2018 SciDAC-4 Principal Investigator Meeting

July 23rd, 2018

Ceren Susut & Randall Laviolette
Advanced Scientific Computing Research
U.S. Department of Energy

U.S. DEPARTMENT OF ENERGY

Bottom Line from SciDAC-3 COV Report, 2014

❖ SciDAC remains the gold standard for fostering interaction between disciplinary scientists and HPC. The PMs are to be commended on continuing the excellence of the SciDAC "brand."

❖ Informal conversations of the reviewers with overseas colleagues indicate that SciDAC is seen as a model program, which they wish could be replicated in their home countries.

Bottom Line from ASCR COV Report, 2017

❖ The SciDAC program is widely known within the computational sciences communities. The COV finds that SciDAC is highly respected nationally and is highly admired in Europe and in Asia.
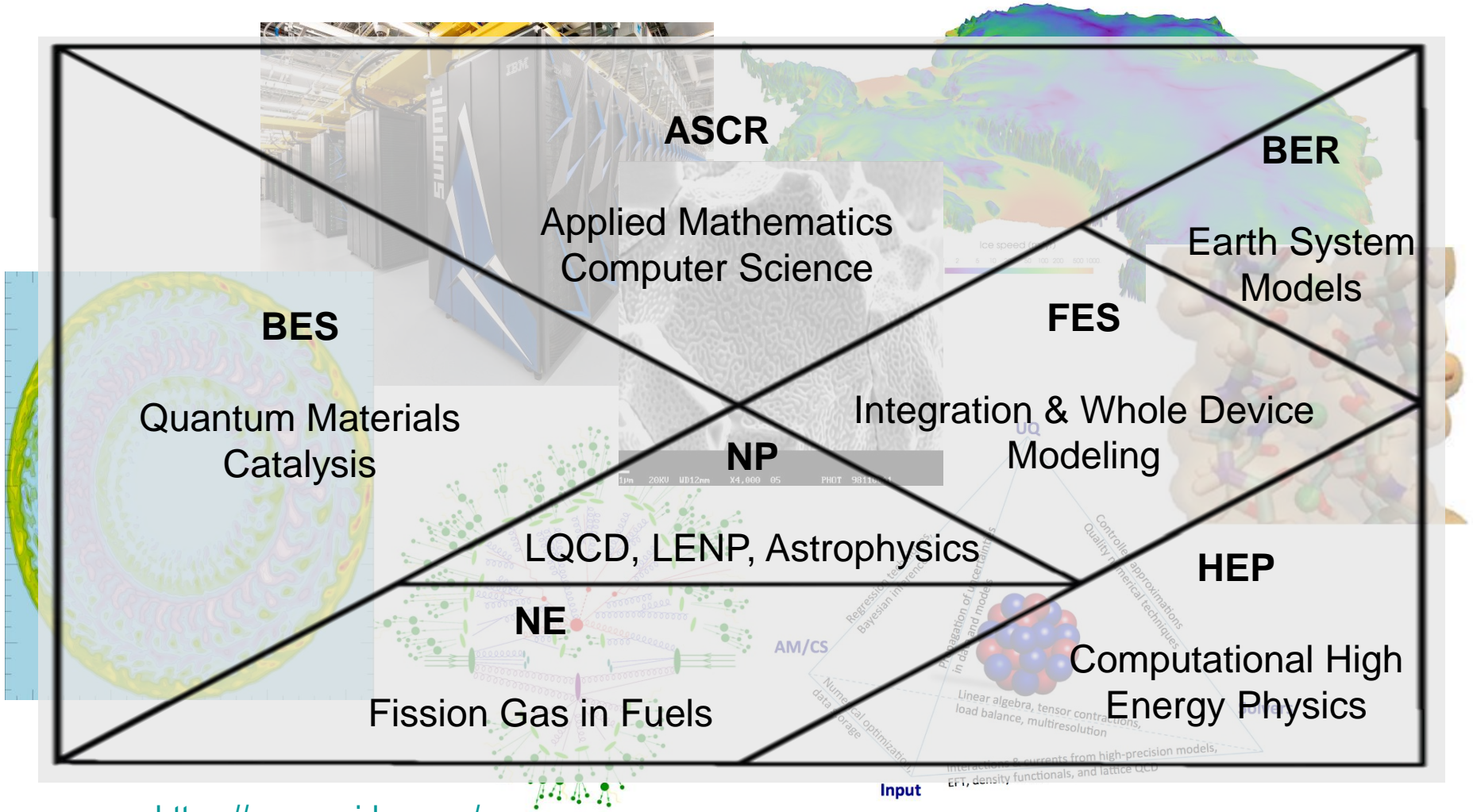
SciDAC
Scientific Discovery through Advanced Computing

https://www.scidac.gov/

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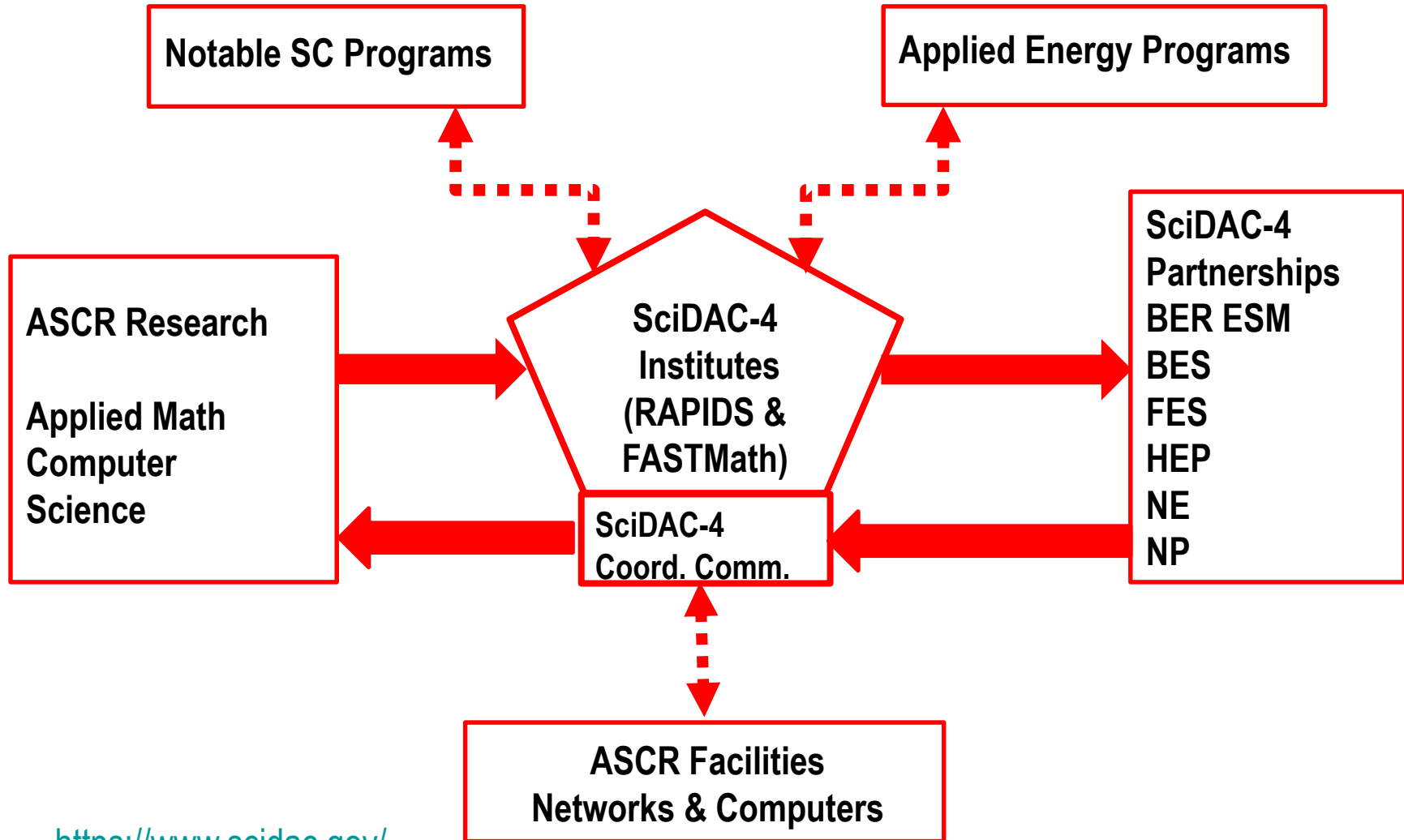
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ASCR

Applied Mathematics
Computer Science

BER

Earth System
Models

BES

Quantum Materials
Catalysis

FES

Integration & Whole Device
Modeling

NP

LQCD, LENP, Astrophysics

HEP

Computational High
Energy Physics

NE

Fission Gas in Fuels

https://www.scidac.gov/

SciDAC is an Evolving Program

Program	Time Frame	Description	Result
SciDAC-1	2001 – 2006	Created scientific software infrastructure for parallel computing; Funded collaborations in DOE science domains	Science at the Terascale
SciDAC-2	2006 – 2011	Added DOE science domains; Enhanced university involvement; Outreach to broader scientific community; Added Data&Visualization	Science to the Petascale
SciDAC-3	2011 – 2016	Improved collaborations among SciDAC Institutes and between ASCR-SC programs; Enhanced architecture- and applications-awareness within each Institute; Added Uncertainty Quantification	Science on multi-core and emerging hybrid architectures
SciDAC-4	2017-2021	Outreach to broader scientific community; First connection to Applied Energy; Built-in flexibility; Added Machine Learning	Science on pre-exascale architectures

https://www.scidac.gov/

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Notable SC Programs

Applied Energy Programs

ASCR Research

Applied Math Computer Science

SciDAC-4 Institutes (RAPIDS & FASTMath)

SciDAC-4 Coord. Comm.

SciDAC-4 Partnerships BER ESM BES FES HEP NE NP

ASCR Facilities Networks & Computers

https://www.scidac.gov/

Goals

❖ Coordinate interactions between SciDAC-4 Institutes and Partnerships

❖ Assess emerging needs across SciDAC-4 projects

❖ Junction point for SciDAC-4, ASCR facilities and broader DOE computational science community

Activities

❖ Kick-off meeting on December 7th, 2017

❖ RAPIDS Webinar on February 13th, 2018

❖ FASTMath Webinar on March 14th, 2018

❖ NE Partnership Telecom on April 16th, 2018

❖ BER Partnership Telecom on May 30th, 2018

❖ Face-to-face meeting on July 25th, 2018

❖ More to come…

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Committee

Rob Ross (ANL, RAPIDS Director, chair)

Lori Diachin (LLNL, FASTMath Director)

Katherine Evans (ORNL, BER POC)

Teresa Head-Gordon (LBNL, BES POC)

David Hatch (U. Texas-Austin, FES POC)

Jim Amundson (FNAL, HEP POC)

Brian Wirth (ORNL, NE POC)

Martin Savage (U. Washington, NP POC)

DOE

Randall Laviolette (ASCR)

Ceren Susut (ASCR)

Dorothy Koch (BER)

James Davenport (BES lead)

John Mandrekas (FES)

Lali Chatterjee (HEP)

Brian Wirth (ORNL, NE POC)

Dan Funk (NE)

Ted Barnes (NP)

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- **SC & NE Program Overview [no questions]: now**
- **Poster session (Mark Pederson): Today and tomorrow in Atrium (8:00 AM-5:30 PM)**
- **Plenary Institutes session, parallel Partnership break-out sessions**
- **Lunches included in the registration fee (Roosevelt, Foyer)**
- **SciDAC-4-ASCR Facilities discussion tomorrow at 8:15 AM here**

https://www.scidac.gov/

s://www.ornl.gov/content/long-term-scidac-investments-provide-ecosystem-quantum-breakthrough

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COMPUTING AND COMPUTATIONAL SCIENCES

Research Highlight

Long Term SciDAC Investments Provide Ecosystem for Quantum Breakthrough

Scott Jones
July 20, 2018

A team of computing researchers and physicists from the Department of Energy's (DOE's) Oak Ridge National Laboratory (ORNL) has become the first group to successfully simulate an atomic nucleus using a quantum computer.

While the discovery is currently making waves across the quantum computing and nuclear communities, the rise of computing as a third pillar next to experiment and theory in low-energy nuclear physics can be traced back to 2006. It was then that an ORNL team led by David Dean, now ORNL's Associate Laboratory Director for Physical Sciences, participated in the SciDAC-2 Universal Nuclear Energy Density Functional (UNEDF) project that aimed to develop a universal density functional for the description of atomic nuclei. UNEDF was jointly funded by DOE's Advanced Scientific Computing Research (ASCR) and Nuclear Physics (NP) programs via the Scientific Discovery through Advanced Computing (SciDAC) program.

Since then, ORNL's Nuclear Theory Group has been a key participant in the SciDAC-3 NUclear Computational Low Energy Initiative (NUCLEI) and SciDAC-4 NUCLEI-2 projects. These projects

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