Argonne National Laboratory

Marc Snir

Department of Energy

- 3 weapon labs, managed by NNSA: LLNL, LANL, SNL

- 18 science labs, managed by the Office of Science

- Perform open, non classified research and have international collaborations

- 3 major CS and applied math divisions: ANL, LBNL, ORNL

Direct descendent of Enrico Fermi's Metallurgical Laboratory

- Opened in Feb 1943 (as new site for Chicago's Metallurgical Laboratory)
- Became Argonne National Laboratory in July 1946 (first national laboratory)

Argonne provides a vital ecosystems for major DOE scientific user facilities

APS

Protein facility

Nanoscience

Chemical engineering

Chemistry

Accelerator physics

Materials and energy sciences

Biology

High performance computing & data

Argonne provides a vital ecosystems for major DOE scientific user facilities

Employees

FTEs	3,375
Joint Faculty	149
Postdocs	273
Grad/Undergrad	874
Annual Facility	4,289
Visiting Scientists	477

FY11 Budget: $680M

Computing at ANL

60 Years of Computing at ANL

1953 – AVIDAC

1957 – Applied Mathematics Division spun off
  Numerical algorithms, math SW (…PACK)

1982 – Mathematics and Computer Science Division
(same year as first CS department in the US) ~25 staff
  Theorem proving, source-to-source, viz

1984 – Advanced Computing Research Facility
  CM-2, DAP-510, BBN TC-2000, Intel iPSC/d5,
Sequent Balance 21000, Encore Multimax, Alliant FX/
8, Ardent Titan

1992 – High-Performance Computing Research Center
  IBM SP1

2005 – Argonne Leadership Computing Facility spun
off

Math libraries (Lapack, PETSc, Nek5000, TAO),
Meshing (MOAB) , Parallel software (MPICH, PVFS),
Grid (Globus), Cloud (Nimbus)

Production Systems at ALCF

Mira – *BG/Q system*
- 49,152 nodes / 786,432 cores
- 786 TB of memory
- Peak flop rate: 10 PF

Vesta - *BG/Q system*
- 4,096 nodes / 65,536 cores
- 64 TB of memory
- Peak flop rate: 832 TF

Cetus - *BG/Q system*
- 2,048 nodes / 32,768 cores
- 32 TB of memory
- Peak flop rate: 416 TF

Tukey – *NVIDIA system*
- 100 nodes / 1600 x86 cores
- 200 M2070 GPUs
- 6 TB x86 memory / 1.1TB GPU memory
- Peak flop rate: 220 TF

Storage - Scratch: 28.8 PB raw capacity, 240 GB/s bw (GPFS); Home: 1.8 PB raw capacity
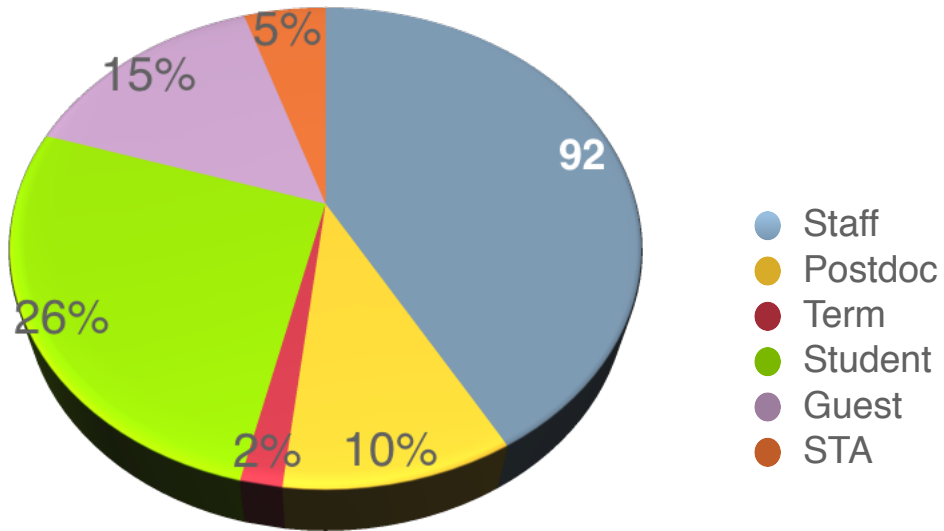
MCS

MCS in Numbers

People

Total: 209 (118 long term)

Legend:
- Staff
- Postdoc
- Term
- Student
- Guest
- STA

Pie chart values: 92, 10%, 2%, 26%, 15%, 5%

MCS Division Areas

Extreme Computing

Pete Beckman

Data

Rob Ross

Applied Math

Paul Hovland

Applications

Ray Bair

People (4/2013)

- EC
- DATA
- APP MA
- APPS
- Support

16 | 20% | 36% | 16% | 16%
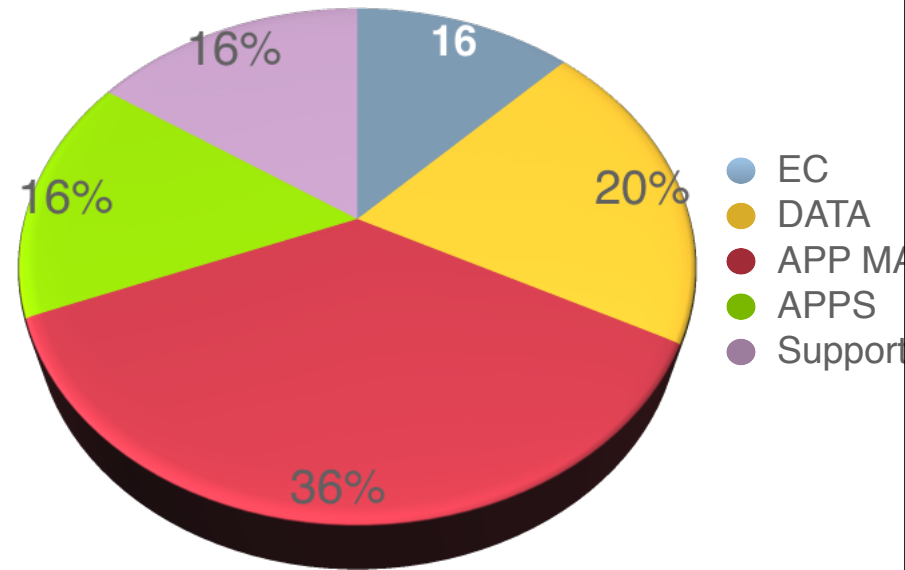
Money (SC, FY 2012)

Research Topics

Applied Math	Extreme Computing	Data	Applications
Paul Hovland	Pete Beckman	Rob Ross	Ray Bair
Optimization Mihai Anitescu / Sven Leyffer	Operating Systems Pete Beckman	Storage Systems Rob Ross	Molecular Science Ray Bair
Numerical PDEs Barry Smith	Programming Models Pavan Balaji	Collaboration Systems Ian Foster	Climate Modeling Rob Jacob
Comp Fluid Dynamics Paul Fischer	Runtime Systems Rajeev Thakur	Visualization Mark Hereld	Reactor Simulation Andrew Siegel
Meshes Tim Tautges	Performance Modeling Boyana Norris	Data Analysis Stefan Wild	Bioinformatics Folker Meyer
	Resilience Franck Cappello		Cosmology Salman Habib

Software Releases (2010-2012) [a]

1. **ADLB** –Asynchronous Dynamic Load Balancing MPI-Library (used by GFMC)
2. **ADIC2** – Tool for the automatic differentiation of programs written in ANSI C. (>1000 users)
3. **CGMA –** The Common Geometry Module, Argonne provides geometry functionality for mesh generation and other applications.
4. **CIFTS –** CIFTS provides coordinated and improved fault tolerance for high-performance computing systems.
5. **C-MPI –** Content-MPI is an implementation of a distributed hash table
6. **Darshan** – a scalable HPC I/O characterization tool.
7. **DCMP –** The Data Domain to Model Domain Conversion Package addresses evaluation of high-end climate models.
8. **ExM –** ExM provides support for extreme-scale, many-task applications.
9. **Falkon –** Fast and lightweight task execution framework.
10. **Globus Toolkit** 5 –: security, communication, information infrastructure, fault detection, resource management, portability, and data management for the grid (> 15M transfers per day,1 PB/day; 6000 registered users)
11. **IOFSL –** I/O forwarding scalability layer.
12. **MINOTAUR** – Open-source toolkit for solving mixed-integer nonlinear optimization problems.
13. **MPICH2 (soon MPICH3)** (>1500 downloads a month, deployed on all top supercomputers)

Software Releases (2010-2012) [b]

14. **MOAB –** Component for representing and evaluating mesh data.
15. **Model Coupling Toolkit** – Coupler technology in the Community Earth System Model.
16. **NekCEM** –electromagnetic solver that uses the spectral-element discontinuous Galerkin method on a conformal spectral-element mesh.
17. **NekLBM** – NekLBM is a spectral-element discontinuous Galerkin lattice Boltzmann fluid solver.
18. **Nek5000** – Nek5000 simulates unsteady incompressible fluid flow with thermal and passive scalar transport.
19. **NEOS** – Network-enabled problem-solving environment for a wide class of applications in business, science, and engineering.
20. **Nimbus** – Integrated set of tools for scientific computing on clouds. (> 50,000 downloads/year, 200 subscribers to support list)
21. **OpenAD** – Tool for automatic differentiation (AD) of numerical computer programs.
22. **OpenAD/F** –Tool for automatic differentiation of Fortran codes.
23. **OpenAnalysis** – The OpenAnalysis toolkit seeks to separate analysis from the intermediate representation in a way that allows the orthogonal development of compiler infrastructures and program analysis.
24. **OSPRI** – OSPRI is an optimized one-sided communication runtime for leadership-class machines.

Software Releases (2010-2012) [c]

25. **Parallel netCDF** – Library providing high-performance I/O while still maintaining file-format compatibility with Unidata's NetCDF.
26. **PETSc** – The Portable, Extensible Toolkit for Scientific computation is a suite of uni- and parallel-processor codes for solving large-scale problems modeled by partial differential equations. (>50,000 downloads a year)
27. **PMI --** Scalable process-management interface for extreme-scale systems.
28. **PVFS** – The Parallel Virtual File System (PVFS) project brings state-of-the-art parallel I/O concepts to production parallel systems.
29. **RGG** – Reactor Geometry (and mesh) Generator is an open source tool to generate several types nuclear reactor assembly/core geometry and mesh.
30. **ROMIO** – ROMIO is a high-performance, portable implementation of MPI-IO.
31. **SISIPHUS** – SISPHUS is a model and software infrastructure for climate simulations related to the dynamics of ice sheets.
32. **Swift** – Swift is a parallel scripting language that runs on multicores, clusters, clouds, and supercomputers.
33. **TACO** – The Toolkit for AMPL Control Optimization provides a set of extensions to the AMPL modeling language to conveniently model mixed integer optimal control problems for ODE or DAE dynamic processes.
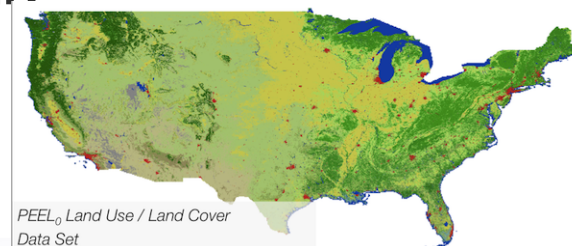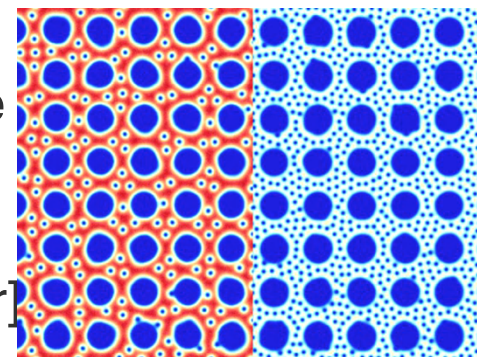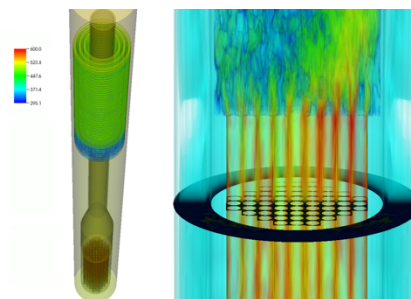
Software Releases (2010-2012) [d]

34. **TAO** – The Toolkit for Advanced Optimization focuses on the design and implementation of component-based optimization software for the solution of large-scale optimization applications. (> 1000 users)

35. **TUNE** – TUNE provides technology for compiler-directed automatic performance tuning, currently targeted at the Cray XT3 system.

36. **UNIC** – UNIC is an unstructured, deterministic neutron transport code that allows a highly detailed description of a nuclear reactor core in our numerical simulations.

Recent Large Projects

- **CESAR** – Center for Exascale Simulation of Advanced Reactors [co-design center, Andrew Siegel, director]
- **M²ACS** -- Multifaceted Mathematics for Complex Energy Systems [ASCR, Mihai Anitescu, director]
- **ARGO*** -- Exascale OS/R [ASCR, Pete Beckman, director]
- **Computation-Driven Discovery for the Dark Universe** – [SciDAC-3, Salman Habib]
- **SDAV -** Scalable Data Management, Analysis, and Visualization Institute [ASCR, Rob Ross, deputy director]
- **RDCEP** -- Center for Robust Decision Making on Climate and Energy [NSF, University of Chicago, Ian Foster, PI]
- Pariticipation in SciDAC Institutes: **FASTMath, SUPER**
- Participation in SciDAC partneships: **OSCon, PSI, NUCLEI**

PEEL$_0$ Land Use / Land Cover Data Set

The Push-Pull Model

- Slow-down of Moore's Law
- New IC technologies
- Massive data (sensors, computers)

- New software stack for future systems
  - From system software to numerical algorithms
- New tools and methods for scientific data management & analysis New coupling methods (CS & applied math support for --)
- New approaches to the development of math software
  - Leverage its mathematical structure
- Integrated solutions
-

Collaborate

- Integration of simulation & analysis
- Study of complex systems (using complex systems)
- Design & decision support

Collaborate with industry

Collaborate with domain scientists