networks, Detecting Forest Threats, and Understanding Climate Change Predictions

Neutrons and Computing

## The Speakers

Prof. Marco Buongiorno Nardelli,  
University of North Texas

Prof. Suresh Babu,  
University of Tennessee/ORNL

Dr. Forrest Hoffman, ORNL

Prof. Jeremy Smith,  
University of Tennessee/ORNL

# High-throughput materials discovery and development: Breakthroughs and challenges in the mapping of the materials genome



- The design of complex materials is being driven by
  - High-throughput data generation frameworks that exploit hardware architectures and massive supercomputing resources
  - Computational data-processing methodologies to distill the complex interactions at the origin of specific materials properties.

**Marco Buongiorno Nardelli**, Professor of Physics and Chemistry, University of North Texas

# Delivering Breakthrough Science through High-Performance Computing: Relevance to Additive Manufacturing Computational End-Station (ACE)



- Additive Manufacturing (AM) has the promise to revolutionize manufacturing providing an approach focus on “dream, design, and create,” without being impeded by the constraints of traditional manufacturing with standard shapes, limited material systems, and properties.
- **Suresh Babu**, Governor’s Chair in Advanced Manufacturing, University of Tennessee/ORNL

# Big Data in the Geosciences: Data Mining Methods for Characterizing Ecoregions, Designing Sampling Networks, and Detecting Forest Health Threats



- Describe analytical methods applied to *in-situ* measurements, large-scale satellite observations, and climate model output.
- Delineated continental and global land areas, creating customized ecoregions as a framework for understanding plant and animal habitats and projecting species shifts under environmental change.

**Forrest Hoffman**, a computational climate scientist in the Climate Change Science Institute (CCSI) at Oak Ridge National Laboratory.

# Neutrons and Computing

- Simulation and Analysis Interface between Leadership-Class Supercomputing and Neutron Scattering of Molecular Systems to enable more impactful science

**Jeremy Smith**, Governor's Chair in Biophysics at UT and Director of UT/ORNL Center for Molecular Biophysics

