U.S. DEPARTMENT OF ENERGY | Office of Science

Overview of Research Division: Advanced Scientific Computing Research (ASCR)

ASCR Extreme Heterogeneity Workshop

January 23, 2018

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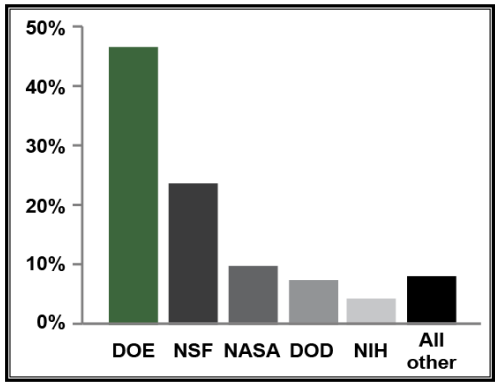
Office of Science
By the numbers

Shown is a portion of SLAC's two-mile-long linear accelerator (or linac), which provides the electron beam for the new Linac Coherent Light Source (~~LCLS~~) – the world's first hard x-ray, free-electron laser. For nearly 50 years, SLAC's linac had produced high-energy electrons for physics experiments. Now researchers use the very intense X-ray pulses (more than a billion times brighter than the most powerful existing sources) much like a high-speed camera to take stop-motion pictures of atoms and molecules in motion, examining fundamental processes on femtosecond timescales.

SC delivers scientific discoveries and tools to transform our understanding of nature and advance the energy, economic, and national security of the U.S.

Research

- Provides about half of the U.S. Federal support for basic research in the physical sciences;
- Supports about 19,000 Ph.D. scientists, graduate students, engineers, and support staff at over 300 institutions and 10 DOE national laboratories;
- Maintains U.S. and world leadership in high-performance computing and computational sciences;
- Continues to be the major U.S. supporter of physics, chemistry, materials sciences, and biology for discovery and for energy sciences.



Support for basic research in the physical sciences by agency.

Source: *NSF Science and Engineering Indicators 2012*

Scientific User Facilities

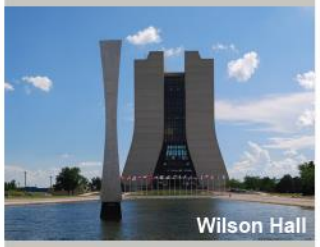
- SC maintains the world's largest collection of scientific user facilities (aka research infrastructure) operated by a single organization in the world, used by more than 27,000 researchers each year.

The DOE Office of Science Laboratories

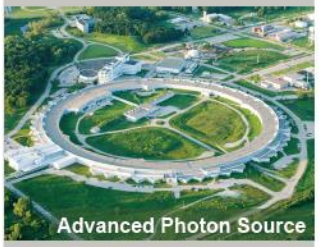
Berkeley, California
202 acres and 97 buildings
3,396 FTEs
950 students & postdocs
9,320 facility users
www.lbl.gov

Richland, Washington
346 acres and 19 buildings
4,344 FTEs
550 students & postdocs
1,733 facility users
www.pnnl.gov

Ames, Iowa
8 acres and 12 buildings
308 FTEs
158 students & postdocs
www.ameslab.gov



Batavia, Illinois
6,800 acres and 354 buildings
1,720 FTEs
55 students & postdocs
2,097 facility users
www.fnal.gov



Argonne, Illinois
1,517 acres and 100 buildings
3,460 FTEs
1,054 students & postdocs
6,547 facility users
www.anl.gov

Menlo Park, California
426 acres and 151 buildings
1,596 FTEs
213 students & postdocs
4,474 facility users
www.slac.stanford.edu

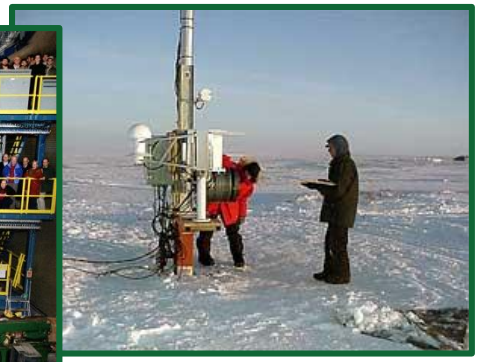
Oak Ridge, Tennessee
4,421 acres and 194 buildings
4,586 FTEs
1,080 students & postdocs
3,215 facility users
www.ornl.gov

Newport News, Virginia
169 acres and 72 buildings
729 FTEs
60 students & postdocs
1,261 facility users
www.jlab.org

Princeton, New Jersey
89 acres and 34 buildings
429 FTEs
54 students & postdocs
290 facility users
www.pppl.gov

Upton, New York
5,322 acres and 310 buildings
2,882 FTEs
642 students & postdocs
4,134 facility users
www.bnl.gov

Office of Science: User Facilities portfolio



- **supercomputers,**
- **high intensity x-ray, neutron, and electron sources,**
- **nanoscience facilities,**
- **genomic sequencing facilities,**
- **particle accelerators,**
- **fusion/plasma physics facilities, and**
- **atmospheric monitoring capabilities.**

- **Open access; allocation determined through peer review of proposals**

- **Free for non-proprietary work published in the open literature**

- Full cost recovery for proprietary work

Office of Science: Research portfolio

Advanced Scientific Computing Research	• **Delivering world leading computational and networking capabilities to extend the frontiers of science and technology**
Basic Energy Sciences	• **Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels**
Biological and Environmental Research	• **Understanding complex biological, climatic, and environmental systems**
Fusion Energy Sciences	• **Building the scientific foundations for a fusion energy source**
High Energy Physics	• **Understanding how the universe works at its most fundamental level**
Nuclear Physics	• **Discovering, exploring, and understanding all forms of nuclear matter**

ASCR Research Programs

Mission

Advance applied mathematics and computer science; deliver, in partnership with disciplinary science, the most advanced computational scientific applications; advance computing and networking capabilities; and develop, in partnership with U.S. industry, future generations of computing hardware and tools for science.

A particular challenge of this program is fulfilling the science potential of emerging computing systems and other novel computing architectures, which will require numerous and significant modifications to today's tools and techniques to deliver on the promise of exascale science.

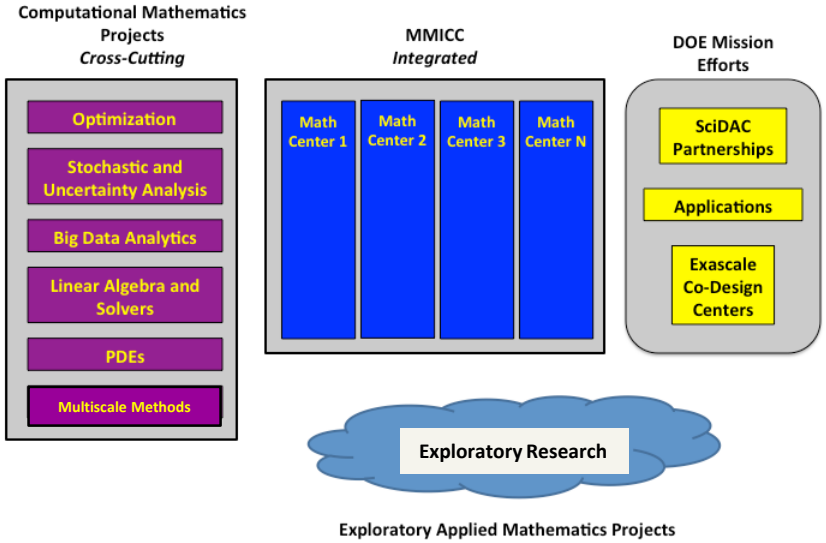
- Applied Mathematics - basic research and development of applied mathematical models, methods, and algorithms for understanding complex natural and engineered systems related to DOE's mission.
- Computer Science - basic research in utilization of computing at extreme scales; understanding extreme scale data from both simulations and experiments
- Computational Partnerships -
  - SciDAC Institutes - methods, algorithms, libraries & methodologies for achieving portability and interoperability of complex scientific software packages; software tools and support for application performance; tools for data analytics & visualization spanning the full range of SciDAC applications
  - SciDAC Partnerships - enable computational scientists to effectively and confidently utilize multi-petaflop computing systems to advance science.

ASCR Applied Mathematics: Program Components and Synergies

Basic research and development of applied mathematics models, methods and algorithms for understanding complex natural, physical and engineered systems relevant to the DOE mission.

Long-term goals:

- Mathematics research that 5-10+ years out will impact DOE mission efforts such as DOE Applications and Pipeline for SciDAC Program
- New Mathematical Multifaceted Integrated Capability Centers (MMICCs) directly enhances impact of applied math on DOE mission



- Cross-cutting computational mathematics projects: Addresses foundational, algorithmic and extreme-scale mathematical challenges
- Exploratory Research (EXPRESS): New mechanism to bring in highly innovative research

ASCR Applied Mathematics
Base Renewal Projects (1 of 2)

Title	Lead PI	Institution
High-Order Methods for High-Performance Multiphysics Simulations	Paul Fischer	ANL
Efficient Error Estimation & Propagation in Complex ODE/DAE/PDE Simulations	Barry Smith	ANL
Simulation and Analysis of Reacting Flows	John Bell	LBNL
High-Resolution and Adaptive Numerical Algorithms for PDEs	Phil Colella	LBNL
Multilevel Iterative Temporal Integration and Time Parallelism for PDEs	Michael Minion	LBNL
Frontiers in Computation: New Methods for Fluids, Structures and Interfaces, Advanced Materials, and Stochastics	James Sethian	LBNL
High-Resolution Methods for Phase Space Problems in Complex Geometries	Milo Dorr & Phil Colella	LLNL LBNL
New Multigrid Advances for Highly Concurrent Architectures	Rob Falgout	LLNL
Formulation, Analysis and Computation of Heterogeneous Numerical Methods	Pavel Bochev	SNL
Enabling Multiphysics Plasma Simulations by the Development of Stable, Accurate, and Scalable Computational Formulations and Solution Methods	John Shadid & Luis Chacon	SNL LANL

Lab Base Math Portfolio sustains foundational research projects in PDEs, Multiphysics modeling & simulation, Time integration, Multigrid methods, & Computational mathematics.

ASCR Applied Mathematics
Base Renewal Projects (2 of 2)

Title	Lead PI	Institution
Data-Driven Optimization for Complex Dynamical Systems	Mihai Anitescu	ANL
Automatic Differentiation for Extreme-Scale Data Analysis & Machine Learning	Paul Hovland	ANL
Nonlinear Robust Optimization	Sven Leyffer	ANL
Extending PETSc's composable Hierarchically Nested Linear Solvers	Lois McInnes	ANL
Stochastic Hybrid Models and Algorithms for Fluids	John Bell	LBNL
Adaptive Dimension Reduction via Coarsening & Multilevel Solvers	Panayot Vassilevski	LLNL
High-order Unstructured Mesh Optimization for Accurate & Efficient Simulations	Tzanio Kolev	LLNL
Uncertainty Quantification for Complex Systems	Alex Tartakovsky	PNNL
Unstructured Primal-Dual Mesh Improvement & Generation	Scott Mitchell	SNL
Mathematics of Tensor Decompositions and Applications	Tammy Kolda	SNL
Specialized Multigrid Methods for Semi-Structured Finite Element Meshes	Ray Tuminaro	SNL

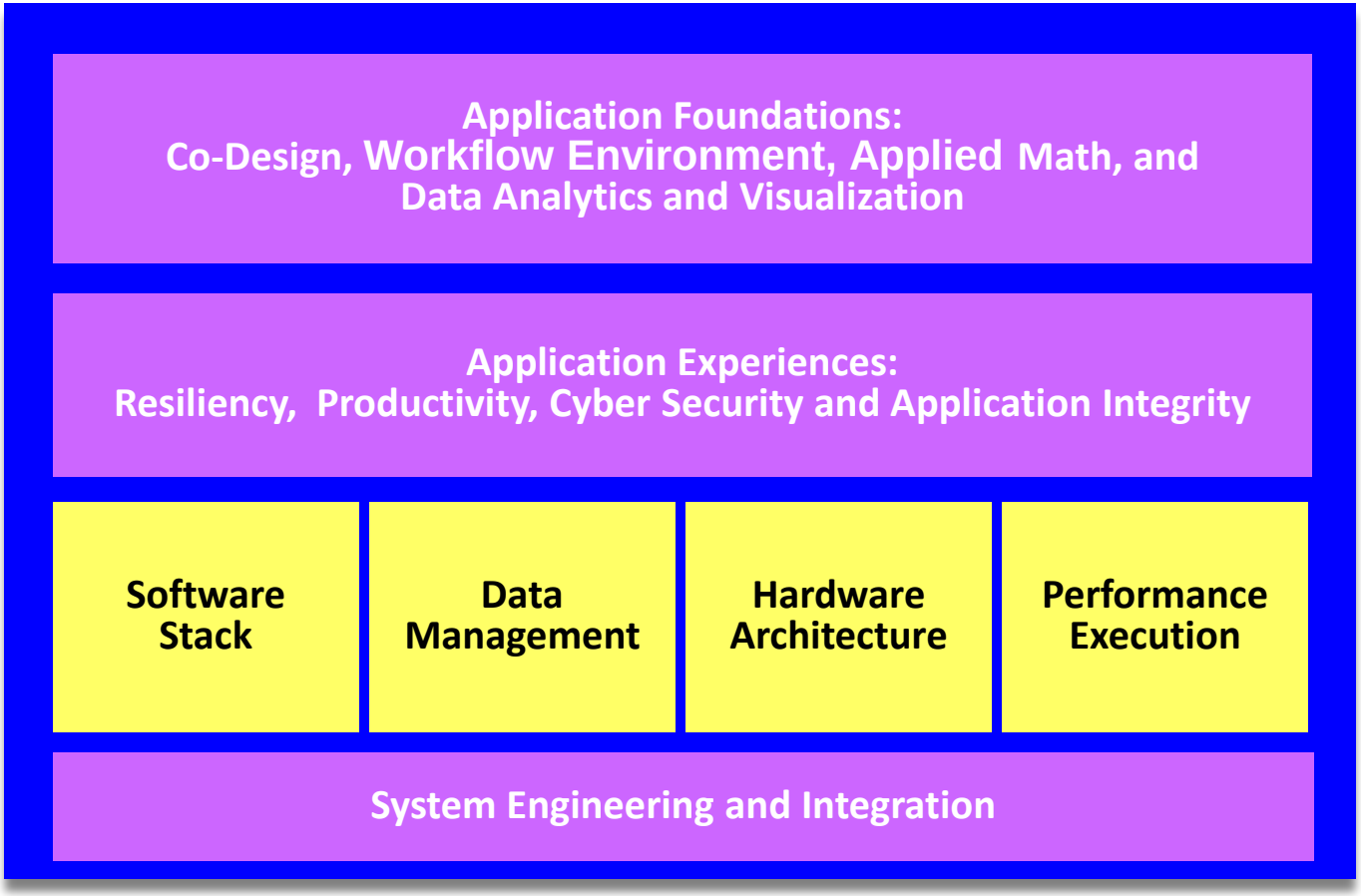
Lab Base Math Portfolio sustains foundational research projects in PDEs, Multiphysics modeling & simulation, Time integration, Multigrid methods, & Computational mathematics.

Mathematical Multifaceted Integrated Capability Centers (MMICCs)

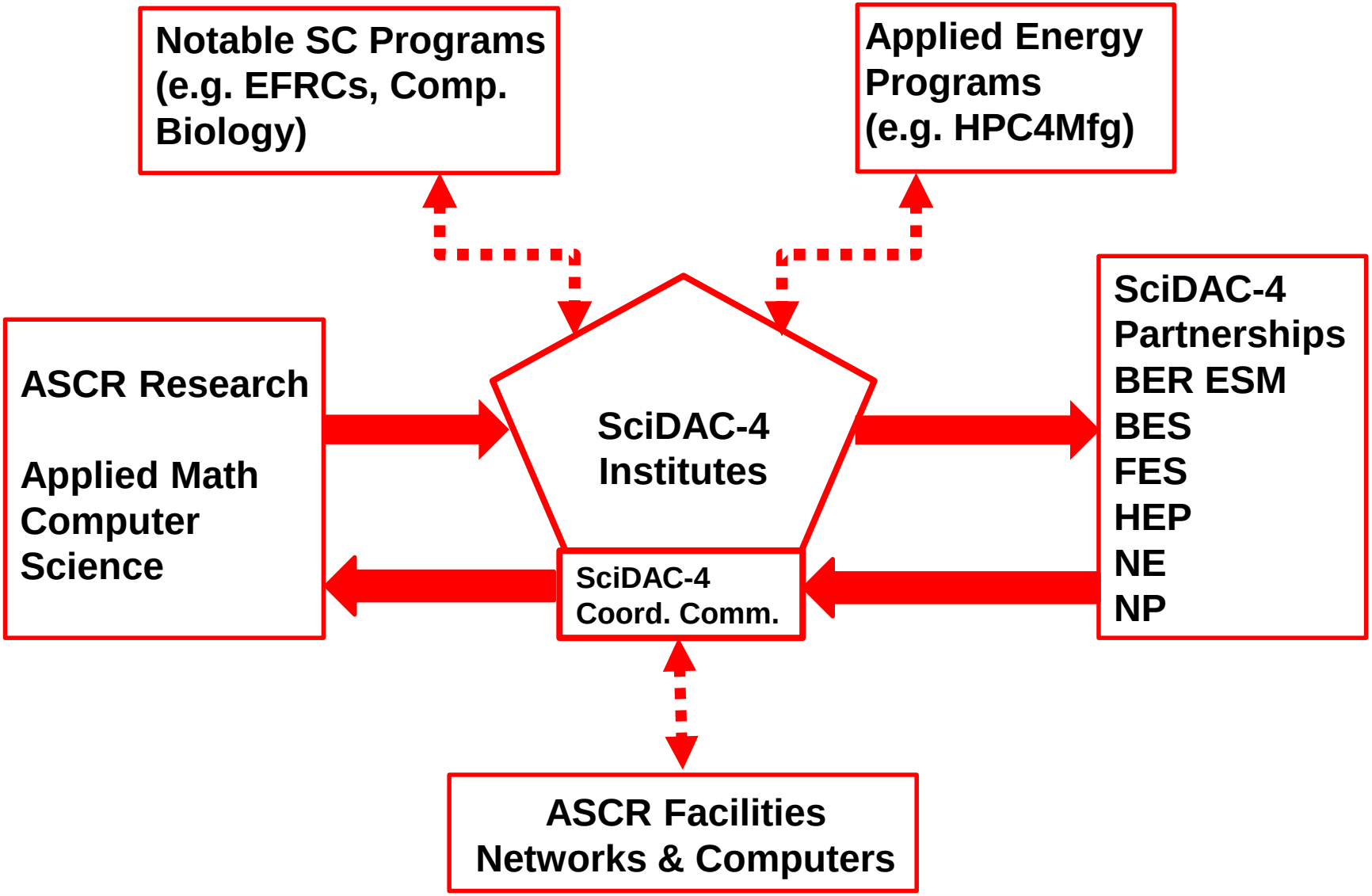
- **Integration of mathematical sub-disciplines:**
  - Allow applied mathematics researchers to take a broader view of the problem as a whole, and devise solution strategies that attack the problem in its entirety by building fundamental, multidisciplinary mathematical capabilities and tools
  - Requires applied mathematics researchers to work together in large, collaborative teams to more effectively address grand challenge problems
- **Careful balance with DOE applications**
  - Motivated by DOE grand challenge problems, but this does not have tight coordination and application-focus of SciDAC Partnership efforts
- **A 5-year research roadmap:**
  - Annual individual research goals and integration goals with metrics of success
- **Annually reviewed by program manager and external review committee:**
  - Evaluate technical progress against 5-year roadmap
  - Evaluate effectiveness of integration toward long-term challenge problems
- **Outreach to research community**
  - Serve as entry points for external researchers to more readily understand the mathematical challenges of DOE-relevant problems.

ASCR Computer Science - Snapshot: Program Components and Synergies

Programmatic structure for the ASCR Computer Science Research & Foundation for Next-Generation



ASCR Scientific Discovery through Advanced Computing: SciDAC-4 Overview



Representative SciDAC-4 Partnership Topics

- **BES:** catalysis, quantum materials
- **BER:** atmosphere dynamics, component-coupling and performance; hi-res. sea ice; ice-land-sea interaction; sensor placement; atmospheric physics convergence
- **FES:** tokamak WDM, energetic particles in burning plasmas, core & edge dynamics, injection & RF coupling, plasma-materials interactions, disruptions
- **HEP:** accelerator physics, cosmology, event analysis & simulation
- **NP:** LQCD, supernovae (II) & mergers, nuclear structure of elements
- **NE:** radiation effects in materials & fuels

- **Equations**
  - –CFD, solid mechanics, gyrokinetic, Newton's, Maxwell's, Schrödinger's, kinetics, QCD, ill-posed inversion
- **Applied Math**
  - –numerical optimization, linear algebra, PDE, ODE, SDE (solvers & theory), MC, FFT/wavelets, UQ, statistics, quadrature
  - –code coupling for multi-scale/-physics
- **Computer Science**
  - –code coupling, memory management, in-situ data movement, auto-tuning, resilience
  - –portability (between LCF swim lanes)

ASCR support for SciDAC-4 Partnerships is widely distributed

Partner	#	ANL	BNL	FNAL	INL	LBNL	LLNL	LANL	ORNL	PNNL	PPPL	SNL	SLAC	TJNAF
BES	3					☒			☒				☒	
BER	6	☒				☒	☒	☒	☒	☒		☒		
FES	7	☒				☒	☒	☒	☒	☒	☒	☒		
HEP	5	☒	☒	☒		☒		☒					☒	
NP	3	☒	☒			☒		☒	☒	☒				☒
NE	1	☒			☒				☒			☒		

- 22 collaborations are Laboratory-led
  - Some Laboratory budgets provide subcontracts for additional Universities and companies
- ASCR supports 62 PIs at 20 institutions (in 25 collaborations)
  - 53 PIs at 13 DOE (SC, NNSA, NE) Laboratories w/ support from ASCR
  - 9 PIs (at UMD, MIT, MSU, RPI, UTn-K, UTx-A & GA) receive direct support from ASCR grants

ASCR SciDAC-4 Institutes

Purpose: To provide intellectual resources in applied mathematics and computer science, expertise in algorithms and methods, and scientific software tools to advance scientific discovery through modeling & simulation in areas of strategic importance to the SC & DOE

Emphasis:

Application-aware: Support SciDAC-4 Partnerships and equipped to interact with other communities (e.g. EFRC's, HPC4Mfg, Computational Biosciences);

Architecture-aware: Existing and emerging DOE HPC systems such as those existing and planned for at OLCF, ALCF and NERSC over the next 3 years. Application-portability and software engineering best practices;

Institutes-aware: Processes for effectively leveraging basic research advances from applied math and computer science & expertise and results from the other Institute.

Management structure: Built-in flexibility, no duplication within the Institute.

Timeline & Proposals: A DOE National Laboratory Announcement was issued in June 2017. 3 proposals were received in July 2017.

2 SciDAC-4 Institutes:

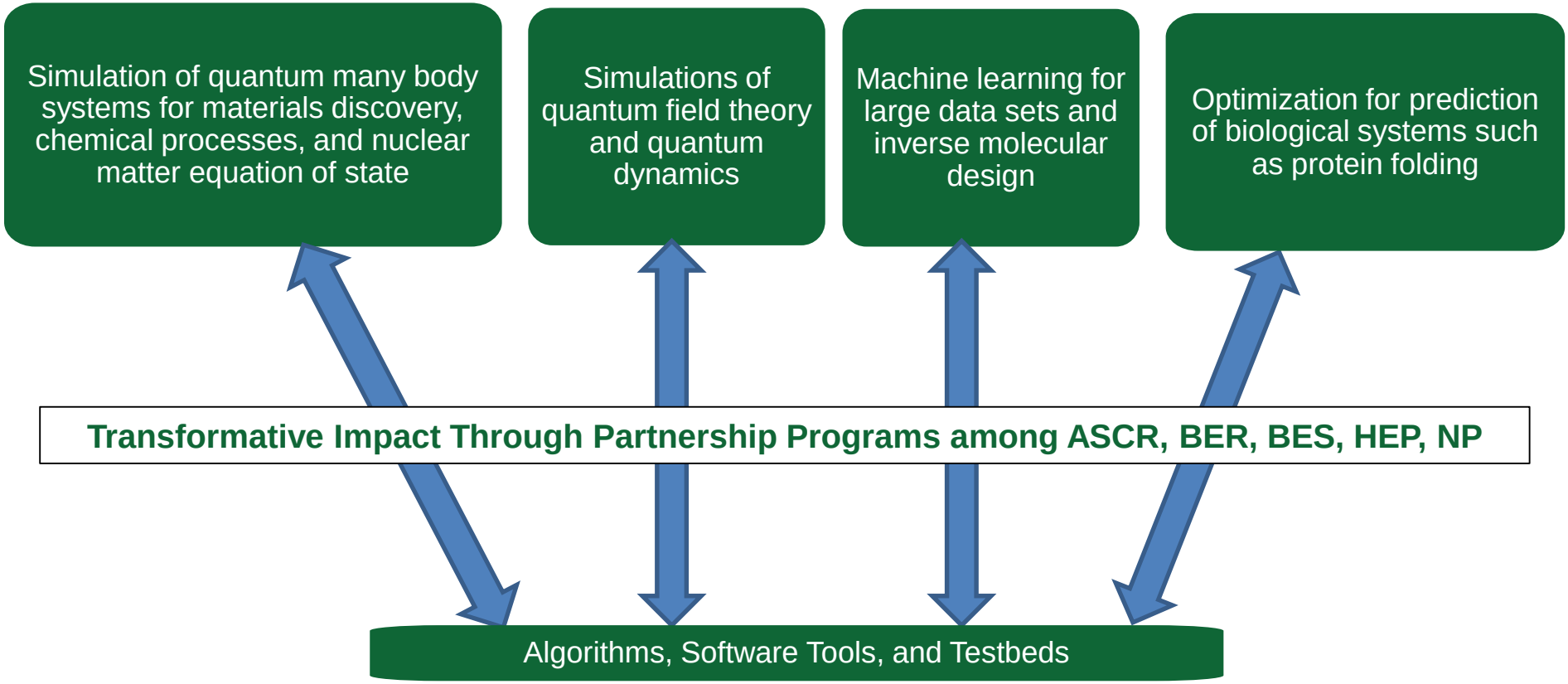
RAPIDS-Resource and Application Productivity through Computation, Information, and Data Science. Director: Rob Ross, ANL, Deputy Director: Lenny Oliker, LBNL;

FASTMath-Frameworks, Algorithms and Scalable Technologies for Mathematics. Director: Lori Diachin, LLNL, Deputy Director: Esmond Ng, LBNL.

Awards to 7 Labs; support to 11 universities and 2 companies through subcontracts.

Quantum Computing Applications for SC Grand Challenges

QIS Task Force identified SC-wide grand challenges that will potentially be transformed by quantum computing applications.



Science Internet of Things (S-IoT)

Purpose: To exploit the next wave of Internet evolution (IoT) to develop advanced capabilities that will define a new paradigm of interactions between scientists and machines in hyper-connected smart environment for science

Technologies Trends
- IoT, SDN, Smart Sensors
- BigData analytics
- Autonomic computing
- Machine Learning

→

Proposed Capabilities
- Self-Management
- IoT Software Stack
- Embedded ML
- IoT security

→

Smart Science Things
- Smart Instruments
- Self-aware Networks
- Intelligent Workflows
- Smart edge computing

→

Smart Superfacility
(Science Internet of Things)

Benefits

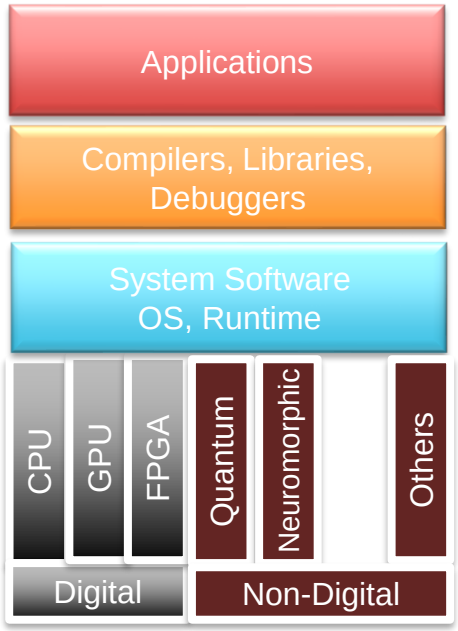
- Improve access and utilization of connected scientific resources
- Reduce scientific resources management and operation complexities
- Simplify complex scientific workflow automation
- Enable machine –to – machine communication

Project Title: **Architecture and Management for Autonomic Science Ecosystems (AMASE).** Lead: ANL (Pete Beckman), Collaborator: LBNL (Alex Sim), Northwestern University (Alok Choudhary)

What does the Future Hold: Strategic Vision for ASCR's Research Program

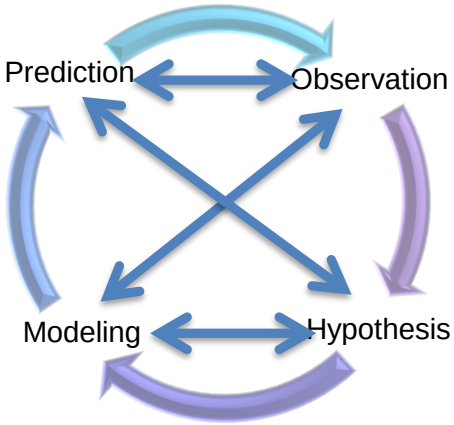
Emerging trends are pointing to a future that is increasingly

1. **Instrumented**: Sensors, satellites, drones, offline repositories
2. **Interconnected**: Internet of Things, composable infrastructure, heterogeneous resources
3. **Automated**: Complexity, real-time, machine learning
4. **Accelerated**: Faster &flexible research pathways for science & research insights



What is the role of ASCR's Research Program in transforming the way we carry out energy & science research?

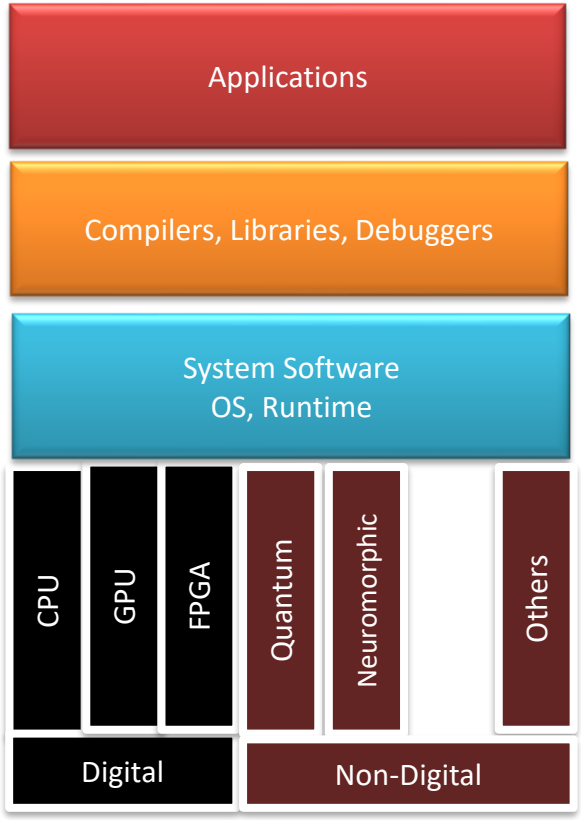
1. **Post-Moore technologies**: Need basic research in new algorithms, software stacks, and programming tools for quantum and neuromorphic systems
2. **Extreme Heterogeneity**: Need new software stacks, programming models to support the heterogeneous systems of the future
3. **Adaptive Machine Learning, Modeling, & Simulation for Complex Systems**: Need algorithms and tools that support automated decision making from intelligent operating systems, in situ workflow management, improved resilience and better computational models.
4. **Uncertainty Quantification:** Need basic research in uncertainty quantification and artificial intelligence to enable statistically and mathematically rigorous foundations for advances in science domain-specific areas.
5. **Data Tsunami:** Need to develop the software and coordinated infrastructure to accelerate scientific discovery by addressing challenges and opportunities associated with research data management, analysis, and reuse.



ASCR Extreme Heterogeneity Workshop

January 23-25, 2018 Virtual Meeting

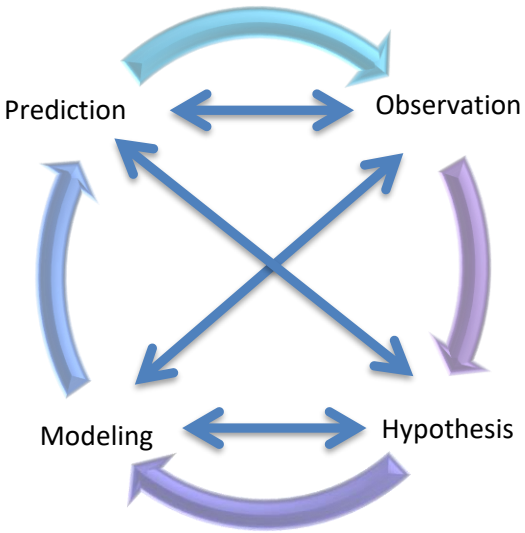
- **POC: Lucy Nowell (Lucy.Nowell@science.doe.gov)**
- **Goal: Identify Priority Research Directions for Computer Science** needed to make future supercomputers *usable, useful and secure* for science applications in the 2025-2035 timeframe
- Primary focus on the software stack and programming models/environments
- 120 expected participants: DOE Labs, academia, & industry
- Observers from DOE and other federal agencies
- Planning: Factual Status Document (FSD) is under development, with outreach planned.
  - White papers to be solicited to contribute to the FSD, identify potential participants, and help refine the agenda
  - Report due early May 2018



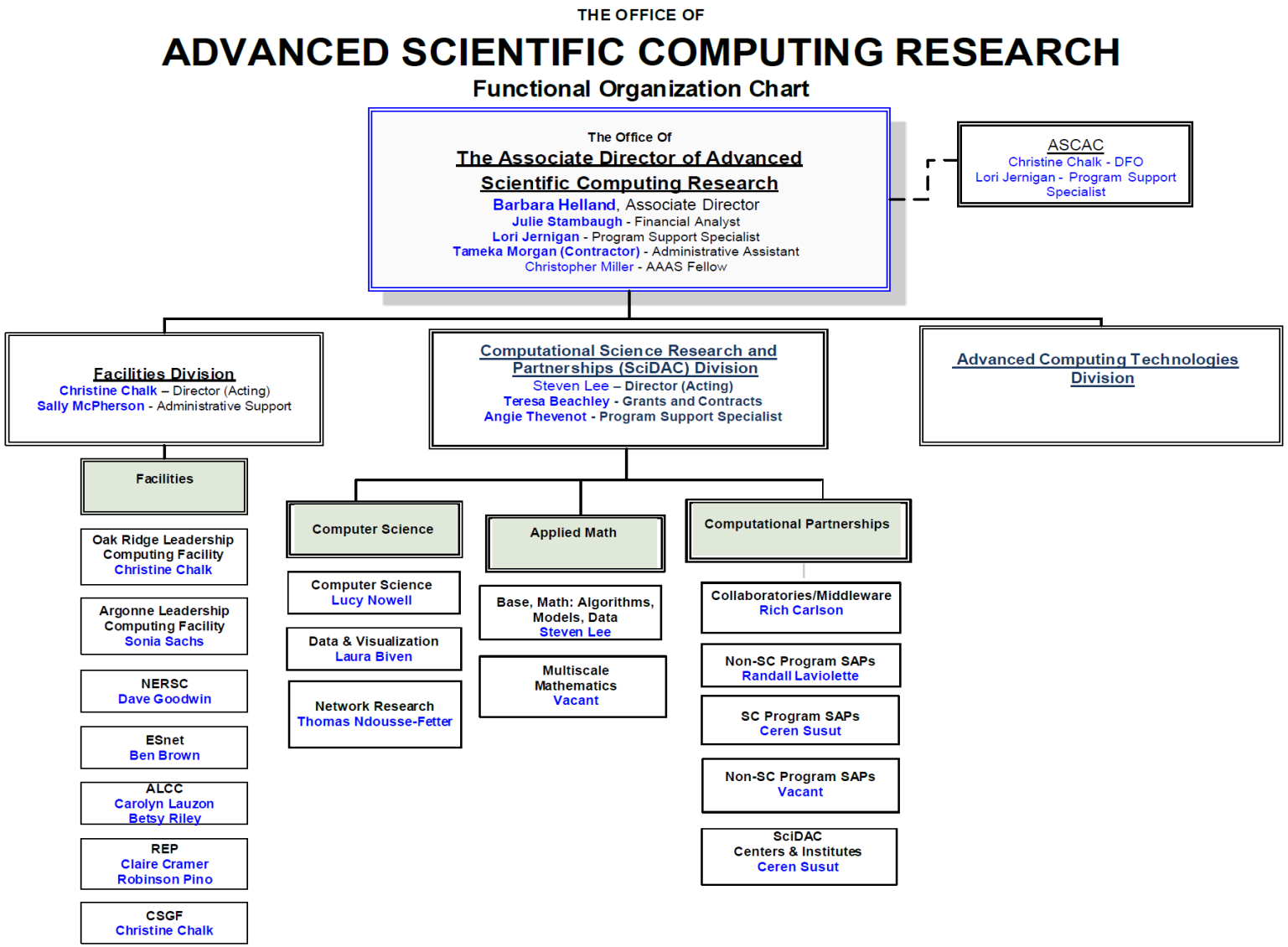
ASCR Scientific Machine Learning Workshop

January 30 – Feb 1, 2018 in DC-area

- **POC**: Steven Lee (Steven.Lee@science.doe.gov)
- **Purpose**: Identify Priority Research Directions and the role of applied mathematics in enabling greater machine learning capabilities for DOE-mission challenges.
- Factual Status Document – Status and recent trends in the underlying mathematical, statistical, and computational foundations of HPC machine learning techniques for scientific data analysis. Identify challenges and opportunities for high-impact through fundamental advances in mathematical modeling and algorithms.
- **Cross-cutting research themes:** optimization, linear algebra, UQ, discrete (tensors, graphs, networks), statistical approaches, ensembles, game theory, validation, scientific method
- **Number of participants:** About 80-100 researchers.
- Call for Position Papers for broad community input (140 received!)
- Observers from DOE and other federal agencies.
- Final Workshop Report due in March-April 2018



Questions?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Lori Jernigan - Program Support Specialist
Tameka Morgan (Contractor) - Administrative Assistant
Christopher Miller - AAAS Fellow
ASCAC
Christine Chalk - DFO
Lori Jernigan - Program Support Specialist
Facilities Division
Christine Chalk – Director (Acting)
Sally McPherson - Administrative Support
Computational Science Research and Partnerships (SciDAC) Division
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Laura Biven
Network Research
Thomas Ndousse-Fetter
Applied Math
Base, Math: Algorithms, Models, Data
Steven Lee
Multiscale Mathematics
Vacant
Computational Partnerships
Collaboratories/Middleware
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