The World Effort on High Performance Computing in Fusion

From Petascale to Exascale

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Office of Fusion Energy Sciences

U.S. DEPARTMENT OF ENERGY
Office of Science

Fusion Power Associates
37th Annual Meeting and Symposium
December 13-14, 2016
Washington, DC

Outline

- **HPC and Fusion**
    - ***Current U.S. capabilities and priorities***
- **The DOE Exascale Computing Project (ECP)**
- **Survey of International Efforts and Connections with the U.S. Program**

With many thanks to:

CS Chang, Bill Harrod, Frank Jenko, Doug Kothe, Lang Lao, Randall Laviolette, Zhihong Lin, Bill Tang, and many others

High Performance Computing Potential

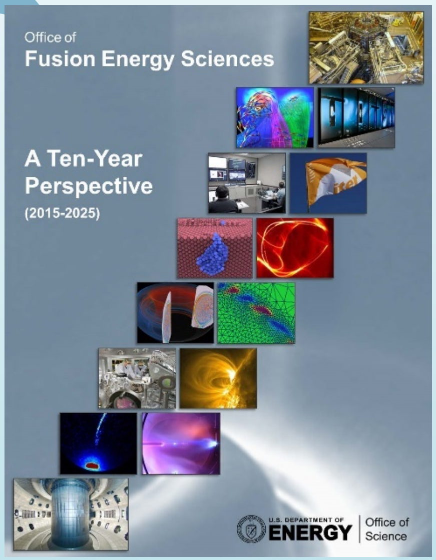
- Advances in computing hardware and computational science over the last decade have firmly established simulations as an equal partner in scientific discovery, along with theory and experiment.
  - Solve problems when experiments are impossible, dangerous, or very costly
  - Enhance economic competitiveness
  - **In fusion**: accelerate scientific discovery and predictive understanding; confidently explore regimes unattainable in current experiments; reduce risk in the design of future devices shortening the path toward the realization of a sustainable fusion energy source
- Recognizing the potential of High Performance Computing (HPC), in 2015 the President established the **National Strategic Computing Initiative** (NSCI) which aims to maximize the benefits of HPC for U.S. economic competitiveness and scientific discovery.

HPC & the Fusion Program

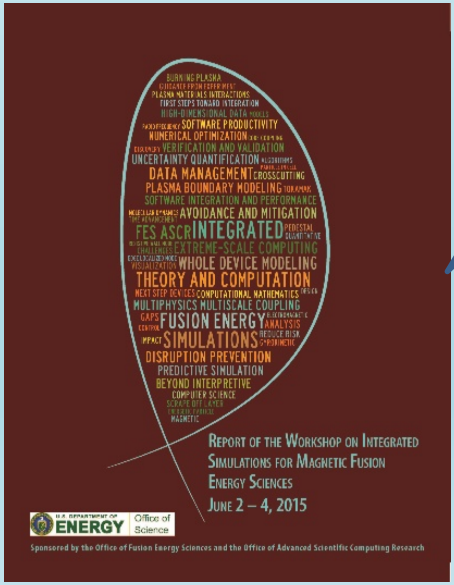
Major themes of the FES strategic plan

– ***Massively parallel computing*** with the goal of validated whole-fusion-device modeling will enable a transformation in predictive power, which is required to minimize risk in future fusion energy development steps.

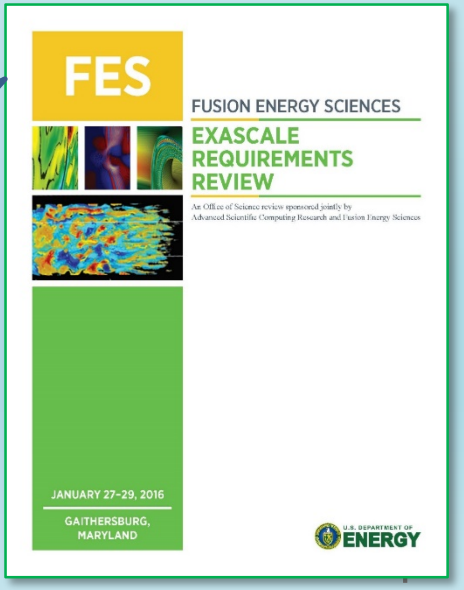
– ***Materials scie***... as it relates to plasma and fusion ...



2015 FES/ASCR Community Workshop on Integrated Simulations (summary presented by Paul Bonoli at last year's FPA Meeting)



January 2016: FES / ASCR Exascale Requirements Review
Identify forefront scientific challenges and opportunities in fusion energy and plasma sciences whose resolution is essential to meeting the FES mission and could be aided by exascale computing over the next decade.



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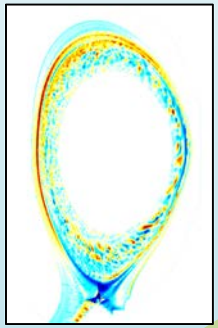
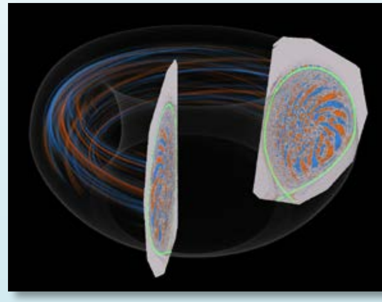
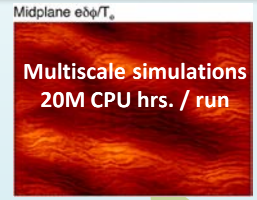
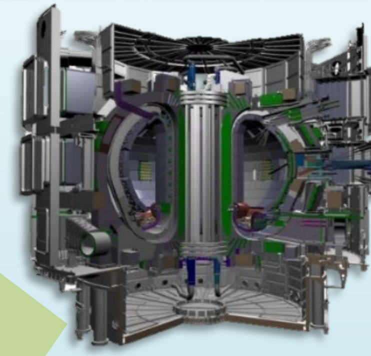
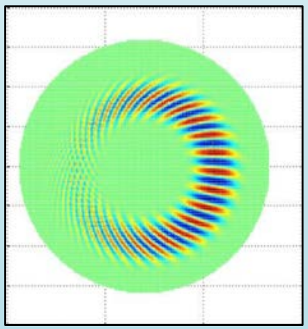
Motivation for the Exascale











Gigaflops

Perturbative (*δf*) 5D electrostatic gyrokinetic single-species (ion) simulation with adiabatic electrons in model geometry

Teraflops

Non-perturbative (full *f*) 5D electrostatic gyrokinetic single-species (ion) simulation with adiabatic electrons of the tokamak edge region in realistic geometry, including background plasma effects

Petaflops

Non-perturbative multiscale 5D electrostatic / electromagnetic gyrokinetic simulations with multiple kinetic species, integrating the edge and core regions

Exaflops

Multiscale, multiphysics 5D / 6D electromagnetic kinetic simulation of ITER plasma, including effects of fusion reactions; whole-device modeling

CS Chang, PPPL, EPSI SciDAC
N. Howard, MIT

Petaflop-level HPC Resources Available to Fusion Scientists

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NERSC The *mission* HPC Center for DOE SC (over 5,000 users)

BERKELEY LAB
Lawrence Berkeley National Laboratory

Cori @ NERSC, > 30 PF

Edison @ NERSC, 2.57 PF

DOE Leadership Computing Facilities at ORNL & ANL

Highly competitive user allocation programs

OAK RIDGE National Laboratory | OAK RIDGE LEADERSHIP COMPUTING FACILITY

Both facilities scheduled to be updated in ~2017—2018 with > 100 PF systems

Argonne NATIONAL LABORATORY

Titan @ OLCF, 27 PF

Mira @ ALCF, 10 PF

The DOE Exascale Computing Project (ECP)

The DOE Exascale Computing Project (ECP)

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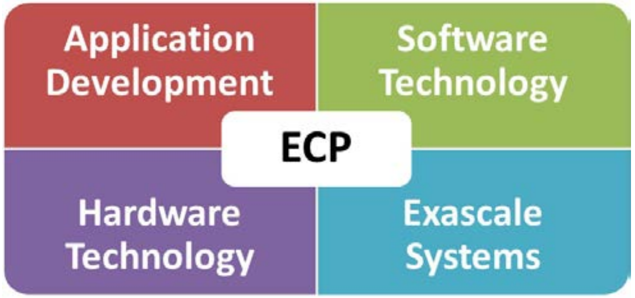
- The President's 2015 National Strategic Computing Initiative (**NSCI**) aims to maximize the benefits of HPC for U.S. economic competitiveness and scientific discovery.
- DOE, along with DoD and NSF, co-lead the NSCI.
- DOE SC and NNSA are executing a joint effort on advanced simulation through a **capable exascale computing program** emphasizing sustained performance on relevant applications and data analytic computing.
- The Exascale Computing Project (ECP) is the vehicle for this effort.

Delivers 50× the performance of today's 20 PF systems, supporting applications that deliver high-fidelity solutions in less time and address problems of greater complexity

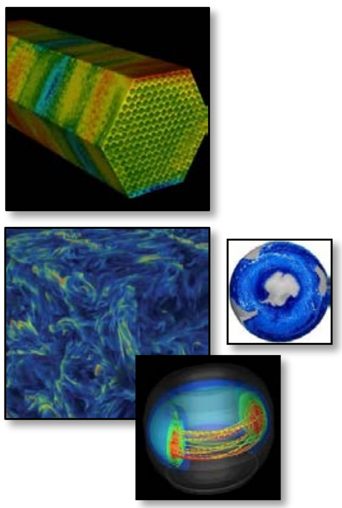
- **Operates in a power envelope of 20–30 MW**
- **Is sufficiently resilient (average fault rate: ≤1/week)**
- **Includes a software stack that supports a broad spectrum of applications and workloads**

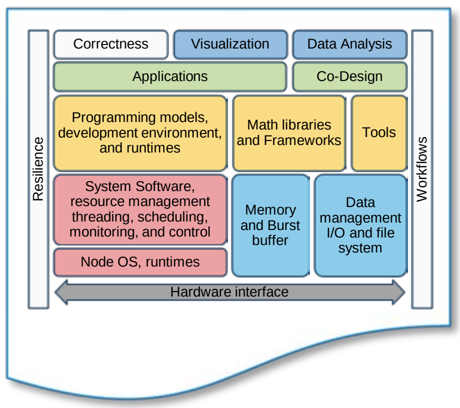
A holistic project approach is needed that uses co-design to develop new platform, software, and computational science capabilities

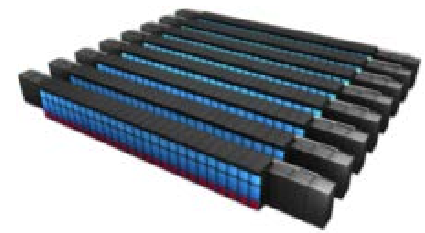


ECP has formulated a holistic approach that uses co-design and integration to achieve capable exascale

Application Development	Software Technology	Hardware Technology	Exascale Systems
Science and mission applications	Scalable and productive software stack	Hardware technology elements	Integrated exascale supercomputers







ECP's work encompasses applications, system software, hardware technologies and architectures, and workforce development

Doug Kothe, SC16

EXASCALE COMPUTING PROJECT

ECP application, co-design center, and software project awards

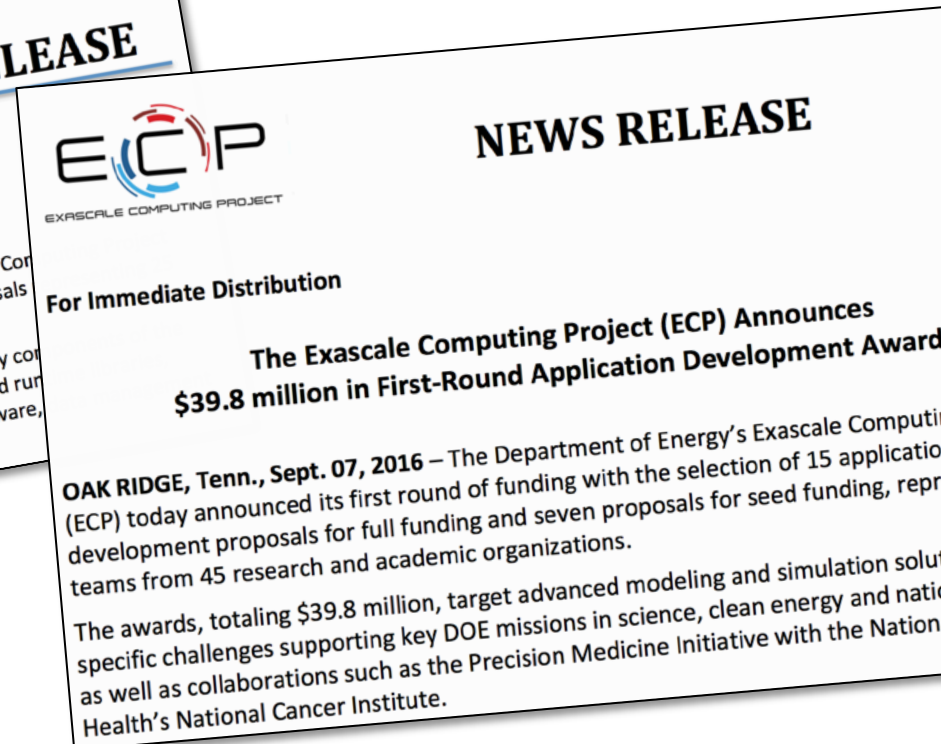
NEWS RELEASE

EXASCALE COMPUTING PROJECT

The Exascale Computing Project Awards $34 Million for Software Development

OAK RIDGE, Tenn., Nov. 10, 2016 – The Department of Energy's Exascale Com
(ECP) today announced the selection of 35 software development proposals
research and academic organizations.

The awards for the first year of funding total $34 million and cover many co
software stack for exascale systems, including programming models and run
mathematical libraries and frameworks, tools, lower-level system software,
and I/O, as well as in situ visualization and data analysis.



EXASCALE COMPUTING PROJECT

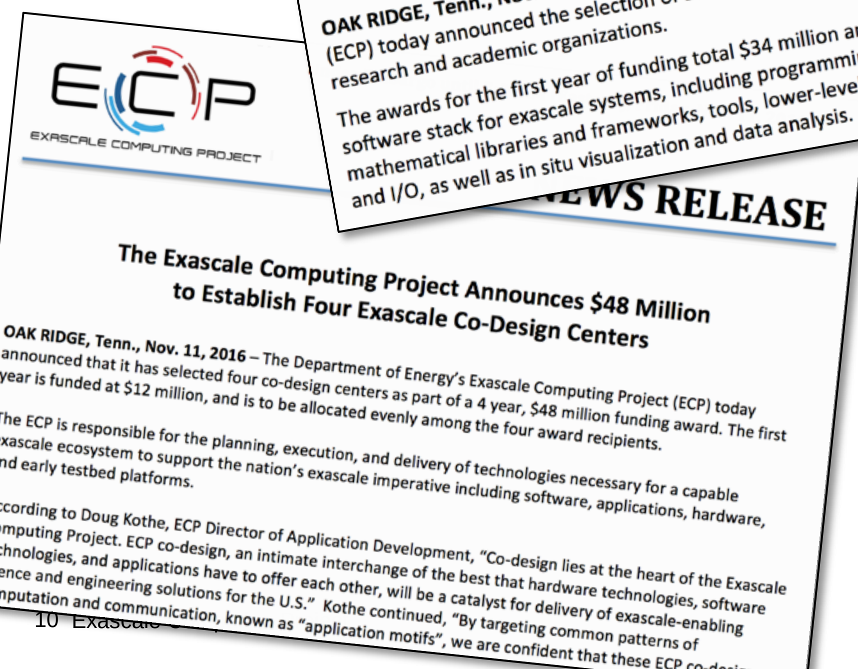
NEWS RELEASE

For Immediate Distribution

The Exascale Computing Project (ECP) Announces $39.8 million in First-Round Application Development Award

OAK RIDGE, Tenn., Sept. 07, 2016 – The Department of Energy's Exascale Computi
(ECP) today announced its first round of funding with the selection of 15 applicatio
development proposals for full funding and seven proposals for seed funding, repr
teams from 45 research and academic organizations.

The awards, totaling $39.8 million, target advanced modeling and simulation solu
specific challenges supporting key DOE missions in science, clean energy and natio
as well as collaborations such as the Precision Medicine Initiative with the Nation
Health's National Cancer Institute.



EXASCALE COMPUTING PROJECT

NEWS RELEASE

The Exascale Computing Project Announces $48 Million to Establish Four Exascale Co-Design Centers

OAK RIDGE, Tenn., Nov. 11, 2016 – The Department of Energy's Exascale Computing Project (ECP) today announced that it has selected four co-design centers as part of a 4 year, $48 million funding award. The first year is funded at $12 million, and is to be allocated evenly among the four award recipients.

he ECP is responsible for the planning, execution, and delivery of technologies necessary for a capable xascale ecosystem to support the nation's exascale imperative including software, applications, hardware, nd early testbed platforms.

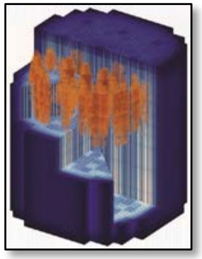
ccording to Doug Kothe, ECP Director of Application Development, "Co-design lies at the heart of the Exascale mputing Project. ECP co-design, an intimate interchange of the best that hardware technologies, software chnologies, and applications have to offer each other, will be a catalyst for delivery of exascale-enabling ence and engineering solutions for the U.S." Kothe continued, "By targeting common patterns of nputation and communication, known as "application motifs", we are confident that these ECP co-design

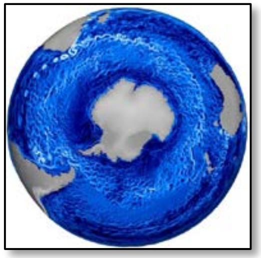
Doug Kothe, SC16

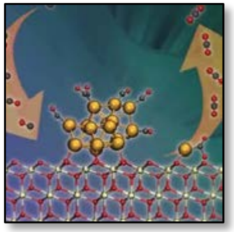
Exascale Applications Will Address National Challenges

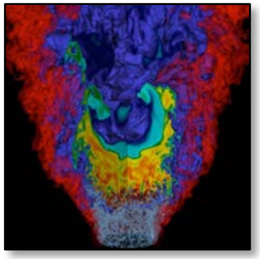
Summary of current DOE Science & Energy application development projects

Nuclear Energy (NE)	Climate (BER)	Chemical Science (BES, BER)	Wind Energy (EERE)	Combustion (BES)
Accelerate design and commercialization of next-generation small modular reactors*	Accurate regional impact assessment of climate change*	Biofuel catalysts design; stress-resistant crops	Increase efficiency and reduce cost of turbine wind plants sited in complex terrains*	Design high-efficiency, low-emission combustion engines and gas turbines*
Climate Action Plan; SMR licensing support; GAIN	Climate Action Plan	Climate Action Plan; MGI	Climate Action Plan	2020 greenhouse gas and 2030 carbon emission goals









* Scope includes a discernible data science component

Doug Kothe, SC16

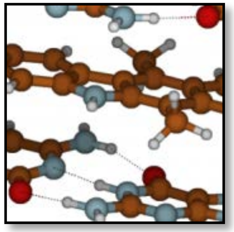
Exascale Applications Will Address National Challenges

Summary of current DOE Science & Energy application development projects

Materials Science (BES)

Find, predict, and control materials and properties: property change due to hetero-interfaces and complex structures

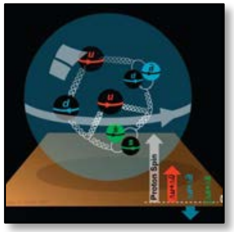
MGI



Nuclear Physics (NP)

QCD-based elucidation of fundamental laws of nature: SM validation and beyond SM discoveries

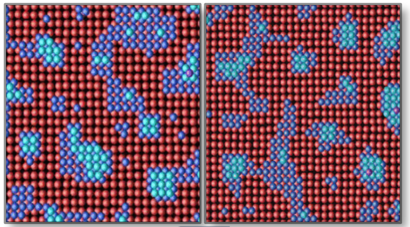
2015 Long Range Plan for Nuclear Science; RHIC, CEBAF, FRIB



Nuclear Materials (BES, NE, FES)

Extend nuclear reactor fuel burnup and develop fusion reactor plasma-facing materials*

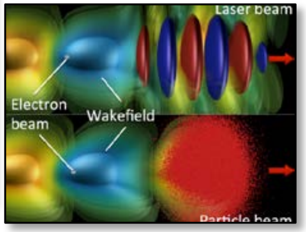
Climate Action Plan; MGI; Light Water Reactor Sustainability; ITER; Stockpile Stewardship Program



Accelerator Physics (HEP)

Practical economic design of 1 TeV electron-positron high-energy collider with plasma wakefield acceleration*

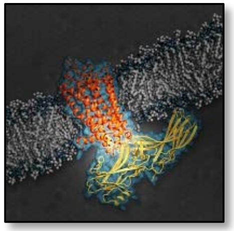
>30k accelerators today in industry, security, energy, environment, medicine



Materials Science (BES)

Protein structure and dynamics; 3D molecular structure design of engineering functional properties*

MGI; LCLS-II 2025 Path Forward



Molecular Dynamics at the Exascale: Spanning the Accuracy, Length and Time Scales for Critical Problems in Materials Science
PI: Arthur Voter (LANL) with:
SNL, UTK

* Scope includes a discernible data science component

Doug Kothe, SC16

Exascale Applications Will Address National Challenges

Summary of current DOE Science & Energy and Other Agency application development projects

Magnetic Fusion Energy (FES)

Predict and guide stable ITER operational performance with an integrated whole device model*

ITER; fusion experiments: NSTX-U, DIII-D, Alcator C-Mod

Advanced Manufacturing (EERE)

Additive manufacturing process design for qualifiable metal components*

NNMIs; Clean Energy Manufacturing Initiative

Cosmology (HEP)

Cosmological probe of standard model (SM) of particle physics: Inflation, dark matter, dark energy*

Particle Physics Project Prioritization Panel (P5)

Geoscience (BES, BER, EERE, FE, NE)

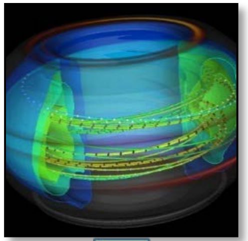
Safe and efficient use of subsurface for carbon capture and storage, petroleum extraction, geothermal energy, nuclear waste*

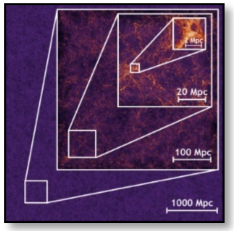
EERE Forge; FE NRAP; Energy-Water Nexus; SubTER Crosscut

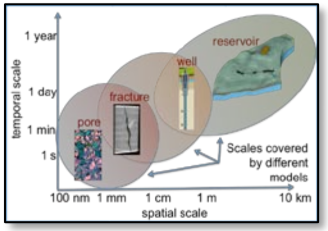
Precision Medicine for Cancer (NIH)

Accelerate and translate cancer research in RAS pathways, drug responses, treatment strategies*

Precision Medicine in Oncology; Cancer Moonshot







High-Fidelity Whole Device Modeling of Magnetically Confined Fusion Plasma
PI: Amitava Bhattacharjee (PPPL) with:
ANL, ORNL, LLNL, Rutgers, UCLA, University of Colorado

* Scope includes a discernible data science component

Doug Kothe, SC16

International HPC Activities & Connections with US Efforts

Japan – Current Capabilities

K computer at RIKEN

- **K (京) Computer** at RIKEN
- 10.5 PF, 7th on TOP-500 list (11/2016)
- Most powerful supercomputer in Japan
- A number of Japanese gyrokinetic codes have been optimized to scale on the K computer

- **Helios: Broader Approach** (BA) Activity
- Operated since 2012 and used extensively by JA and EU researchers
- 1.23 PF peak performance
- Scheduled to be decommissioned at the end of the year

Helios system at Rokkasho site

Plasma Simulator at NIFS

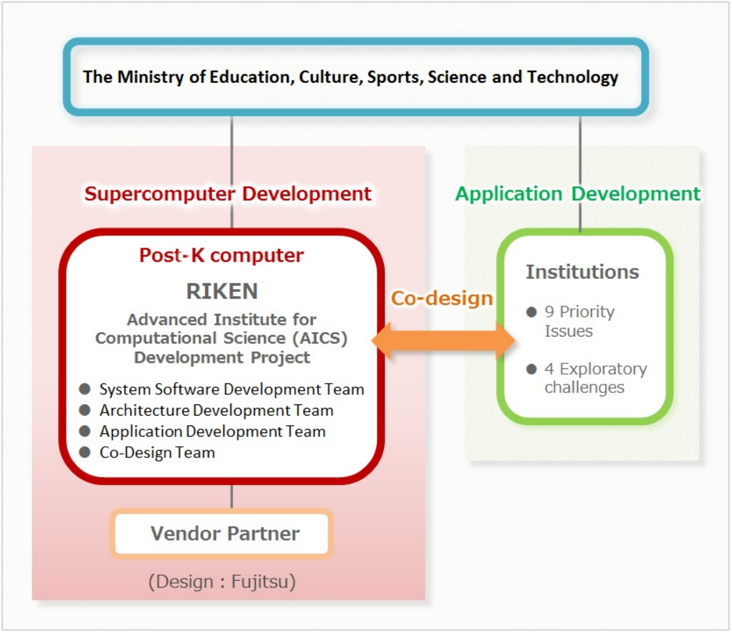
- The **Plasma Simulator** computer at NIFS has been developed and periodically updated
- **Current version**: 2.62 PF Fujitsu FX-100 system
- Addresses the needs of the **Numerical Simulation Reactor Research Project** (NSRP) which aims at integration and on the construction of the Numerical Test Reactor (NTR)

Japan – Exascale Plans

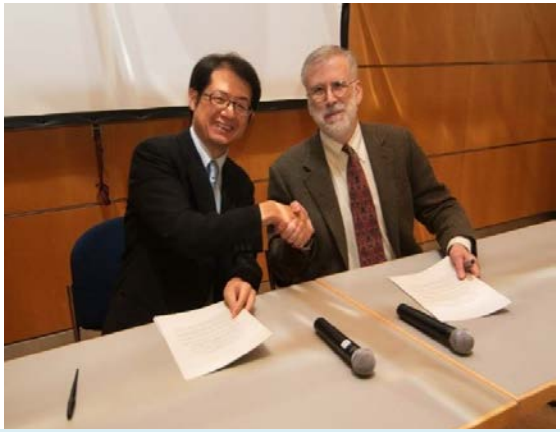
FLAGSHIP 2020 Project

- Started in 2014, aims at the development of the next Japanese flagship supercomputer, "**Post-K**"
- Led by **RIKEN** Advanced Institute of Computational Science (AICS)
- Budget of about **$1.1B**
- Follows a "**co-design**" approach, similar to the U.S.
- **Fujitsu** was selected as a vendor partner
- Applications are selected via the **Strategic Programs for Innovative Research** (SPIRE) project
  - *Fusion is a subcategory of Priority Issue #6 "Accelerated Development of Innovative Clean Energy Systems"*
- International collaborations, including collaboration between **DOE** and **MEXT** under an implementing agreement.

http://www.aics.riken.jp/en/postk/project



Post-K Development Organization

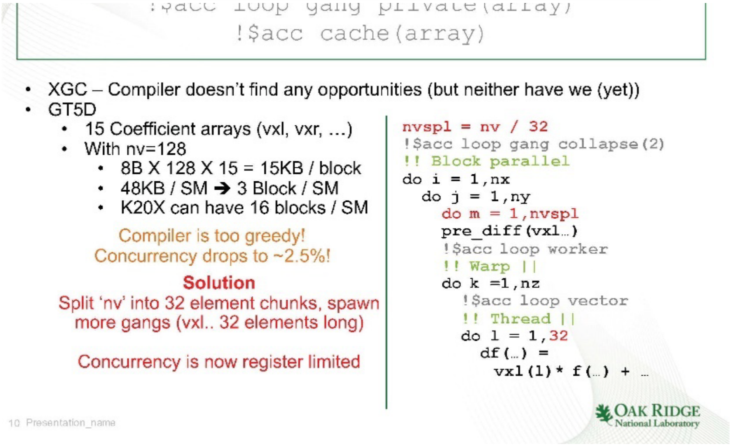


Yoshio Kawaguchi (MEXT, Japan)
and William Harrod (DOE / ASCR, USA), 2014

Japan – US Exascale Collaborations in Fusion

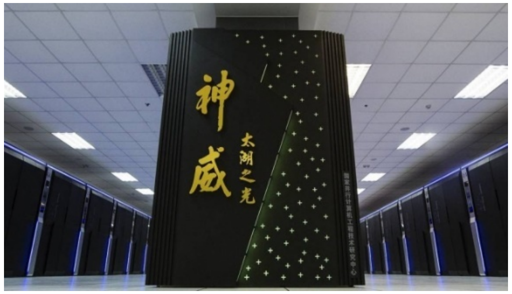
- Since 2014, a series of annual workshops was initiated to promote collaborations between the U.S. and Japanese fusion simulation projects.
- This activity is organized by the U.S. – Japan Joint Institute for Fusion Theory (JIFT) and aims to identify gaps in the scalable U.S. and Japanese fusion simulation codes and enable collaborations for addressing the common challenges in getting to the exascale.
- Current focus is on gyrokinetic (GK) codes or extended MHD codes with GK closures for energetic particle research.
- Some of the core codes included in this exercise: XGC1 (US), GENE (US), GTC (US), GKV (JP), GT5D (JP); other codes in extended MHD, RF, & materials science have also participated.

2016 workshop participants at ORNL



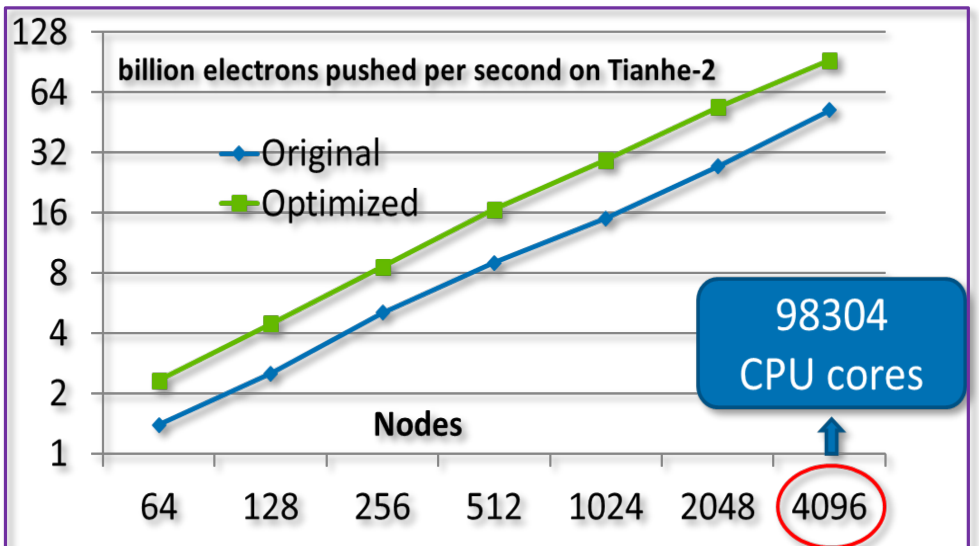
Discussions are fairly technical…

China – HPC & US Collaborations



Sunway TaihuLight, 93 PF

Tianhe-2 (TH-2), 33.6 PF



GTC weak scaling up to the full TH-2

- Although replaced as number one on the November TOP 500 list by the new 93 PF **Sunway TaihuLight** system, the 33.6 PF **Tianhe-2** system at the National Supercomputing Center in Guangzhou is a major computational resource for fusion scientists.
- The UCI-led **Gyrokinetic Toroidal Code (GTC)** group has ported the GTC code on TH-2 and benefited from collaborations with the ITER-CN Simulation Project.
  - *In 2013, GTC was highlighted as one of only two applications running at scale on TH-2*
  - *35 joint US-CN papers were published*
- Collaborations will continue to port GTC on other multi-petascale and, eventually, exascale systems.
- A version of the **GTC** code (GTC-P) has already been ported on **TaihuLight**.
- China plans to develop one exascale machine and 2-3 software centers by 2020 relying on domestic technologies.

HPC Activities in EU

Software / Application Developments*:

- The **ITER Integrated Modeling** (IM) Program developed the **Integrated Modelling & Analysis Suite** (IMAS) framework
  - *Uses the U.S.-developed* Kepler *scientific workflow application*
- **EUROfusion** established a 5-year Integrated Modeling (EU-IM) program
  - 100 scientists ~ 18 PPY + Core Support Team ~ 8 PPY
  - strong commitment to IMAS (full adoption & convergence in 2017)
- **U.S. near term plans to contribute to IMAS**:
  - Continue integration of *TRANSP* and *NUBEAM* into IMAS
  - Continue adaptation of *EFIT*, *ELITE*, *GACODE*, and *OMFIT* within IMAS
  - Apply *SOLPS-ITER* to DIII-D experiments and other applications.
- 6 **ITER Scientist Fellows** in the IM area were selected.
- Exascale planning efforts are also under way.

* *Lang Lao, 8th IMEG Meeting Report*

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EU Hardware& US Collaborations

EUROfusion secured three partitions on the Marconi Supercomputer (Marconi-Fusion)

EUROfusion

14 SEPTEMBER 2016

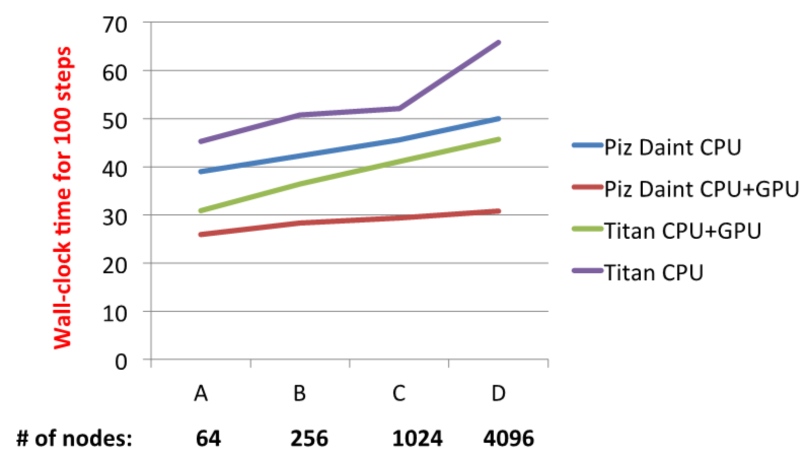
EUROFUSION: MARCONI SELECTED TO SUPPORT EUROPEAN RESEARCH ON FUSION

An all-Italian partnership between ENEA and CINECA has been selected by EUROfusion, the European Consortium for the development of fusion energy, to deliver high-performance computing and data storage to support European research on fusion.

U.S. codes scale well on Europe's fastest supercomputer

Piz Daint @ Swiss National Supercomputing Center (~9.8PF)

Weak scaling of GTC-P on Titan and Piz Daint



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Thank you!