# Computing and Computational Sciences

## Computational Sciences and Engineering

The Computational Sciences and Engineering Division focuses on transdisciplinary computational science and analytics at scale to enable scientific discovery across the physical sciences, engineered systems, and biomedicine and health sciences. It provides foundations and advances in quantum computation and information science and develops community applications, data assets, and technologies to advance crosscutting science outcomes.

**Advanced Computing Methods for Physical Sciences**

*Delivers multiscale, multifidelity computational models and systems developing algorithms and analytics for the physical sciences.*

*1.* Computational Earth Sciences — Develops extreme-scale models and data analytics methods applied to Earth systems modeling. Examples include E3SM and ILAMB, among others.

*2. Computational Chemistry and Nanomaterials Sciences* — Delivers nanomaterials and chemical science at the forefront of the field through HPC. Leads and contributes to the development of Quantum Monte Carlo and Hubbard applications, and machine-learning methods for experimental data. Application examples include QMCPACK and DCA++, among others.

*3. Multiscale Materials* — Delivers multiscale material models to a broad range of energy, transportation, and advanced manufacturing applications. Houses specific strengths in thermomechanics, phase-field modeling, molecular dynamics, and Density Functional Theory.

*4. Quantum Computational Science* — Develops the fundamental quantum computer science, algorithms, and software interfaces needed to leverage quantum accelerators to advance scientific discovery.

*5. Quantum Information Science* — Leverages experimental expertise in the implementation of quantum sensors, networks, and algorithms in quantum hardware platforms and testbeds.

**Advanced Computing Methods for Engineered Systems**

*Develops scalable and coupled algorithms for engineering, cybernetics, autonomous and complex systems applications.*

*1. Scalable Algorithms and Coupled Physics* — Creates performance portable applications and supports algorithms and libraries for coupled physics simulations at scale. Leads in development for programming models, frameworks, and data mapping standards.

*2. Computational Systems Engineering and Cybernetics* — Leads modeling for large-scale dynamical systems with applications in scalable control systems. Develops solutions for sensor data aggregation and methods for approaches to learning, control, and optimization.

*3.* Multiphysics Modeling and Flows — Leads high-fidelity modeling and numerical tools development for fluid dynamics and complex flow physics, including turbulent, multiphase and reacting flows, fluid structure interactions, and computational mechanics and shock wave propagation.

*4. Autonomous and Complex Systems* — Develops and deploys disruptive technologies at the extreme scale, such as multimodal sensing and pioneering algorithms for large laser arrays, signal processing algorithms, and online computing for sensing platforms.

*5. Computational Urban Sciences* — Creates data-driven understanding of complex urban systems at all scales and leads in the development of related data analytics.

**Advanced Computing for Health Sciences**

*Delivers scalable computational solutions to biomedical and healthcare delivery challenges*

*1. Biostatistics and Multiscale Systems* — Develops statistical, machine-learning, and deep-learning methodologies for large-scale genomics, text, and imaging applications. Develops and incorporates AI and data-driven approaches at the intersections of molecular dynamics simulations that exploit the unique capabilities of the OLCF and the experimental validation capabilities at the Spallation Neutron Source, both Department of Energy Office of Science User Facilities.

2. *Multimodal Data Analytics* — Leverages expertise in large-scale biomedical informatics and statistical genetics to build and use tools for healthcare needs. Creates scalable AI and machine-learning solutions for multidimensional, multimodal data in HPC environments applied to biomedicine and bioengineering. Includes privacy and biomedical informatics for supervised and unsupervised learning with healthcare data, specifically phenotyping, information extraction, medical imaging, and new outcomes such as recurrence.

## Computer Science and Mathematics

The Computer Science and Mathematics Division delivers fundamental and applied research capabilities in applied mathematics and computer science, experimental computing systems, scalable algorithms and systems, artificial intelligence and machine learning, data management, workflow systems, analysis and visualization technologies, programming systems and environments, and systems science and engineering.

**Mathematics in Computation**

*Delivers scalable and architecture-aware algorithms*

*1. Discrete Algorithms* — Algorithms and foundations for discrete structures, including graph algorithms and discrete optimization.

*2. Data Analysis and Machine Learning* — Algorithms and foundations for data analysis and machine learning.

*3. Multiscale Methods* — Algorithms and foundations for methods spanning multiple time and length scales.

*4. Systems and Decision Sciences* — Algorithms and foundations for engineered systems.

**Computing Systems**
*Explores the impact that fundamental changes in computing technologies and systems will have on the DOE and ORNL mission*

*1. Beyond Moore* — Explores the applicability of novel computing technologies for science.

*2. Architectures and Performance* — Develops tools and methods for evaluating emerging computing architectures.

*3. Intelligent Systems and Facilities* — Addresses the challenges associated with managing computing resources and facilities at scale.

*4. Programming Systems* — Explores programming models, languages, and translation tools.

*5. Software Engineering* — Engineers the next generation of scientific software to ensure quality, including reliability, trustworthiness, and usability.

*6. Application Engineering* — Delivers advanced scientific applications with best-in-class methods, design, and implementation.

**Data and AI Systems**
*Manages and gains knowledge from data*

*1. Visualization* — Develops methods, tools, and technologies for visual data analysis.

*2. Learning Systems* — Creates scalable tools to build models from data.

*3. Workflow Systems* — Develops methods, tools, and technologies for the coordinated management of data movement.

*4. Performance Engineering* — Rebuilds and optimizes data applications and systems, with an emphasis on scalability and advanced platforms to accelerate discovery.

*5. Data Engineering* — Engineers data assets and systems, including data wrangling and system design, to drive scientific innovation.

## National Center for Computational Sciences

The National Center for Computational Sciences Division (NCCS) provides state-of-the-art computational and data science infrastructure for technical and scientific professionals to accelerate scientific discovery and engineering advances across a broad range of disciplines. As an important part of the broader High-Performance Computing (HPC) infrastructure, the division also hosts the Oak Ridge Leadership Computing Facility (OLCF), a Department of Energy Office of Science User Facility.

**Systems**
*Administers and supports the division's computing, networking, and storage systems.*

*1. HPC Infrastructure Operations* — Provides continuous monitoring, issue triaging and escalation, and general support of critical computational and facilities-related infrastructure.

*2. HPC Computing* — Administers and supports system installation, deployment, acceptance, performance testing, upgrades, problem diagnosis, and troubleshooting.

*3. HPC Storage and Archive* — Administers and supports high-speed parallel file systems and archive capabilities, which support the overall mission of leadership-class and scalable computing programs.

*4. HPC Infrastructure and Networking* — Designs, implements, and operates all networking and system services common to all HPC and storage services in the division.

*5. HPC Clusters* — Administers and supports the division's HPC computing infrastructure, which includes system installation, deployment, acceptance, performance testing, upgrades, problem diagnosis, and troubleshooting.

*6. HPC Cybersecurity and Information Engineering* — Develops tools and administers data management platforms to extract and analyze telemetry, event logs, and system state information to ensure security, operational, and laboratory policy compliance.

**Operations**

*Provides support to the division's infrastructure users and acquaints the public with the work conducted at the OLCF.*

1. *User Assistance - Production Systems* — Provides technical support, training, documentation and tools to NCCS users for systems that have entered full user operations.

2. *User Assistance – Pre-Production Systems* — Ensures the functionality, performance, and usability of new NCCS systems through activities such as test development, acceptance, software installation, documentation, and early user support for all NCCS pre-production systems.

3. *Application Development and User Access* — Develops and maintains large software applications and tools used by the staff and users of the division's computational ecosystem. Provides access through these applications to the computational resources inside of the division. Ensures systems are compliant with laboratory and DOE User Facility policies.

4. *Platforms* — Provides platforms as a service to NCCS users and staff so that they can develop, manage, and deliver their own applications that run on NCCS systems.

5. *Outreach and Communications* — Develops and maintains communication materials for use with and by the NCCS sponsors and program managers that showcase NCCS capabilities and user research accomplishments.

**Science Engagement**

*Partners NCCS users with experts in scientific domains and computation to obtain optimal scientific results from the center's computational resources and systems.*

1. *Advanced Computing for Chemistry and Materials* —Partners with HPC and data analytics users in the chemical and materials sciences.

2. *Advanced Computing for Nuclear, Particles, and Astrophysics* — Partners with HPC and data analytics users in nuclear physics, such as nuclear structure and quantum chromodynamics; high energy physics, such as particle physics; and astrophysics, such as stellar evolution and cosmology.

3. *Advanced Computing for Life Sciences and Engineering*— Partners with HPC and data analytics users in climate science, geophysics, biology, biomedical sciences, and engineering.

4. *Algorithms and Performance Analysis* — Partners with HPC and data analytics users on algorithmic and performance improvements and characterizes application performance and application requirements.

**Advanced Technologies**

*Offers scientific, technical, operational, and thought leadership by developing, hardening, and deploying solutions for compute and data intensive computing environments.*

1. *AI Analytics Scalable Methods* — Develops and deploys emerging large-scale data science and AI methods for scientific user programs and enables innovation through operational data analytics.

2. *Data Lifecycle and Scalable Workflows* — Enables data stewardship and enriched scalable data access capabilities. Develops end-to-end scientific workflow technologies to user programs.

3. *Technology Integration* — Identifies technical gaps in the computing and data sciences ecosystems and evaluates, develops, and deploys systems and solutions to enable scientific discovery.