

# ORNL Participation in SciDAC and Related Projects

ORNL researchers participate in 18 SciDAC efforts. To learn more about particular projects, please visit us in the ORNL (R1971) and SciDAC (R1872) booths.

Climate Astrophysics **Applications** Chemistry Fusion

• **Chemistry Advanced Methods for Electronic Structure**

- Institutions: ORNL, University of Colorado
- ORNL PI: Robert J. Harrison

*Approaches to one- and two-electron quantum chemical models that eliminate basis set error and scale correctly with system size*

• **Scientific Application Pilot in Chemistry: Fundamental Algorithms for Advanced Applications in Science and Technology (FAAFAST)**

- Institutions: ORNL, PNNL, University of Colorado
- ORNL PI: George Fann

*Fast, O(N), spectrally accurate, multiwavelet, and low separation methods for computational chemistry*

• **Climate Change Prediction: Collaborative Design and Development of the Community Climate System Model**

- Institutions: ANL, LANL, LBNL, LLNL, NASA-Goddard, NCAR, PNNL, ORNL
- ORNL PI: John Drake



*Building comprehensive, fully-coupled models of the Earth's climate system*

• **High-Energy and Nuclear Physics: Shedding New Light on Exploding Stars: TeraScale Simulations of Neutrino-Driven Supernovae and their Nucleosynthesis (aka TeraScale Supernova Initiative, TSI)**

- Institutions: Clemson University, Florida Atlantic University, Indiana University at Indianapolis, NCSA, NC State University, ORNL, SUNY-SB, University of California San Diego, University of Illinois, University of Washington
- ORNL PI: Anthony Mezzacappa



*Understanding explosions of massive stars (core collapse supernovae) and their associated phenomenology (element production, neutrino, and gravitational wave signatures)*

• **Fusion Energy Sciences: Numerical Computation of Wave-Plasma Interactions in Multi-Dimensional Systems**

- Institutions: CompX Corp., Lodestar Corp., Mission Research Corp., MIT, ORNL, PPPL
- ORNL PI: Don Batchelor

• **Fusion Energy Science: TeraScale Atomic Physics for Controlled Fusion Energy**

- Institutions: Auburn University, Daresbury Laboratory (UK), Drake University, Queens University (Belfast), ORNL, Rollins College, Sheffield-Hallam University (UK), University of Strathclyde (UK)
- ORNL PI: David R. Schultz

*Implement state-of-the-art atomic collision codes on the next generation of terascale computing facilities*

• **Scientific Application Pilot in Fusion Energy Sciences**

- Institution: ORNL
- ORNL PI: Leonard Gray

*Developing a quantitatively accurate predictive understanding of electromagnetic wave processes, which support important heating, current drive, and stability and transport applications in fusion-relevant plasmas*

**Integrated Software Infrastructure**  
Applied Math **Centers** Computer Science

• **Optimal PDE Simulations (TOPS)**

- Institutions: ANL, LBNL, LLNL, CMU, NYU, ODU, University of California-Berkeley, University of Colorado-Boulder, University of Tennessee
- ORNL PI: Jack Dongarra (UT/ORNL)



*Developing, implementing, and supporting optimal or near-optimal schemes for partial differential equation-based simulations and closely related tasks, as well as core implicit linear and nonlinear solvers*

• **Terascale Simulation Tools and Technologies Center (TSTT)**

- Institutions: ANL, BNL, LLNL, ORNL, PNNL, RPI, SNL, SUNY-SB
- ORNL PI: Eduardo F. D'Azevedo



*The TSTT Center has as its central goal to address the technical and human barriers preventing the effective use of powerful adaptive, composite, and hybrid methods.*

• **Center for Component Technology in Terascale Simulation Software (aka Common Component Architecture, CCA)**



- Institutions: ANL, Indiana University, LANL, LLNL, ORNL, PNNL, SNL, University of Utah
- ORNL PIs: David E. Bernholdt and James A. Kohl

*Developing the tools and technologies to bring the benefits of component-based software development to high-performance scientific computing*

• **Scientific Data Management (SDM)**

- Institutions: ANL, BNL, Georgia Tech University, LLNL, NC State University, Northwestern University, ORNL, University of California San Diego
- ORNL PIs: Randy Burris, Tom Potok, and Nagiza Samatova



*Provide a coordinated framework for the unification, development, deployment, and reuse of scientific data management software*

• **High-End Computer System Performance: Science and Engineering (aka Performance Evaluation Research Center, PERC)**



- Institutions: ANL, University of Illinois, LBNL, University of Maryland, LLNL, University of Tennessee, SDSC
- ORNL PIs: Thomas H. Dunigan, Jr. and Patrick H. Worley

*Developing a science for understanding of scientific applications on high-end computer systems and developing engineering strategies for improving performance on these systems*

• **Scalable Systems Software Enabling Technology Center**

- Institutions: Ames Lab, ANL, LANL, LBNL, NCSA, ORNL, PNNL, SNL
- ORNL PIs: AI Geist and Stephen Scott



*Producing an integrated suite of systems software and tools for the effective management and utilization of terascale computational resources, particularly those at the DOE facilities*

**Collaboratories**

• **DOE Science Grid**

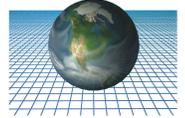
- Institutions: ANL, LBNL, ORNL, PNNL
- ORNL PI: AI Geist



*Computing and data infrastructure for large-scale science*

• **The Earth System Grid II**

- Institutions: ANL, LBNL, LLNL, NCAR, ORNL, University of Southern California
- ORNL PI: David E. Bernholdt



*Turning climate model datasets into community resources*

• **Scientific Annotation Middleware (SAM)**

- Institutions: ORNL, PNNL
- ORNL PI: AI Geist

*A lightweight, flexible middleware to support the creation and use of metadata annotations*

**Hardware Infrastructure and Related Projects**

• **Net100: Development of Network-aware Operating Systems**

- Institutions: LBNL, ORNL, PSC
- ORNL PIs: Thomas H. Dunigan, Jr. and Nagi Rao



*The project seeks to measure and understand end-to-end network and application performance, and apply that knowledge to tuning networks and applications.*

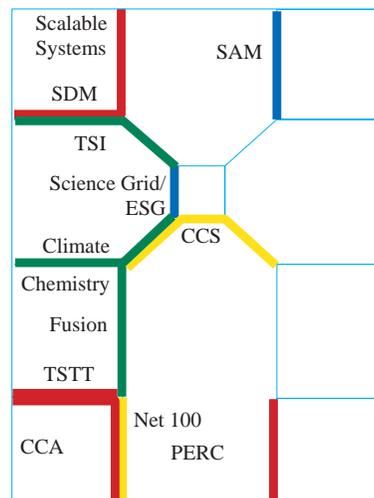
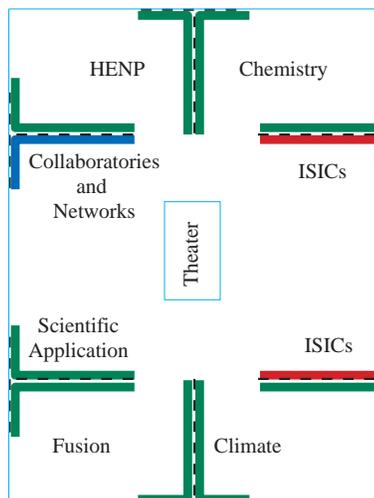
• **SciDAC Computational Infrastructure**

- Institutions: ORNL Center for Computational Sciences (CCS)
- ORNL PI: Buddy Bland



*The CCS is designated as the primary computational resource for SciDAC projects.*

SciDAC (R1872) Floor Plan



ORNL (R1971) Floor Plan

