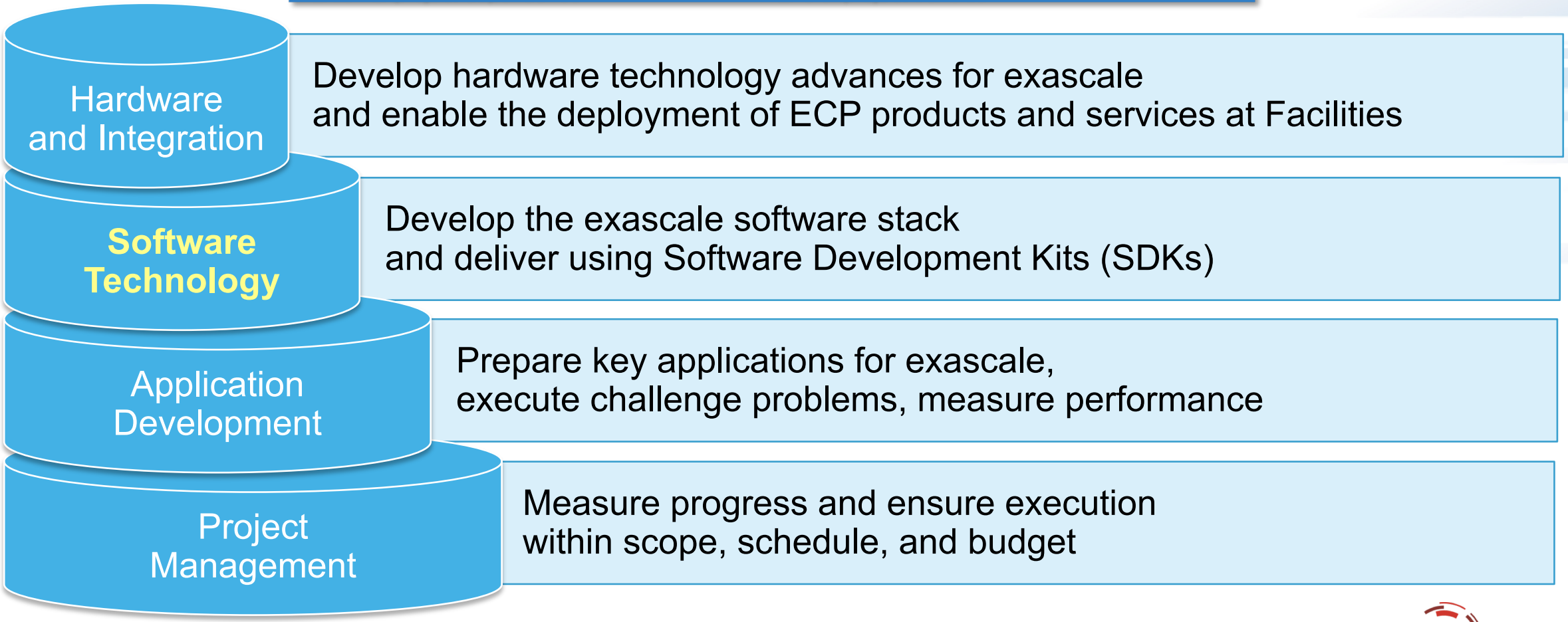
ECP Update

Douglas B. Kothe (ORNL), Director, ECP

DOE Advanced Scientific Computing Advisory Committee (ASCAC)
Washington, DC
September 17, 2018

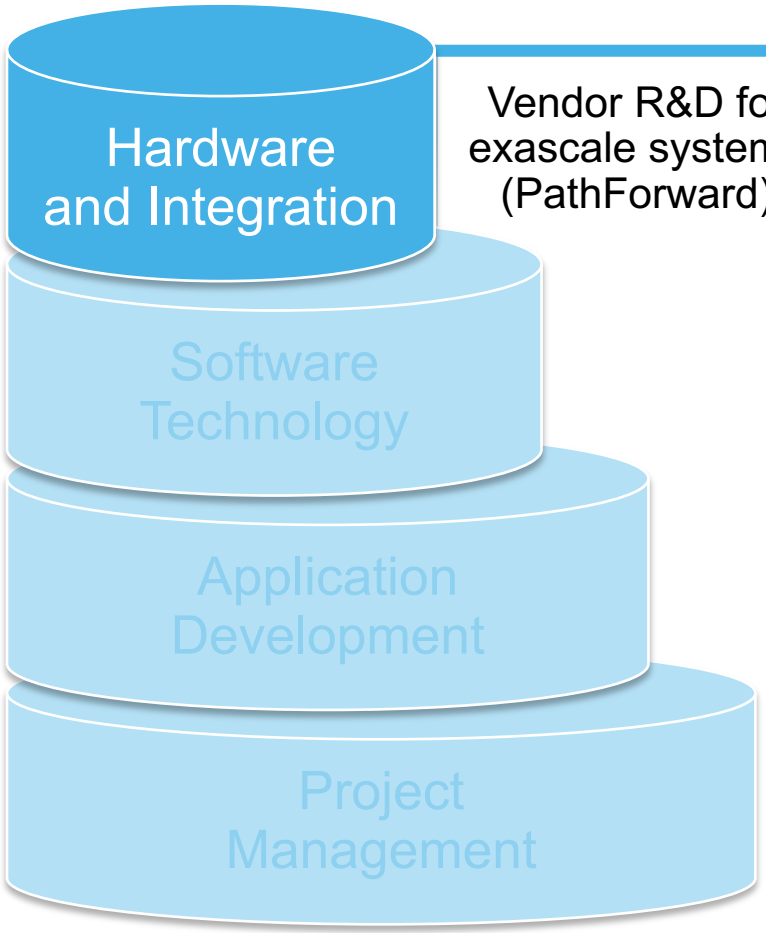
ECP is a large and complex project

ECP is Unique and Complex	
RD&D and software development nature	Broad and qualitative mission need requirements
Two sponsoring DOE programs	Outcomes both products and solutions
Numerous participating institutions	Key performance parameters require innovation
Decentralized cost system	Application of scope contingency
External project dependence	End of project transition



Hardware and Integration (HI)

Develop technology advances for exascale and deploy ECP products



Vendor R&D for exascale systems (PathForward)

Evaluation of hardware technology and performance

Software deployment and application integration at HPC facilities

Pre-exascale and exascale system utilization measurement and tracking

Community training and productivity

HI Elements

- 15 WBS L4 subprojects executing RD&D
- 141 L4 subproject milestones delivered in FY17-18

Challenges: Ensuring PathForward commitments are timely and adequate for exascale systems; deploying impactful application performance engineers; implementing co-dependent HPC facility engagement plans; deploying production-hardened software stack

Relevant US Pre-Exascale and Exascale Systems for ECP

Pre-Exascale Systems

2013

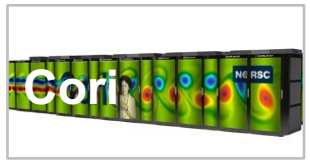
ANL
IBM BG/Q

ORNL
Cray/NVIDIA K20

LLNL
IBM BG/Q

2016

ANL
Cray/Intel KNL



LBNL
Cray/Intel
Xeon/KNL

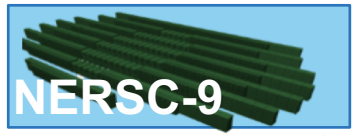
LANL/SNL
Cray/Intel
Xeon/KNL

2018

ORNL
IBM/NVIDIA
P9/Volta

LLNL
IBM/NVIDIA
P9/Volta

2020



LBNL
TBD

LANL/SNL
TBD

Exascale Systems

2021-2024

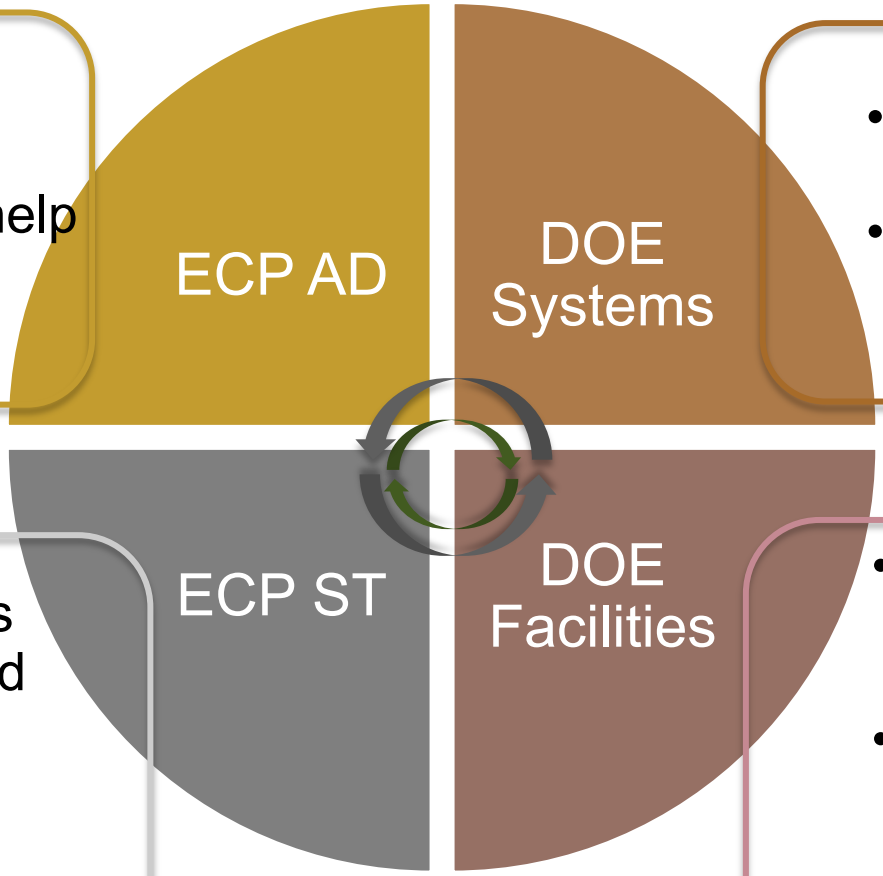
ANL
Intel/Cray TBD

ORNL
TBD

LLNL
TBD

HI provides technical capabilities to deploy and integrate ECP software and applications at the facilities and has a major role in partnering with the facilities

- Provides ASCR and vendor application performance help
- Offers training / best practices help
- Facilitates access to ASCR systems



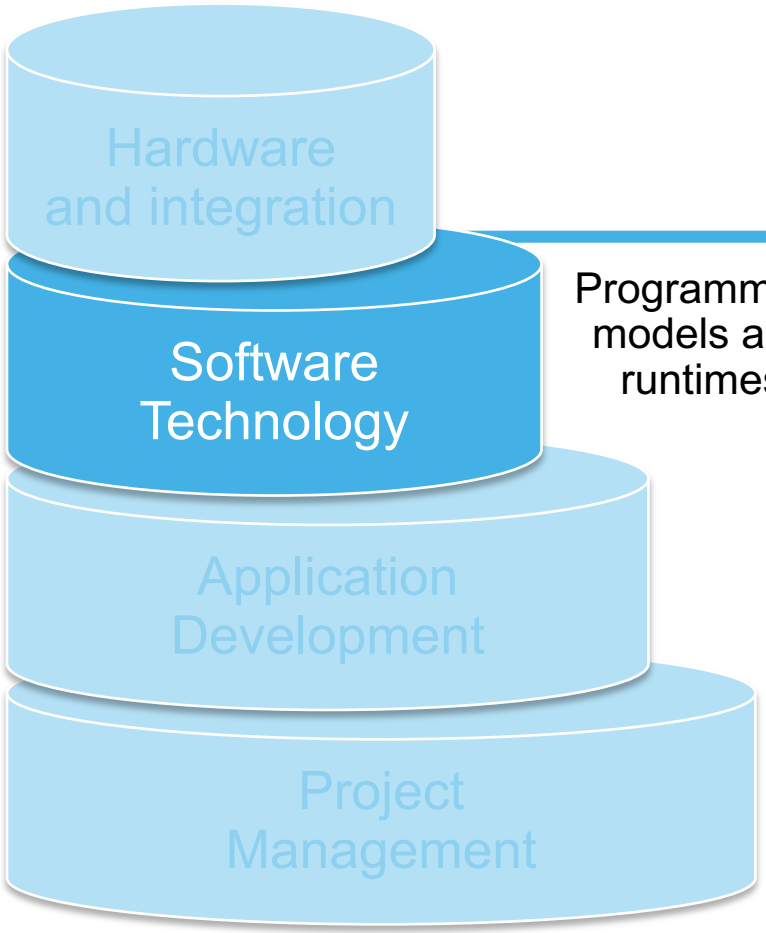
- Accelerates hardware innovations for systems
- Assesses the value of specific hardware innovations

- Deploys ST products at facilities
- Provides testing, packaging, and integration support
- Offers training / best practices
- Facilitates access to ASCR systems

- Provides add'l ASCR staff to deploy and integrate ECP ST products
- Provides additional ASCR and vendor staff to prepare ECP AD apps
- Partners with the facilities

Software Technology

Develop the exascale software stack and deliver using Software Development Kits (SDKs)



Programming models and runtimes

Development tools

Mathematical libraries

Data and visualization

Software ecosystem and delivery

ST Elements

- 55 WBS L4 subprojects executing RD&D
- ST efforts currently contribute to 89 unique products

Challenges: Qualitative changes: Massive concurrency; Multi-scale, multi-physics, data-driven science; Ecosystem integration

Software Development Kits (SDKs): A Key ST Design Feature

An important delivery vehicle for software products with a direct line of sight to AD applications

ECP software projects

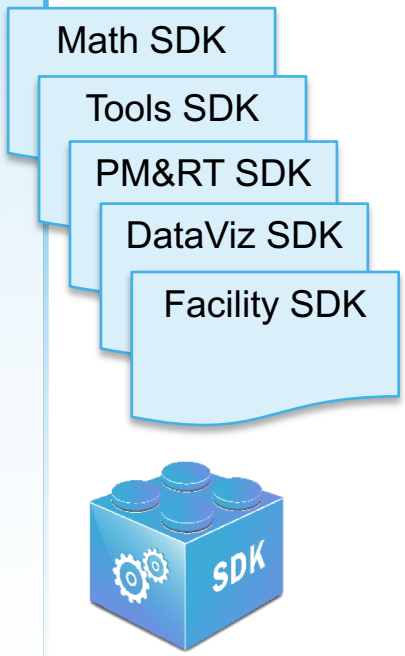
Each project to define (at least 2) release vectors

More projects ⟵ ⟶ Fewer projects

SDKs

Reusable software libraries embedded in applications; cohesive/interdependent libraries released as sets modeled on xSDK

- Regular coordinated releases
- Hierarchical collection built on Spack
- Products may belong to >1 SDK based on dependences
- Establish community policies for library development
- Apply Continuous Integration and other robust testing practices



OpenHPC

Potential exit strategy for binary distributions

- Target similar software to existing OpenHPC stack
- Develop super-scalable release targeting higher end systems

Direct2Facility

Platform-specific software in support of a specified 2021–2023 exascale system

- Software **exclusively** supporting a specific platform
- System software, some tools and runtimes

Assume all releases are delivered as “build from source” via Spack – at least initially

Focus on ensuring that software compiles robustly on all platforms of interest to ECP (including testbeds)

ECP Software Technology (ST) Capability Assessment Report

Document scope

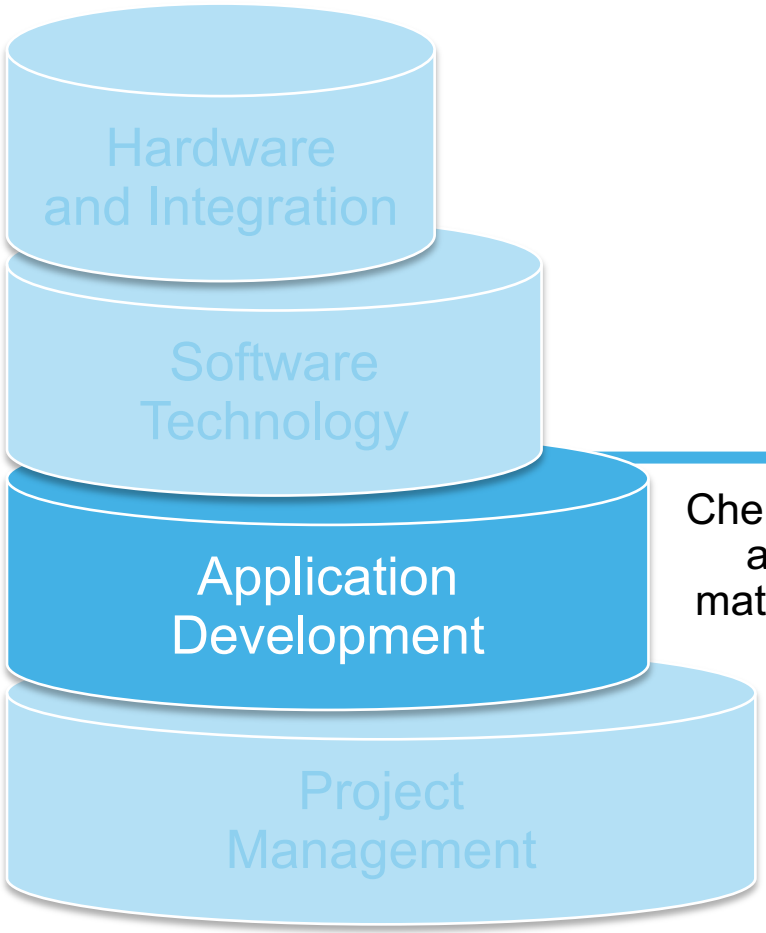
1. **Executive summary**
2. **ST approach**
   - SDKs, delivery strategy, project restructuring, new projects
3. **ST WBS L3 areas**
   - Scope, assumptions, objectives, plan, risks
4. **ST deliverables**
   - Products, standards committees, contributions to external products
5. **ST WBS L3 project summaries (55)**
   - Overview, challenges, strategy, recent progress, next steps
6. **Appendix – ECP/Stakeholder content**
   - Impact goals/metrics framework
   - **Gap and overlap analysis**
   - ASC-ASCR leverage tables

Plans to update every other quarter

Available
https://www.exascaleproject.org

Application Development

Prepare key applications for exascale, execute challenge problems, measure performance



AD Elements

- 33 WBS L4 subprojects executing RD&D
- 135 L4 subproject milestones delivered in FY17, 181 milestones in FY18

Challenges: Adopting and co-designing programming models that portably expose critical system features to attain portable, efficient performance. Dealing with extreme parallelism, increased faults, and complex node architectures.

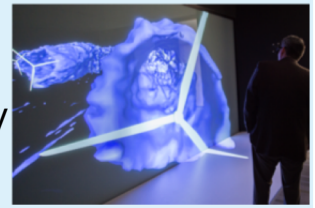
Chemistry and materials | Energy | Earth and space science | Data analytics and optimization | National security | Co-design centers

Exascale apps can deliver transformative products and solutions

Challenge problem target and impact, lead institution, stakeholder

ExaWind: Turbine Wind Plant Efficiency

Harden wind plant design and layout against energy loss susceptibility; higher penetration of wind energy



Lead: NREL
DOE EERE

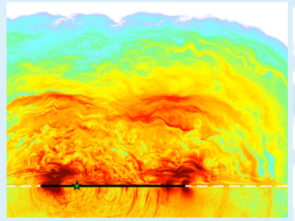
ExaAM: Additive Manufacturing of Qualifiable Metal Parts

Accelerate the widespread adoption of AM by enabling routine fabrication of qualifiable metal parts

Lead: ORNL
DOE NNSA / EERE

EQSIM: Earthquake Hazard Risk Assessment

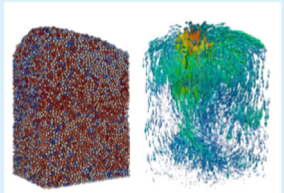
Replace conservative and costly earthquake retrofits with safe purpose-fit retrofits and designs



Lead: LBNL
DOE NNSA / NE, EERE

MFIX-Exa: Scale-up of Clean Fossil Fuel Combustion

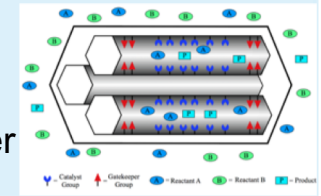
Commercial-scale demo of transformational energy technologies - curbing CO_2 emissions at fossil fuel power plants by 2030



Lead: NETL
DOE EERE

GAMESS: Biofuel Catalyst Design

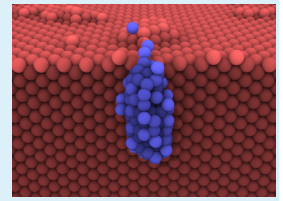
Design more robust and selective catalysts orders of magnitude more efficient at temperatures hundreds of degrees lower



Lead: Ames
DOE BES

EXAALT: Materials for Extreme Environments

Simultaneously address time, length, and accuracy requirements for predictive microstructural evolution of materials



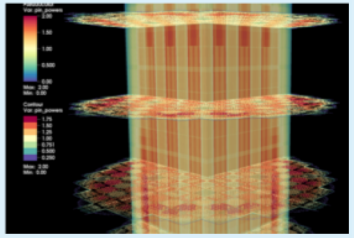
Lead: LANL
DOE BES, FES, NE

Exascale apps can deliver transformative products and solutions

Challenge problem target and impact, lead institution, stakeholder

ExaSMR: Design and Commercialization of Small Modular Reactors

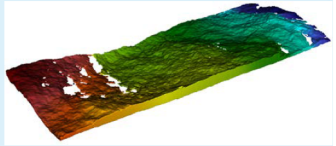
Virtual test reactor for advanced designs via experimental-quality simulations of reactor behavior



Lead: ORNL
DOE NE

Subsurface: Carbon Capture, Fossil Fuel Extraction, Waste Disposal

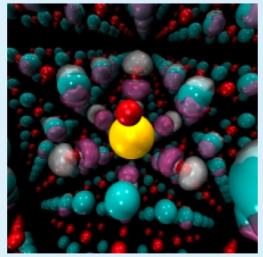
Reliably guide safe long-term consequential decisions about storage, sequestration, and exploration



Lead: LBNL
DOE BES, EERE, FE, NE

QMCPACK: Find, Predict, Control Materials & Properties at Quantum Level

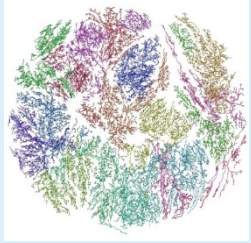
Design and optimize next-generation materials from first principles with predictive accuracy



Lead: ORNL
DOE BES

ExaSGD: Reliable and Efficient Planning of the Power Grid

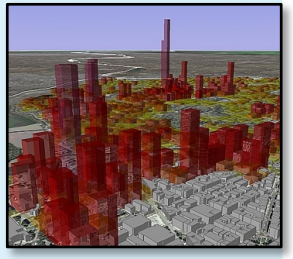
Optimize power grid planning, operation, control and improve reliability and efficiency



Lead: PNNL
DOE EDER, CESER, EERE

Urban: Urban Systems Science

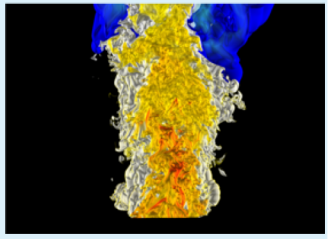
Evaluate energy codes and integration, retrofits, transportation, financing; integrate microgrids and renewables



Lead: ANL
DOE EERE, BER

Combustion-PELE: High-Efficiency, Low-Emission Combustion Engine Design

Reduction or elimination of current cut-and-try approaches for combustion system design



Lead: SNL
DOE BES, EERE

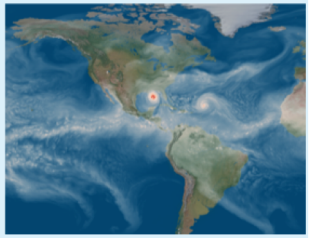
Exascale apps can deliver transformative products and solutions

Challenge problem target and impact, lead institution, stakeholder

E3SM-MMF: Accurate Regional Impact Assessment in Earth Systems

Forecast water resources and severe weather with increased confidence; address food supply changes

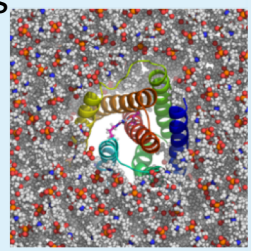
Lead: SNL
DOE BER



NWChemEx: Catalytic Conversion of Biomass-Derived Alcohols

Develop new optimal catalysts while changing the current design processes that remain costly, time consuming, and dominated by trial-and-error

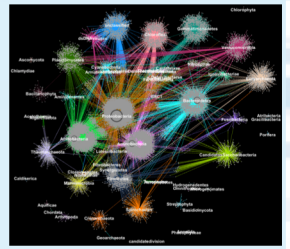
Lead: PNNL
DOE BER, BES



ExaBiome: Metagenomics for Analysis of Biogeochemical Cycles

Discover knowledge useful for environmental remediation and the manufacture of novel chemicals and medicines

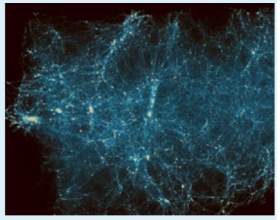
Lead: LBNL
DOE BER



ExaSky: Cosmological Probe of the Standard Model of Particle Physics

Unravel key unknowns in the dynamics of the Universe: dark energy, dark matter, and inflation

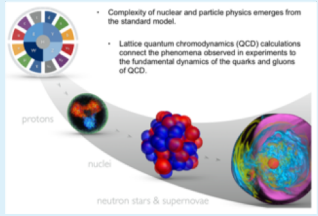
Lead: ANL
DOE HEP



LatticeQCD: Validate Fundamental Laws of Nature

Correct light quark masses; properties of light nuclei from first principles; <1% uncertainty in simple quantities

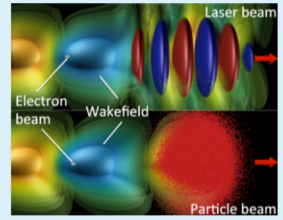
Lead: FNAL
DOE NP, HEP



WarpX: Plasma Wakefield Accelerator Design

Virtual design of 100-stage 1 TeV collider; dramatically cut accelerator size and design cost

Lead: LBNL
DOE HEP

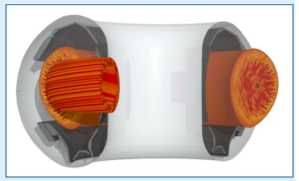


Exascale apps can deliver transformative products and solutions

Challenge problem target and impact, lead institution, stakeholder

WDMApp: High-Fidelity Whole Device Modeling of Magnetically Confined Fusion Plasmas

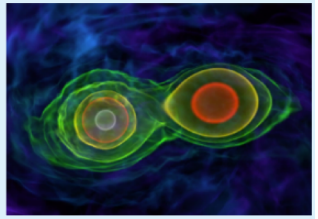
Prepare for ITER experiments and increase ROI of validation data and understanding; prepare for beyond-ITER devices



Lead: PPPL
DOE FES

ExaStar: Demystify Origin of Chemical Elements

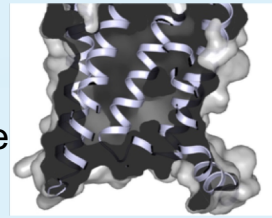
What is the origin of the elements? Behavior of matter at extreme densities? Sources of gravity waves?



Lead: LBNL
DOE NP

ExaFEL: Light Source-Enabled Analysis of Protein and Molecular Structure and Design

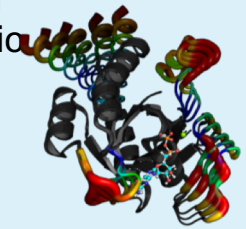
Process data without beam time loss; determine nanoparticle size & shape changes; engineer functional properties in biology and material science



Lead: SLAC
DOE BES

CANDLE: Accelerate and Translate Cancer Research

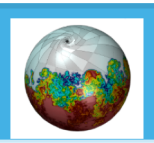
Develop predictive pre-clinical models & accelerate diagnostic and targeted therapy thru predicting mechanisms of RAS/RAF driven cancers



Lead: ANL
NIH

Exascale Multiphysics Applications for National Security Mission

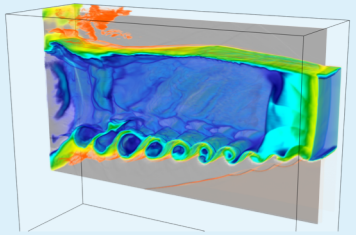
ECP application projects in the NNSA ASC ATDM program element



The MARBL Multi-physics Code

Multi-physics simulations of high energy-density physics and focused experiments driven by high-explosive, magnetic or laser based energy sources

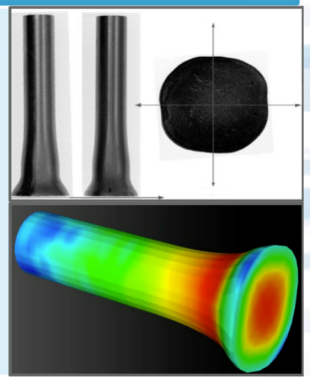
- Magneto-radiation-hydrodynamics at the exascale
- Next-generation pulsed power / ICF modeling
- High-order numerical methods



Lead: LLNL

Ristra: Next-Generation Multi-physics for National-Security Applications

– 3D multi-physics for national-security mission
– Mesoscale insight for extreme-condition materials
– Exascale high energy density physics simulations



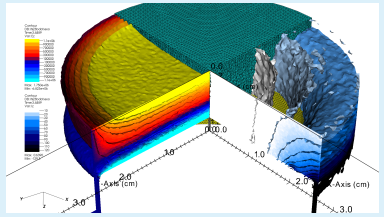
A Ristra hydrodynamics code with an advanced grain-structure-aware material model captures the asymmetric deformation in Taylor-Anvil experiments

Lead: LANL

EMPIRE for Electromagnetic Plasma Physics

Computing electronic effects induced by ionizing radiation interacting with materials under various re-entry flight conditions

Self-consistent plasma simulation including the radiation output of a hostile builder device, radiation transport, plasma generation and propagation down through the effects on ND system electronics

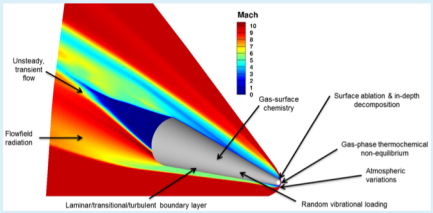


Lead: SNL

SPARC for Virtual Flight Testing

Virtual flight test of re-entry vehicles from exo-atmospheric bus separation to target for normal and hostile environments.

State-of-the-art hypersonic flight simulation capability on next-generation hardware, including thermo-chemical non-equilibrium gas ablation models, and hybrid RANS-LES turbulence models.



Lead: SNL

ExaLearn: New ECP Center for ML Co-Design

PI Frank Alexander, BNL
Members: ANL, LANL, LBNL, LLNL, ORNL, PNNL, SNL

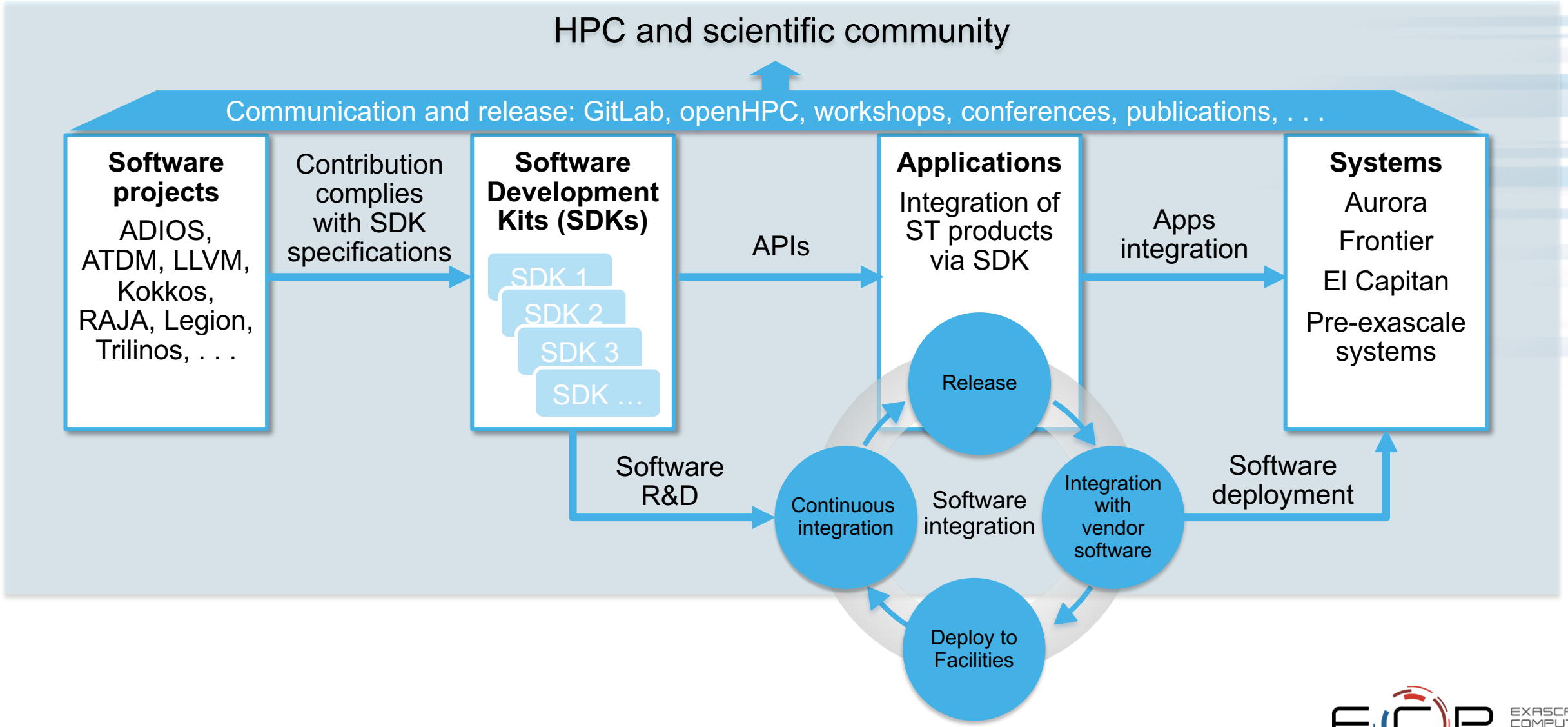
- AI, as a form a data analytics focused on model building, has the potential to accelerate scientific discovery or enable prediction in areas currently too complex for direct simulation
- Some AI use cases
  - Classification and regression, including but not limited to image classification and analysis, e.g. scientific data output from DOE experimental facilities or from national security programs.
  - Surrogate models in high-fidelity and multiscale simulations, including uncertainty quantification and error estimation.
  - Structure-to-function relationships, including genome-to-phenome, the prediction of materials performance based on atomistic structures, or the prediction of performance margins based on manufacturing data.
  - Control systems, e.g., for wind plants, nuclear power plants, experimental steering and autonomous vehicles.
  - Inverse problems and optimization. This area would include, for example, inverse imaging and materials design.
- Areas in need of research
  - Data quality and statistics
  - Learning algorithms
  - Physics-Informed AI
  - Verification and Validation
  - Performance and scalability
  - Workflow and deployment

Expected Work Product

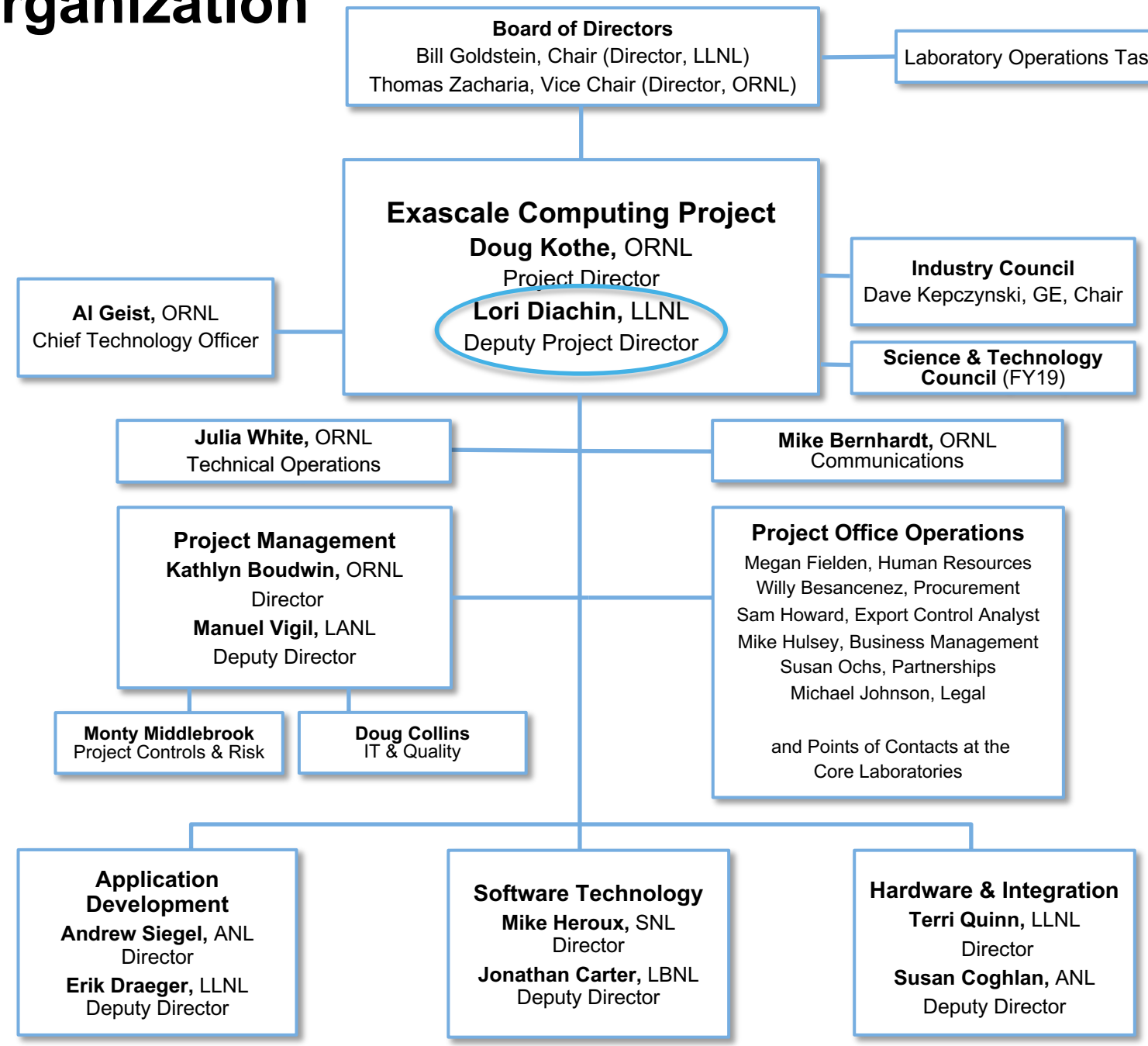
A toolset that . . .

- Is applicable to multiple problems within the DOE mission
- Has a line-of-sight to exascale computing, e.g. through using exascale platforms directly, or providing essential components to an exascale workflow
- Does not replicate capabilities easily obtainable from existing, widely-available packages

ECP's Flow of Product Delivery and Deployment



ECP Organization



Core Laboratories

OAK RIDGE National Laboratory

Argonne NATIONAL LABORATORY

BERKELEY LAB Lawrence Berkeley National Laboratory

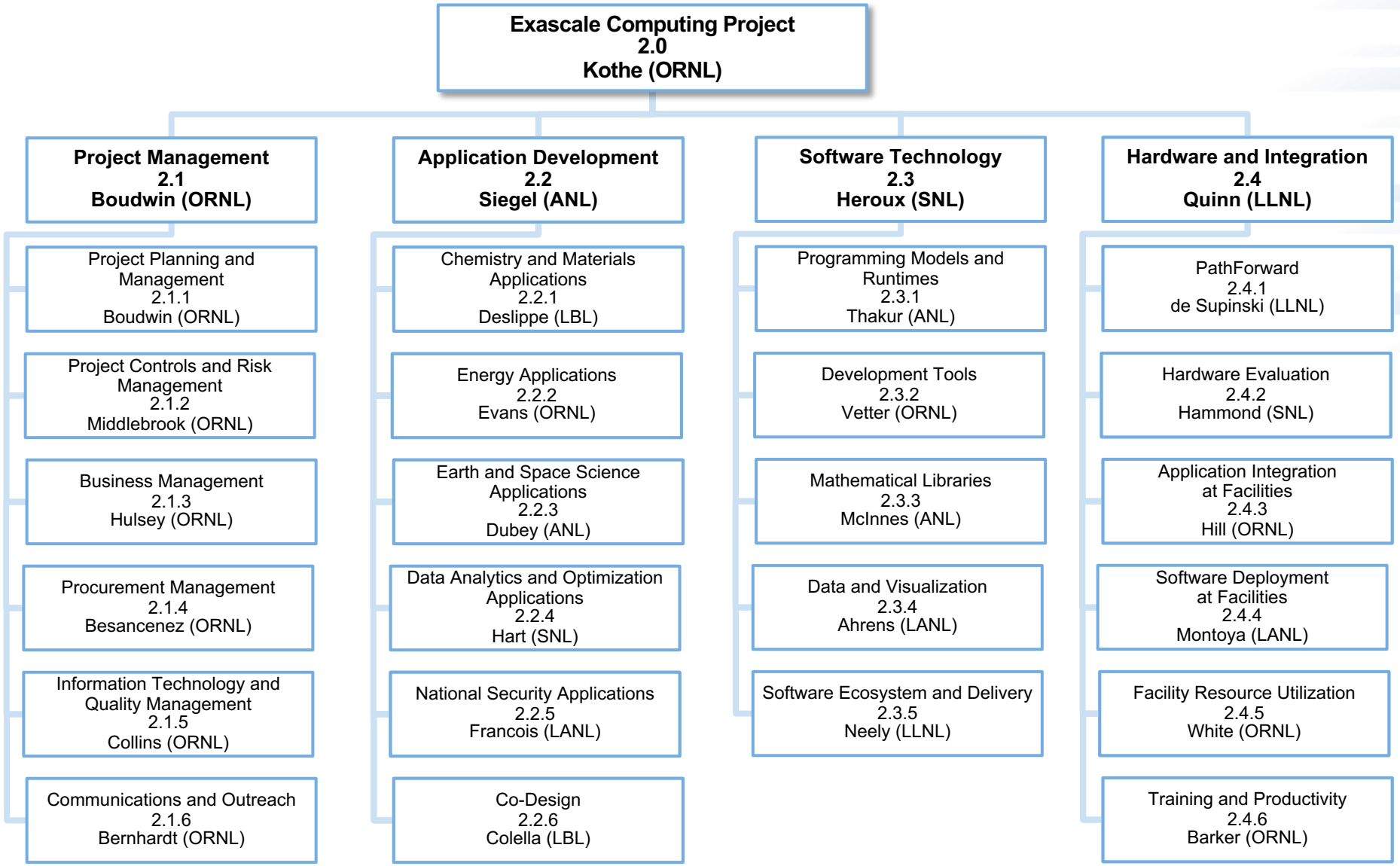
Lawrence Livermore National Laboratory

Los Alamos NATIONAL LABORATORY

Sandia National Laboratories

ECP EXASCALE COMPUTING PROJECT

ECP Work Breakdown Structure



WBS L2 and L3 leadership unchanged over the last year

ECP Progress in past 10 Months: Summary

Technical Accomplishments

- Revised and refined timeline and FY19 – FY23 plans
- AD: Apps in full swing, with measurable progress; Co-Design Centers making impact; all apps with better defined challenge problems and performance metrics
- ST: SDKs moving with 1st release scheduled; deep dive assessment performed; WBS L4 impact goals/metrics defined; 89 products tracked as they evolve
- HI: Tangible PathForward progress; apps priorities being established at Facilities; SDKs CI plan underway

Technical Accomplishments

- Numerous milestones delivered and subjected to expert scrutiny (including external reviews)
- HI Key Milestone milestone delivered (Q2 FY18) – PathForward assessment
- ST Key Milestone delivered (Q3 FY18) – comprehensive Capability Assessment Report
- Key Performance Parameters refined, quantified, on track, and on project dashboard – see clear path to convergence by CD-2 review (Q4 FY19)

Project Management

- Implemented performance measurement plan and associated project dashboard
- WBS L4 milestone lifecycle (creation, definition, tracking, review) defined, documented, understood
- Addressed mission need gaps and mitigated selected risks with cost contingency
- Formulated and implemented proactive responses to recommendations from recent reviews
- Close and constructive Project Office working relationships established with L2/L3 technical leadership

Stakeholder Relations

- Selected ECP leaders participated in CORAL2 RFP
- Co-authored Facilities engagement plan and co-dependent milestones
- Collaborations with DOE sponsors/stakeholders, other federal agencies (NSF, DoD, NASA), participating institutions, Industry Council, BOD, LOTF, WBS L4 PIs