# The Exascale Computing Project

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**HPC User Forum**

September 7, 2016, 2016

# What is the Exascale Computing Project?

- Who in this room has heard of the Exascale Computing Project?

- When we say the Exascale Computing Project – what comes to mind?
  - Hardware / systems / platforms?
  - Software / software stack?
  - Applications?

*If you were thinking ‘all the above’ – you were right.*

# What is the Exascale Computing Project?

- The ECP is a collaborative effort of two US Department of Energy (DOE) organizations – the Office of Science (DOE-SC) and the National Nuclear Security Administration (NNSA).
- As part of President Obama's National Strategic Computing initiative, ECP was established to accelerate delivery of a capable exascale computing system that integrates hardware and software capability to deliver approximately 50 to 100 times more performance than today's petaflop machines.
- ECP's work encompasses applications, system software, hardware technologies and architectures, and workforce development to meet the scientific and national security mission needs of DOE.

# The Role of ECP within NSCI

- DOE is a lead agency within NSCI, along with DoD and NSF
- In particular: DOE SC and NNSA will execute a joint effort on advanced simulation through a **capable exascale** computing program emphasizing sustained performance on relevant applications
  - This is ECP's role
- Deployment agencies: NASA, FBI, NIH, DHS, NOAA

# Approach to executing that DOE role in NSCI

- Starting this year, the Exascale Computing Project (ECP) was initiated as a DOE-SC/NNSA-ASC partnership, using DOE's formal project management processes
- The ECP is a ten-year project led by DOE laboratories and executed in collaboration with academia and industry
- The ECP leadership team has staff from six U.S. DOE labs
  - Staff from most of the 17 DOE national laboratories will take part in the project
- The ECP will collaborate with the facilities that operate DOE's most powerful computers

# Exascale Computing Project goals are derived from CD-0 mission need

| Develop scientific, engineering, and large-data applications that exploit the emerging, exascale-era computational trends caused by the end of Dennard scaling and Moore's law | Create software that makes exascale systems usable by a wide variety of scientists and engineers across a range of applications | Enable by 2023 two diverse computing platforms with up to 50× more computational capability than today's 20 PF systems, within a similar size, cost, and power footprint | Help ensure continued American leadership in architecture, software and applications to support scientific discovery, energy assurance, stockpile stewardship, and nonproliferation programs and policies |
|---|---|---|---|
| Foster application development | Ease of use | Two diverse architectures | US HPC leadership |

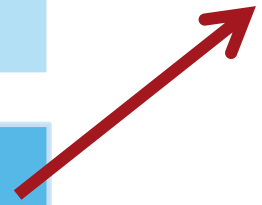
# Applications Development activities

- Fund applications development teams
  - Each aiming at capability and specific challenge problems
  - Following software engineering practices
  - Tasked to provide software and hardware requirements
  - Execute milestones jointly with software activities
- Establish co-design centers for commonly used methods
    - E.g., Adaptive Mesh Refinement, Particle-in-Cell
- Developer training

# Today We Are Pleased to Announce

Develop scientific, engineering, and large-data applications that exploit the emerging, exascale-era computational trends caused by the end of Dennard scaling and Moore's law

Foster application development



September 7, 2016

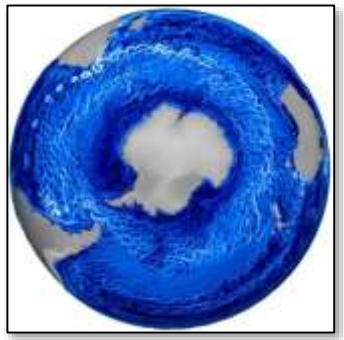
## The Exascale Computing Project (ECP) Announces $39.8 Million in First-Round Application Development Awards

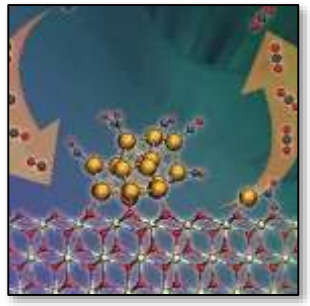
Selected 22 proposals representing teams from 45 research and academic organizations

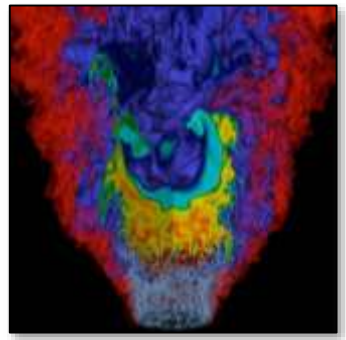
# Exascale Applications Will Address National Challenges

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 |





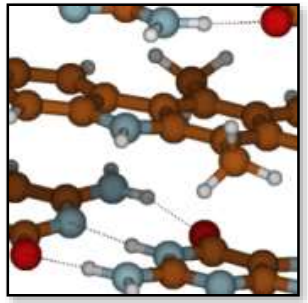


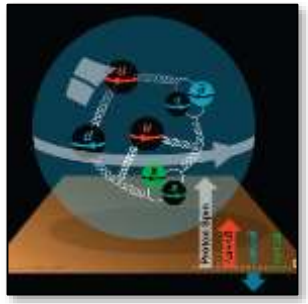
EXASCALE COMPUTING PROJECT

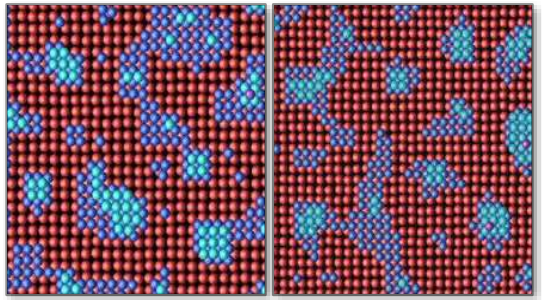
# Exascale Applications Will Address National Challenges

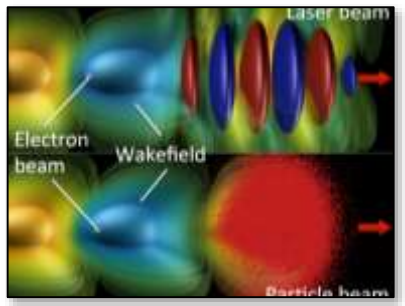
Summary of current DOE Science & Energy application development projects

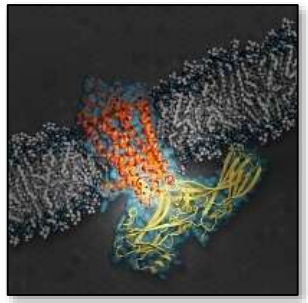
| Materials Science (BES) | Nuclear Physics (NP) | Nuclear Materials (BES, NE, FES) | Accelerator Physics (HEP) | Materials Science (BES) |
|---|---|---|---|---|
| Find, predict, and control materials and properties: property change due to hetero-interfaces and complex structures | QCD-based elucidation of fundamental laws of nature: SM validation and beyond SM discoveries | Extend nuclear reactor fuel burnup and develop fusion reactor plasma-facing materials | Practical economic design of 1 TeV electron-positron high-energy collider with plasma wakefield acceleration | Protein structure and dynamics; 3D molecular structure design of engineering functional properties |
| MGI | 2015 Long Range Plan for Nuclear Science; RHIC, CEBAF, FRIB | Climate Action Plan; MGI; Light Water Reactor Sustainability; ITER; Stockpile Stewardship Program | >30k accelerators today in industry, security, energy, environment, medicine | MGI; LCLS-II 2025 Path Forward |









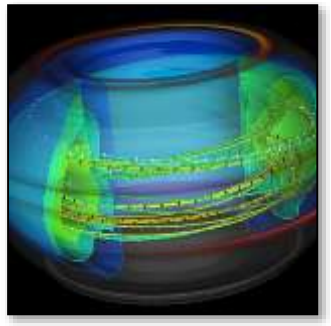


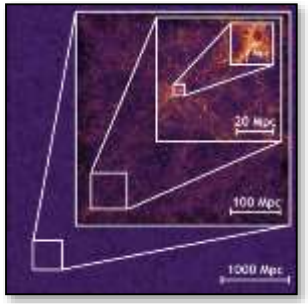
EXASCALE COMPUTING PROJECT

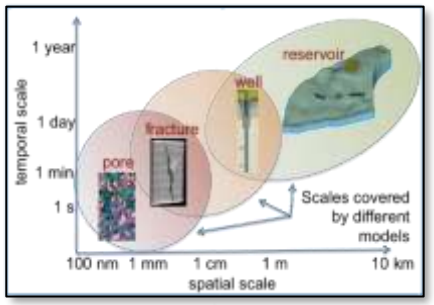
# Exascale Applications Will Address National Challenges

Summary of current DOE Science & Energy application development projects

| Magnetic Fusion Energy (FES) | Advanced Manufacturing (EERE) | Cosmology (HEP) | Geoscience (BES, BER, EERE, FE, NE) |
|---|---|---|---|
| Predict and guide stable ITER operational performance with an integrated whole device model | Additive manufacturing process design for qualifiable metal components | Cosmological probe of standard model (SM) of particle physics: Inflation, dark matter, dark energy | Safe and efficient use of subsurface for carbon capture and storage, petroleum extraction, geothermal energy, nuclear waste |
| ITER; fusion experiments: NSTX, DIII-D, Alcator C-Mod | NNMIs; Clean Energy Manufacturing Initiative | Particle Physics Project Prioritization Panel (P5) | EERE Forge; FE NRAP; Energy-Water Nexus; SubTER Crosscut |





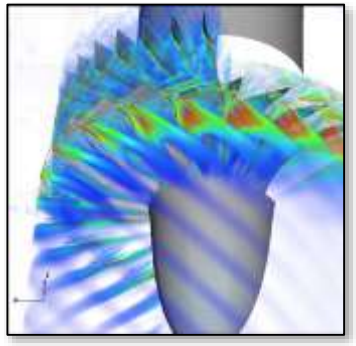


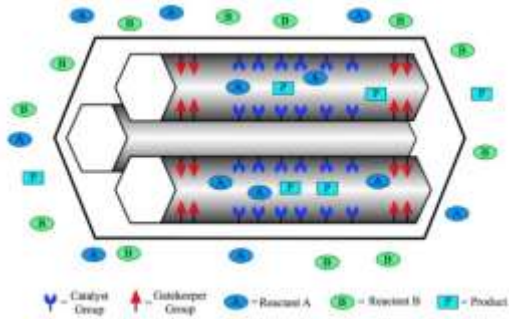

EXASCALE COMPUTING PROJECT

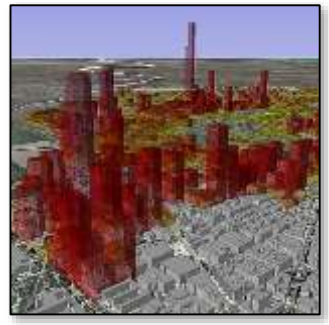
# Exascale Applications Will Address National Challenges

Summary of current DOE Science & Energy application development seed projects

| Seismic (EERE, NE, NNSA) | Carbon Capture and Storage (FE) | Chemical Science (BES) | Urban Systems Science (EERE) |
|---|---|---|---|
| Reliable earthquake hazard and risk assessment in relevant frequency ranges | Scaling carbon capture/storage laboratory designs of multiphase reactors to industrial size | Design catalysts for conversion of cellulosic-based chemicals into fuels, bioproducts | Retrofit and improve urban districts with new technologies, knowledge, and tools |
| DOE Critical Facilities Risk Assessment; urban area risk assessment; treaty verification | Climate Action Plan; SunShot; 2020 greenhouse gas/2030 carbon emission goals | Climate Action Plan; SunShot Initiative; MGI | Energy-Water Nexus; Smart Cities Initiative |







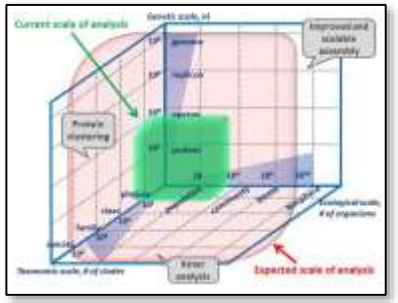


EXASCALE COMPUTING PROJECT

# Exascale Applications Will Address National Challenges

Summary of current DOE Science & Energy application development seed projects

| Metagenomics (BER) | Astrophysics (NP) | Power Grid (EERE, OE) |
|---|---|---|
| Leveraging microbial diversity in metagenomic datasets for new products and life forms | Demystify origin of chemical elements (> Fe); confirm LIGO gravitational wave and DUNE neutrino signatures | Reliably and efficiently planning our nation's grid for societal drivers: rapidly increasing renewable energy penetration, more active consumers |
| Climate Action Plan; Human Microbiome Project; Marine Microbiome Initiative | 2015 Long Range Plan for Nuclear Science; origin of universe and nuclear matter in universe | Grid Modernization Initiative; Climate Action Plan |



# Exascale Applications Will Address National Challenges

Summary of current DOE NNSA application development projects

## Stockpile Stewardship

### Gaps and Opportunities

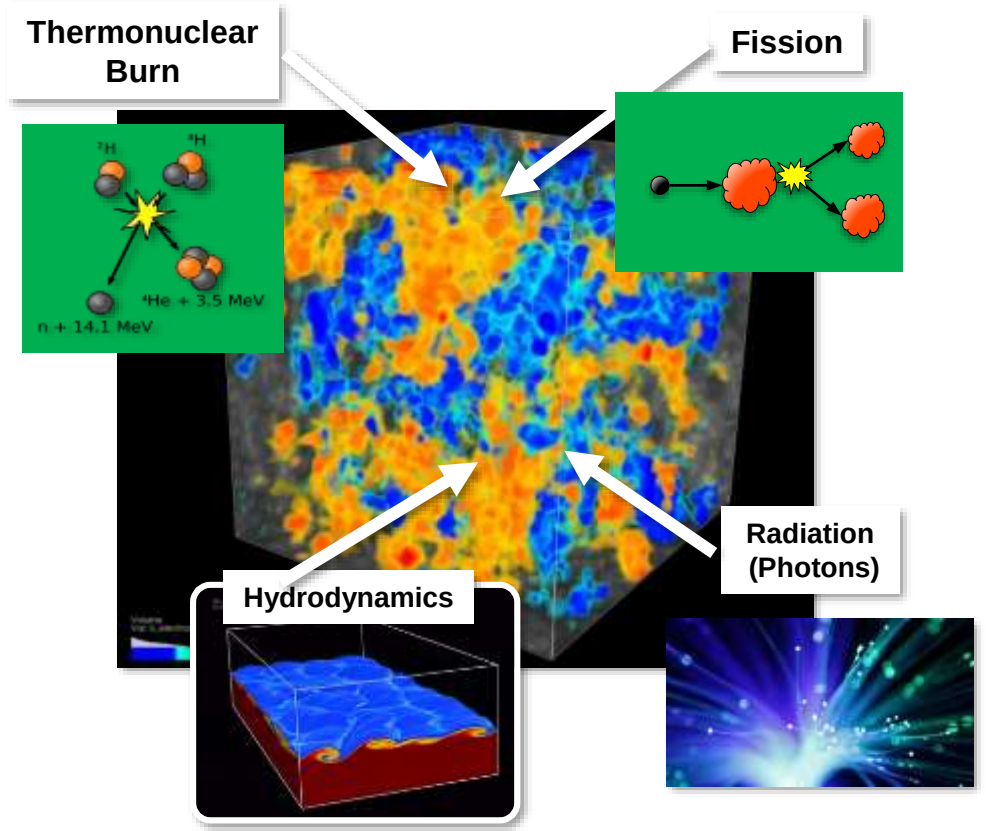
- Complete understanding of thermonuclear boost
- Resolution of important length scales with appropriate fidelity

### Simulation Challenge Problems

- 3D boost simulations with multiple coupled physical processes at unprecedented resolution
- Detailed highly resolved 3D nuclear safety simulations
- UQ performed in 3D at lower resolution with sub-grid models to capture unresolved physics

### Prospective Outcomes and Impact

- Simulation of appropriately complex material at engineering scale through formal and rigorous validation of sub-grid models
- Improved interpretation and understanding of nuclear test data
- High-confidence predictions of thermonuclear boost less dependent upon 2D calibrations



# Exascale Applications Will Address National Challenges

Summary of current Other Agency application development projects

**Precision Medicine for Cancer (NIH)**

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

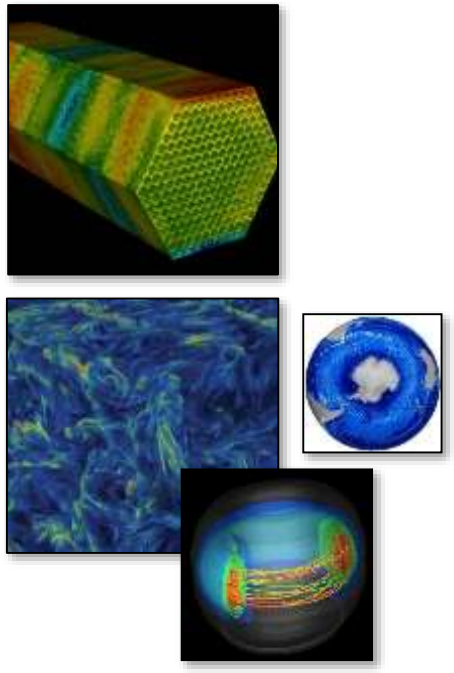
Precision Medicine in Oncology; Cancer Moonshot

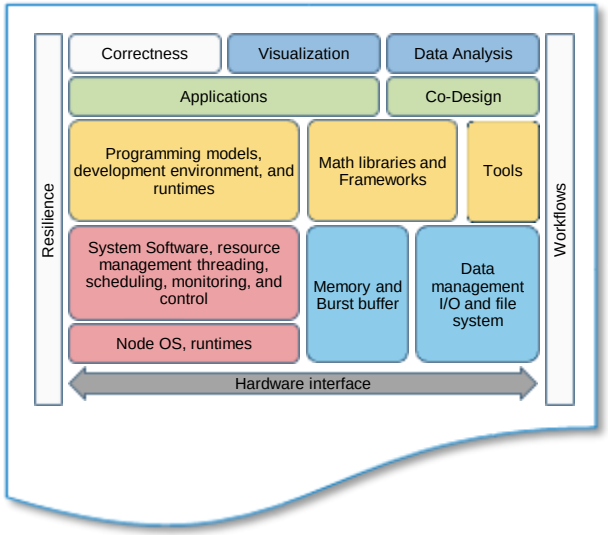
# Achieving *capable* exascale computing

- Support applications solving science problems 50× faster or more complex than today's 20 PF systems
- Operate in a power envelope of 20–30 MW
- Be sufficiently resilient (average fault rate no worse than weekly)
- At least two diverse system architectures
- Possess a software stack that meets the needs of a broad spectrum of applications
- A holistic project approach is needed that uses co-design to develop new platform, software, and computational science capabilities at heretofore unseen scale
  - Essential for tackling much deeper challenges than those that can be solved by hardware scale alone

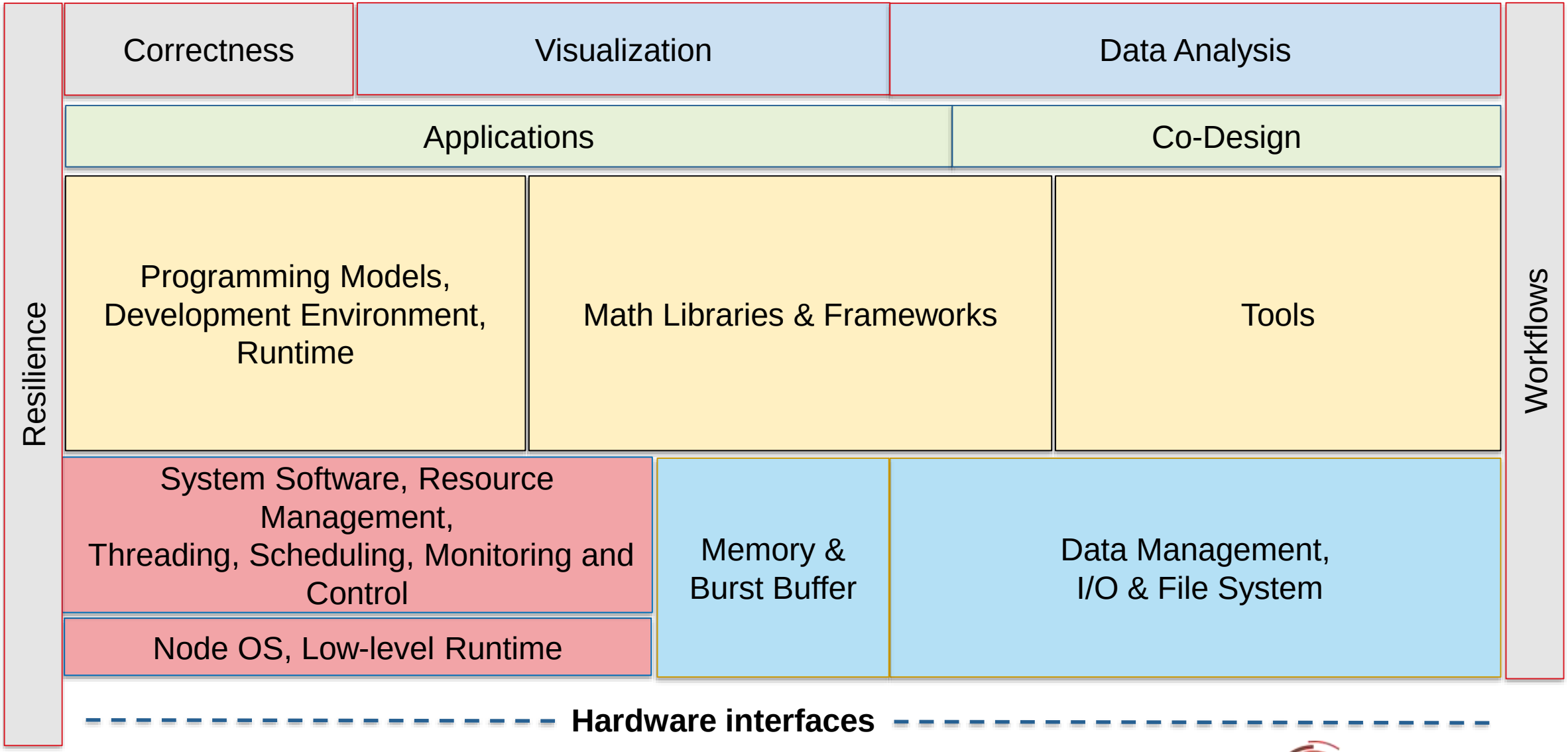
# ECP has formulated a holistic approach that uses co-design and integration to achieve capable exascale

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






# Conceptual ECP Software Stack



# Hardware Technology Activities

- PathForward: support DOE-vendor collaborative R&D activities required to develop exascale systems with at least two diverse architectural features; quote from RFP:
  - PathForward seeks solutions that will improve application performance and developer productivity while maximizing energy efficiency and reliability of exascale systems.
- Design Space Evaluation
  - Apply laboratory architectural analysis capabilities and Abstract Machine Models to PathForward designs to support ECP co-design interactions

# ECP phases

- 2016 – 2019
  - Develop applications, conduct R&D&D on software technologies
    - Use current systems, CORAL systems as testbeds
  - Vendor R&D on node and system designs that are better suited for HPC applications
- 2019
  - **ECP insights are used in formulation of RFP for exascale systems**
  - DOE and NNSA laboratories issue RFP for exascale systems, select offers, award build and NRE contracts
- 2019-2023
  - ECP Applications and software technologies are modified with knowledge of systems
  - Software technologies are “productized”
- 2023-2025
  - Exascale systems are in production, applications and software deal with actual system behavior

# ECP status

- Solicited and received proposals for
  - applications development,
  - co-design centers, and
  - software technology activities
  - Hardware technology R&D
- 22 application proposals have been selected for funding
- Co-design centers and software technology proposals are being evaluated
- Initial awards will be made this FY
- Responses to PathForward RFP (Hardware Technology R&D by vendors) have been evaluated and proposals selected for funding
  - Contracts expected to be put in place this fall

# Thank you!