EXASCALE COMPUTING PROJECT

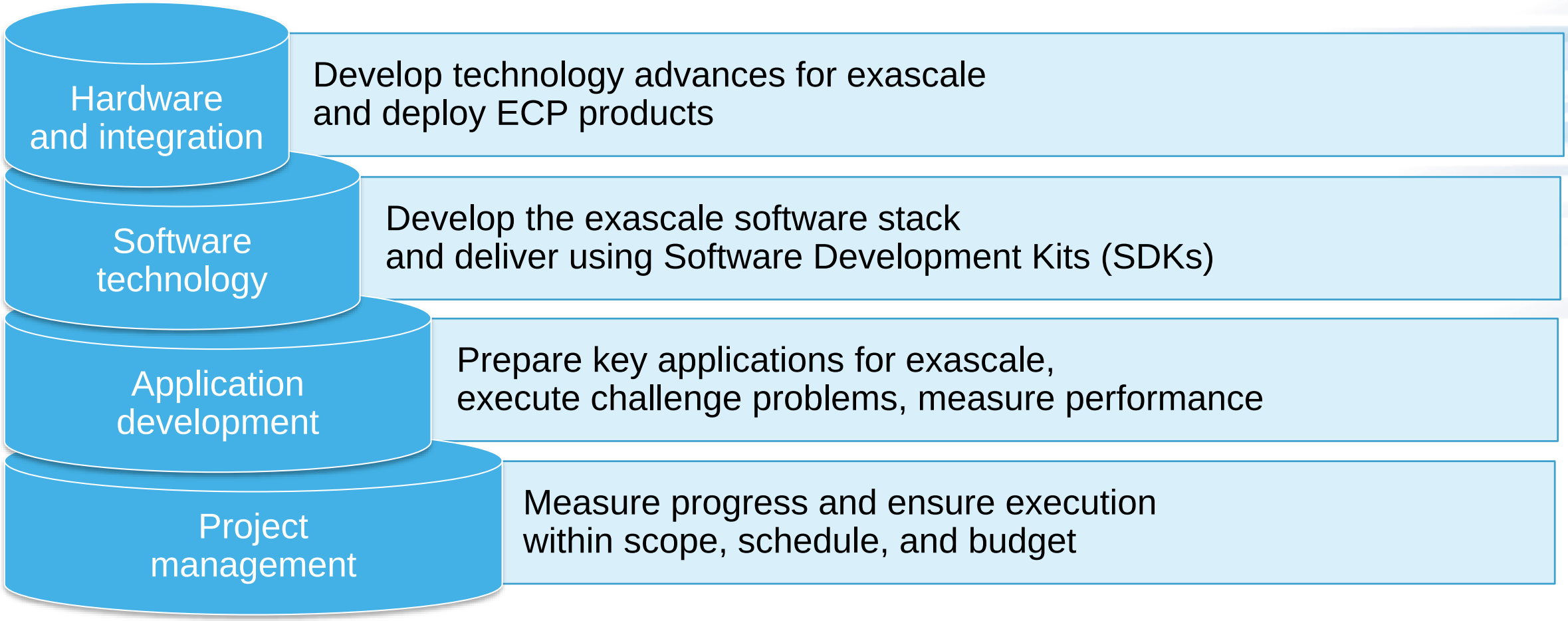
The Exascale Computing Project Software Stack

Michael A. Heroux, Sandia National Laboratories
Director of Software Technology, Exascale Computing Project

High End Computing (HEC) Interagency Working Group (IWG)
July 19, 2018

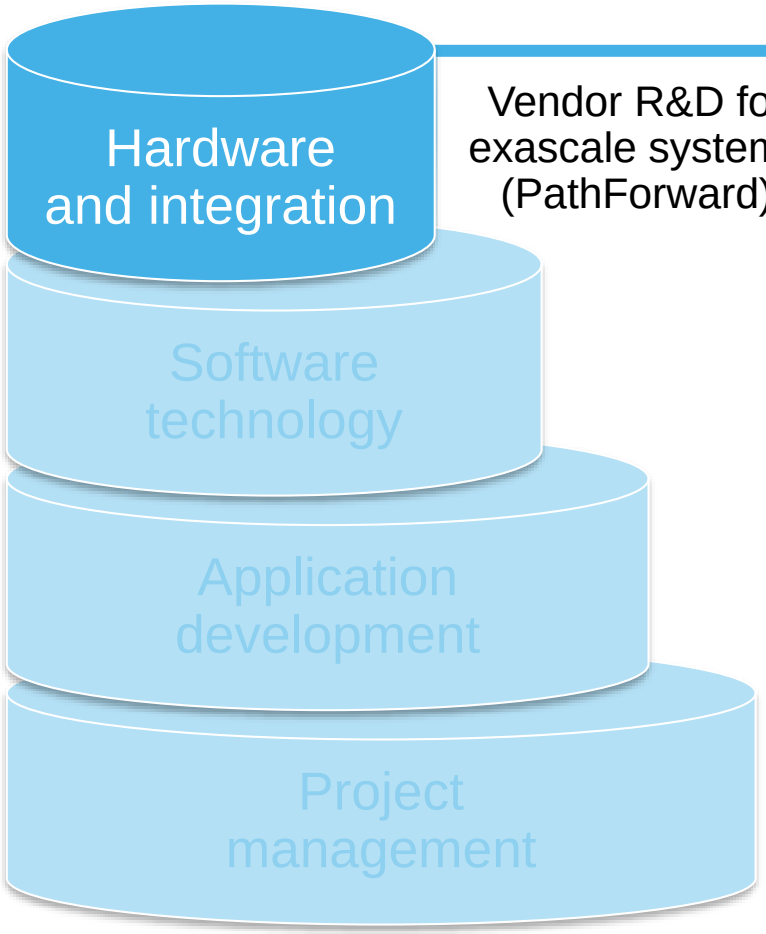
U.S. DEPARTMENT OF ENERGY | Office of Science
National Nuclear Security Administration

ECP is a large, complex project
Spanning the nation and structured for success



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

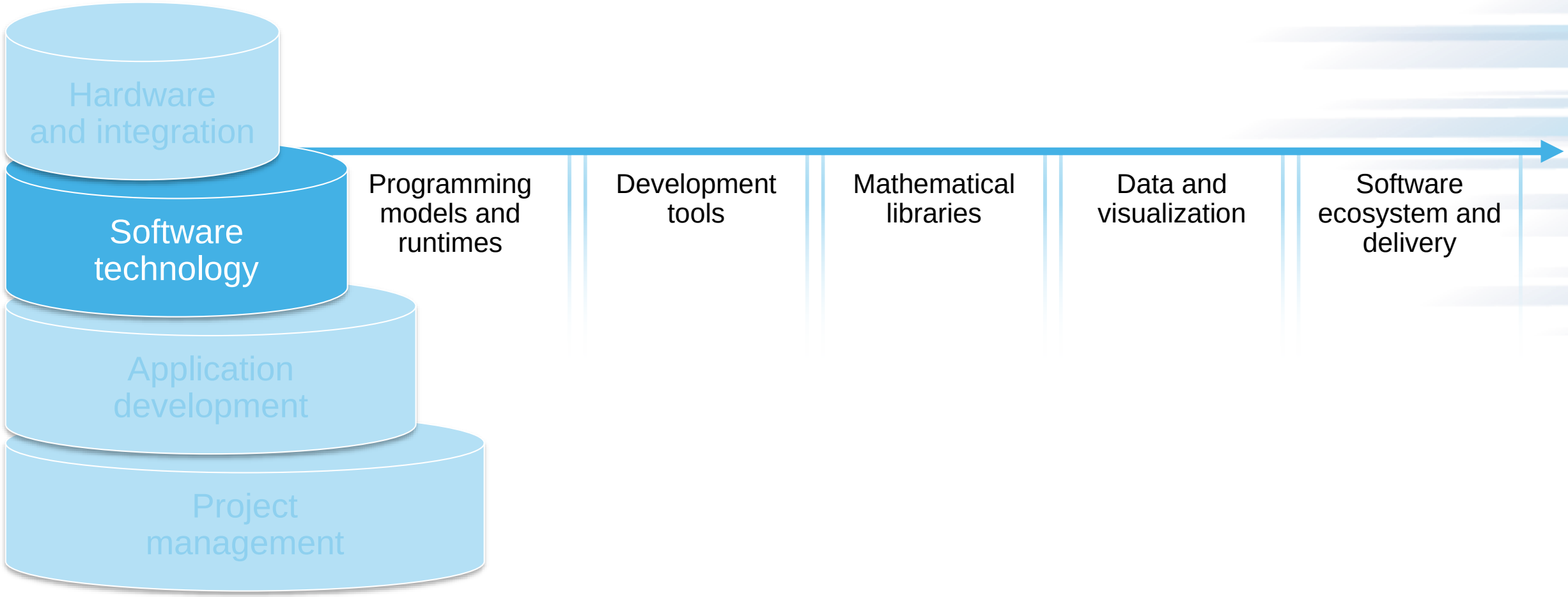
Software deployment and application integration at HPC facilities

Pre-exascale and exascale system utilization measurement and tracking

Community training and productivity

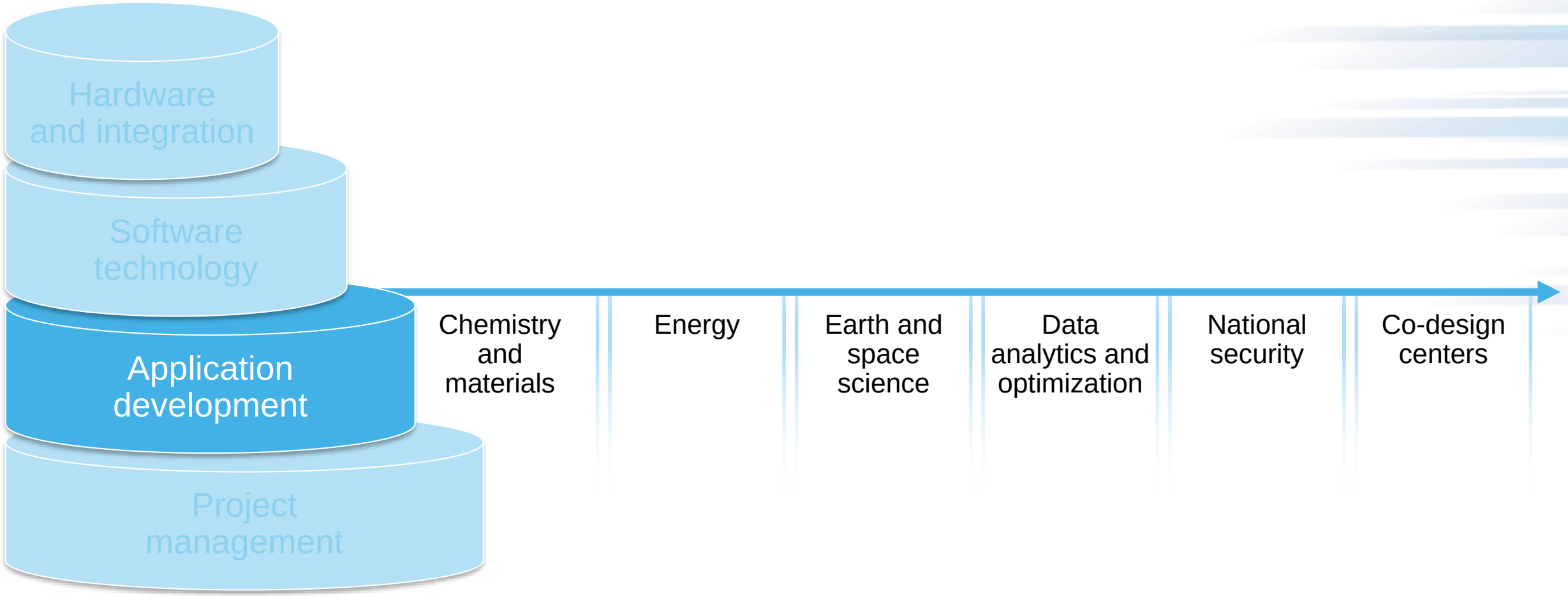
Software technology (ST)

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



Application development (AD)

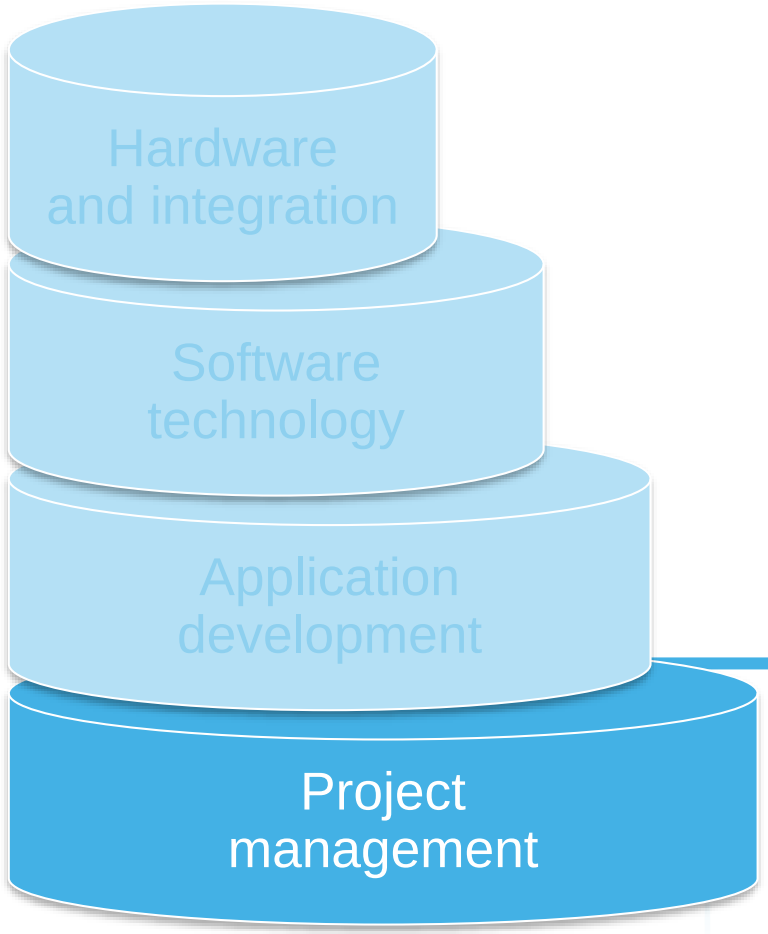
Prepare key applications for exascale, execute challenge problems, measure performance



EXASCALE COMPUTING PROJECT

Project management (PM)

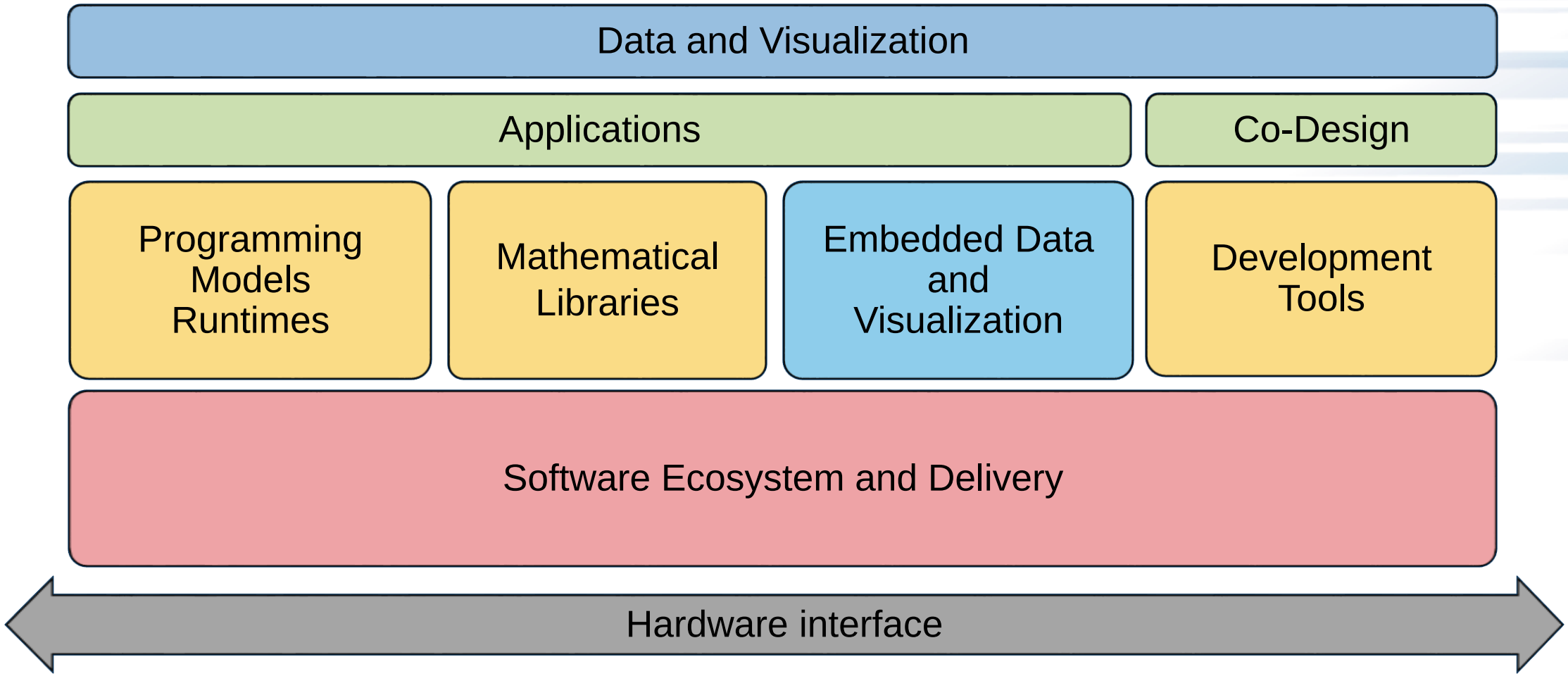
Measure progress and ensure execution within scope, schedule, and budget



- Project planning
- Project controls and risk
- Business manage-ment
- Procure-ment manage-ment
- Information technology and quality manage-ment
- Commun-ication and outreach

Overview of ECP Software Technology

ECP SW Stack: Strategic Alignment and Synergies



ECP Software: Productive, sustainable ecosystem

Goal

Build a comprehensive, coherent software stack that enables application developers to productively write highly parallel applications that effectively target diverse exascale architectures

- Extend current technologies to exascale where possible

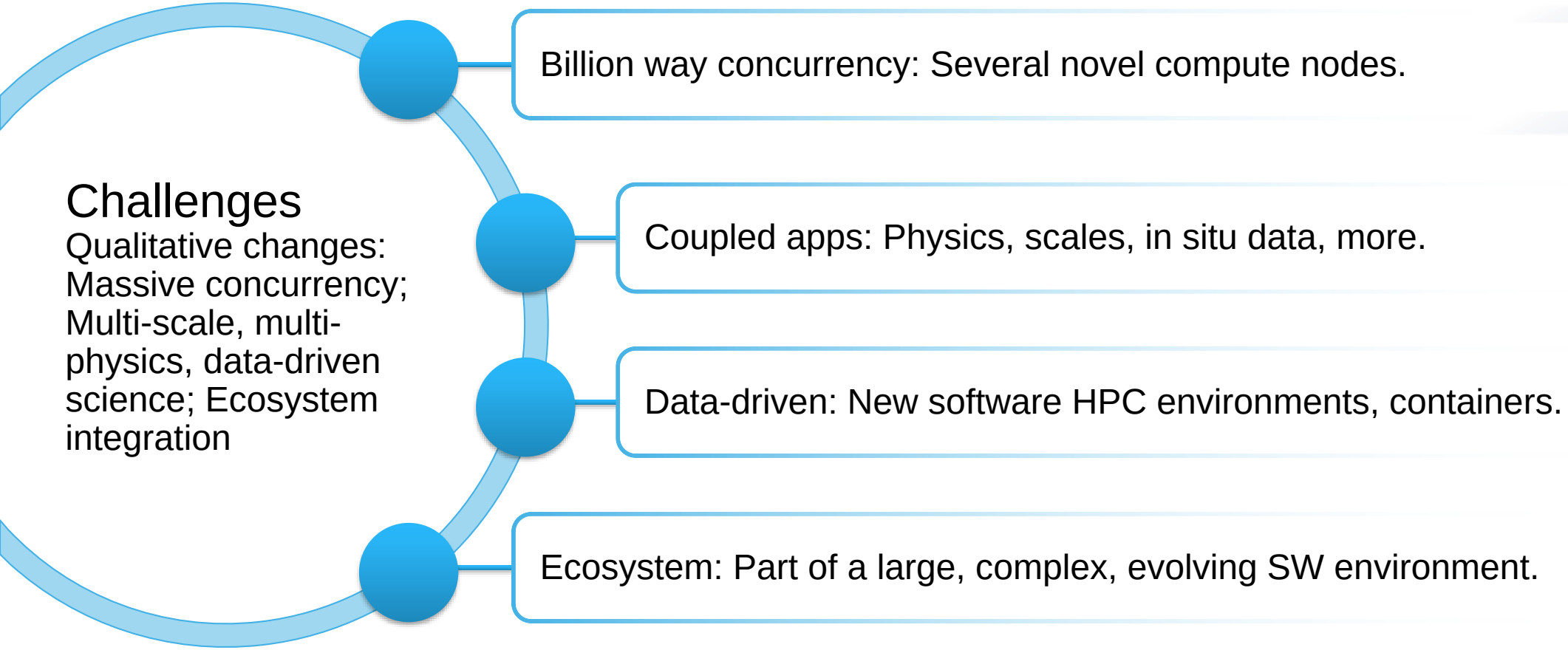
- Perform R&D required for new approaches when necessary

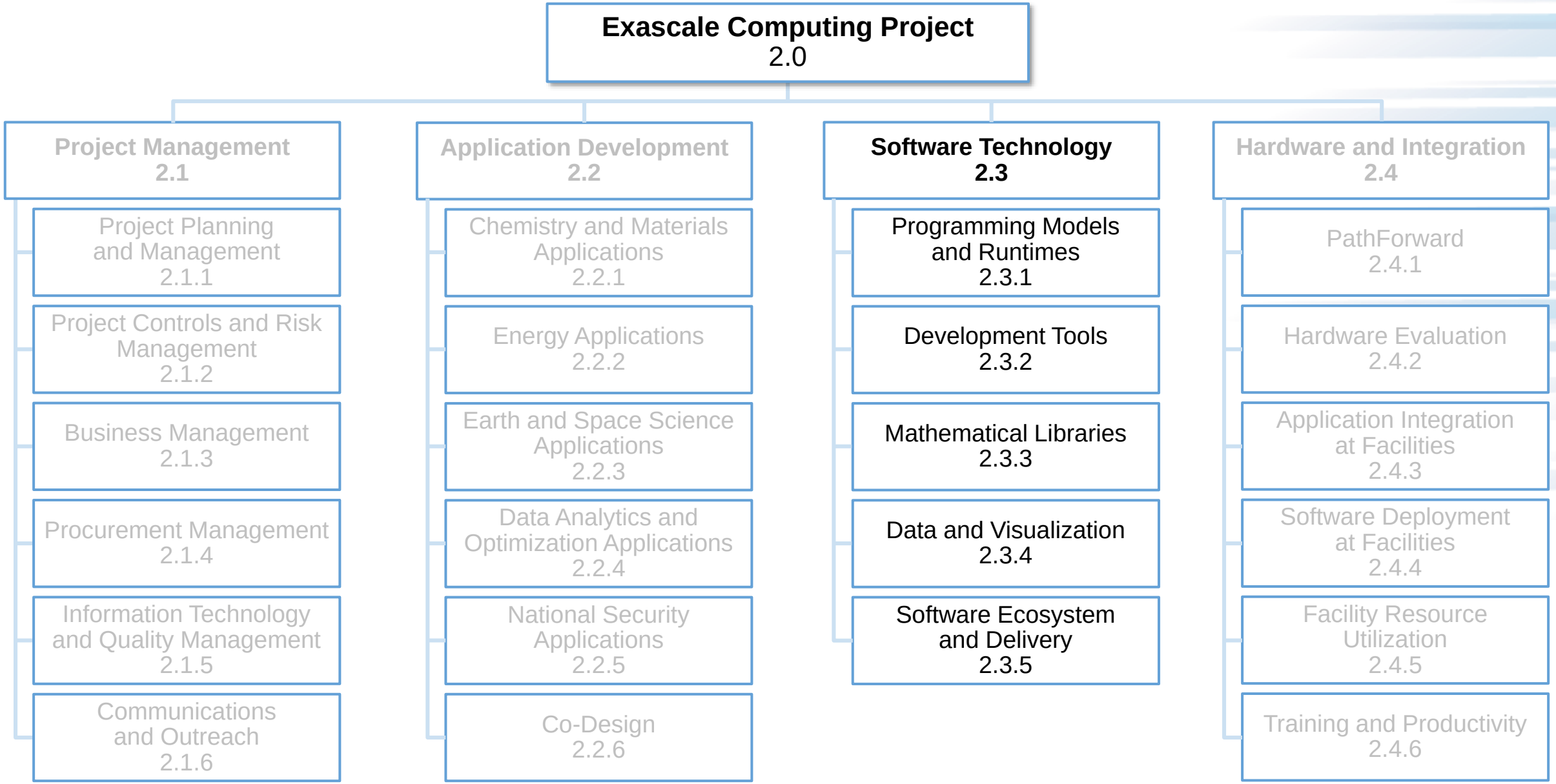
- Coordinate with and complement vendor efforts

- Develop and deploy high-quality and robust software products

55 WBS L4 subprojects executing RD&D
185 L4 subproject (P6) milestones delivered in FY17
67 delivered so far in FY18, 77 in progress right now
564 L4 subproject (P6) milestones planned in FY18-19

ECP software: Challenges




Exascale Computing Project
2.0
Project Management
2.1
Project Planning and Management
2.1.1
Project Controls and Risk Management
2.1.2
Business Management
2.1.3
Procurement Management
2.1.4
Information Technology and Quality Management
2.1.5
Communications and Outreach
2.1.6
Application Development
2.2
Chemistry and Materials Applications
2.2.1
Energy Applications
2.2.2
Earth and Space Science Applications
2.2.3
Data Analytics and Optimization Applications
2.2.4
National Security Applications
2.2.5
Co-Design
2.2.6
Software Technology
2.3
Programming Models and Runtimes
2.3.1
Development Tools
2.3.2
Mathematical Libraries
2.3.3
Data and Visualization
2.3.4
Software Ecosystem and Delivery
2.3.5
Hardware and Integration
2.4
PathForward
2.4.1
Hardware Evaluation
2.4.2
Application Integration at Facilities
2.4.3
Software Deployment at Facilities
2.4.4
Facility Resource Utilization
2.4.5
Training and Productivity
2.4.6

ECP Software Technology Leadership Team

Mike Heroux, Software Technology Director
Mike has been involved in scientific software R&D for 30 years. His first 10 were at Cray in the LIBSCI and scalable apps groups. At Sandia he started the Trilinos and Mantevo projects, is author of the HPCG benchmark for TOP500, and leads productivity and sustainability efforts for DOE.

Jonathan Carter, Software Technology Deputy Director
Jonathan has been involved in the support and development of HPC applications for chemistry, the procurement of HPC systems, and the evaluation of novel computing hardware for over 25 years. He currently a senior manager in Computing Sciences at Berkeley Lab.

Rajeev Thakur, Programming Models and Runtimes (2.3.1)
Rajeev is a senior computer scientist at ANL and most recently led the ECP Software Technology focus area. His research interests are in parallel programming models, runtime systems, communication libraries, and scalable parallel I/O. He has been involved in the development of open source software for large-scale HPC systems for over 20 years.

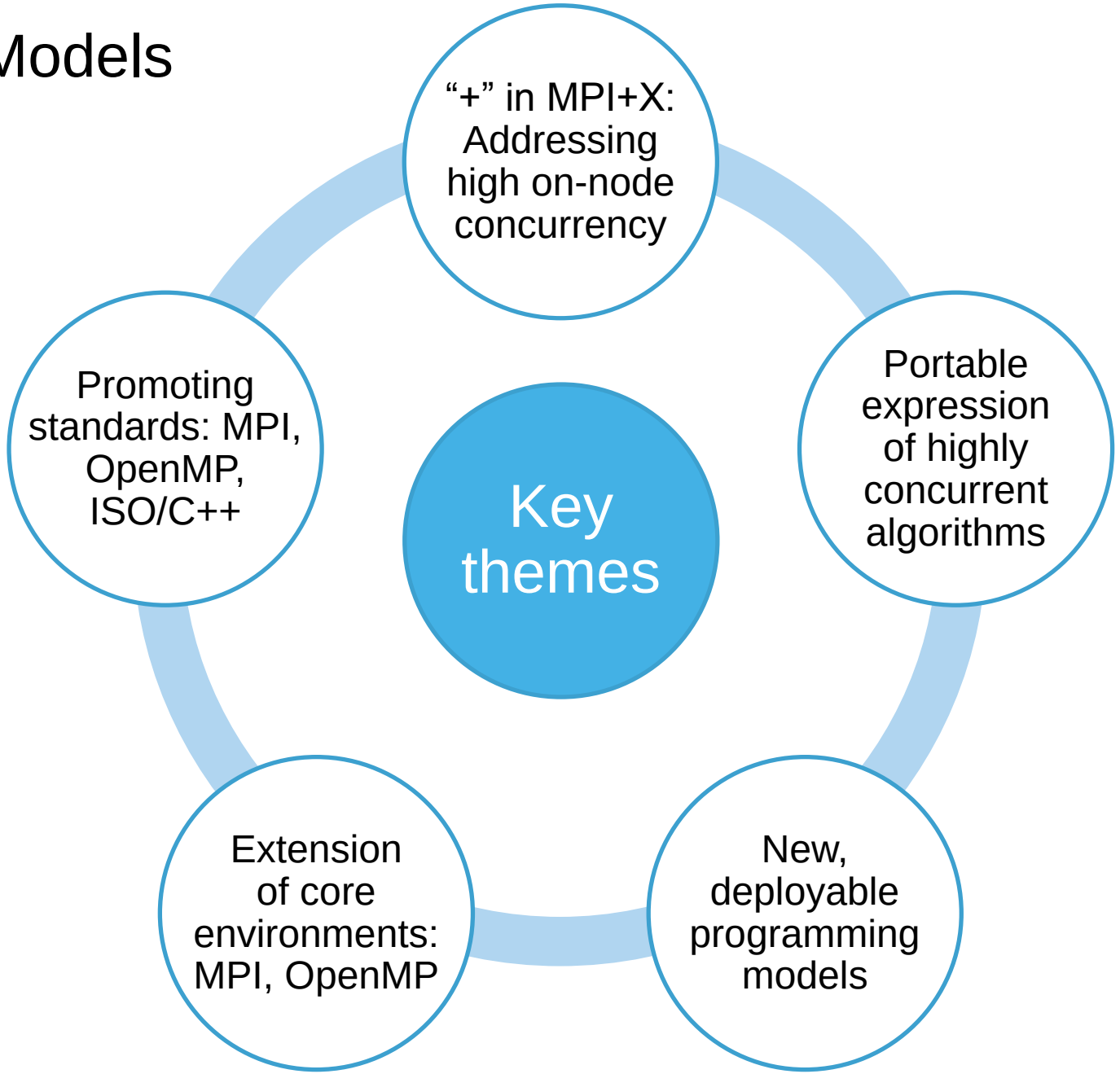
Jeff Vetter, Development Tools (2.3.2)
Jeff is a computer scientist at ORNL, where he leads the Future Technologies Group. He has been involved in research and development of architectures and software for emerging technologies, such as heterogeneous computing and nonvolatile memory, for HPC for over 15 years.

Lois Curfman McInnes, Math Libraries (2.3.3)
Lois is a senior computational scientist in the Mathematics and Computer Science Division of ANL. She has over 20 years of experience in high-performance numerical software, including development of PETSc and leadership of multi-institutional work toward sustainable scientific software ecosystems.

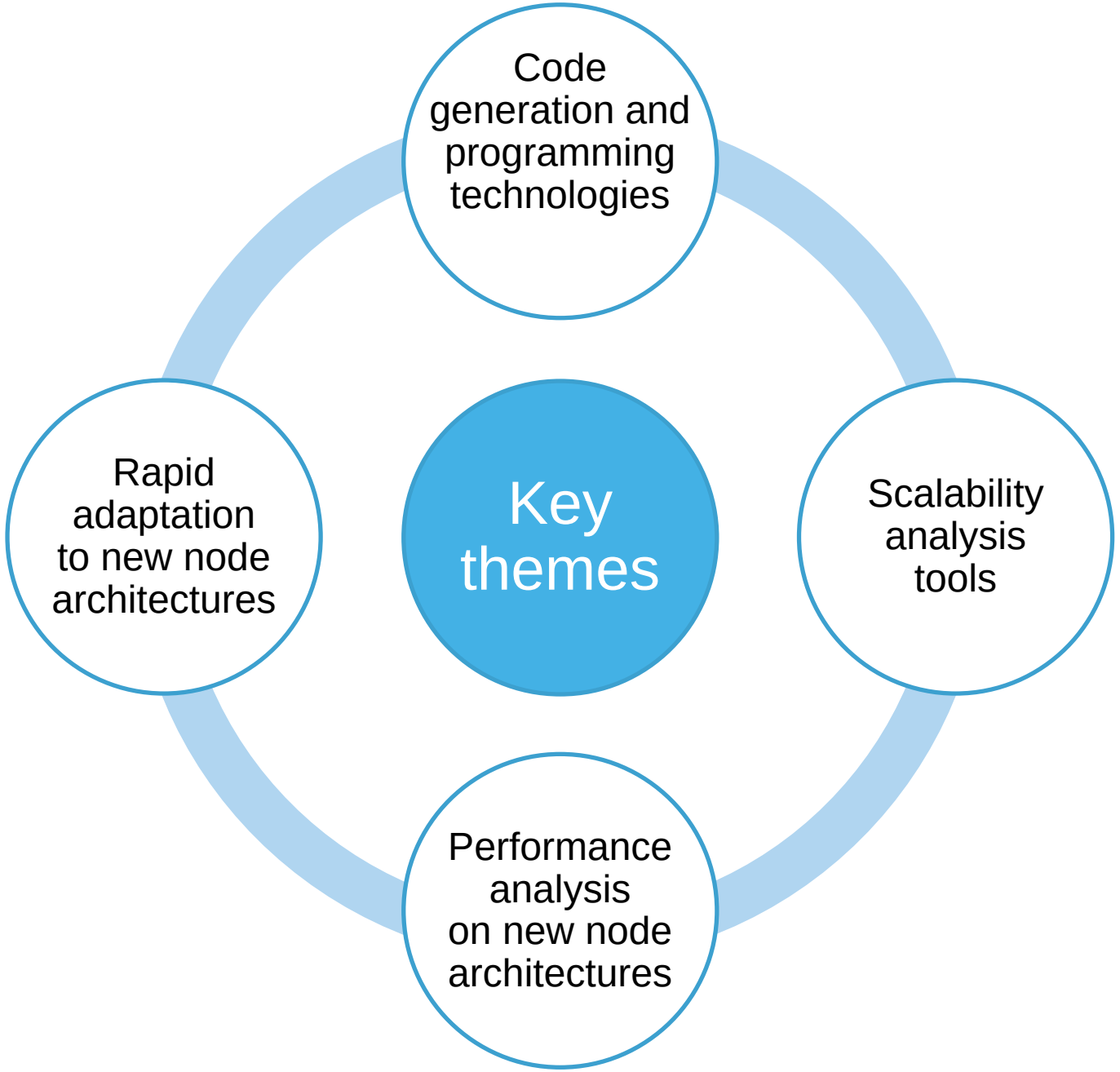
Jim Ahrens, Data and Visualization (2.3.4)
Jim is a senior research scientist at the Los Alamos National Laboratory (LANL) and an expert in data science at scale. He started and actively contributes to many open-source data science packages including ParaView and Cinema.

Rob Neely, Software Ecosystem and Delivery (2.3.5)
Rob has several leadership roles at LLNL spanning applications, CS research, platforms, and vendor interactions. He is an Associate Division Leader in the Center for Applied Scientific Computing (CASC), chair of the Weapons Simulation and Computing Research Council, and the lead for the Sierra Center of Excellence.

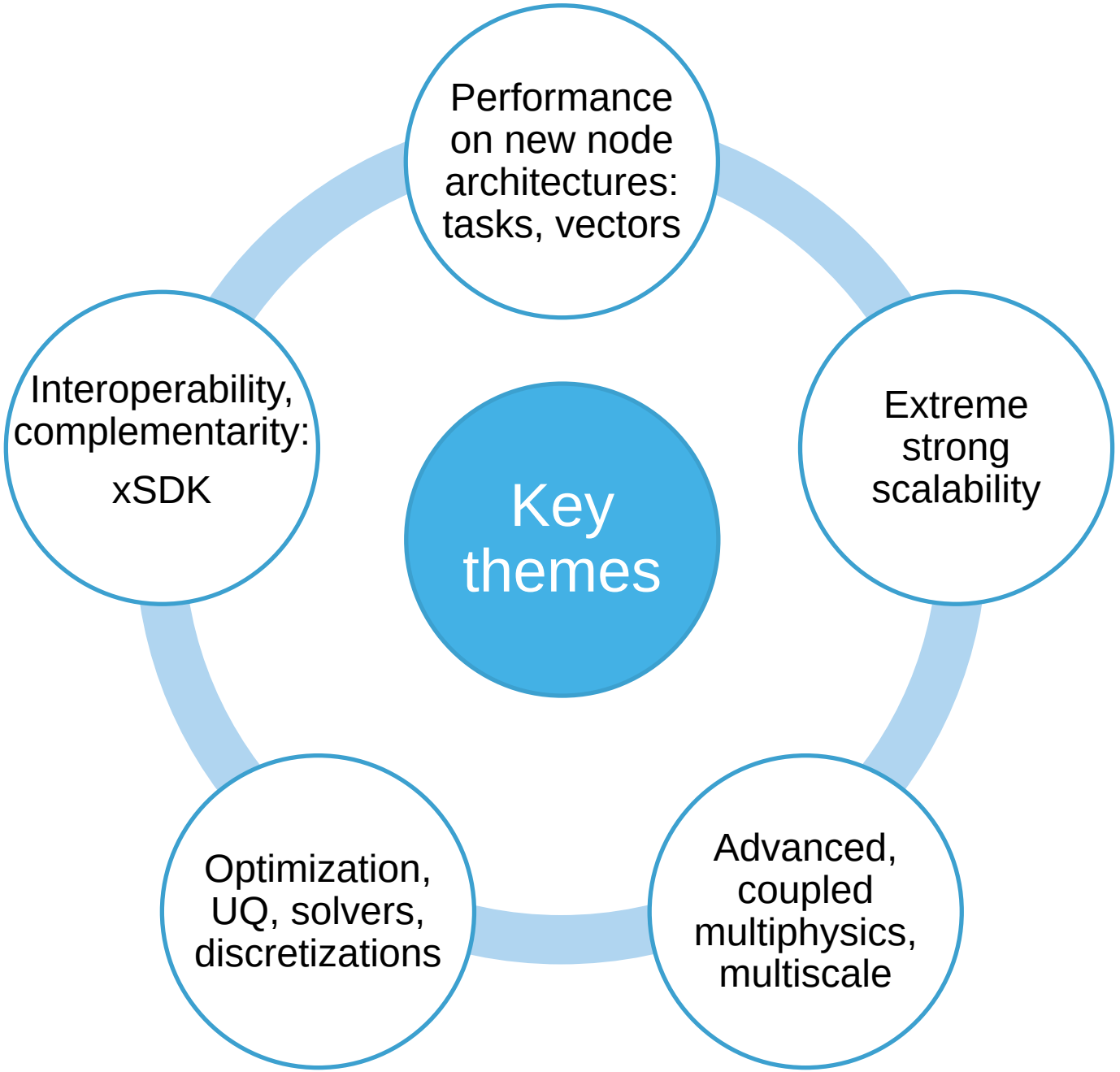
Programming Models and Runtimes



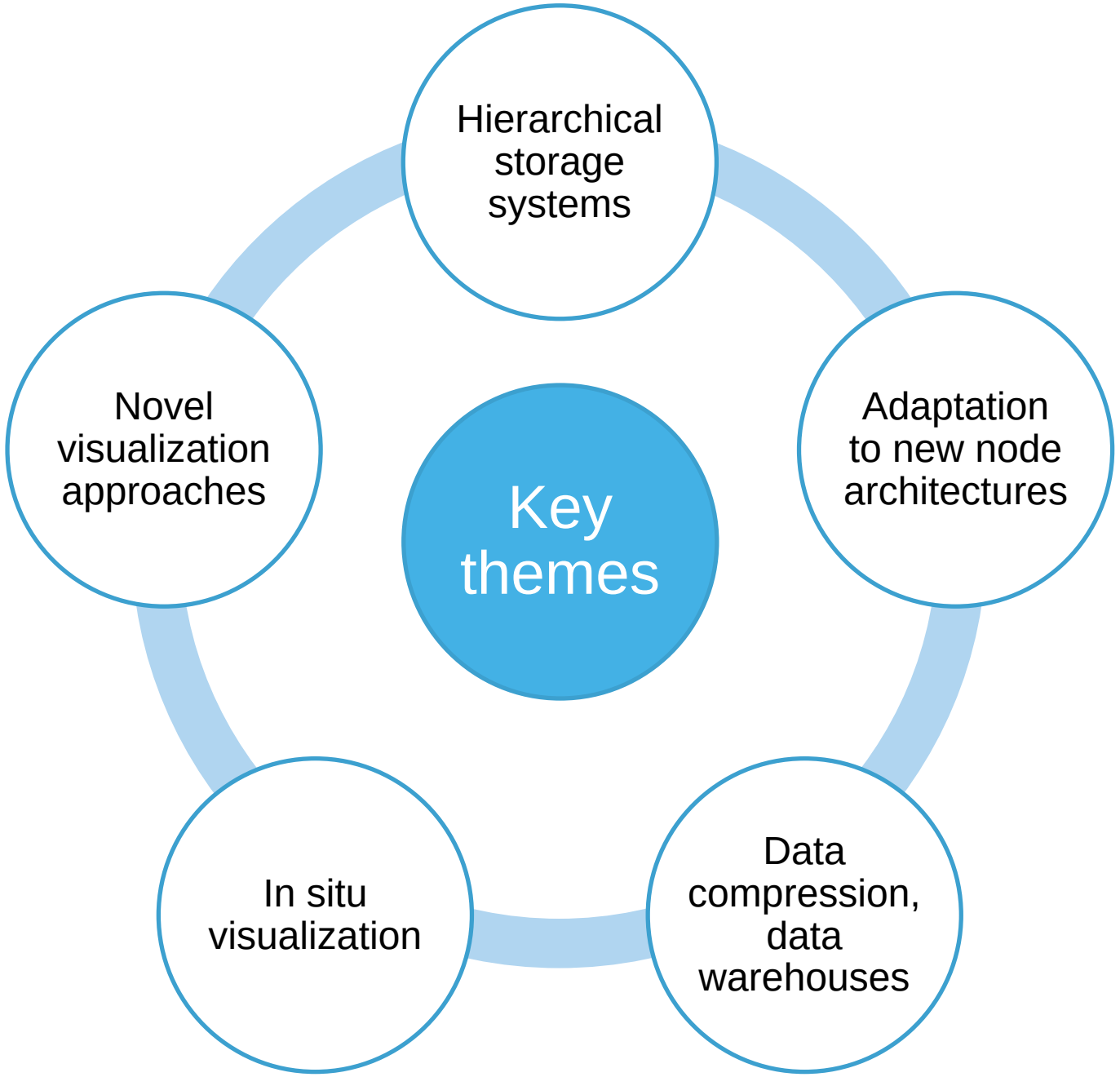
Development Tools



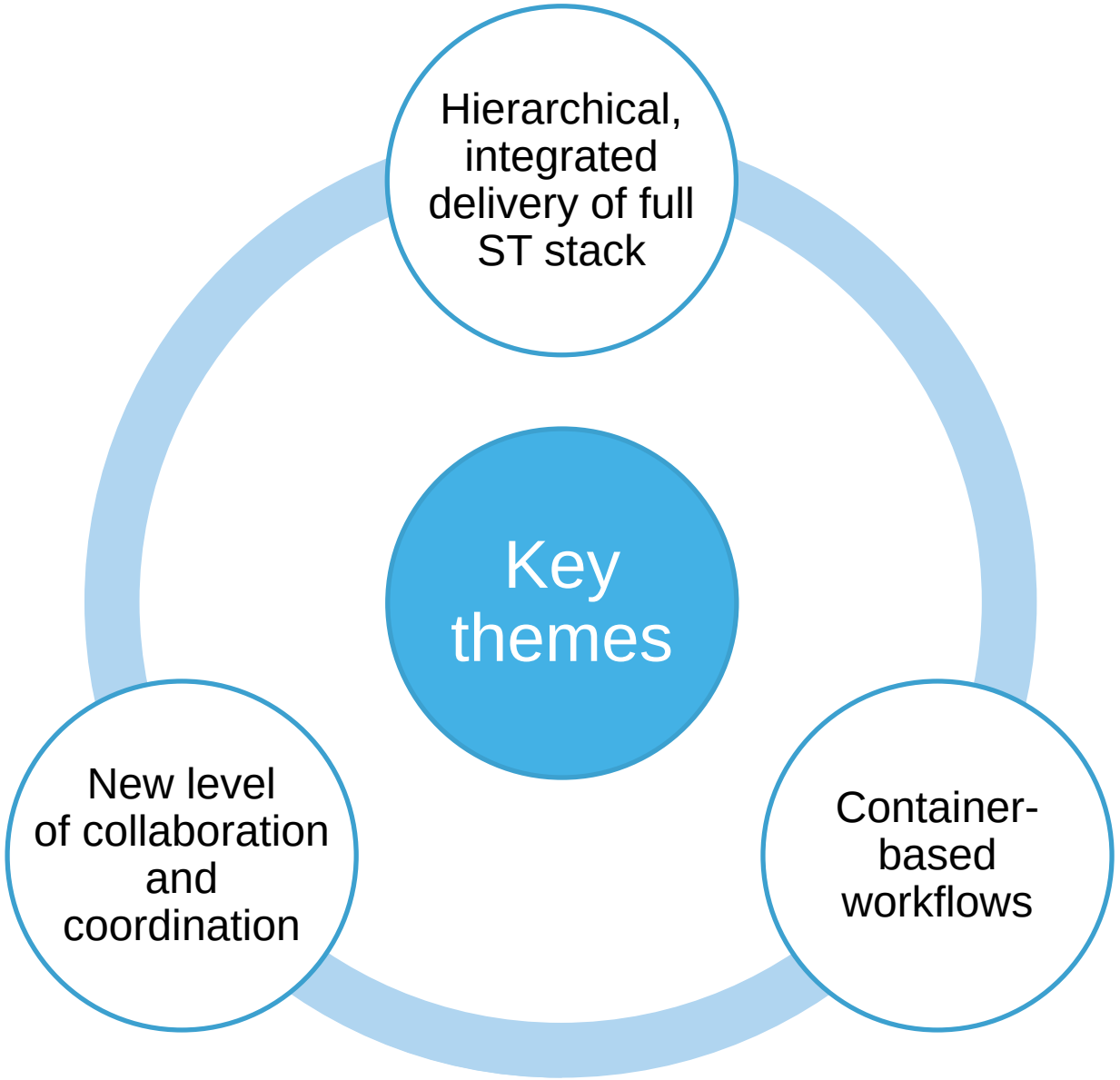
Math Libraries



Data and Visualization



Software Ecosystem and Delivery



ECP ST Products

ECP ST Products:
55 Projects contribute to 89 Unique Products

Spack Package Support	
Have Spack Package	43
Spack Package in progress	21

Source Build System	
Cmake	44
Configure/Make (autotools)	32
Custom	4

Delivery	
Direct to users from source	81
Vendor stack	11
ALCF	19
OLCF	20
NERSC	20
LLNL	18
LANL	17
OpenHPC	9
Containers (Docker)	3+

User Support	
Documentation	81
Tutorials	50
Support staff training	21
Email/phone contact	70
User-access issue tracking	65

- 48% support Spack.
- 24% Spack in progress.

➢ **Requirement for Q1FY19 participation.**

- Most users directly manage ST software from source.

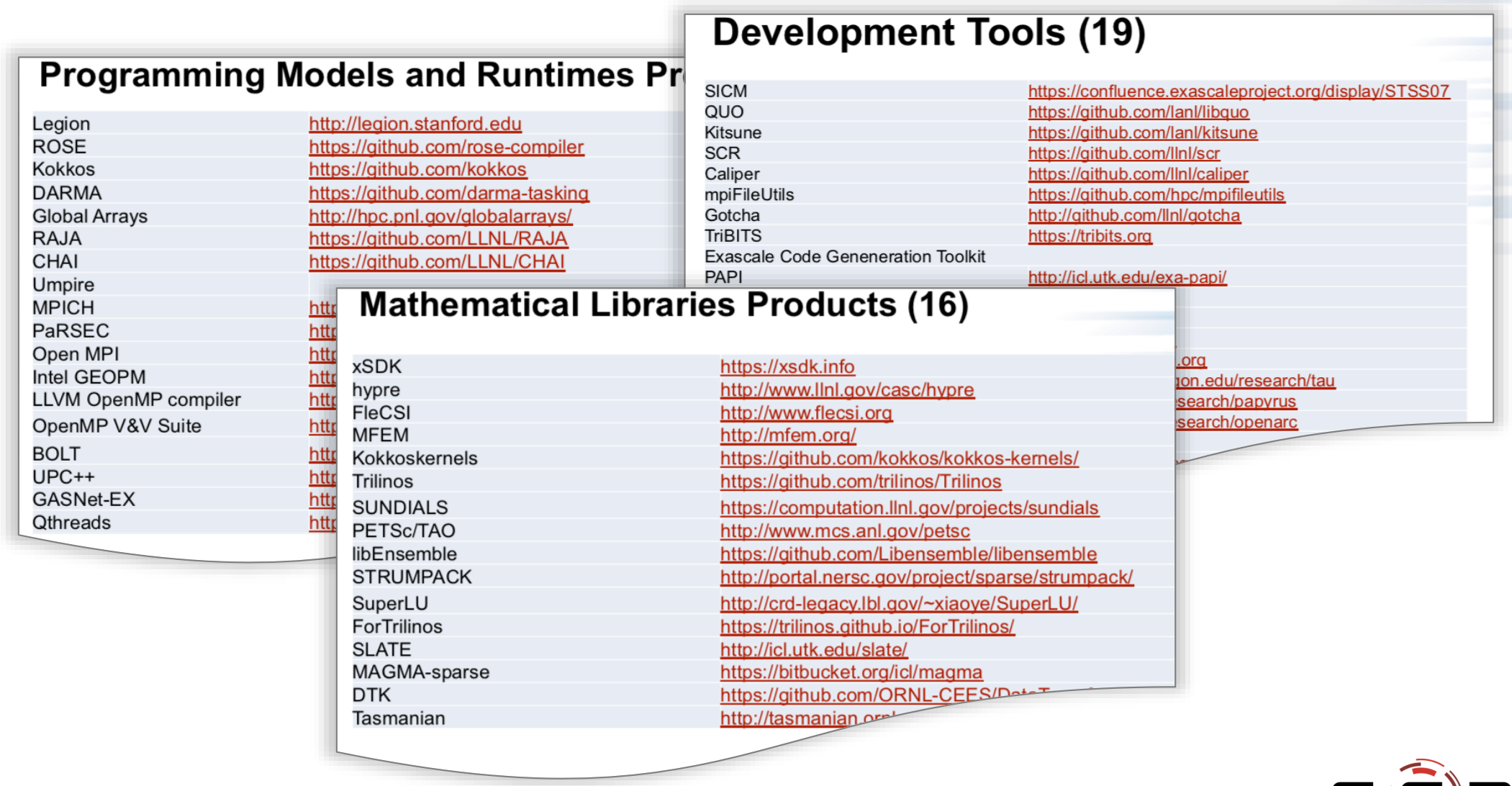
➢ **Spack packages, SDKs will improve access and management.**

- ST projects have diverse delivery experience with:
  - vendors,
  - leadership facilities,
  - binary release,
  - Containers

➢ **Can leverage across other projects.**

Stats collected April 2018

ECP ST efforts currently contribute to 89 unique products



Programming Models and Runtimes Pr

Legion	http://legion.stanford.edu
ROSE	https://github.com/rose-compiler
Kokkos	https://github.com/kokkos
DARMA	https://github.com/darma-tasking
Global Arrays	http://hpc.pnl.gov/globalarrays/
RAJA	https://github.com/LLNL/RAJA
CHAI	https://github.com/LLNL/CHAI
Umpire	
MPICH	http
PaRSEC	http
Open MPI	http
Intel GEOPM	http
LLVM OpenMP compiler	http
OpenMP V&V Suite	http
BOLT	http
UPC++	http
GASNet-EX	http
Qthreads	http

Development Tools (19)

SICM	https://confluence.exascaleproject.org/display/STSS07
QUO	https://github.com/lanl/libquo
Kitsune	https://github.com/lanl/kitsune
SCR	https://github.com/llnl/scr
Caliper	https://github.com/llnl/caliper
mpiFileUtils	https://github.com/hpc/mpifileutils
Gotcha	http://github.com/llnl/gotcha
TriBITS	https://tribits.org
Exascale Code Genereration Toolkit	
PAPI	http://icl.utk.edu/exa-papi/

.org
on.edu/research/tau
search/papyrus
search/openarc

Mathematical Libraries Products (16)

xSDK	https://xsdk.info
hypre	http://www.llnl.gov/casc/hypre
FleCSI	http://www.flecsi.org
MFEM	http://mfem.org/
Kokkoskernels	https://github.com/kokkos/kokkos-kernels/
Trilinos	https://github.com/trilinos/Trilinos
SUNDIALS	https://computation.llnl.gov/projects/sundials
PETSc/TAO	http://www.mcs.anl.gov/petsc
libEnsemble	https://github.com/Libensemble/libensemble
STRUMPACK	http://portal.nersc.gov/project/sparse/strumpack/
SuperLU	http://crd-legacy.lbl.gov/~xiaoye/SuperLU/
ForTrilinos	https://trilinos.github.io/ForTrilinos/
SLATE	http://icl.utk.edu/slate/
MAGMA-sparse	https://bitbucket.org/icl/magma
DTK	https://github.com/ORNL-CEES/Data
Tasmanian	http://tasmanian.org

Programming Models and Runtimes Products (18)

Legion	http://legion.stanford.edu
ROSE	https://github.com/rose-compiler
Kokkos	https://github.com/kokkos
DARMA	https://github.com/darma-tasking
Global Arrays	http://hpc.pnl.gov/globalarrays/
RAJA	https://github.com/LLNL/RAJA
CHAI	https://github.com/LLNL/CHAI
Umpire	
MPICH	http://www.mpich.org
PaRSEC	http://icl.utk.edu/parsec/
Open MPI	https://www.open-mpi.org/
Intel GEOPM	https://geopm.github.io/
LLVM OpenMP compiler	https://github.com/SOLLVE
OpenMP V&V Suite	https://bitbucket.org/crpl_cisc/sollve_vv/src
BOLT	https://github.com/pmodels/argobots
UPC++	http://upcxx.lbl.gov
GASNet-EX	http://gasnet.lbl.gov
Qthreads	https://github.com/Qthreads

Development Tools (19)

SICM	https://confluence.exascaleproject.org/display/STSS07
QUO	https://github.com/lanl/libquo
Kitsune	https://github.com/lanl/kitsune
SCR	https://github.com/llnl/scr
Caliper	https://github.com/llnl/caliper
mpiFileUtils	https://github.com/hpc/mpifileutils
Gotcha	http://github.com/llnl/gotcha
TriBITS	https://tribits.org
Exascale Code Geneneration Toolkit	
PAPI	http://icl.utk.edu/exa-papi/
CHiLL Autotuning Compiler	
Search using Random Forests (SuRF)	
HPCToolkit	http://hpctoolkit.org
The Dyninst Binary Tools Suite	http://www.paradyn.org
Tau	http://www.cs.uoregon.edu/research/tau
Papyrus	https://ft.ornl.gov/research/papyrus
openarc	https://ft.ornl.gov/research/openarc
LLVM	http://llvm.org/
Program Database Toolkit (PDT)	https://www.cs.uoregon.edu/research/pdt/home.php

Mathematical Libraries Products (16)

xSDK	https://xsdk.info
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FleCSI	http://www.flecsi.org
MFEM	http://mfem.org/
Kokkoskernels	https://github.com/kokkos/kokkos-kernels/
Trilinos	https://github.com/trilinos/Trilinos
SUNDIALS	https://computation.llnl.gov/projects/sundials
PETSc/TAO	http://www.mcs.anl.gov/petsc
libEnsemble	https://github.com/Libensemble/libensemble
STRUMPACK	http://portal.nersc.gov/project/sparse/strumpack/
SuperLU	http://crd-legacy.lbl.gov/~xiaoye/SuperLU/
ForTrilinos	https://trilinos.github.io/ForTrilinos/
SLATE	http://icl.utk.edu/slate/
MAGMA-sparse	https://bitbucket.org/icl/magma
DTK	https://github.com/ORNL-CEES/DataTransferKit
Tasmanian	http://tasmanian.ornl.gov/

Data & Visualization Products (25)

HXHIM	http://github.com/hpc/hxhim.git
Cinema	https://datascience.lanl.gov/Cinema.html
MarFS	https://github.com/mar-file-system/marfs
GUFI (The Grand Unified File Index)	https://github.com/mar-file-system/GUFI
Siboka	
ROVER	
C2C	
TuckerMPI	
ParaView	https://www.paraview.org/
Catalyst	https://www.paraview.org/in-situ/
VTK-m	http://m.vtk.org
FAODEL	https://github.com/faodel/faodel
IOSS	https://github.com/gsjaardema/seacas
VeloC	https://xgitlab.cels.anl.gov/ecp-veloc
SZ	https://github.com/disheng222/SZ
UnifyCR	https://github.com/LLNL/UnifyCR
HDF5	https://www.hdfgroup.org/downloads/
ADIOS	https://github.com/ornladios/ADIOS2
Parallel netCDF	http://cucis.ece.northwestern.edu/projects/PnetCDF/
Darshan	http://www.mcs.anl.gov/research/projects/darshan/
ROMIO	http://www.mcs.anl.gov/projects/romio/
Mercury (part of Mochi suite)	http://www.mcs.anl.gov/research/projects/mochi/
zfp	https://github.com/LLNL/zfp
VisIt	https://wci.llnl.gov/simulation/computer-codes/visit
ASCENT	https://github.com/Alpine-DAV/ascent

SW Ecosystem & Delivery Products (11)

BEE	
FSEFI	
Spack	https://github.com/spack/spack
Sonar	
Secure JupyterHub	
Kitten Lightweight Kernel	https://github.com/HobbesOSR/kitten
AML	https://xgitlab.cels.anl.gov/argo/aml
ArgoContainers	https://xgitlab.cels.anl.gov/argo/containers
COOLR	https://github.com/coolr-hpc
NRM	https://xgitlab.cels.anl.gov/argo/nrm
Flang/LLVM Fortran compiler	http://www.flang-compiler.org

ECP ST SDKs

SDKs are a key delivery vehicle for ECP

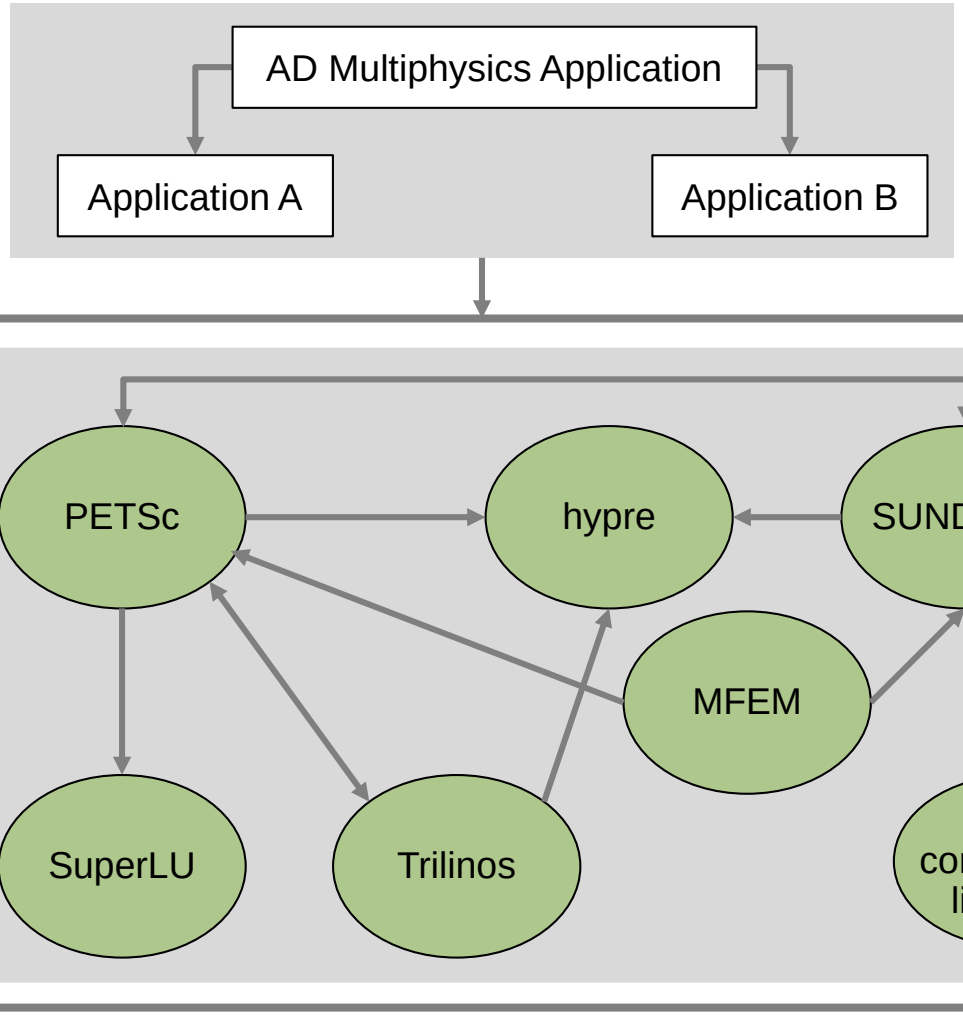
- A collection of related software products (called packages) where coordination across package teams will improve usability and practices and foster community growth among teams that develop similar and complementary capabilities
- Attributes
  - Domain scope: Collection makes functional sense
  - Interaction model: How package interact; compatible, complementary, interoperable
  - Community policies: Value statements; serve as criteria for membership
  - Meta-infrastructure: Encapsulates, invokes build of all packages (Spack), shared test suites
  - Coordinated plans: Inter-package planning. Does not replace autonomous package planning
  - Community outreach: Coordinated, combined tutorials, documentation, best practices
- Overarching goal: Unity in essentials, otherwise diversity

ECP's Math SDK (xSDK)

Key interactions with apps, packages, Spack

Notation: A → B:

A can use **B** to provide functionality on behalf of **A**



xSDK functionality, November 2017

Tested on key machines at ALCF, NERSC, OLCF, also Linux, Mac OS X

ECP ST SDK community policies:
Important team building, quality improvement, membership criteria.

xSDK compatible package: Must satisfy mandatory xSDK policies:

M1. Support xSDK community GNU Autoconf or CMake options.
M2. Provide a comprehensive test suite.
M3. Employ user-provided MPI communicator.
M4. Give best effort at portability to key architectures.
M5. Provide a documented, reliable way to contact the development team.
M6. Respect system resources and settings made by other previously called packages.
M7. Come with an open source license.
M8. Provide a runtime API to return the current version number of the software.
M9. Use a limited and well-defined symbol, macro, library, and include file name space.
M10. Provide an accessible repository (not necessarily publicly available).
M11. Have no hardwired print or IO statements.
M12. Allow installing, building, and linking against an outside copy of external software.
M13. Install headers and libraries under <prefix>/include/ and <prefix>/lib/.
M14. Be buildable using 64 bit pointers. 32 bit is optional.
M15. All xSDK compatibility changes should be sustainable.
M16. The package must support production-quality installation compatible with the xSDK install tool and xSDK metapackage.

Also specify **recommended policies**, which currently are encouraged but not required:

R1. Have a public repository.
R2. Possible to run test suite under valgrind in order to test for memory corruption issues.
R3. Adopt and document consistent system for error conditions/exceptions.
R4. Free all system resources it has acquired as soon as they are no longer needed.
R5. Provide a mechanism to export ordered list of library dependencies.

xSDK member package: Must be an xSDK-compatible package, *and* it uses or can be used by another package in the xSDK, and the connecting interface is regularly tested for regressions.

Prior to defining and complying to these policies, a user could not correctly, much less easily, build hypre, PETSc, SuperLU and Trilinos in a single executable: a basic requirement for some ECP app multi-scale/multi-physics efforts.

https://xsdk.info/policies

Version 0.3.0, Nov 2017

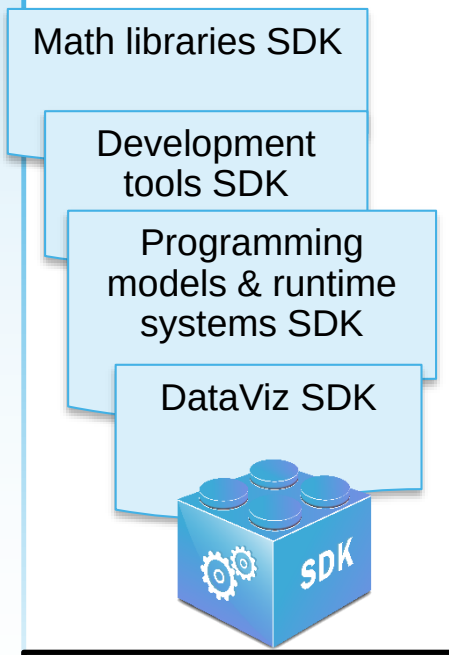
ECP Software Projects

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

SDK Leadership Team: Decades of Software Experience

- **Jim Willenbring – SDK Coordinator and Release Manager**
- **Sameer Shende – Programming Models & Runtimes**
- **Bart Miller – Development Tools**
- **Lois McInnes – Math Libraries**
- **Chuck Atkins - Data & Viz**

We are extending the SDK approach to all ECP domains

- First concrete effort: Spack target to build all packages in an SDK
  - Decide on good groupings
  - Not necessarily trivial: version compatibility issues, coordination of common dependencies
- SDKs will help reduce complexity of delivery:
  - Hierarchical build targets
  - Distribution of software integration responsibilities
- Longer term:
  - Establish community policies, enhance best practices sharing
  - Provide a mechanism for shared infrastructure, testing, training, etc
  - Enable community expansion beyond ECP

Other Important ECP ST Contributions

ECP ST Staff Contribute to ISO and *de facto* standards groups: Assuring Sustainability through standards

Standards Effort	ECP ST Participants
MPI Forum	15
OpenMP	15
BLAS	6
C++	4
Fortran	4
OpenACC	3
LLVM	2
PowerAPI	1
VTK ARB	1

- **MPI/OpenMP:** Several key leadership positions.
- Heavy involvement in all aspects.

- **C++:** Getting HPC requirements considered, contributing working code.

- **Fortran:** Flang front end for LLVM.

- ***De facto:*** Specific HPC efforts.

- **ARB*:** Good model for SDKs.

*Architecture Review Board

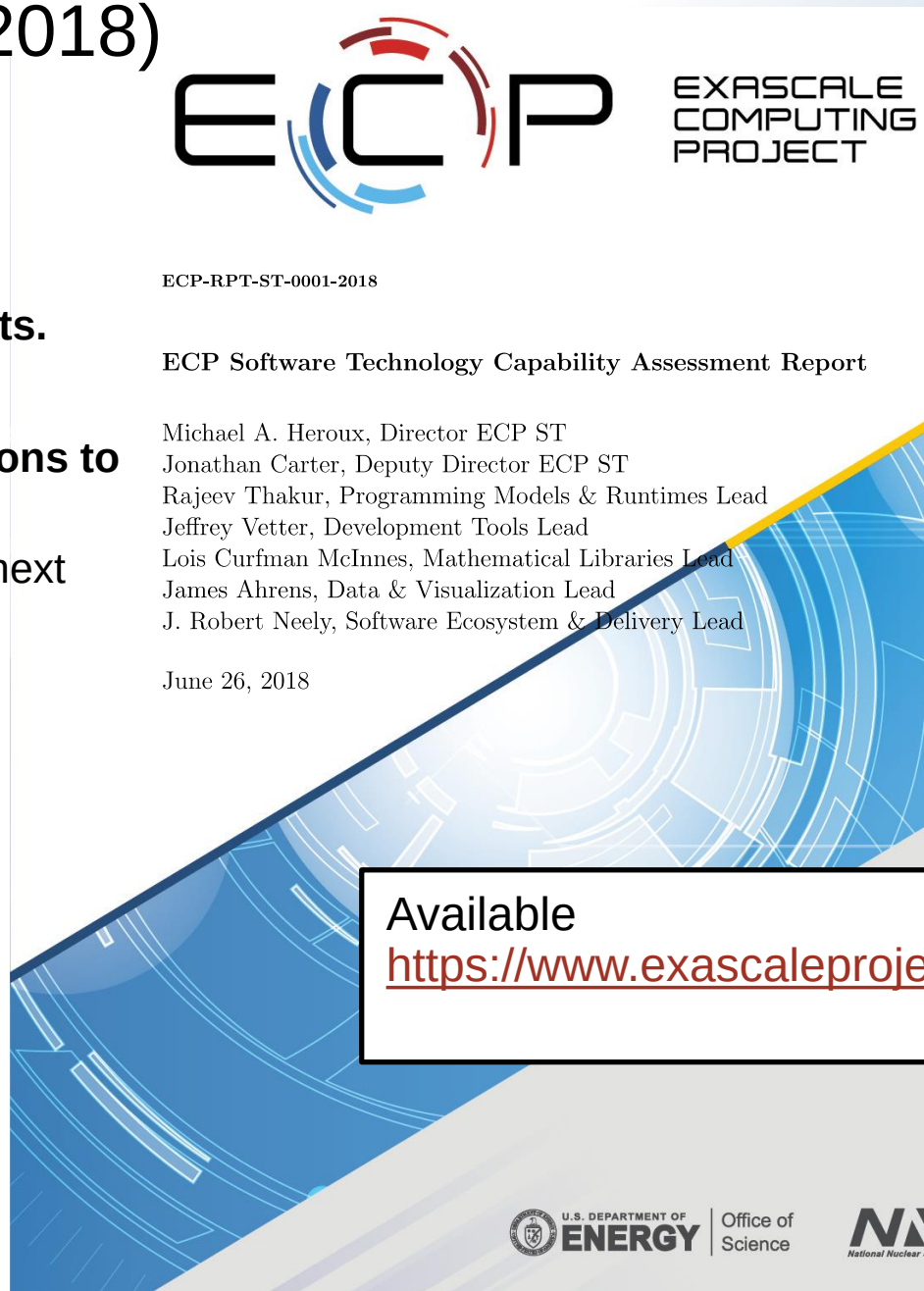
External Product Impact

Product	Contribution
MAGMA	ECP ST math libraries eorts inform the design, implementation, and optimization of numerical linear algebra routines on NVIDIA GPUs
Vendor/community compilers and runtimes	The Validation and Verication Suite (on-going effort) for the SOLLVE project has helped uncover bugs in OpenMP implementations provided by Cray, LLVM and XL.
SWIG	The ECP ST ForTrilinos eorts contributes the capability to generate automatic Fortran bindings from C++ code.
TotalView Debugger	ECP ST sta are engaged in co-design of OMPD, the new debugging interface for OpenMP programs, along with RogueWave engineers. This eort helps RogueWave improve their main debugging product, TotalView, by making it aware and compatible with recent advances in OpenMP debugging.
MPI Forum	ECP ST sta maintain several chapters of the MPI Forum, effort that require a constant involvement with the other authors, as well as participation to the online discussions related to the chapter and regular attendance of the MPI Forum face-to-face activities. An ECP ST staff member belongs to several working group related to scalability and resilience where, in addition to the discussions, implements proof-of-concept features in OpenMPI.
Cray MPICH MPI-IO	As part of the ExaHDF5 ECP project, the ALCF worked with Cray MPI-IO developers to merge the upstream ROMIO code into the downstream proprietary Cray MPICH MPI-IO, leveraging Crays extensive suite of IO performance tests and further tuning the algorithm. Cray is currently targeting its deployment in an experimental release.
OpenHPC	An ECP ST staff member serves on the OpenHPC Technical Steering Committee as a Component Development representative.
LLVM	An ECP ST staff member is co-leading design discussions around the parallel IR and loop-optimization infrastructure.

Some of our best work is to provide input to software we don't productize or support.

ECP Software Technology Capability Assessment Report (Released July 2018)

- Three document elements:
  1. Executive summary – Public content.
  2. Project Description - Public content.
     - **SDKs, Delivery strategy, project restructuring, new projects.**
     - Technical areas overview.
     - **Deliverables: Products, Standards committees, contributions to external products.**
     - Project two-pages: 55 with description, activities, challenges, next steps.
  3. **Appendix – ECP/Stakeholder content.**
     - **Impact goals/metrics framework.**
     - **Gaps and Overlaps.**
     - **ASC-ASCR leverage tables.**
- LaTeX, separate contributors, easily updated.
- 212 pages (191 public), update twice a year.



Summary

- ECP Software Technology contributes to a broad spectrum of HPC software products:
  - 89 products total.
  - 33 broadly used in HPC.
    - Require substantial investment and transformation in preparation for exascale architectures
  - Additional 23 important to some existing applications,
    - Typically represent new capabilities that enable new usage models for realizing the potential that Exascale platforms promise.
  - Remaining products are in early development phases
    - Addressing emerging challenges and opportunities that Exascale platforms present.
- ECP SW Development Kits (SDKs) are a key focus:
  - Enables hierarchical leadership, management deployment.
  - Defines membership criteria through community policies.
  - Defines boundaries of responsibilities: ECP, Facilities, Other communities.

"Any opinions, findings, conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Networking and Information Technology Research and Development Program."

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