

# The Scientific Computing Group

Tammy Welcome, Group Leader

## Mission

The Scientific Computing Group will facilitate development of scientific applications than run on NERSC capability platforms and promote optimal use of NERSC resources.

## Responsibilities

- Collaborate with strategic users to port and develop scientific applications
- Evaluate, integrate, and create new hardware and software technologies
- Evaluate, integrate, and create new new numerical and non-numerical algorithms
- Aid in procurement of new capability systems
- Serve as internal NERSC quality control and user advocate
- Bridge gap between new technology and research scientists
- Bridge gap between research scientists and staff

## Early tasks focus on preparing facility, staff, and users for T3E

### Now - T3E Delivery:

- Learn T3E architecture and performance
- Educate NERSC users and staff; prepare users (User Services)
- Plan for T3E arrival (Large Systems)
- Evaluate ERCAP proposals for MPP allocations (ERSUG)
- Develop "terms of engagement" for collaborations
- Arrange early access for staff and users (CRI, other Vendors)
- Staff to 3+ group leader

## Later, focus on demonstrating viability of T3E to meet needs of ER researchers

### T3E Delivery - Optional Upgrade:

- Collaborate with small number of strategic projects (Scientific Visualization/User Services)
- General development and porting support (User Services)
- ensure CRI meets production status requirements for optional upgrade
- Educate NERSC users (User Services)
- Contingency planning/follow on procurement planning
- Staff to 10+ group leader

## Future tasks are more pathfinding in nature

### Optional Upgrade -- ?

- Development of advanced capability applications that stress systems
  - Hardware
  - Software
  - Numerical Algorithms
- Integration of research into production environment
- Identify areas for research in response to unmet user needs
- Set direction for high-end computing

## NPAPs (NERSC Parallel Algorithm Prototypes) will aid users in developing parallel applications

- Repository of parallel algorithm prototypes
  - computational techniques

- tradeoffs
- performance
- program development tools
- Range from kernels to state-of-the-art computational techniques used as building blocks

**NPAPs will enable NERSC to impact a larger number of users than a one-on-one approach**

- Ease burden of getting started on parallel systems
- Reduce lag time between development of new algorithms and introduction into applications
- use to develop parallel applications and save in program development costs

**Group composed of 10 scientists with broad-base knowledge of scientific computing on capability platforms**

- **Discipline-specific knowledge** (Office of Fusion Energy, High Energy and Nuclear Physics, Basic Energy Sciences, Health & Environmental Research, Computational & Technology Research)
- **Computational Science knowledge** (ODEs, PDEs, linear and non-linear solvers, image processing, particle methods, etc.)
- **Parallel Computing** (architecture, software systems, performance, etc.)
- **Computer Science** (scientific databases, object-oriented design and development, distributed computing, etc.)

**Members of the Scientific Computing Group**

Tammy Welcome, Group Leader

Sisira Weeratunga

Adrian Wong

Sherry Li

Youngbae Kim

Chris Ding

Osni Marques

Andrew Canning

+ 2 openings