

Oak Ridge National Laboratory
Computer Science and Mathematics Division

FY 2003 Level 2 Plan

Jeff Nichols
July 2002

FY2003 Level 2 Plan

Computer Science and Mathematics Division

Organizational Description

The Computer Science and Mathematics Division (CSM) is ORNL's premier source of basic and applied research in high-performance computing, applied mathematics, and intelligent systems. Basic and applied research programs are focused on computational sciences, intelligent systems, and information technologies.

Mission

Our mission includes basic research in computational sciences and application of advanced computing systems, computational, mathematical and analysis techniques to the solution of scientific problems of national importance. We seek to work collaboratively with universities to enhance science education and progress in the computational sciences.

Vision

The Computer Science and Mathematics Division (CSMD) seeks to become the premier location among DOE laboratories where outstanding scientists, computer scientists and mathematicians can perform interdisciplinary computational research.

Core Functions/Focus Areas

Climate Dynamics

The Computational Climate Dynamics group conducts research in climate sensitivity, computational methods of global and regional climate modeling. An emphasis is placed on the atmospheric dynamics coupled with chemical and hydrological processes. Research areas include spectral methods for fluid flow, parallel algorithms, performance models, atmospheric chemistry, river transport and hydrological coupling, air-sea interactions and climate analysis techniques.

Complex Systems

The Complex Systems group conducts fundamental research in engineering sciences in support of the goals and priorities of the DOE Office of Science. Its unique technologies and facilities also contribute to the missions of the US national security community. Research areas include:

- Global optimization
- Nonlinear dynamical systems, including neural networks, time series analysis, and chaos
- Massively parallel, asynchronous computing
- Automated computer code differentiation with application to sensitivity and uncertainty analysis
- Quantum information science, including quantum optics, entangled systems, quantum algorithms, and quantum cryptography
- Optical science, with emphasis on laser array synchronization for application to directed energy weapons, deep-space optical communications, interferometric nanolithography, and optical radars
- Architectures and algorithms for petascale optical computing

- Computer networks, including analysis and control of network dynamics, performance optimization of network transport protocols, and cyber warfare
- Advanced sensor systems, with emphasis on information fusion, mobile ad-hoc sensor networks and hyperspectral remote sensing
- Robotics, with focus on mobile, heterogeneous cooperating intelligent systems
- Optimal control of distributed systems
- Bioengineering applications

Computational Biology

The Computational Biology group develops computational methods and capabilities to advance understanding of complex biological systems and predict their behavior particularly those required by the DOE Genomes to Life Initiative.

Computational Materials Science

The Computational Materials Science group conducts research ranging from nano-science to full-size engineering applications. Research areas include:

- Engineering and transportation technology
- Engineering sciences
- Nano science
- Applied mathematics
- Soft materials (polymers)
- Surface science (catalysis)
- Magnetism and magnetotransport in nanostructures
- Light-weight materials
- Carbon based nanostructures (Carbon nano-tubes and molecular electronics)
- Advanced mathematical and computational tools for design and analysis of functionally graded materials

Computational Mathematics

The Computational Mathematics Group is devoted to the development, analysis and application of efficient numerical algorithms for solving large-scale scientific and engineering problems on advanced computer architectures. The Computational Mathematics Group is home to the Alston F. Householder Postdoctoral Fellowship. Principal research areas include:

- boundary element method
- dense matrix computations
- direct methods for sparse matrix computations
- iterative methods for linear systems
- algorithms for solving differential equations
- large eigenvalue computations
- computational geometry and mesh generation

Network and Cluster Computing

The Network and Cluster Computing group performs basic research in component technologies, super-scalar algorithms, fault tolerant distributed computing, cluster computing, networking, computational steering, and distributed data analysis. Tools and software are developed to make high performance computing more effective and accessible for scientists and engineers working on problems of national importance.

Scientific Applications Support

Members of the Scientific Applications Support group are research scientists who provide a liaison between the users of the high performance computers of the Center for Computational Sciences (CCS) and the CCS itself. They actively participate as part of the research teams, and help administer the computers in the CCS and other CSM computing systems.

Statistics and Data Science

The Statistics and Data Sciences group conducts research in the analysis and exploration of data, the collection and organization of data, and decisions based on data. Our work is relevant from the design phase of an experiment or study to the final phase of analysis and interpretation. Our collaborations with other scientists cut across many areas, including the physical sciences, computational sciences, environmental sciences, biological sciences, epidemiology, engineering, and chemistry.

Systems and Operations

The Systems and Operations group provides 24/7 operations coverage of the CCS high performance computing and storage systems and the ORNL mass storage systems. The group also provides systems administration, configuration, and management for the CCS high performance computing systems and for CSM workstations and servers.

Strategic Intent

Strategic goals supporting division missions are to:

- Support the Lab agenda for Excellence in Operations, Environment Safety & Health (ES&H), and Community Service
- Maintain and grow integrated computer and computational science research programs that incorporate leading edge fundamental and applied R&D
- Maintain leadership roles in R&D program management for ORNL and DOE
- Form internal and external partnerships to maximize scientific and technological impacts
- Maintain and expand a high performance computing capability for DOE and ORNL
- Participate in educational outreach programs

Strategic Objectives

Strategy #1 - Support the Lab agenda for Excellence in Operations, Environment Safety & Health (ES&H), and Community Service

- Maintain safe and compliant working conditions
- Maintain implementation of ISMS
- Comply with all environmental regulations
- Conduct operations that are cost-effective and efficiently utilize allocated space
- Maintain high quality staff

Strategy #2 - Maintain and grow integrated computer and computational science research programs that incorporate leading edge fundamental and applied R&D

- **Neutron Sciences:** Develop innovative research programs that take advantage of unique capabilities; support SNS design needs through HPC access; expand ongoing collaboration in application of CSMD's (CESAR) unique laser technology to accelerator physics
- **Complex Biological Systems:** Integrate and extend ORNL's resources in computational biology and bioinformatics to advance modeling of complex biological systems in support of the Genomes to Life Program

- **Advanced Materials:** Expand ORNL capabilities and programs in nanoscale science, engineering, and technology; expand division participation in NSET initiative
- **Climate Dynamics:** Study the climate sensitivity to new chemical, carbon and hydrological processes and contribute model components to a comprehensive software engineering design of coupled climate models.
- **Computational Mathematics:** Maintain and grow computational research into fast transform algorithms such as wavelet, fast multipole or nonuniform FFT and specialized techniques in support of important scientific applications such as fusion or nanotechnology.
- **Quantum Computing:** Grow ORNL capabilities and programs in quantum information science, engineering, and technology

Strategy #3 - Maintain leadership roles in R&D program management for ORNL and DOE

- Maintain high quality S&T programs
- Develop new programs and program directions; in particular, based on existing strengths, focus on DOD, NASA, and the Intelligence Community
- Review available information to determine customer satisfaction

Strategy #4 - Form internal and external partnerships to maximize scientific and technological impacts

- **High-Performance Computing:** Enhance accessibility of high-performance computing power within ORNL and for external partners; enhance network connectivity to ORNL from ESnet
- **High-Performance Computing:** Expand the scope of the Joint Institute for Computational Sciences; devise ways to include core universities in JICS

Strategy #5 - Maintain and expand a high performance computing capability for DOE and ORNL

- **High-Performance Computing:** Secure a multi-teraflops computational platform and infrastructure; upgrade present system to 10 teraflops capability
- **Facilities Modernization:** Implement Facilities Revitalization Project to design and construct new facilities and renovate, replace, and dispose of existing facilities in support of ORNL mission assignments and objectives.
CSM will contribute in design, furnishing, and move-in process for new Computational Sciences and JICS Buildings
- **High-Performance Computing:** Increase Laboratory expertise in modeling, simulation, numerical methods, and future architectures; develop and deploy algorithms, libraries tools and collaborative problem solving environments; expand division participation in SciDAC Initiative, Genomes to Life Initiative, and Topical Centers.

Strategy #6 - Participate in educational outreach programs

- **Research Alliance for Minorities (RAM):** to encourage African American, Hispanic American, and Native American (AAHANA) students to pursue advanced degrees in science, mathematics, engineering and technology with the long-term goal of addressing underutilizations in the workforce

Implementing Actions

Program Overview and Division Integration

The Laboratory Agenda contains ORNL's strategic objectives and critical outcomes agreed to by the Leadership Team and the Department of Energy (DOE). These are documented in the Laboratory's Performance Evaluation Plan. The Computing and Computational Sciences Directorate Leadership Team worked together to develop a Level 1 Plan for the Directorate to support the Laboratory Agenda. The CSMD Leadership Team, in turn, utilized the Directorate Level 1 plan to develop a level 2 Plan for the Division. Thus, the Laboratory Agenda and the Directorate key outcomes for FY2003 provide the framework for the CSMD's performance assessment program. The Level 2 Plan outlines the FY 2003 strategies, implementing actions, and expected outcomes.

Prioritized implementing actions resulting from the strategic planning process becomes the action plan for the Division's new major projects during the year. The FY2003 Plan is reviewed with Division staff. The high level milestones for the implementing actions are entered into the ORNL Assessment Tracking System. The plan is assessed at regular monthly meetings with the CSMD Extended Leadership Team.

Roles and Responsibilities

Division Director

- Develop a Division Performance Assessment Plan and implementation process in order to assess performance of organization.
- Work with Group Leaders, Task/Project Managers, and Staff to determine performance-assessment areas for review.
- Lead efforts to identify appropriate division-level lessons learned resulting from performance assessment activities
- Work with Group Leaders, Task Project Managers, and Staff to ensure that any needed corrective actions resulting from the performance assessment effort are identified, attributed to the actual cause, and tracked to completion to prevent recurrence

Group Leaders/Supervisors:

- Work with Division Director, Task/Project Managers, and Staff to determine performance assessment areas for review.
- Identify performance assessment areas to review to ensure the quality of products and services meet customer requirements and to ensure a safe working environment.
- Conduct performance assessment activities (e.g. walk throughs) within assigned areas.
- Share applicable lessons learned with assigned staff personnel

Task/Project Manager:

- Work with Division Director, Group Leaders, and Staff to suggest performance-assessment areas for review.
- Identify performance assessment areas to review to ensure that the products or services meet customer requirements.
- Identify performance assessment areas to review to Identify hazards on task/projects.

Staff:

- Work with Division Director, Group Leaders, and Task/Project Managers to suggest performance-assessment areas for review

Formatted

- Identify performance assessment areas to review in order to perform work effectively, efficiently, safely, and securely in support of the Laboratory Agenda and organizational goals and objectives.
- Provide feedback to Project Leaders, Group Leaders, or Division Director regarding performance assessment process.
- Provide feedback to Project Leaders, Group Leaders, or Division Director regarding performance-assessment process.

Actions

Strategy #1 - Support the Lab agenda for Excellence in Operations, Environment Safety & Health (ES&H), and Community Service

- Maintain safe and compliant working conditions
 - Coordinate with ORNL ES&H staff to ensure compliance with all relevant metrics relating to workplace safety
 - Conduct periodic workplace reviews for self-identification of significant ESH issues
 - Assess staff training needs and ensure required training completed
- Maintain implementation of ISMS
 - Apply SBMS to existing and new work
 - Review all off-site subcontracts by ESH&Q SME and division requestor for ESH&Q (SBMS) issues
 - Communicate SBMS principles to staff by Management
- Comply with all environmental regulations
 - Consider pollution prevention and waste minimization for all new work
- Conduct operations which are cost-effective and efficiently utilize allocated space
 - Conduct assessments of division activities supported by organizational burden to determine opportunities for further reduction
 - Evaluate space utilization for all activities with the goal of efficiently utilizing existing space
- Maintain high quality staff
 - Assess staff retention and hiring (employees and postdoctoral staff) to determine potential issues
 - Hire at least 8 new staff members as supported by program funding

Strategy #2 - Maintain and grow integrated computer and computational science research programs that incorporate leading edge fundamental and applied R&D

- **Neutron Sciences:** Develop innovative research programs that take advantage of unique capabilities; support SNS design needs through HPC access
 - Assist SNS design team on the CSM supercomputers
- **Complex Biological Systems:** Integrate and extend ORNL's resources in computational biology and bioinformatics to advance modeling of complex biological systems
 - Lead proposals in the Genomes to Life Initiative
 - Create strategic partnerships with universities, and other labs.
- **Advanced Materials:** Expand ORNL capabilities and programs in nanoscale science, engineering, and technology; expand division participation in NSET initiative
 - ***Formalize Computational Materials Research topical focus within CCS (CCS-CMR)***
 - Contribute to the completion of ORNL proposal for the Center for Nanophase Materials Sciences
 - Participate in proposals to DOE-BES for NSET research funding

- **Climate Dynamics:** Broaden the science funding base for climate research in order to build more comprehensive climate models. Also, incorporate key collaborations from the mathematical/algorithm research programs of MICS and SciDAC into ongoing model development efforts
- **Computational Mathematics:**
 - Although ORNL has world class expertise in BEM, this is not well known outside a small research community. We will develop BEM library software "BEMPACK" similar to successfully LAPACK to more widely disseminate this technology and apply BEM in new areas such as modeling coupled CFD, thermal and mechanical analysis in MEMS.
 - Conduct research in new areas and complementary to SciDAC ISIC, such as fast transform methods, that will be used in 5 to 10 years
 - Fulfill mission in supporting the advancement of science in key areas such as fusion, or NSET and participate in proposals to DOE for funding through SciDAC Science Application Pilot Centers

Strategy #3 - Maintain leadership roles in R&D program management for ORNL and DOE

- Maintain high quality S&T programs
 - Exceed historic publication rates
 - Succeed in nominations of staff for external recognition
- Develop new programs and program directions
 - Participate in major sponsor planning activities and program assessments
 - Attain at least a factor of 2 ROI for ORNL program development investments
- Review available information to determine customer satisfaction
 - Attain scores and feedback indicating high quality will be maintained
 - Retain current funding levels and/or market share for major programs

Strategy #4 - Form internal and external partnerships to maximize scientific and technological impacts

- **High-Performance Computing:** Enhance accessibility of high-performance computing power within ORNL and for external partners; enhance network connectivity to ORNL from ESnet
 - Provide OC48 connection to ORNL from ESnet
- **High-Performance Computing:** Expand the scope of the Joint Institute for Computational Sciences; devise ways to include core universities in JICS
 - Develop a program plan for JICS to include all core universities

Strategy #5 - Maintain and expand a high performance computing capability for DOE and ORNL

- **High-Performance Computing:** Secure a multi-teraflops computational platform and infrastructure; upgrade present system to 10 teraflops capability
 - Secure funding for a major computer upgrade
 - Prepare a response to the Japanese Earth Simulator
- **Facilities Modernization:** Implement Facilities Revitalization Project to design and construct new facilities and renovate, replace, and dispose of existing facilities in support of ORNL mission assignments and objectives; contribute in design process for new Computational Sciences and JICS Buildings
 - Coordinate ORNL input into specifications for CSB
 - Provide functional specifications for JICS building
 - Coordinate ORNL input for furniture for the CSB
 - Coordinate move of all CCS computing resources into the CSB

- **High-Performance Computing:** Increase Laboratory expertise in modeling, simulation, numerical methods, and future architectures; develop and deploy algorithms, libraries tools and collaborative problem solving environments; expand division participation in SciDAC Initiative, and lead ORNL proposals for Topical Centers
 - Hire expert staff in modeling, simulation, numerical methods, and future architectures
 - Evaluate emerging technologies
 - Evaluate availability of algorithms, libraries tools and collaborative problem solving environments
 - Lead several SciDAC projects
 - Lead ORNL proposals for Genomes to Life
 - Organize workshops to develop Topical Center goals
 - Lead DOE response to the Earth Simulator computer

Strategy #6 - Participate in educational outreach programs

- Facilitate collaborative efforts by faculty and ORNL research staff to mentor students

Staff Development and Key Hires

Leadership and needed expertise to deliver on the strategic intent and address key issues are being developed in two key ways: development of current personnel (internal to ORNL) and strategic hires.

The following strategic hires are planned for 2003:

- 1) A Technical Group Leader (TGL) for the Computational Biology group
- 2) An outstanding senior scientist or TGL for the Computational Math group
- 3) An outstanding senior scientist for the Network and Cluster Computing group
- 4) A visualization expert to galvanize ORNL's science visualization research
- 5) Four people to support ORNL's response to the Earth Simulator:
 - two expert system programmers
 - two expert application support programmers
- 6) Six critical hires to support the new programs in the Complex Systems group:
 - Optical Computing (with emphasis on digital optics)
 - Quantum Computing (with emphasis on algorithms for cryptography or for search)
 - Ultrafast lasers (with focus on material science)
 - Massively parallel computing (with expertise in concurrently asynchronous systems)
 - Optical radars (with applications to missile tracking and target discrimination)
 - High performance networks

FY 2003 Outcomes

The following represents specific outcomes to be delivered by the end of FY 2003:

- 1) Submit technical publications in excess of the FY02 rate
- 2) Deliver computing resources to science programs
- 3) Establish a Genomes to Life research program
- 4) Move the CCS from the 4500N computer center to the CSB
- 5) Establish core of a topical center for computational materials research within CCS
- 6) Connect ORNL to Atlanta with state-of-the-art OC192 network
- 7) Establish a computational chemistry program
- 8) Evaluate new experimental computer systems

- 9) Hire Householder fellow
- 10) Hire distinguished defense science advisor
- 11) Ensure financial health and integrity of division
- 12) Maintain excellence in Environment Safety & Health (ES&H),

CSM Performance Assessment Outcomes and Schedule for FY 2003

- 1. Technical publications submission rate exceeds that of FY02 (Jeff Nichols) 9/30/03**
Publication submission rate reviewed quarterly (CPPR) and compared with rate for FY03
- 2. Computing resources are delivered to science programs (Buddy Bland) 9/30/03**
Deliver agreed computing to SciDAC program (29,450,000 MPP) 9/30/03
Deliver agreed resources to OBER programs (2,500,000 MPP) 9/30/03
- 3. Genomes to Life research program is established (Al Geist) 9/30/03**
Get GTL-1 funding to ORNL and into CSMD 01/31/03
Submit at least two proposals to DOE for the second round of GTL funding 05/31/03
Staff up GTL program in CSM with at least two new postdocs 09/30/03
- 4. Experimental computer systems are evaluated (Buddy Bland) 9/30/03**
Evaluation Plan for Cray X1 3/1/03
Participate in IBM Federation Early Ship program 7/31/03
Meet with at least three additional vendors for briefings 9/30/03
- 5. CCS moved from 4500N to the new CSB (Buddy Bland) 9/30/03**
Move coordinator assigned 2/28/03
Move plan complete 3/31/03
Move completed 9/30/03
- 6. Core of topical research centers for Climate, Materials, and Fusion are established (Thomas Schulthess) 09/30/03**
Hold workshop on Ultrascale simulations (all three centers) 03/31/03
Establish presence on the WWW 07/31/03
Organize joint international workshops with Center for Nanophase Materials Science 08/31/03
Assure continuity in the future (share funding responsibility with Jeff Nichols) 09/30/03
- 7. ORNL and Atlanta connected by state-of-the-art OC192 network (Bill Wing) 12/31/02**
Establish OC192 hardware link from ORNL to Atlanta 12/31/02
- 8. Computational Chemistry program established (Robert Harrison)**
- 9. Householder fellow hired (Ed D'Azevedo) 07/31/03**
Form Selection Committee and identify candidates 11/30/02
Conduct interviews 02/28/03
Select and make offer 03/30/03
Hire 07/31/03
- 10. Distinguished defense science advisor hired (Jacob Barhen) 03/31/03**
Identify candidates 10/31/02
Conduct interviews 02/28/03
Select and make offer 03/15/03
Hire 03/31/03

11. Financial health and integrity of CSMD is assured (Kyle Spence) 09/30/03

Review and report on CSMS financial health Monthly
Conduct assessment of procurement card spending 2/28/03
Prepare and submit annual budget 4/15/03

12. Division Safety Performance is assessed (Ross Toedte) 09/30/03

Conduct quarterly safety assessments and walk-throughs of Division space
Identify, document, and mitigate any identified hazards
Communicate safety issues to Division staff
Develop Division web page(s) regarding ES&H issues and resources