U.S. DEPARTMENT OF ENERGY

DOE Office of Advanced Scientific Computing Research

Presented to the

Advanced Scientific Computing Advisory Committee

by

Barbara Helland
Associate Director

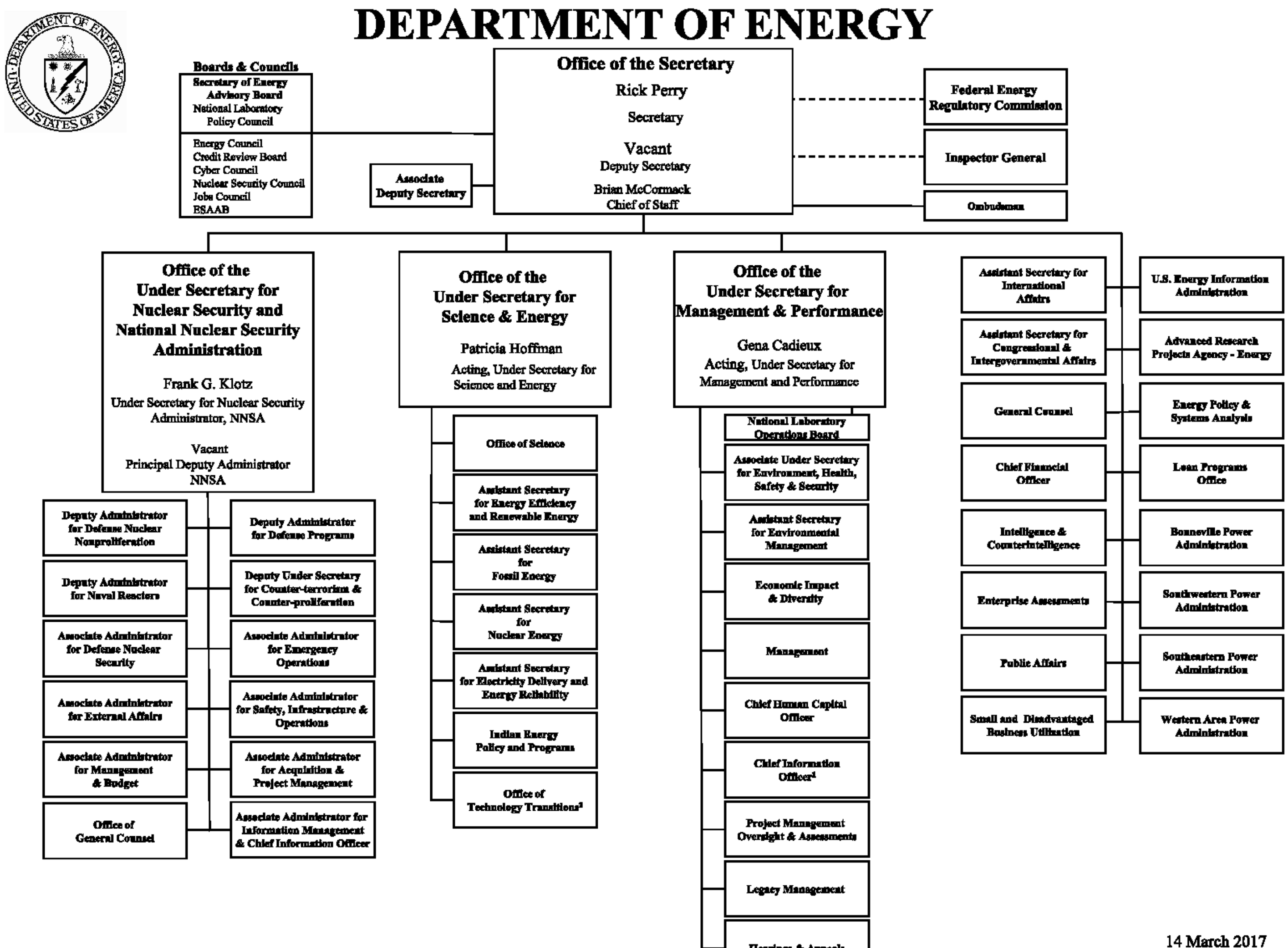
April 18, 2017

Some Agenda Details

- **UPDATE ON THE EXASCALE COMPUTING PROJECT –** *Paul Messina, ECP Director*
- **UPDATE ON CURRENT CHARGES**
  - *Committee of visitors – David Levermore*
  - *LDRD Report – Martin Berzins*
  - *Future Technologies – Vivek Sarkar*
- **ASCR UPDATES**
  - *Math Centers - Abani Patra*
  - *Quantum Workshop – Claire Cramer*
  - *Project Leadership Institute – Ben Brown*
- **UPDATE ON HPC IN ASIA –** *John Shalf, Lawrence Berkeley National Laboratory*
- **CSGF LONGINTUDINAL STUDY –** *John Wells and Tara Dunderdale, Westat*
- **CORI EARLY SCIENCE –** *Jack Deslippe, Lawrence Berkeley National Laboratory*
- **MACHINE LEARNING –** *Shinjae Yoo, Brookhaven National Laboratory*
- **DOWN THE RABBIT HOLE: FROM B3LYP TO X86 –** *Jeff Hammond, DOE CSGF Alumni*
- **SCIDAC – EFRC COLLABORATION –** *Wolfgang Windl, Ohio State University*

Staffing Changes

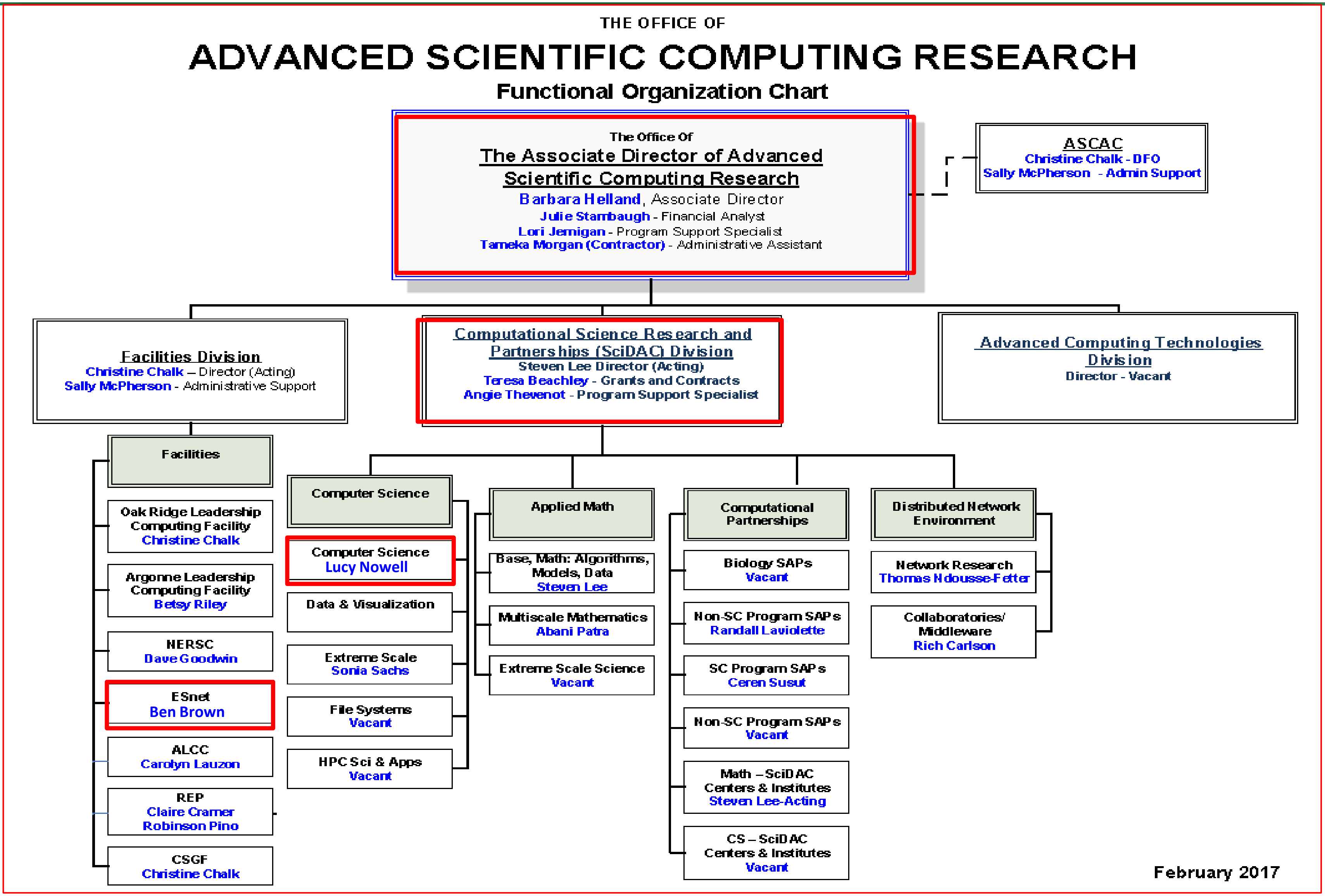
DOE ORG Chart



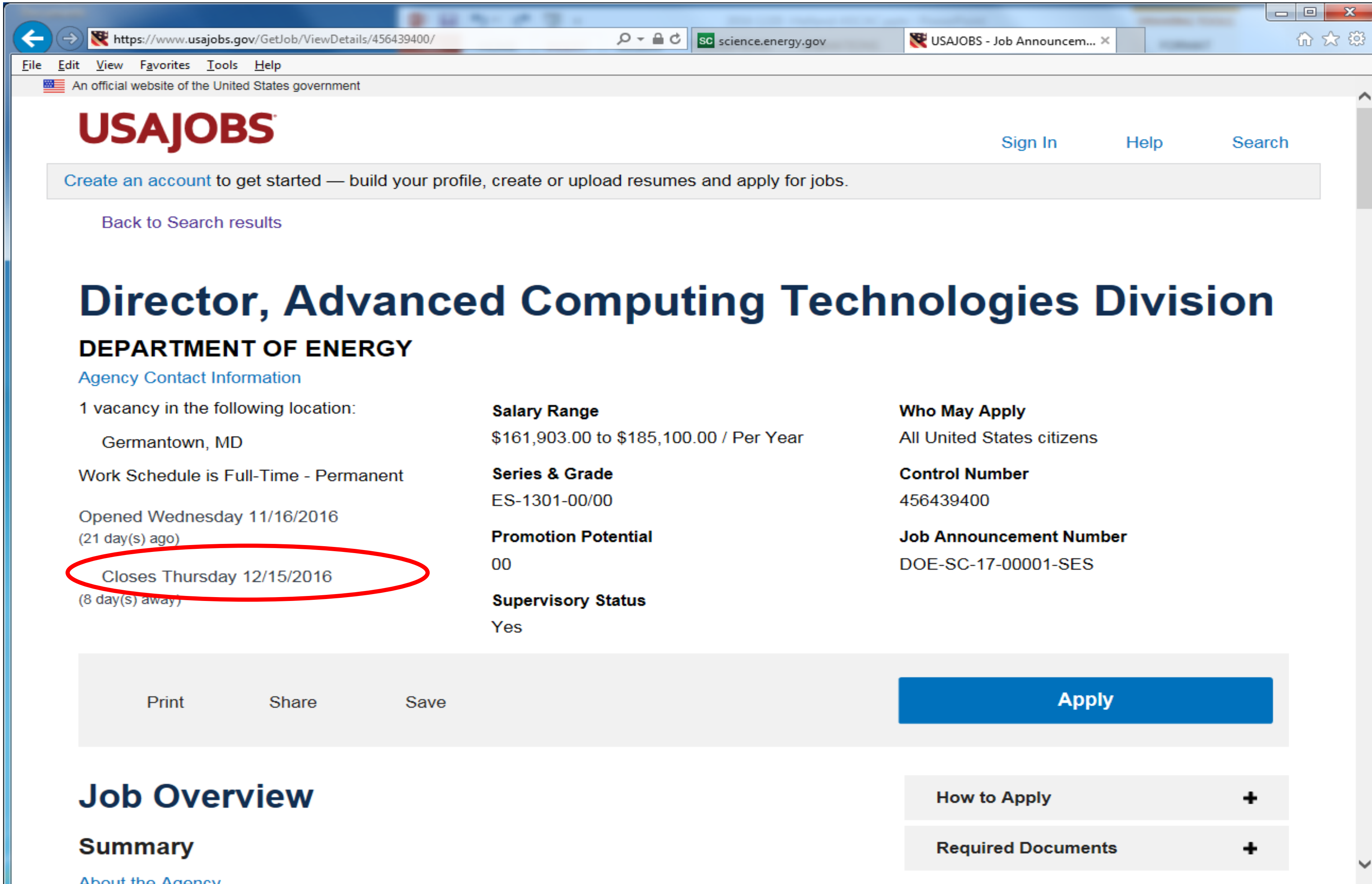
[1] The CIO reports directly to the Secretary for the purposes of carrying out responsibilities under Subchapter 44 U.S.C.§ 3506(a)(2)(A).
[2] The director of the Office of Technology Transitions also serves as DOE's Technology Transfer Coordinator who reports to the Secretary of Energy

SC Transition Leadership

U.S. DEPARTMENT OF ENERGY | Office of Science



Division Director Job Posting



https://www.usajobs.gov/GetJob/ViewDetails/456439400/ | science.energy.gov | USAJOBS - Job Announcem...

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Director, Advanced Computing Technologies Division

DEPARTMENT OF ENERGY

Agency Contact Information

1 vacancy in the following location:

Germantown, MD

Work Schedule is Full-Time - Permanent

Opened Wednesday 11/16/2016
(21 day(s) ago)

Closes Thursday 12/15/2016
(8 day(s) away)

Salary Range
$161,903.00 to $185,100.00 / Per Year

Series & Grade
ES-1301-00/00

Promotion Potential
00

Supervisory Status
Yes

Who May Apply
All United States citizens

Control Number
456439400

Job Announcement Number
DOE-SC-17-00001-SES

Print Share Save Apply

Job Overview

How to Apply +

Required Documents +

Summary

About the Agency

ENERGY

Research Updates

SciDAC-4 Partnerships Status (April 2017)

Partner	Collaborations (proposals)	Closed (open)	Panel Review	Reviewers (reviews)	Requested ($=$1000)	Max. Available* ($=$1000)
NP Barnes	7 (51)	24 Feb. (10 Nov.)	3 April	12 (24)	$53,612	$25,000
HEP[1] Chatterjee	14 (14)	27 Feb. (4 Nov.)	7 April	32 (73)	$75,042	$25,000
FES Mandrekas	17 (96)	21 Feb. (16 Nov.)	*19-21 April*	47 (126)	$201,596	$90,000
BER[2] Koch	30 (98)	15 Mar. (4 Nov.)	*3-4 May*	49 (170)	$120,695	$50,800
NE[3] Funk	5 (12)	5 April (16 Dec.)	*mail-in only*	TBD	$28,492	$7,500
TOTAL	73 (271)				$479,437	$198,300

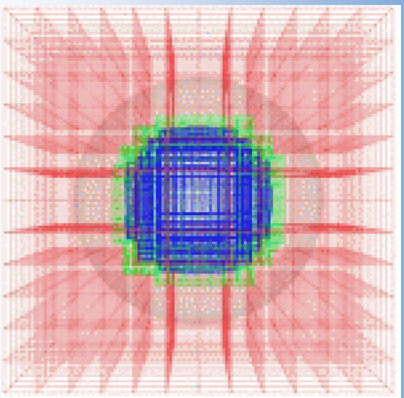
[1]Lab-led multi-institution consortia [2]Combines two solicitations: 5y & 2.5y
[3]Office of Accelerated Innovation in Nuclear Energy, Office of Nuclear Energy

*as stated in solicitations, subject to Budget & Appropriations

Scalable Structured Adaptive Mesh

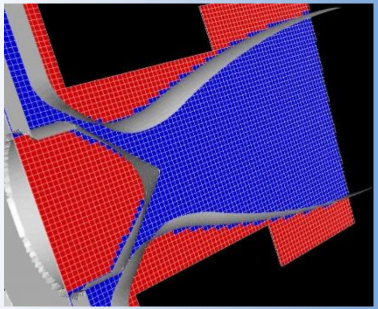
ASCR Base Math

- Efficient algorithms on adaptive hierarchies
- Higher order methods
- Design of new efficient solvers
- High-arithmetic intensity methods

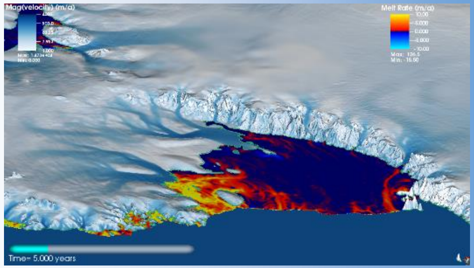


1990s to present

SciDAC Development: APDEC & FASTMath

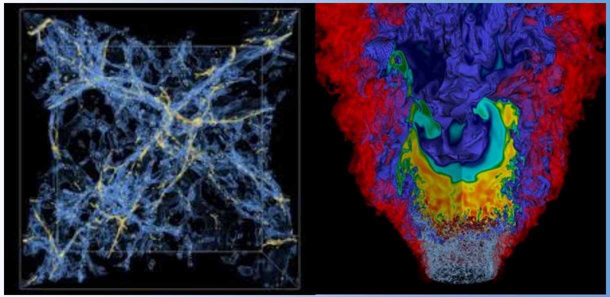


- Complex geometries
- Particles
- Efficient, scalable solvers
- Productive, widely-used software frameworks



2000’s to present

Outcome & Impact



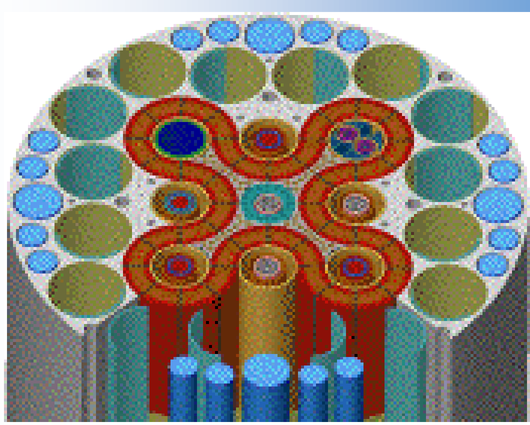
- Widely used in SciDAC applications
  - BISICLES for ice sheets
  - Nyx for cosmology
  - COGENT for fusion
  - ChomboCrunch for subsurface
- ECP: Applications, Co-Design
- HPC4MFG

Contacts: Ann Almgren ASAlmgren@lbl.gov
Dan Martin DFMartin@lbl.gov

Scalable Unstructured Adaptive Meshes

NSF, DoD and DOE

- Fully automatic unstructured automatic mesh generation and adaptation for general geometries
- Started in the 1980's
- High order meshes and methods
- Easily applied to complex geometries of interest in science research and for industrial applications



SciDAC Development

Parallel Unstructured Mesh Infrastructure

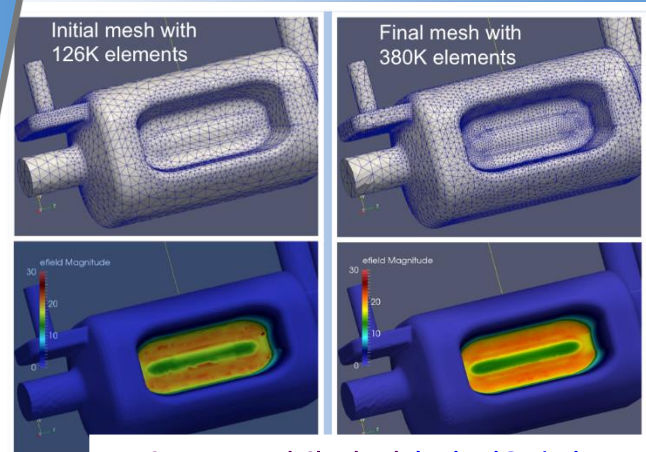
- Fully parallel curved mesh adaptation
- >92 elements on ¾M cores w/ strong scaling
- Many core and GPU versions developed
- Extension to mesh/PIC started
- Full simulation workflow

Parallel Unstructured Mesh Infrastructure

- Domain Topology
- Mesh Topology/Shape
- Partition Control
- Dynamic Load Balancing
- Mesh Adaptation
- Simulation Fields

Outcome & Impact

- Mesh infrastructure used in several fusion and accelerator SciDAC apps
- Adaptive mesh refinement methods used in ice sheets, nuclear & solid mechanics applications
- Scales to full DOE systems
- ~10 Phase II SBIR/STTR grants
- IBM, Boeing, Corning, etc.



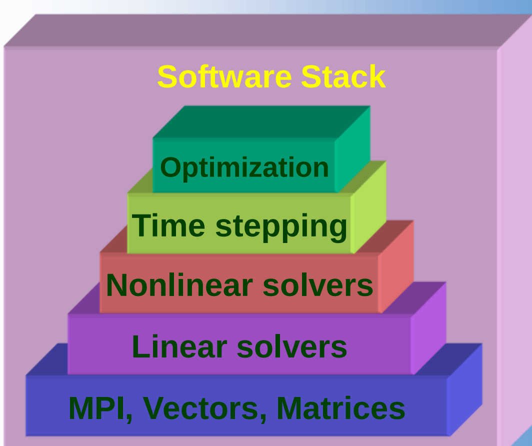
Contacts: Mark Shephard shephard@rpi.edu

PETSc: Integrators & Solvers for Scalable Simulations

ASCR Base Math

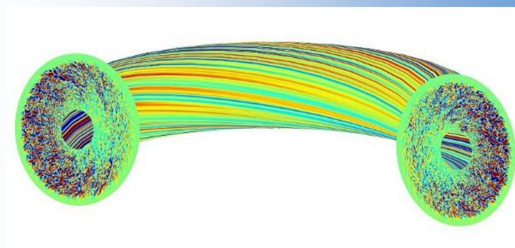
PETSc: Scalable, composable hierarchical algebraic solvers and integrators for PDE-based simulations.

- Begun 1994: research on advanced algorithms
- Provides numerical infrastructure needed by many physical simulations



Contacts: Lois Curfman McInnes curfman@mcs.anl.gov, Barry Smith bsmith@mcs.anl.gov

SciDAC Development



2000's to present

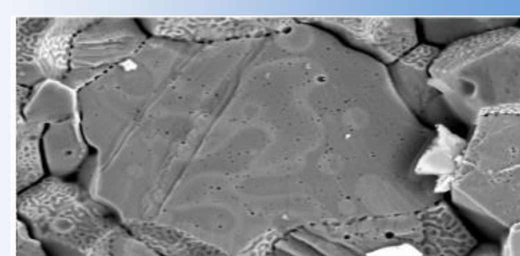
TOPS and FASTMath

Various fusion partnerships, e.g.,

Plasma Surface Interactions (PI: Wirth): Highly scalable simulations of cluster dynamics for materials

Outcome & Impact

- PETSc used by 2015 & 2016 Gordon Bell Prize winners
- DOE subsurface flow codes: Pflotran & Chombo-Crunch
  - Power systems modeling
  - MOOSE package: multiphysics simulations for nuclear reactors
  - Materials science: NE-funded project: *Understanding of Fission Gas Behavior in Nuclear Fuel*, 2017

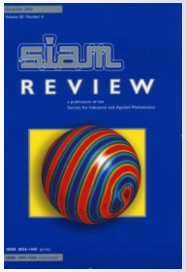


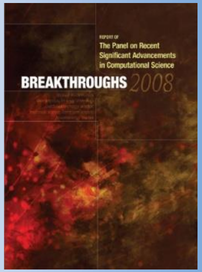
Contact: Barry Smith bsmith@mcs.anl.gov

Scalable Algebraic Multigrid Preconditioners in *hypre*

ASCR Base Math

- Fundamental algorithmic development of algebraic multigrid methods (AMG)
- Adaptive AMG
  - Chosen to appear in SIAM Review as an outstanding research contribution
- Auxiliary-space Maxwell Solver (AMS)
  - Selected for ASCR's top ten "Breakthroughs 2008" report
- AMG theoretical framework and ultra-parallel smoother theory and development



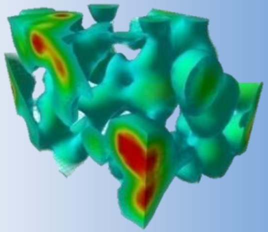


SciDAC Development: TOPS and FASTMath

- Theory into practice
  - Application-specific AMG algorithm development
  - Implementation in *hypre*
  - Parallel algorithms research

hypre R&D 100

- Adaptive AMG is first ever QCD solver to avoid critical slowing down

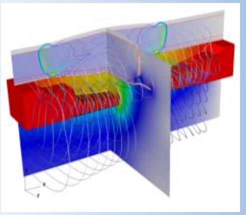


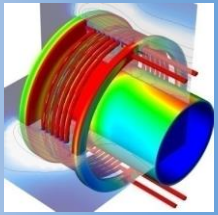
Quantum Chromodynamics

- Novel complexity-reducing AMG methods create speedups to 10x

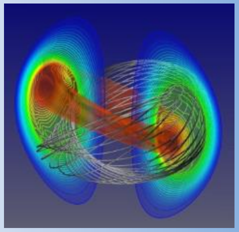
Outcome and Impact

- AMG algorithms and *hypre* play a key role in a wide array of DOE simulations
- AMS and new smoothers enable huge EM simulations





- ASC codes at LLNL / LANL
- PETSc / Trilinos
- SciDAC applications



Magnetic Fusion Energy

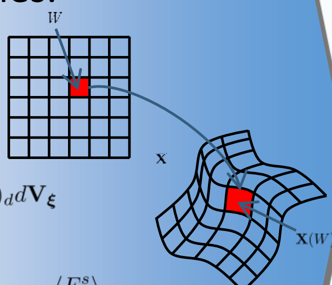
Contacts: Rob Falgout rfalgout@llnl.gov
Ulrike Yang umyang@llnl.gov

Interfacing High-Resolution Discretization with Fast Solvers

ASCR Base

Developed a general formalism for high-order, mapped-multiblock (MMB), finite-volume discretization

A systematic approach for efficient discretization of conservative systems in block-structured geometries.



$$\int_{\mathbf{X}(W)} \nabla_{\mathbf{X}} \cdot \mathbf{F} d\mathbf{x} = \sum_{d=0}^{D-1} \sum_{\alpha=0,1} (-1)^{1+\alpha} \int_{V_d^\alpha} (\mathbf{N}^T \mathbf{F})_d d\mathbf{V}_\xi$$

$$\frac{1}{h^{D-1}} \int_{V_d^\alpha} (\mathbf{N}^T \mathbf{F})_d d\mathbf{V}_\xi \equiv \sum_{s=1}^{D} \langle N_d^s \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} \langle F^s \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}$$

$$+ \frac{h^2}{12} \sum_{s=1}^{D} \left(\mathbf{G}_0^{\perp,d} \langle N_d^s \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d} \right) \cdot \left(\mathbf{G}_0^{\perp,d} (\langle F^s \rangle_{\mathbf{i}+\frac{1}{2}\mathbf{e}^d}) \right) + O(h^4)$$

Accuracy and free-stream preservation is achieved for general conservative systems:

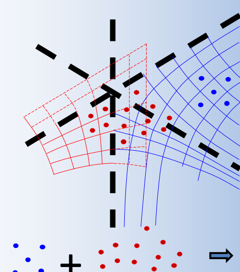
P. Colella, M. R. Dorr, J. A. F. Hittinger and D. F. Martin, J. Comput. Phys. 230 (2011), pp. 2952-2976

P. McCorquodale, M. R. Dorr, J. A. F. Hittinger, P. Colella, J. Comput. Phys. 288 (2015), pp. 181-195

SciDAC3 Development

Developed an interface between FASTMath PDE and solver frameworks:

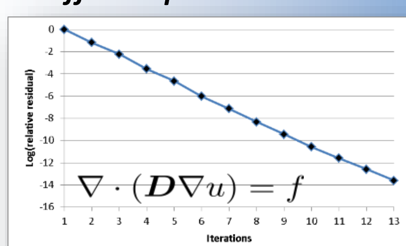
- Uses Chombo MMB support for linear system build
- Uses *hypre* and PETSc state-of-the-art linear solvers



Simplifies the construction of <u>complex</u> MMB linear operators

$Ax = b$

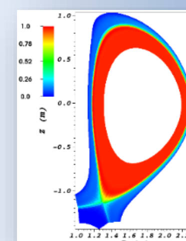
Efficient convergence of BoomerAMG for an MMB tensor diffusion problem:

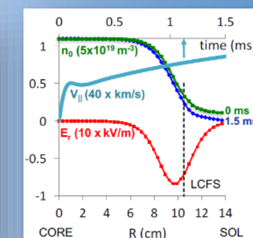


Outcome & Impact

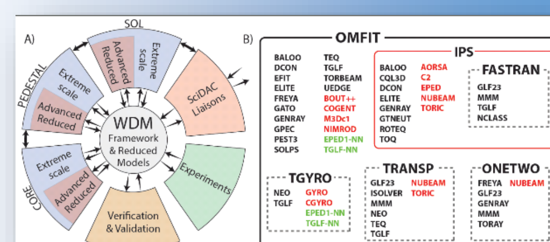
Enabled the solution of problems with fast time scales in an important fusion application:

Edge plasma simulation using COGENT





Contributing to SciDAC FES application partnerships (e.g., Advanced Tokamak Modeling): http://scidac.github.io/atom/



Contact: Milo Dorr dorr1@llnl.gov

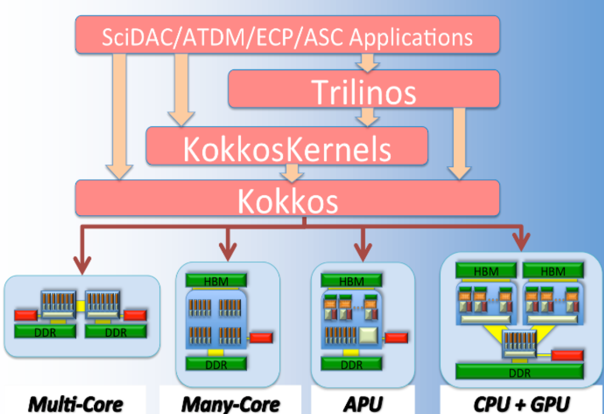
KokkosKernels: Performance-Portable Sparse, Dense, and Graph Kernels

FASTMATH

Sandia National Laboratories

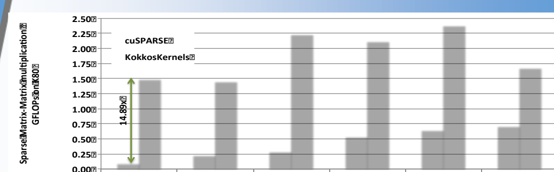
Initial Development

- Multithreaded sparse/dense linear algebra and graph kernels
- Performance-portable algorithms, and implementations using Kokkos programming model
- Begun as part of FASTMath and ATDM

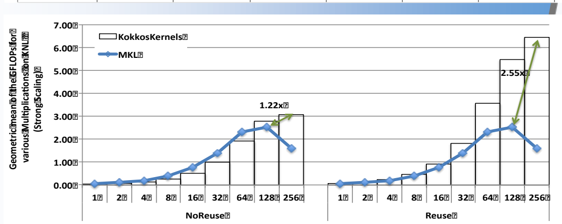


SciDAC3 Development

- Thread Scalable Graph Coloring, Graph partitioning, component finding and ordering methods
- Performance-portable preconditioners and linear algebra kernels
- Impact in scientific simulations and data analysis problems



	Laplace AxP	Laplace RX(AP)	Brick AxP	Brick RX(AP)	Empire AxP	Empire RX(AP)
cuSPARSE	0.100	0.229	0.291	0.542	0.646	0.715
KokkosKernels	1.489	1.458	2.234	2.118	2.381	1.678



Outcome & Impact

- Foundational library for several SciDAC, NNSA and ECP applications for performance-portable kernels
- Enabling multigrid methods by providing thread-scalable algorithms for both setup and solve phases
- Matrix-Matrix multiplication that is significantly faster than vendor kernels both on KNLs and GPUs

POC: S. Rajamanickam srajama@sandia.gov

SciDAC QUEST Institute: Dakota software

DAKOTA

Explore and predict with confidence

Research: LDRD, ASC V&V, ASCR UQ

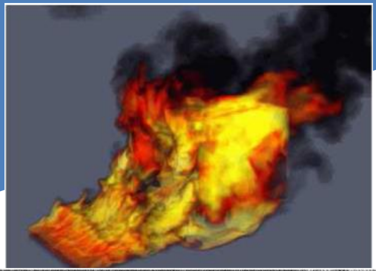
- Dakota initiated as LDRD (FY95-97)
- ASC V&V has been primary steward (FY98-present)
- ASCR UQ (FY11-13)

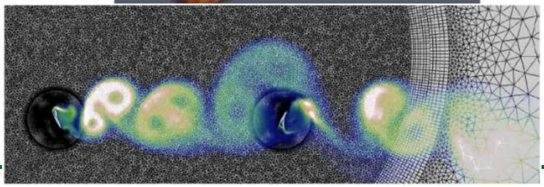
Further Development: SciDAC QUEST, CASL

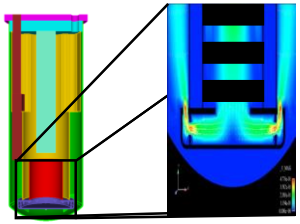
- Investments in Bayesian methods, random fields, multifidelity
- QUEST: FY12-16
  CASL FY10-present

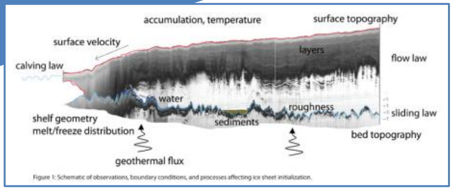
Outcome& Impact

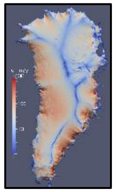
- SciDAC/EFRC Partnerships: PISCEES, WastePD, CHWM
- DOD/DARPA: ARL, EQUiPS
- SBIR: Intelligent Light
- Industry CRADAs: Lockheed Martin, Goodyear, Caterpillar, et al.

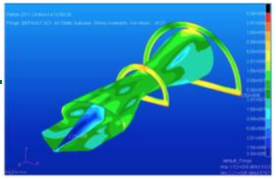












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QUEST UQ toolkit (UQTk) http://www.sandia.gov/UQToolkit

BES, LDRD, DARPA, ASCR Base Math Research

- Key algorithms for intrusive and non-intrusive PC-based UQ
- Fortran and C++
- 2001 – 2011

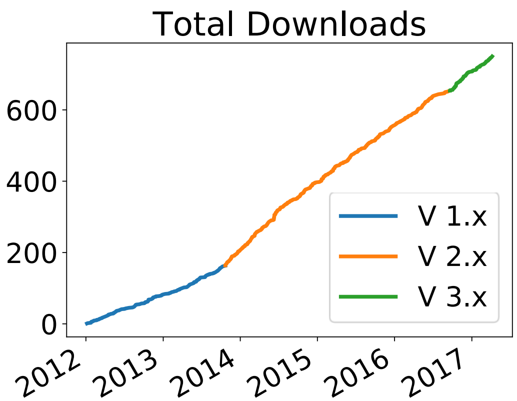
Further Development (SciDAC)

- Significantly expanded range of methods for forward and inverse UQ
- Better software engineering
- C++ with Python interface
- Growing list of tutorial examples
- Target use: UQ Research, prototyping, teaching
- 2011 – 2017

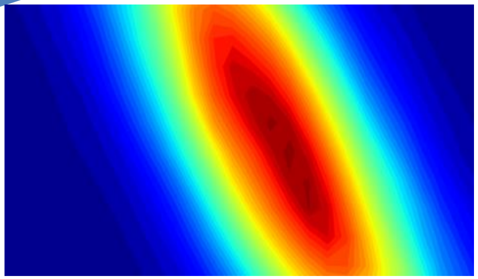
Outcome & Impact

UQTk widely used:

- SciDAC Partnerships (BER, FES, BES, EFRC)
- Other DOE (ACME, ASC) & DARPA (EQUiPS) projects
- Sandia LDRD projects
- Multiple university collaborators
- 700+ downloads from academia, industry, research labs



"Using UQTk, the time required for computing multidimensional triple products for intrusive SSFEM is reduced from an hour to a couple of minutes.", Ajit Desai, Carleton University, Canada

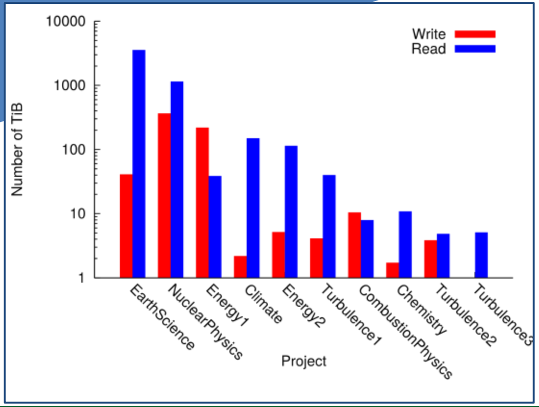


Darshan: I/O characterization for data-intensive science

SDAV Scalable Data Management, Analysis, and Visualization

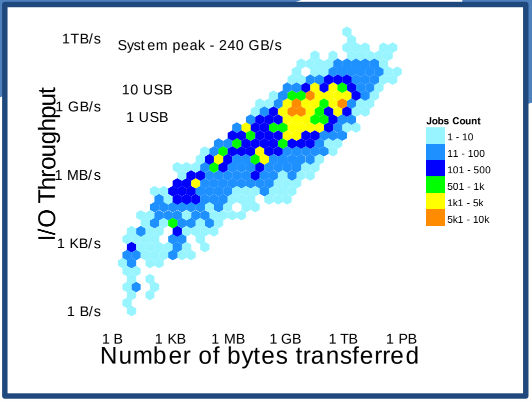
ASCR Base (2008-2011)

- Darshan was conceived to address the need for greater understanding of I/O behavior in diverse scientific applications
- Enabled unprecedented insight into the behavior of the most data-intensive scientific applications at Argonne National Laboratory



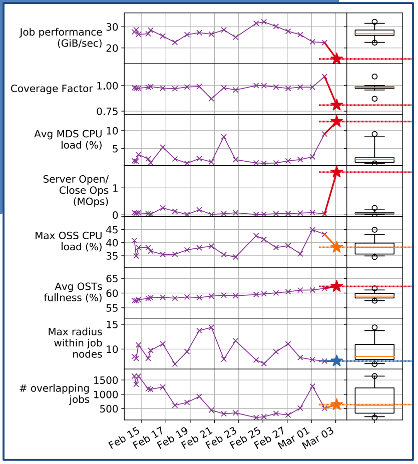
SciDAC (2012-2017)

- Darshan was generalized and ported to multiple computational platforms (IBM BG/Q, Cray XE and XC, Linux clusters) and deployed at every major ASCR facility
- Widespread deployment enabled both cross-platform studies and targeted optimizations to improve the scientific productivity of numerous applications



Impact Going Forward

- Darshan is supported by the ALCF, NERSC, and OLCF computing facilities on their largest systems
- Vendors such as Intel are contributing major features



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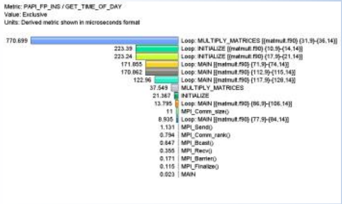
TAU: Tuning and Analysis Utilities

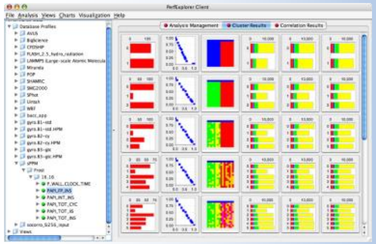
Allen D. Malony (PI), Sameer Shende (Co-PI), University of Oregon

Prior Funding

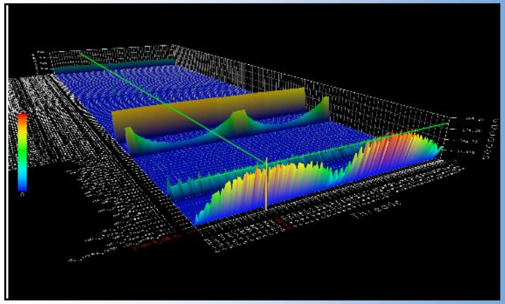
Parallel Profiling and Tracing : 1994-2011:

Application measurement system for a broad array of parallel programming models, languages, platforms. Instrumentation automation, library wrapper support, sampling. Visual and automated analysis tools.





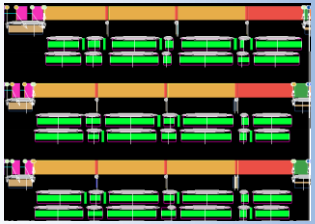
Measurement and analysis for numerous models, platforms and languages: MPI, OpenMP, Posix Threads, CUDA, C/C++, Fortran, Python, Java, UPC, Cray, IBM BG/L,P,Q



SciDAC3 Development

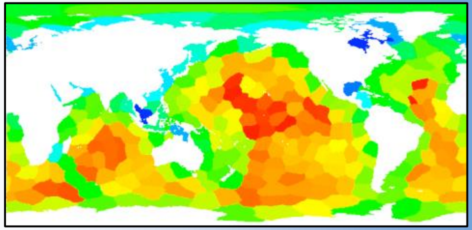
TAU activities under SciDAC3 : 2011-2016:

- **Collaboration with SDAV institute**
- **Extended support as driven by hardware, application requirements – OMPT (OpenMP), Cupti (CUDA), Intel® Xeon® Phi, Manycore CPUs**
- **Engaged with SciDAC 3 application teams to assist in performance engineering efforts**



TAU measurment of CUDA trace (XGC)

TAU used to assist performance engineering for DOE and SciDAC codes.



TAU performance data visualized in application context (MPAS-Ocean)

Outcome & Impact

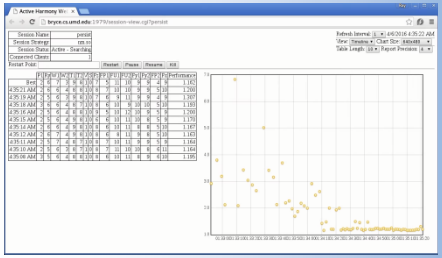
- **TAU is installed as package/module at most DOE computing centers**
- **Contributed to OpenMP Tools (OMPT) included in OpenMP 5.0 specification under review**
- **Ready for deployment on current and planned HPC systems**
- **Identified and eliminated scaling limits, enabling profile measurements of 768k+ processes/threads of execution**
- **Will be leveraged as part of Exascale Computing Project (ECP) “Programming Toolchain for Emerging Architectures and Systems (PROTEAS)**
- **http://tau.uoregon.edu**

Auto-tuning: Automating Performance Portability

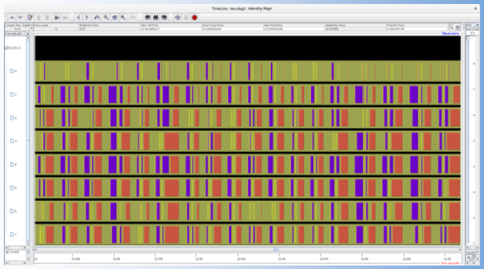
ASCR Base & LDRD

Developed Components 2004-2012:

Separate Tools Developed:
Active Harmony: Tuning Search Engine
Orio: Auto-tuning pragmas
TAU: Performance Measurement
Chill: Flexible Compiler Transformations



Active Harmony Search



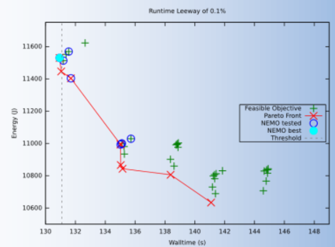
TAU Visualization

Proof of concept showed that each component can work in isolation.

SciDAC3 Development

Integrated Techniques & Demonstrated Successes 2013-2017

- **Combined Active Harmony, Chill, Orio and TAU**
- **Added multi-objective auto-tuning for power and performance**
- **TAU Performance database integrated for storing auto-tuning information**
- **Evaluated auto-tuning with SciDAC3 applications and libraries**

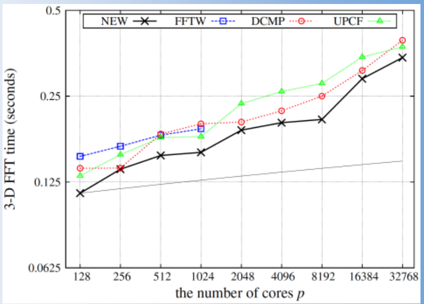


Tuning for Energy vs. Performance (Lulesh)

Outcome & Impact

- **Auto-tuning in PETSC (1.5-2.0x faster for tested application)**

- **OFFT : online auto-tuned FFT library with 2-d decomposition (1.8X faster than FFTW)**

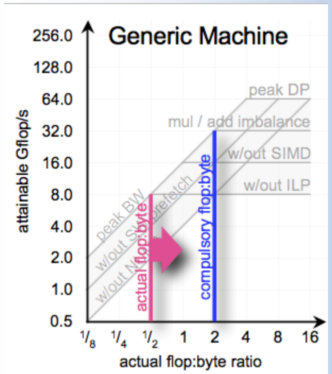


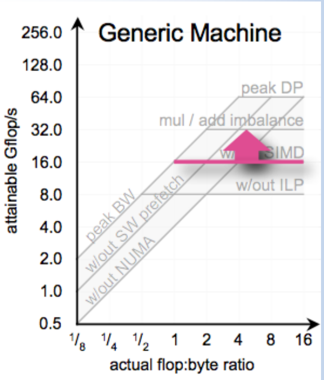
- **Auto-tuning part of Exascale Computing Project (ECP) in build process**

Roofline: Insightful Visual Performance Modeling

ASCR Base & LDRD

Developed Roofline concept:
2006-2011:
easy-to-understand, visual performance model that offers insights to programmers and architects on improving parallel software and hardware.



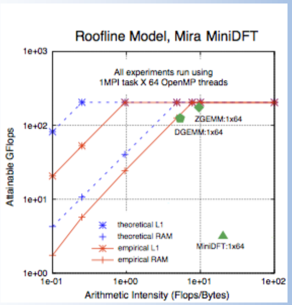


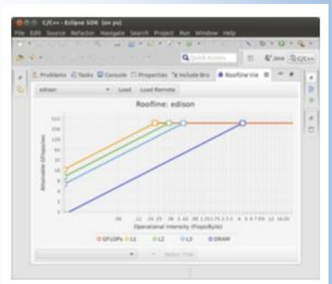
Proof of concept successfully applied to numerous computational kernels and emerging computing systems.

SciDAC3 Development

Roofline augmentation under SciDAC3
2013-2017:

- **Collaboration with FASTMath SciDAC Institute**
- **Developed Empirical Roofline Toolkit (ERT) with public release 03/2015, with Roofline Visualizer**
- **Created community tool for automatic hardware introspection and analysis**

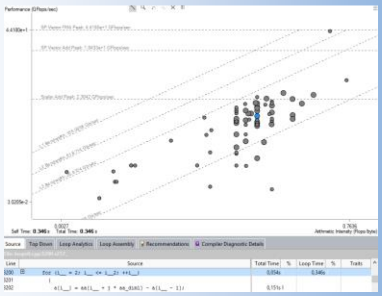




Automated Roofline code used to diagnose performance problems for DOE and SciDAC codes.

Outcome & Impact

- **Roofline has become a broadly used performance modeling methodology across the DOE community**
- **Intel has embraced the approach and integrated it into its production Intel® Advisor**
- **Collaboration with NERSC to instrument and analyze execution of real applications on machines such as Edison and Cori**
- **Will be leveraged as part of Exascale Computing Project (ECP) application assessment**



Snapshot of existing Intel Roofline tool in practice.

- http://tinyurl.com/modynl7

- http://tinyurl.com/n2q76pm

Contact: Sam Williams swwilliams@lbl.gov

SciDAC-EFRC Collaborations in Support of EM and Nuclear Clean-Up Mission

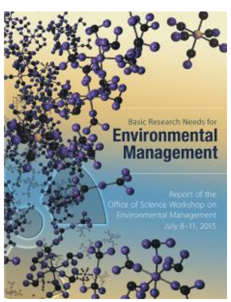
Tools & Expertise of 4 SciDAC Institutes

FASTMATH QUEST SDAV SUPER

Scalable Data Management, Analysis, and Visualization

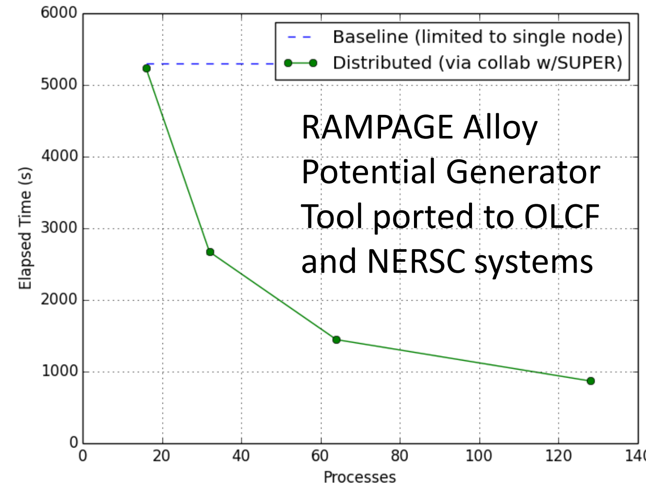
14 Collaborative Pilot Projects

Priority Research Directions of 4 EFRCs



CAST, CHWM, IDREAM, WastePD awarded in FY16

Significant Impact Demonstrated on Scientific Progress



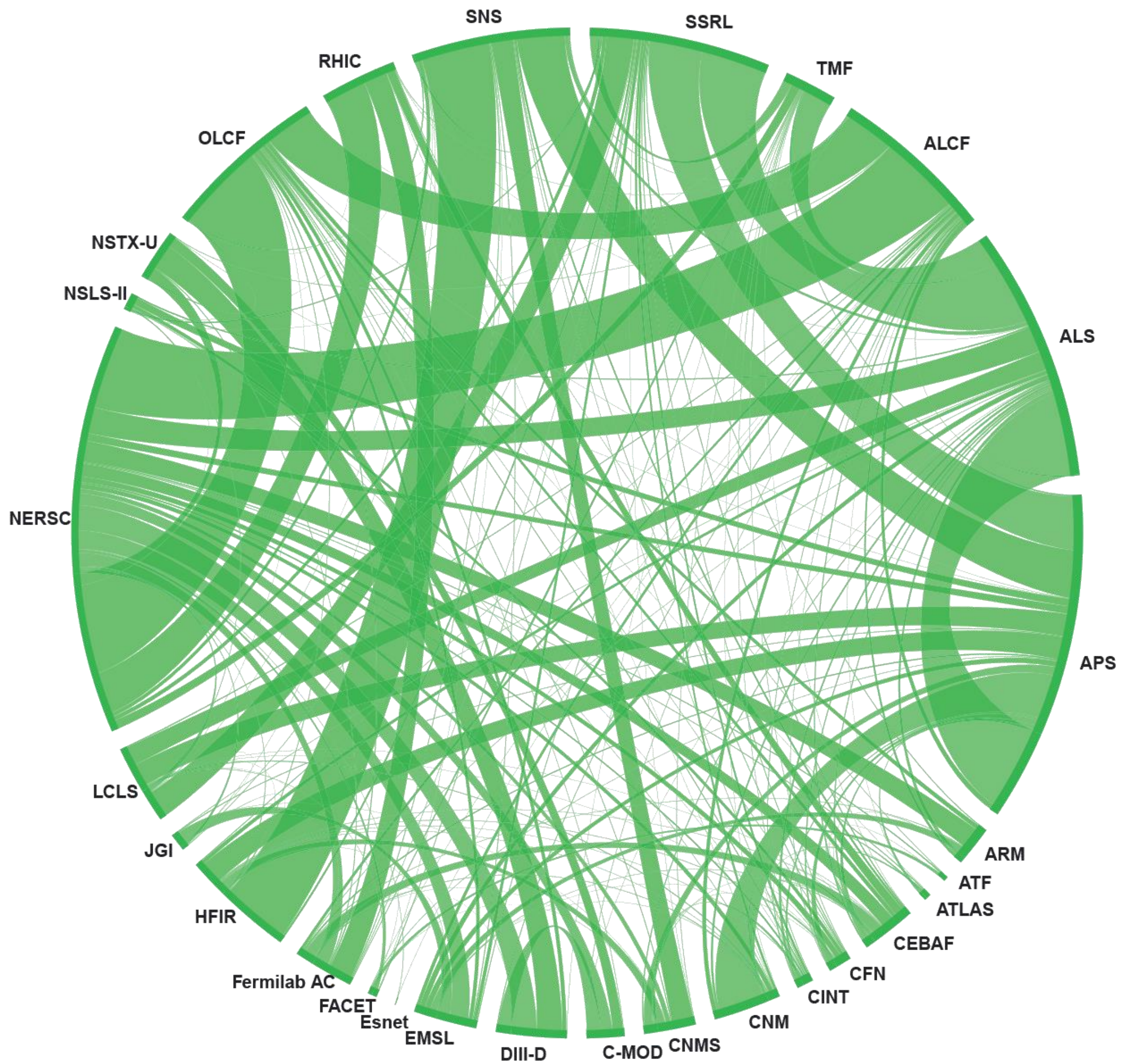
SUPER-WastePD Collaboration

See Wolfgang Windl's talk tomorrow at 4:00 pm

Facility and Project Updates

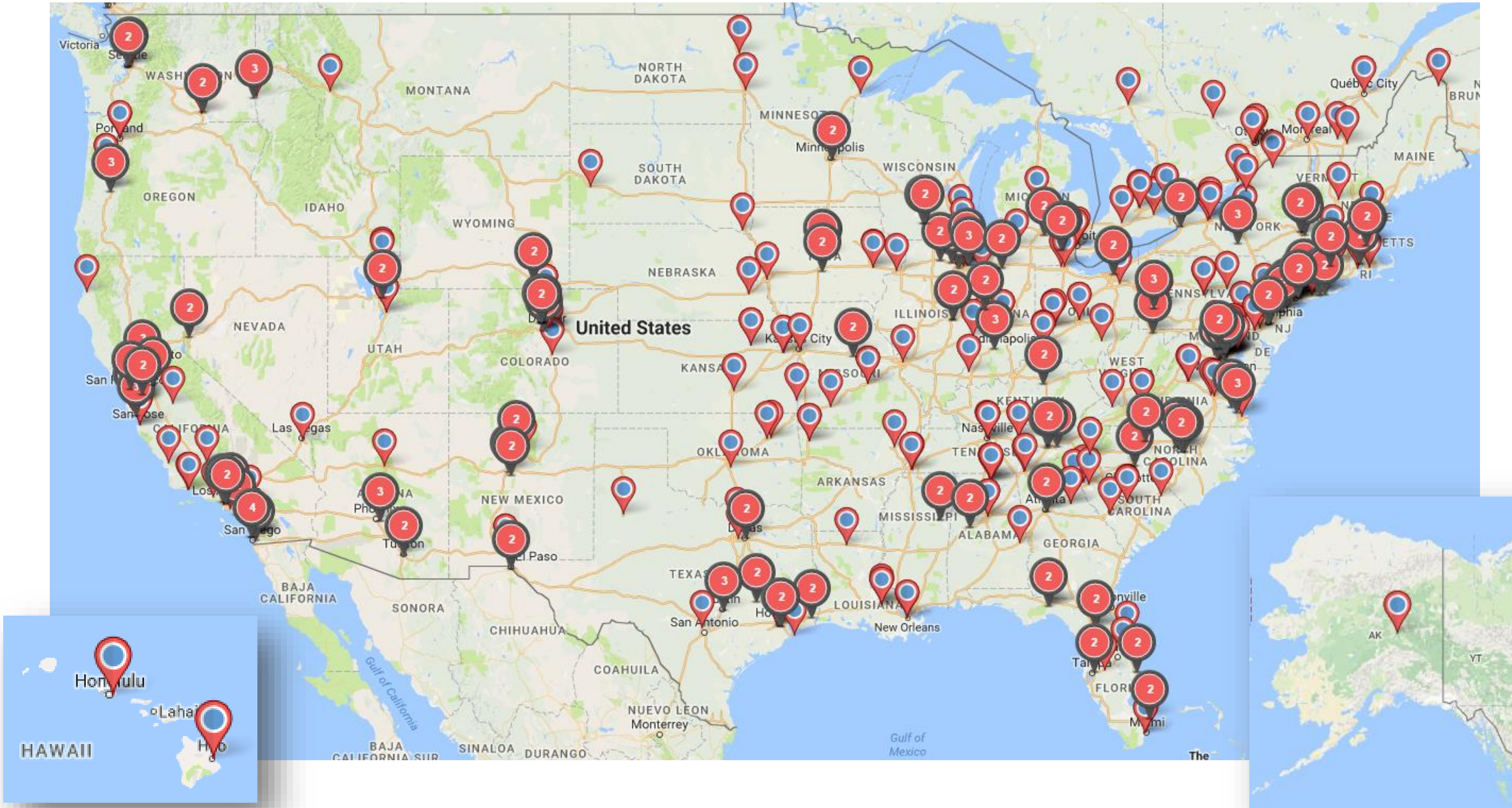
User Crossover Among SC User Facilities, FY 2015

The width of the ribbon connecting two facilities corresponds to the number of users who utilized both of those facilities



ASCR User Facilities

FY 2015 Users by Institution



ASCR Computing Upgrades At a Glance

System attributes	OLCF Now	ALCF Now		NERSC Now		OLCF Upgrade	ALCF Upgrades
Name Planned Installation	**TITAN**	**MIRA**	**Theta 2016**	**Edison**	**Cori**	**Summit 2017-2018**	**Aurora 2018-2019**
System peak (PF)	27	10	>8.5	2.6	~ 31	200	180
Peak Power (MW)	9	4.8	1.7	2	3.5	13.3	13
Total system memory	710TB	768TB	>480 TB DDR4 + High Bandwidth Memory (HBM)	357 TB	~1 PB DDR4 + High Bandwidth Memory (HBM)+1.5PB persistent memory	> 2.4 PB DDR4 + HBM + 3.7 PB persistent memory	> 7 PB High Bandwidth On-Package Memory Local Memory and Persistent Memory
Node performance (TF)	1.452	0.204	> 3	0.460	> 3	> 40	> 17 times Mira
Node processors	AMD Opteron Nvidia Kepler	64-bit Power PC A2	Intel Knights Landing Xeon Phi many core CPUs	Intel Ivy Bridge	Intel Xeon Phi KNL Intel Haswell CPU in data partition	Multiple IBM Power9 CPUs & multiple Nvidia Voltas GPUS	Knights Hill Xeon Phi many core CPUs
System size (nodes)	18,688 nodes	49,152	>2,500 nodes	5,600 nodes	9,300 KNL nodes + 2,000 nodes in data partition	~4,600 nodes	>50,000 nodes
System Interconnect	Gemini	5D Torus	Aries	Aries	Aries	Dual Rail EDR-IB	2nd Generation Intel Omni-Path Architecture
File System	32 PB 1 TB/s, Lustre®	26 PB 300 GB/s GPFS ™	10PB, 210 GB/s Lustre initial	7.6 PB 168 GB/s, Lustre®	28 PB 744 GB/s Lustre®, 1.5 TB/s Burst Buffer	120 PB 1 TB/s GPFS™	150 PB 1 TB/s Lustre®

Innovative and Novel Computational Impact on Theory and Experiment

INCITE promotes transformational advances in science and technology through large allocations of computer time, supporting resources, and data storage at the Argonne and Oak Ridge Leadership Computing Facilities (LCFs) for computationally intensive, large-scale research projects.

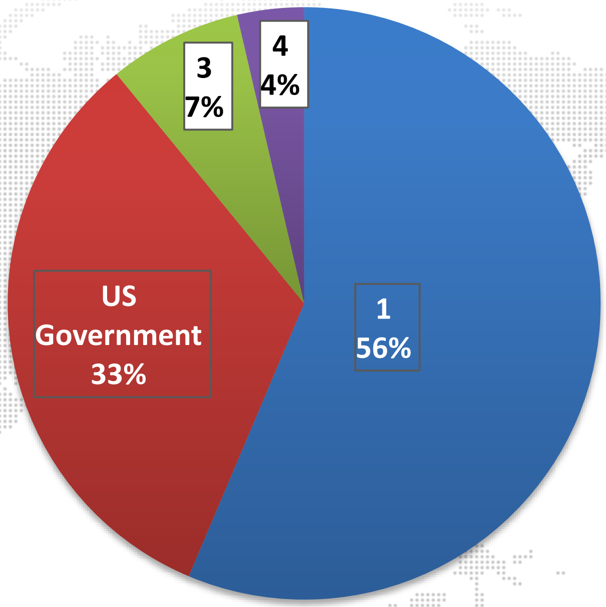
The 2018 INCITE Call for Proposals opened April 17, 2017 and will close June 23, 2017.

For more information visit http://www.doeleadershipcomputing.org/

2017 INCITE award statistics

- Request for Information helped attract new projects
- Call closed June 24th, 2016
- Total requests of more than 13 billion core-hours
- Awards of 5.8 billion core-hours for CY 2017
- **55 projects awarded of which 17 are renewals**

PIs by Affiliation (Awards)



Acceptance rates

45% of nonrenewal submittals and 85% of renewals

Contact information
Judith C. Hill, INCITE Manager
hilljc@DOEleadershipcomputing.org

Objectives of Current "Exascale" Requirements Review (RR)

Goal: Ensure the ability of ASCR facilities to support SC mission science in the exascale regime (2020-2025 timeframe).

Program Office : Identify key computational science drivers from Biological and Environmental Sciences that push exascale and describe **the HPC ecosystem** –HPC machine and related resources- needed to successfully accomplish your science goals

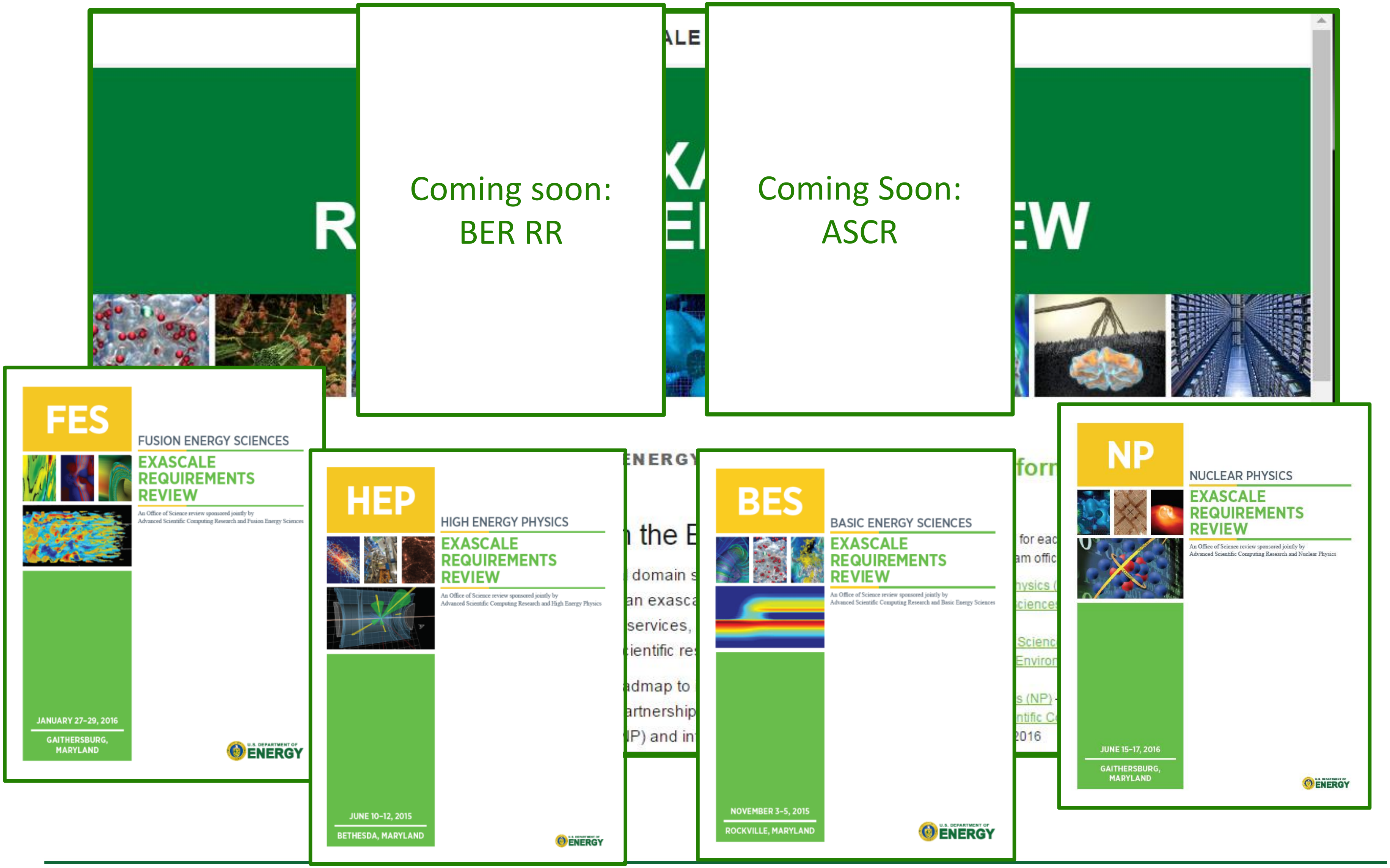
Schedule

June 10-12,2015	HEP
November 3-5 2015	BES
January 27-29, 2016	FES
March 29-31, 2016	BER
June 15-17 2016	NP
Sept. 27-29, 2016	ASCR
March 9-10, 2017	Crosscut

- Capture the whole picture:
  - Identify continuum of computing needs for the program office from institution clusters to Leadership computing.
    - » *Note: ASCR focus is on HPC and Leadership computing*.
  - Include modeling and simulation, scientific user facilities and large experiments needs, data needs, and near real time needs.
- Information gathered will inform the requirements for ecosystems for planned upgrades in 2020-2023 including the pre-exascale and exascale systems, network needs, data infrastructure, software tools and environments, and user services.

ASCR: Communicate to DOE SC scientists the known/fixed characteristics of upcoming compute system in the 2020-2025 timeframe and ask the computational scientists for feedback on proposed architectures

Exascaleage.org



CHARGE to breakouts – day 2

•What are promising areas for partnerships with ASCR and other offices?

•How can HPC be made more productive for science across the Office of Science?

•What are possible paths forward?

•Can we articulate examples where action on a particular crosscut topic could lead to better scientific outcomes?

Cross Cutting Breakouts

- Computing
  - Hardware
  - Allocations, Access, and Policies
- Data
  - Large-Scale Data Storage and Analysis
  - Experimental and Simulation Workflows
  - Data Management, Archiving, and Curation
  - I/O performance
  - Remote access, sharing, and data transfer
- Software & App Development
  - Workflows
  - **Models, Methods, and Algorithms**
  - Common Environment and Sensible Standards
  - Portability, Performance, and Sustainability
- Training & Workforce
  - Partnerships
  - Training for current and next generation systems
  - Workforce

U.S. Leadership in HPC: NSA-DOE Report

U.S. Leadership in High Performance Computing (HPC)

A Report from the NSA-DOE Technical Meeting on High Performance Computing

December 1, 2016

- **Meeting Held September 28-29, 2016**
- **Attendees**
  - 40 representatives from USG agencies: HQ, National Laboratories, NSA-SME, IARPA, NSF and other agencies
  - 10 representatives from industry representing HPC vendors, technology developers and users
  - 10 SMEs from academia and other organizations with background in HPC
- **Addressed following questions**
  - Has the state of HPC leadership changed since 2012? How?
  - What does this mean for U. S. leadership in HPC, which is recognized as a key component of national and economic security?
  - What should we do?

Recommendations

- It is critical to lead exploration of innovative computing architectures that will unleash creativity of the HPC community.
- Workforce development is a major concern in HPC… We must inspire a new generation of students to master the skills for HPC and we must develop “public-private” relationships between the USG and industry to insure that there are rewarding careers for people with these skills.
- NSCI leadership must work to modernize export control practices to account for the new reality of Chinese technological capability and business practices, and develop more efficient contracting regulations to improve public-private partnership in HPC science and technology development.

Questions?