Oak Ridge National Laboratory evolved from the Manhattan Project

ORNL in 1943
The Clinton Pile was the world’s first continuously operated nuclear reactor
Today, ORNL is DOE’s largest science and energy laboratory

- $1.3B budget
- 4,350 employees
- 3,900 research guests annually
- $350 million invested in modernization
- World’s most powerful open scientific computing facility
- Nation’s largest concentration of open source materials research
- Nation’s most diverse energy portfolio
- Operating the world’s most intense pulsed neutron source
- Managing the billion-dollar U.S. ITER project
The University of Tennessee

- An ORNL partner since 1946
- State-funded Science Alliance started in 1982, to build programs with ORNL
- Shared research in many areas
- Joint appointments
- Joint institutes in advanced materials, biological sciences, computational sciences, neutron sciences, nuclear physics

Battelle

- A 65-year relationship with DOE and its predecessors
- Develops and deploys technology worldwide
- Manages or co-manages 6 DOE national laboratories: ORNL (with UT), Brookhaven (with SUNY-Stony Brook), Idaho, Lawrence Livermore (with UC and Bechtel), NREL (with MRI), Pacific Northwest
Leading the development of ultrascale scientific computing

• Leadership Computing Facility:
  – World’s most powerful open scientific computing facility
  – Jaguar XT operating at 1.64 petaflops
  – Exascale system by the end of the next decade
  – Focus on computationally intensive projects of large scale and high scientific impact

• Addressing key science and technology issues
  – Climate
  – Fusion
  – Materials
  – Bioenergy

The world’s most powerful system for open science
Facilities Designed for Exascale Computing

Open Science Center (40,000 ft²)
- Upgrading building power to 15 MW
- 210 MW substation, upgradeable to 280 MW
- Deploying a 6,600 ton chiller plant
- Tripling UPS and generator capability

National Security Center (40,000 ft²)
- Capability computing for national defence
- 25 MW of power and 8,000+ ton chiller

New Computer Facility (100,000+ ft²)
- 100,000 ft² raised floor expandable with modular build out to over 250,000 ft²
- Open and Secure operations
- Lights out facility
State-of-the-art Infrastructure - Power

External grid
- Ft. Loudon
- Bull Run
- Kingston

Local distribution
- 210-MW substation
- Upgradeable to 280 MW
- 4000 substation

Facilities
- Computational Sciences Building
- Multipurpose Research Facility
The Computer Science and Mathematics Division (CSMD) 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 throughout the world to enhance science education and progress in the computational sciences.

**Vision**
The Computer Science and Mathematics Division (CSMD) seeks to maintain our position as the premier location among DOE laboratories and to become the premier location worldwide where outstanding scientists, computer scientists and mathematicians can perform interdisciplinary computational research.
Scale


- Energy and power
- Memory and storage
- Concurrency and Locality
- Resiliency

- Commodity
The Memory Wall

Recommendation: Research thrusts in

• Co-development and optimization of Exascale Hardware Technologies and Architectures
  – new devices must be evaluated in the context of new architectures that can utilize the new features of such devices

• Co-development and optimization of Exascale Architectures and Programming Models
  – explosive growth in concurrency
  – locality-aware and communication-efficient architectures

• Co-development of Exascale Algorithms, Applications, Tools, and Run-times

• Development of a deep understanding of how to architect Resilient Exascale Systems

• Commodity → Interconnects
Observations

- **Programming is resource management**
  - the programming model must reflect the relative costs of using the resources available
  - MPI accurately reflects the current distributed memory systems
    - emphasis is on distributed nature of memory

- **Vertical integration (co-development)**
  - inter-disciplinary teams including mathematicians, computer scientists, and domain scientists
  - from economics: ownership of suppliers (backward integration), distributors (forward integration) or both (balanced integration)
Gordon Bell prize awarded to ORNL team

A team led by ORNL’s Thomas Schulthess received the prestigious 2008 Association for Computing Machinery (ACM) Gordon Bell Prize at SC08.

The award was given to the team for attaining the fastest performance ever in a scientific supercomputing application.

The team achieved 1.352 petaflops on ORNL’s Cray XT Jaguar supercomputer with a simulation of superconductors.

By modifying the algorithms and software design of the DCA++ code, the team was able to boost its performance tenfold.
New algorithm to enable 1+ PFlop/s sustained performance in simulations of disorder effects in high-$T_c$ superconductors

- T. A. Maier
- P. R. C. Kent
- T. C. Schulthess
- G. Alvarez
- M. S. Summers
- E. F. D’Azevedo
- J. S. Meredith
- M. Eisenbach
- D. E. Maxwell
- J. M. Larkin
- J. Levesque

Thomas Schulthess
Conceptual Organization of CSMD

Apply
- Computational Chemistry
- Computational Astrophysics
- Comp Materials Sciences
- Molecular Biophysics
- Computer Science Research
- Future Technologies
- Performance Tools
- Complex Systems
- Computational Engineering and Energy Sciences

Think
- Applied Mathematics
- Statistics and Data Science
- Scale (Massive Parallelism)
Computational Mathematics

• Development of multiresolution analysis for integro-differential equations and Y-PDE
• Boundary integral modeling of Functionally Graded Materials (FGMs)
• Large-scale parallel Cartesian structured adaptive mesh refinement
• Fast Multipole / non-uniform FFTs
• New large-scale first principles electronic structure code
• New electronic structure method
• Fracture of 3-D cubic lattice system
• Adventure system
• Eigensolver with Low-rank Upgrades for Spin-Fermion Models
Statistics and Data Science

- Chemical and Biological Mass Spectrometer Project
- Discrimination of UXO
- Forensics - Time Since Death
- A Statistical Framework for Guiding Visualization of Petascale Data Sets
- Statistical Visualization on Ultra High Resolution Displays
- Local Feature Motion Density Analysis
- Statistical Decomposition of Time Varying Simulation Data
- Site-wide Estimation of Item Density from Limited Area Samples
- Network Intrusion Detection
- Bayesian Individual Dose Estimation
- Sparse Matrix Computation for Complex Problems
- Environmental Tobacco Smoke (ETS)
- Explosive Detection Canines
- Fingerprint Uniqueness Research
- Chemical Security Assessment Tool (CSAT)
- Sharing a World of Data: Scaling the Earth Systems Grid to Petascale
- Group Violent Intent Modeling Project
- ORCAT: A desktop tool for the intelligence analyst
- Data model for end-to-end simulations with Leadership Class Computing
- A Knowledge-Based Middleware and Visualization Framework for the Virtual Soldier Project
- GWAVA: An Information Retrieval Web application for the Virtual Autopsy
Computer Science Research

Perform basic research and develop software and tools to make high performance computing more effective and accessible for scientists and engineers.

- **Heterogeneous Distributed Computing** – PVM, Harness, OpenMPI(NCCS)
- **Holistic Fault Tolerance** – CIFTS
- **CCA Changing the way scientific software is developed and used**
- **Cluster computing management and reliability** – OSCAR, MOLAR
- **Building a new way to do Neutron Science** – SNS portal
- **Building tools to enable the LCF science teams** – Workbench
- **Data-Intensive Computing for Complex Biological Systems** – BioPilot
- **EarthSystem Grid** – Turning climate datasets into community resources (SDS, Climate)
- **Robust storage management from supercomputer to desktop** – Freeloader
- **UltraScienceNet defining the future of national networking**
- **Miscellaneous** – electronic lab notebooks, Cumulvs, bilab, smart dust
Future Technologies

Research Mission - performs basic research in core technologies for future generations of high-end computing architectures and system software, including experimental computing systems, with the goal of improving the performance, reliability, and usability of these architectures for users.

Topics include

- **Emerging architectures**
  - IBM CELL (i.e., Playstation)
  - Graphics Processors (e.g., Nvidia)
  - FPGAs (e.g., Xilinx, Altera, Cray, SRC)
  - Cray XMT Multithreaded architecture

- **Operating systems**
  - Hypervisors
  - Lightweight Kernels for HPC

- **Programming Systems**
  - Portable programming models for heterogeneous systems

- **Parallel IO**
  - Improving Lustre for Cray

- **Performance modeling and analysis**
  - Improving performance on today’s systems
  - Modeling performance on tomorrow’s systems (e.g., DARPA HPCS)
  - Tools for understanding performance

- **Applications**
  - Fusion
  - Physics
  - Bio

- **Visualization**
  - New methods for CNMS

Sponsors include:

- **SciDAC**
  - Performance Engineering Research Institute
  - Scientific Data Management
  - Petascale Data Storage Institute
  - Visualization (VACET)
  - Fusion
  - COMPASS

- **DOE Office of Science**
  - Fast OS - Molar
  - Software Effectiveness

- **DOD**
  - HPC Mod Program

- **NSA**
  - Peta-SSI FASTOS

- **DARPA**
  - Peta-Scale Performance (DARPA HPCS)

- **LDRD**
  - Performance Tools for Large Scale Systems
  - FPGA Programmability
  - Perumullla

- **NCCS**
  - Vendor Interaction Evaluations
  - Scientific Computing
Complex Systems

**Mission:** Support DOD and the Intelligence Community
Theory – Computation – Experiments

**Examples of current research topics:**

- **Missile defense:** C2BMC (tracking and discrimination), NATO, flash hyperspectral imaging
- **Modeling and Simulation:** Sensitivity and uncertainty analysis, global optimization
- **Laser arrays:** directed energy, ultraweak signal detection, terahertz sources, underwater communications, SNS laser stripping
- **Terascale embedded computing:** emerging multicore processors for real-time signal processing applications (CELL, HyperX, …)
- **Anti-submarine warfare:** ultra-sensitive detection, coherent sensor networks, advanced computational architectures for nuclear submarines, Doppler-sensitive waveforms, synthetic aperture sonar
- **Quantum optics:** cryptography, quantum teleportation
- **Computer Science:** UltraScience network (40-100Gb per L)
- **Intelligent Systems:** neural networks, mobile robotics

**Sponsors:** DOD(AFRL, DARPA, MDA, ONR, NAVSEA), DOE(SC), NASA, NSF, IC (CIA, DNI/DTO, NSA)

UltraScience Net
Computational Chemical Sciences

• Application areas
  - Chemistry, materials, nanoscience, electronics

• Major techniques
  - Atomistic and quantum modeling of chemical processes
  - Statistical mechanics and chemical reaction dynamics

• Strong ties to experiment
  - Catalysis, fuel cells (H₂), atomic microscopy, neutron spectroscopy

• Theory
  - Electronic structure, statistical mechanics, reaction mechanisms, polymer chemistry, electron transport

• Development
  - Programming models for petascale computers
  - Petascale applications

Computational Chemical Sciences is focused on the development and application of major new capabilities for the rigorous modeling of large molecular systems found in, e.g., catalysis, energy science and nanoscale chemistry.

Funding Sources: OBES, OASCR, NIH, DARPA
Algorithms Project Overview
It all revolves around the science

Multi-core Aware
Hybrid, Parallel in time

Multi-precision
Krylov, Poisson, Helmholtz

Hierarchical MPI
MPI_Comm_Node, etc

Shared memory
MPI_Alloc_Shared

Extreme Scale
Million node systems

Node level
Detailed kernel studies

Multi-core
Processor affinity
Memory affinity
Scheduling

Memory hierarchy
Future designs

Interconnect
Latency/BW effects

Influence design

Science Applications

Algorithms

Runtime

Simulation

Architecture

Institute for Advanced Architectures and Algorithms
## Extreme Scale System Center (ESSC)

### Application Performance Studies
- Modeling and Analysis of applications and kernels on large SMP’s, large Clusters, SPD’s
  - Selected kernels are supplied by DOD
- Database Analysis (Analytics repository, Data base analysis of sensor data from extreme scale systems to improve resilience of these systems)
- Languages (HPCS (X10, Chapel, Fortress), UPC, OpenSHMEM)
  - Productivity/programmability (all apps/kernels are converted to new languages)

### Networking and I/O Analysis and Deployment (WAN, LAN, Interconnect, Sensors)
- 100 Gb/Lambda Long Haul (Development)
- USN is a “dark fiber” ORNL controls end-to-end technology (unlimited scenarios)
- Cyber Security, Dynamic performance analysis

### System Software Tools
- Development Environments (Compiler analysis, Common Software Infrastructure…)
- Resource Manager/Job Schedulers (Graph Analytics, Optimization, Analytics, Topology and power aware…)

### RAS at Scale (Reliability, Availability, Serviceability)
- System, I/O, Network, Applications, Environment (Power, Space and Cooling and Analytics)
- Power Management, Analysis, Modeling and Prediction (Optimization and Graph Analytics)
- Power/location aware computing (Sensors, Analytics, Databases…)

### Advanced Technologies / Architectures
- SPD’s, Sensor Fusion, Analytics, Hybrid Computing, C64, memory technologies, disruptive technologies, Special Projects