Planning for the Exascale Software Center

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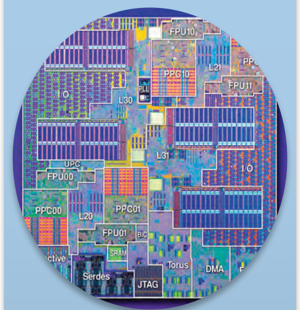
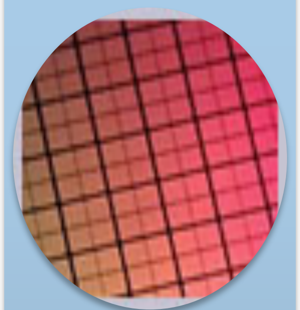
Major Components of DOE Exascale Initiative



Platform R&D

2 Vendor Tracks

- Power
- Integration
- Risk Mitigation



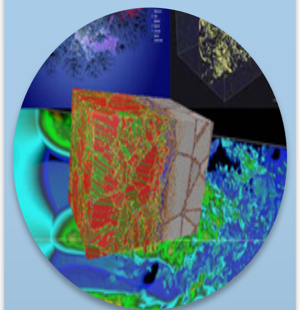
Critical Technologies

(everyone benefits)

- Memory
- Nonvolatile storage
- Optics

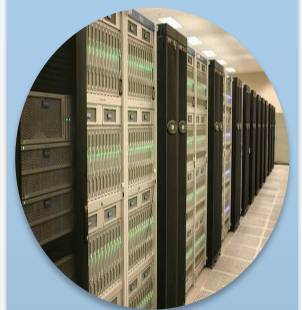
Software and Environments

- Operating environment
- Systems Software
- System reliability
- Programming model



Co-design

- Performance models
- Simulators
- Applications integration with vendors



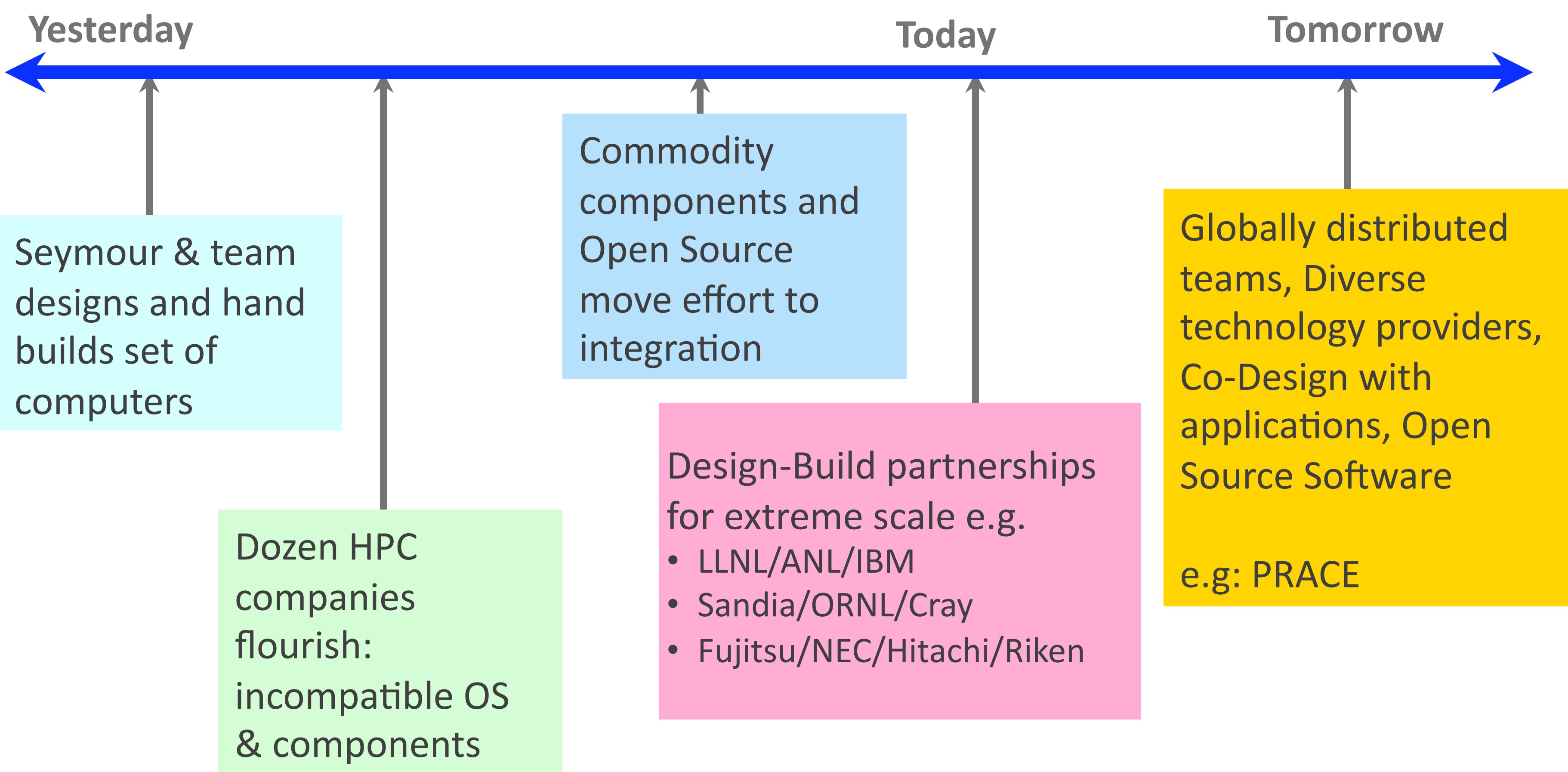
Platforms

- Early prototypes to ensure component integration and usefulness
- Risk mitigation for vendors – Non recoverable engineering cost

Exascale Initiative

Research and development, but also coordination and Quality Assurance.

The Changing Face of Extreme-Scale Platforms



Current HPC software approach needs a reboot

It is our view that complex systems almost always fail in complex ways ...
– Columbia Accident Investigation Board Report, August 2003

- Software development uncoordinated with hardware features
  - (e.g., power mgmt, multicore tools, math libraries, advanced memory models)
- Only basic acceptance test software is delivered with platform
  - UPC, HPCToolkit, Optimized libraries, PAPI, can be YEARS late
- Vendors often “snapshot” key Open Source components and then deliver a stale code branch
- Community codes unprepared for sea change in architectures
- “Coordination via contract” is poor and only involves 2 parties
- No global evaluation of key missing components

Current ESC Planning Team

Coordinating PIs:

Pete Beckman, Argonne National Laboratory
Jack Dongarra, University of Tennessee

Pavan Balaji, Argonne National Laboratory
George Bosilca, University of Tennessee
Ron Brightwell, Sandia National Laboratory
Jonathan Carter, Lawrence Berkeley National Laboratory
Franck Cappello, University of Illinois
Barbara Chapman, University of Houston
James Demmel, University of California Berkeley
Al Geist, Oak Ridge National Laboratory
Bill Gropp, University of Illinois
Paul Hargrove, Lawrence Berkeley National Laboratory
Michael Heroux, Sandia National Laboratory
Kamil Iskra, Argonne National Laboratory
Rusty Lusk, Argonne National Laboratory
Allen Malony, University of Oregon
Arthur Barney Maccabe, Oak Ridge National Laboratory
Terry Moore, University of Tennessee
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Special thanks for feedback and help developing material:

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Mark Seager, Lawrence Livermore National Laboratory
Pat McCormick, Los Alamos National Laboratory
Andy White, Los Alamos National Laboratory
Peg Williams, Cray
Peter Young, Cray
Robert Wisniewski, IBM
Al Gara, IBM
Bill Dally, Nvidia
Steve Parker, Nvidia
David Lombard, Intel
Ed Temple, Argonne National Laboratory

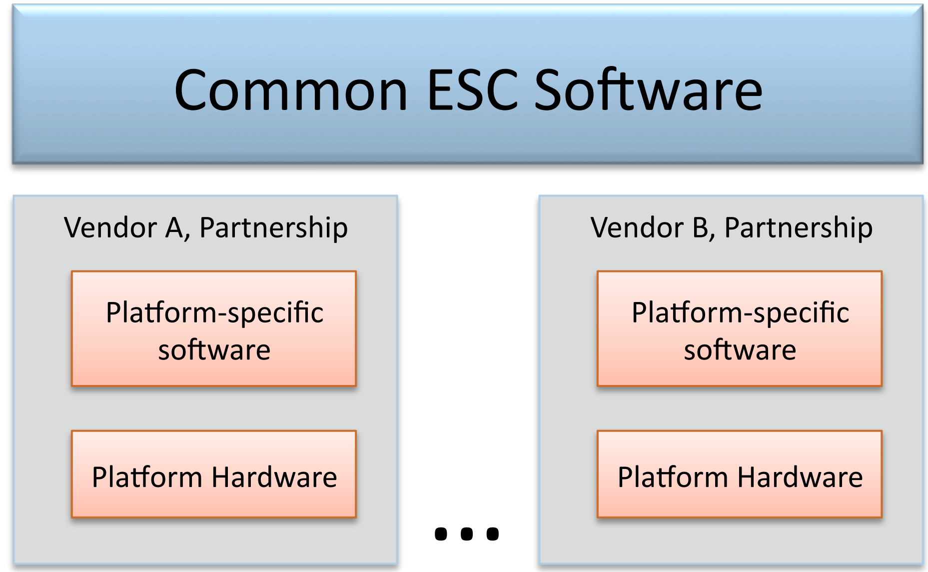
Exascale Software Center (ESC)

Goal: Ensure successful deployment of coordinated exascale software stack on Exascale Initiative platforms.

Ultimately responsible for success of software

- Identify required software capabilities
- Identify gaps
- Design and develop open-source software components
  - Both: evolve existing components, develop new ones
  - Includes maintainability, support, verification
- Ensure functionality, stability, and performance
- Collaborate with platform vendors to integrate software
- Coordinate outreach to the broader open source
- Track development progress and milestones

Assumptions

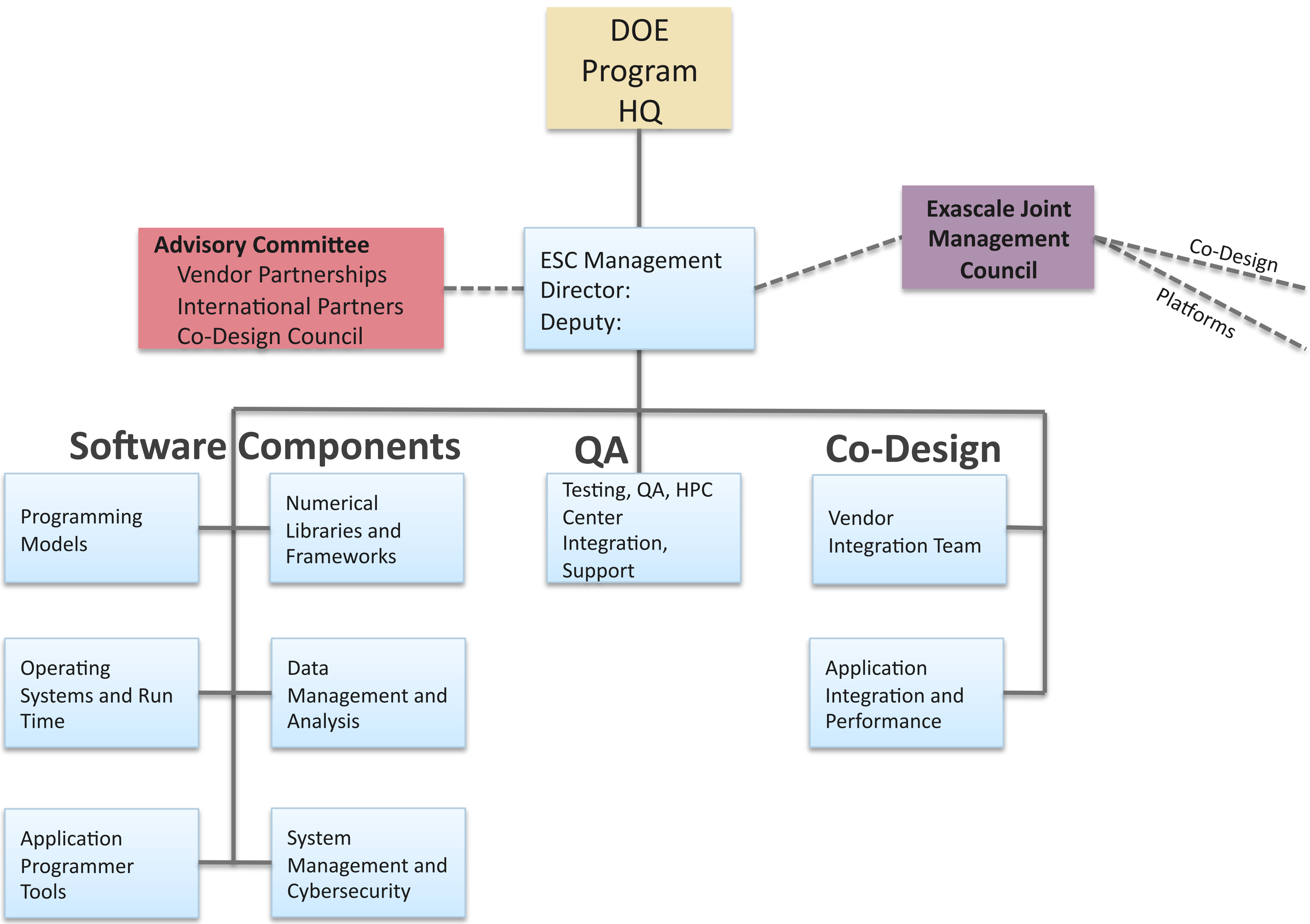


- Several vendor platform partnerships
- ~2015 early scalability demonstration systems
  - Arch 2010-2011 ; System build 2015
- ~2018 exascale system
  - Arch 2014-2015 ; System build 2018
- Co-design centers provide initial applications
- ESC:
  - Partnership funding agencies, labs, and universities
  - Responsible for the common software environment for EI systems
  - All development will be open source
  - Some components will be integrated and supported by vendor, others will be provided atop basic platform, supported by ESC
  - Vendor-specific components will be part of their platform strategy
    - E.g.: system management, RAS, compiler, etc.

The Exascale Software Center in One Slide

- Scope
  - Deliver high quality system software for exascale platforms
    - ~2015, ~2018
  - Identify software gaps, research & develop solutions, test and support deployment
  - Increase the productivity and capability and reduce the risk of exascale deployments
- Cost:
  - Applied R&D: ~10-20 distributed teams of 3 to 7 people each
  - Large, primarily centralized QA, integration, and verification center
- Schedule overview
  - 2010 – Q1 2011: Planning and technical reviews
  - April 2011: *Launch Exascale Software Center!*
  - 2014, 2017: SW ready for integration for 2015, 2018 systems respectively

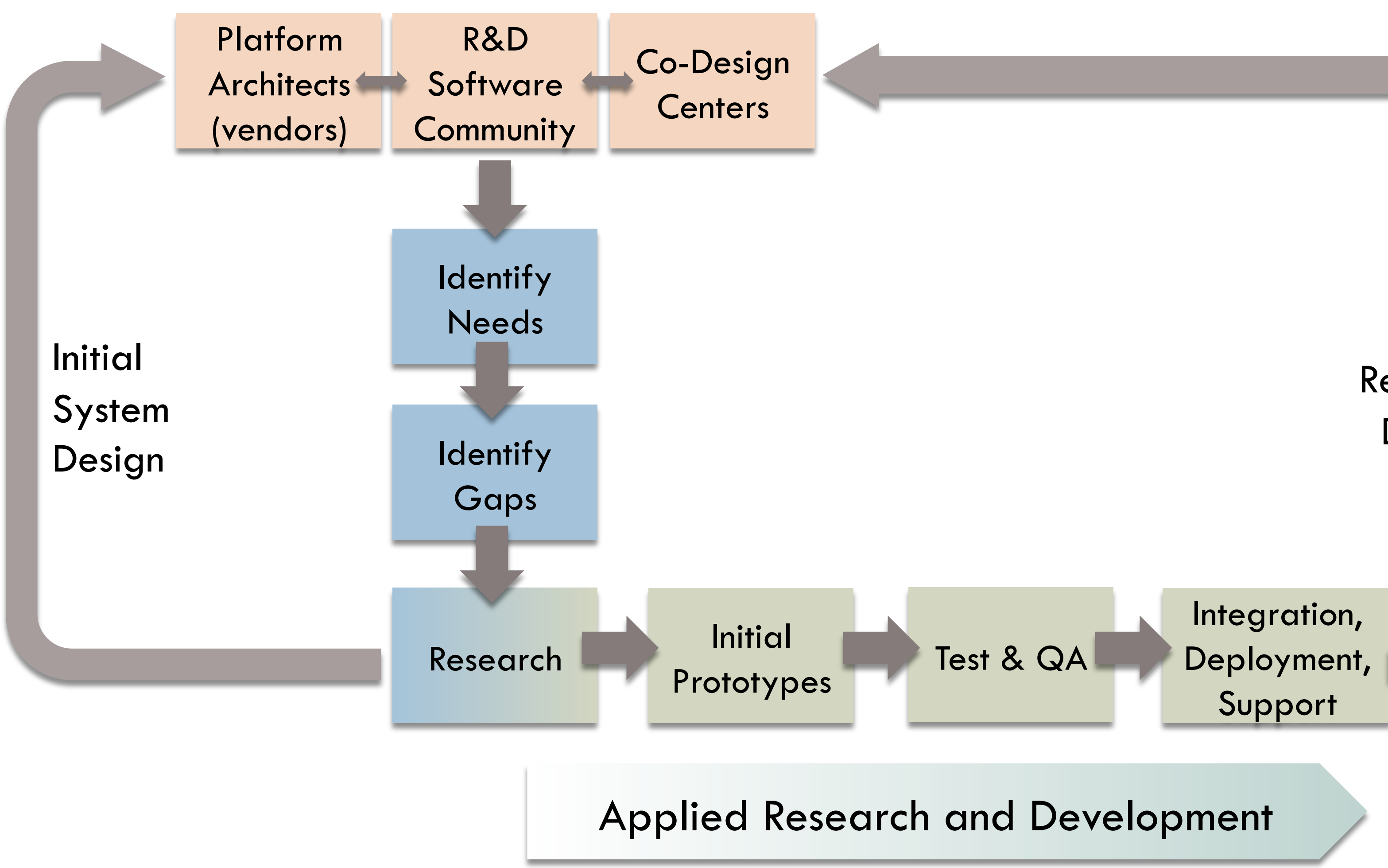
ESC Organization Chart



Specific Challenges for the Center

- How does the Center participate in co-design activities? What are vendors and application teams looking for from the Center?
- Given resource constraints, how does the Center select components to be supported? What does the Center require of these components and the teams that develop them? How does the Center interact with these teams?
- How do we engage with the larger DOE, US, and international communities?

The Exascale Software Center and Co-Design Processes



Co-Design Examples (current successes)

Co-Design Example: Math Libraries

- BLAS, Sca/LAPACK co-design: Well-known, huge success.
- Trilinos, PETSc:
  - Services:
    - Libraries: State-of-the-art libraries for scalable solvers, etc.
    - Framework: Building blocks for app implementations.
    - Kernels (non-BLAS): SpMV, SpSV – good avg. performance.
  - Vendor collaboration:
    - Cray-specific sparse kernels: avg 30% performance boost.
    - Trilinos, PETSc pre-compiled for Crays:
      - module load trilinos/10.4.1
      - module load petsc
    - "Heads-up" on trends:
      - Vendor: Early Sp kernels results for future systems.
      - Trilinos/PETSc teams: Perf-impacting app, algorithm trends.

MPICH Co-design with IBM and Cray

- The MPICH group has for years worked closely with both IBM and Cray in co-designing MPICH for Blue Gene and XT systems
- Specific optimizations were recently added to MPICH to improve its multithreaded performance to attain the high multithreaded message rates needed for BG/Q
- On the 32-bit BG/P architecture, we worked with IBM to make MPI_Aint as a 64-bit quantity to enable HDF-5 and other I/O libraries access files larger than 2GB correctly
- Similarly, various optimizations and features, such as support for checkpoint-restart and improvements to the Nemesis communication layer, were added in collaboration with Cray to better support Cray systems

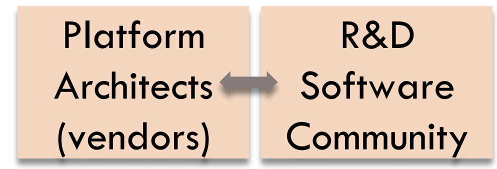
More Examples from Co-Design with IBM

Hardware ▪ Added MMU ▪ # of cores ▪ # of chips ▪ Efficiency and safety improvements in the power module designs	**MPI** ▪ MPI scalability fixes (esp. memory) ▪ Fine-grained locking or lock-free methods for thread safety (open portable atomics lib) ▪ Derived datatype optimizations
Operating System ▪ Smart scheduler ▪ Reduced memory footprint ▪ Performance improvements (python, shr libs) ▪ Speculative multi-threading system programming interface	**Code Development & Tools** ▪ Improved performance counters ▪ Improved behavior for TLS and TM to better match application needs ▪ Flexible programming model - MPI everywhere; flexible task/thread ratio ▪ Increased user level APIs
System Management ▪ Distributed control system ▪ New pervasive security model ▪ Open source, plug-in dynamic allocator ▪ Many RAS usability and performance improvements	**I/O** ▪ Full size, standard PCI-e cards ▪ Debugger interfaces for IO nodes ▪ Persistent memory uses ▪ Page sizes and scalability improvements

Co-Design Examples: System Mgmt

- Blue Gene/Q resource allocation system
  - Collaboration between ANL, LLNL, and IBM
  - Supports dynamic allocation of network and node resources
- Blue Gene/P RAS real-time streaming interface
  - Supports real-time notifications of system failure events
  - Dovetails with existing RAS polling system from BG/L
  - Collaboration between ANL, LLNL, and IBM

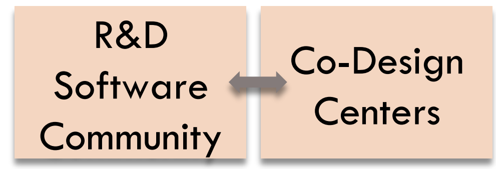
Vendors and Co-Design



- Want something like ESC to coordinate and take *real* responsibility for features and milestones
  - Improved leverage over projects that are currently less responsive than needed
- Do not want "toss over the wall" strategy. "hardening" cannot be done by different team.
- Need to manage risk of final machine functionality, performance, stability and acceptance
- Key ESC models:
  - ESC developed -- vendor integrated and supported
  - ESC developed – ESC provided, and supported
- Formalized roles between ESC and Vendors for development, risk, support, and acceptance
- Feedback and progress tracking between ESC and vendors must be shared
- Application co-design centers should coordinate discussions of system software through ESC
- NDA material for roadmaps, across co-design centers, etc will be difficult to coordinate

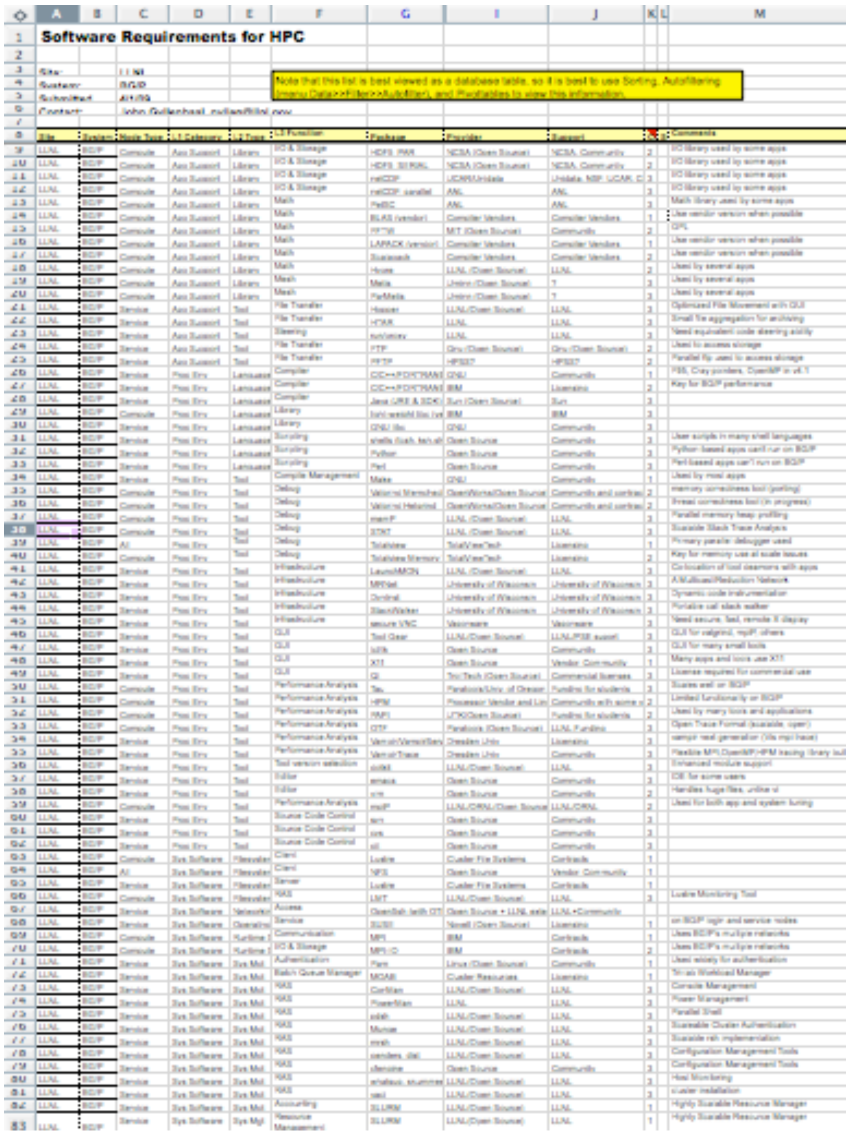
	Examples of software package	Primary developer	First-level Support Provider	Second-level Support Provider
1	RAS, system mgmt, compilers	Vendor	Vendor	Vendor
2	OS, MPI, PAPI, math libraries	ESC	Vendor	ESC
3	Performance tools, I/O libraries	ESC	ESC	ESC
4	Perl, Python	Broader Community	Vendor	
5	Eclipse IDE	Broader Community	Broader Community	

Applications and Co-Design



- Want something like ESC to coordinate and take *real* responsibility for features and milestones
  - Improved leverage over projects that are currently less responsive than needed
- Want to know specifics about hardware and available software
- Applications will provide best estimates of needs for exascale science:
  - Data movement, memory sizes, programming models, etc
- Applications will test and evaluate prototype system software
- Need help managing risk of final machine functionality, performance, stability and acceptance
- Formalized roles between ESC and App Co-Design Centers for development, risk, support, and acceptance
- Feedback and progress tracking between ESC and App Co-Design Centers
- Coordinate discussions of system software through ESC
- NDA material for roadmaps, across co-design centers, etc will be difficult to coordinate

An Overabundance of Software



- Software and functionality fall into variety of categories:
  - I/O Storage
  - Math Libraries
  - Performance Tools
  - Etc.
- Software executes in a number of domains within the system:
  - Service node, I/O nodes, compute nodes, login nodes, etc

Examples: ORNL XT3 I/O and Math Libraries

Software Requirements for HPC

Site:	**ORNL**
System:	**Cray XT3**
Submitted	**8/25/06**
Contact:	**Jeff Vetter, vetter@ornl.gov**

Note that this list is best viewed as a da
(menu Data>>Filter>>Autofilter), and Pi

Site	System	Node Type	L1 Category	L2 Type	L3 Function	Package	Provider
ORNL	Cray XT3	All	App Support	Library	I/O & Storage	HDF5_PAR	NCSA
ORNL	Cray XT3	All	App Support	Library	I/O & Storage	HDF5_SERIAL	NCSA
ORNL	Cray XT3	All	App Support	Library	I/O & Storage	netCDF	UCAR/Unidata
ORNL	Cray XT3	All	App Support	Library	I/O & Storage	netCDF, parallel	ANL
ORNL	Cray XT3	Compute	App Support	Library	Math	PetSC	ANL
ORNL	Cray XT3	Compute	App Support	Library	Math	Aztec	Sandia
ORNL	Cray XT3	Compute	App Support	Library	Math	BLAS	AMD
ORNL	Cray XT3	Compute	App Support	Library	Math	FFTPack	Netlib
ORNL	Cray XT3	Compute	App Support	Library	Math	FFTW	MIT
ORNL	Cray XT3	Compute	App Support	Library	Math	LAPACK	AMD
ORNL	Cray XT3	Compute	App Support	Library	Math	MUMPS	CERFACS

Examples: LLNL BG/P Tools

Site	System	Node Type	L1 Category	L2 Type	L3 Function	Package	Provider
LLNL	BG/P	Service	Prog Env	Tool	Infrastructure	LaunchMON	LLNL (Open Source)
LLNL	BG/P	Service	Prog Env	Tool	Infrastructure	MRNet	University of Wisconsin
LLNL	BG/P	Service	Prog Env	Tool	Infrastructure	DynInst	University of Wisconsin
LLNL	BG/P	Service	Prog Env	Tool	Infrastructure	StackWalker	University of Wisconsin
LLNL	BG/P	Service	Prog Env	Tool	Infrastructure	secure VNC	Vaporware
LLNL	BG/P	Service	Prog Env	Tool	GUI	Tool Gear	LLNL(Open Source)
LLNL	BG/P	Service	Prog Env	Tool	GUI	tcl/tk	Open Source
LLNL	BG/P	Service	Prog Env	Tool	GUI	X11	Open Source
LLNL	BG/P	Service	Prog Env	Tool	GUI	Qt	TrollTech (Open Source)
LLNL	BG/P	Compute	Prog Env	Tool	Performance Analysis	Tau	Paratools/Univ. of Oregon (
LLNL	BG/P	Compute	Prog Env	Tool	Performance Analysis	HPM	Processor Vendor and Linu
LLNL	BG/P	Compute	Prog Env	Tool	Performance Analysis	PAPI	UTK(Open Source)
LLNL	BG/P	Compute	Prog Env	Tool	Performance Analysis	OTF	Paratools (Open Source)
LLNL	BG/P	Service	Prog Env	Tool	Performance Analysis	Vampir/VampirServ	Dresden Univ
LLNL	BG/P	Service	Prog Env	Tool	Performance Analysis	VampirTrace	Dresden Univ
LLNL	BG/P	Service	Prog Env	Tool	Tool version selection	dotkit	LLNL(Open Source)
LLNL	BG/P	Service	Prog Env	Tool	Editor	emacs	Open Source
LLNL	BG/P	Service	Prog Env	Tool	Editor	vim	Open Source
LLNL	BG/P	Compute	Prog Env	Tool	Performance Analysis	mpiP	LLNL/ORNL(Open Source)
LLNL	BG/P	Service	Prog Env	Tool	Source Code Control	svn	Open Source
LLNL	BG/P	Service	Prog Env	Tool	Source Code Control	cvs	Open Source
LLNL	BG/P	Service	Prog Env	Tool	Source Code Control	git	Open Source

Examples: LLNL Visualization and Analysis

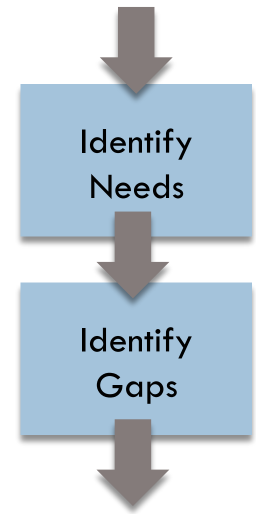
Package	Provider	Support	Criticality
VisIt	LLNL(Open Source)	LLNL	1
OpenGL	Open Source	Community	1
EnSight	CEI	Licensing	2
ImageMagick	Open Source	Open Source	2
Tecplot	Tecplot, Inc.	Licensing	2
IDL	ITT Visual Informations Systems	Licensing	2
gnuplot	Open Source	Open Source	2
POV-Ray	Open Source	Community	2
RasMol	Open Source	Community	2
vmd	UIUC(Open Source)	UIUC	2
ParaView	Open Source	Community	2
NCAR	NCAR(Open Source)	NCAR	3
mplayer	Open Source	Community	3
Blockbuster	LLNL(Open Source)	LLNL	3
GIMP	Open Source	Community	3
xxdiff/tkdiff/meld	Open Source	Community	3

Breadth of Software Capabilities in ESC

- Initial set of types of software capabilities developed based on IESP report, DOE Exascale workshops, and conversations with vendors and application teams
  - Programming Models
  - Operating Systems and Runtime
  - Application Programmer Tools
  - Numerical Libraries and Frameworks
  - Data Management and Analysis
  - System Management and Cybersecurity
- Is this the minimum set that ESC should support?
- Where do we make the cut between vendor-supported and ESC-supported software?
- What can we rely on the co-design centers to support?

Selecting ESC Components to Provide Capability

- ESC is responsible for delivering successful software
  - Technical evaluation:
    - Criticality to successful deployment and key applications
    - Technical risk for achieving goal
  - Project team evaluation:
    - Team history of delivering high-quality, applied software
    - Management and institutional support

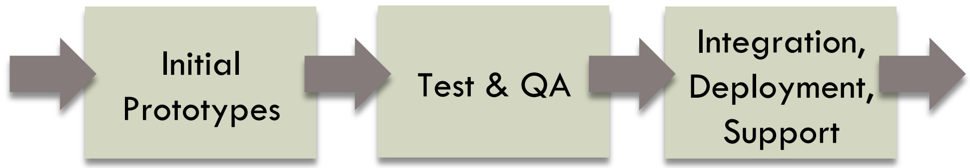


- ESC will make component selection and resource decisions based on criticality and risk
  - Continuous evaluations of progress; adjust resources

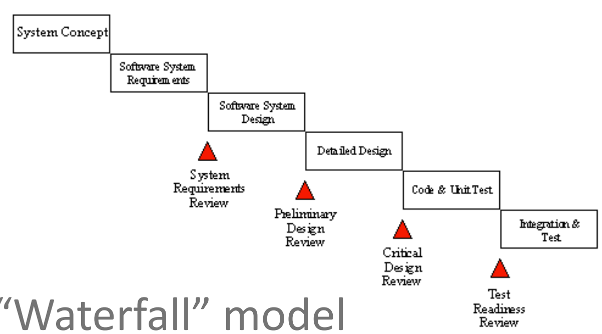
Technical Evaluation Matrix

		Low Risk	**Moderate Risk**
ESC Supported	Important		
Vendor Supported	Critical		
	Most Critical		

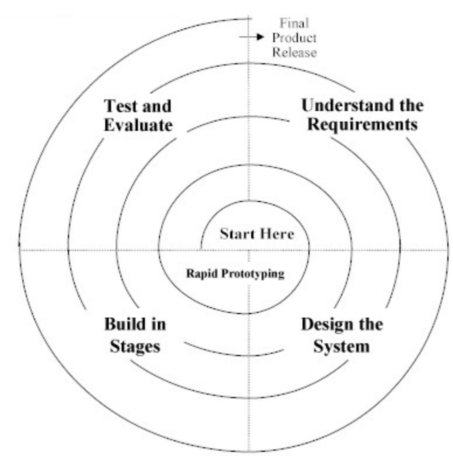
ESC Software Development



- Successful applied R&D teams are built around clear goal of delivering working, supported packages
- Good software hygiene can't be someone else's job
- ESC must **work with successful teams existing processes** or in some cases, boot new teams within institutions with excellent history of deployed software
  - Probably not feasible to launch new team at site without history of software success
- Formal plans and milestones and reviews are necessary for each component
- Co-design feedback and risk-based assessments work well with spiral development discipline for software (common in R&D)



Classic "Waterfall" model



"Spiral" model

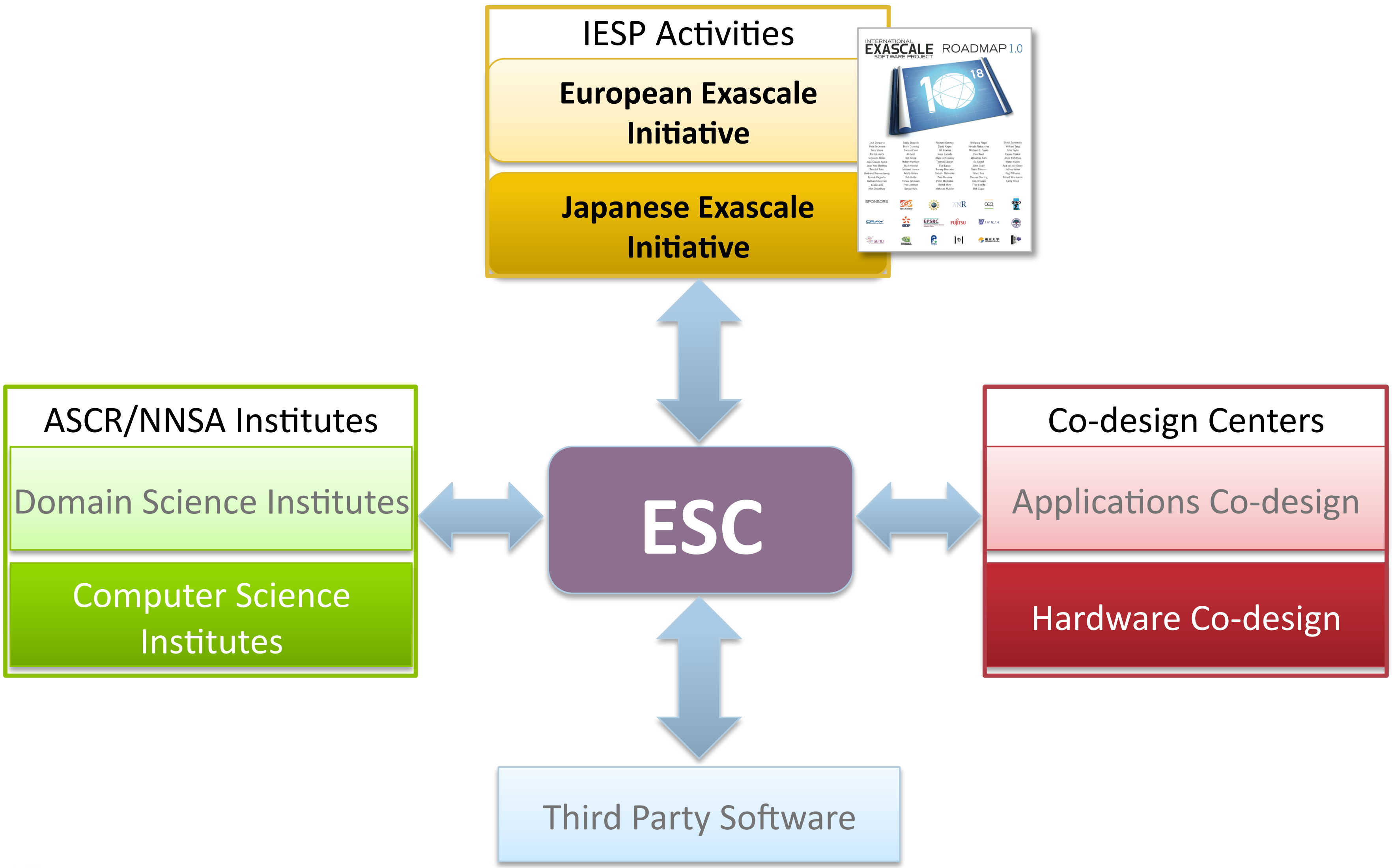
Required Processes for ESC Components

- Formulation of clear deliverables with specific targets for functionality, performance, and stability
- Defined team management plan and risk tracking
- Documented software development plans
  - QA (unit tests, integration, etc)
  - Performance testing
  - Documentation, support
  - Bug and new feature tracking
- Resource accounting
- Technical review schedule
- Release schedule
- Integration plan

Distributed Project Staffing Approach

- "ESC Component Teams" should be located where their center of mass has demonstrated success
  - E.g: Math libraries at UTK, Performance tools at UOregon and Rice
- Each Component Team will have at least one "embedded" QA and testing staff member provided by ESC
  - Position will be held by professional QA/build engineer (i.e., not a student or postdoc)
  - Candidates will be approved by ESC director of QA and have performance appraisal "matrix input"
- Each site must have local ESC team members responsible for integration
  - Will belong to production computing division, not R&D division
- QA, integration, and support team will be primarily at one site
- Resources dedicated to collaboration and software development infrastructure is required

Community Engagement



Next Steps in ESC Planning

- Develop software planning documents:
  - Definition of review materials
  - Formal review in April 2011
- Build application co-design liaisons, develop plan for jointly evaluating key software
- Build links to IESP organizational plan
- Begin technical evaluation and ranking of key software components
- Link to NSF, NASA, DARPA, and other groups

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