Maturing the ARM Software Ecosystem for U.S. DOE/ASC Supercomputing

ARM HPC User Group @ SC17
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Sandia National Laboratories

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Outline

- Vanguard
- Tri-lab ARM Software Stack Effort
- Preliminary Results
- Conclusion

Vanguard: Prototype Systems for Advanced Architectures

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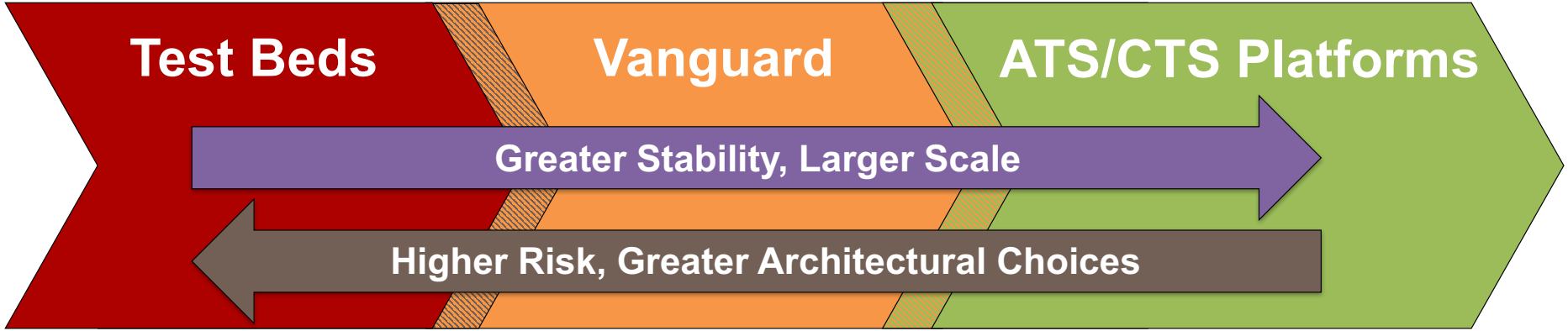
- Expand the HPC ecosystem by developing emerging, yet-to-be-proven, technologies
  - Is technology viable for future ATS/CTS platforms supporting ASC integrated codes?
  - Increase technology choices
- Address hardware and software technologies together
  - If hardware technology is new, gaps in software stack are certain
- Buy down risk before commitment on capability/capacity class investment

Where Vanguard Fits

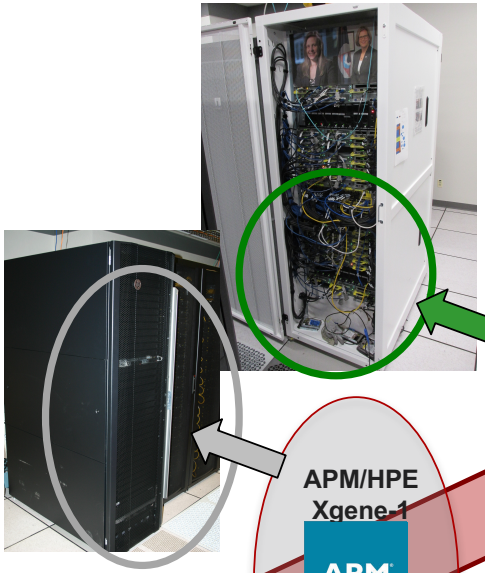


- Small testbeds (~10-100 nodes)
- Breadth of architectures key
- Brave users

- Larger-scale experimental systems
- Focused efforts to mature new technologies
- Broader user-base
- Not targeted for production use

- Leadership-class systems (Petascale, Exascale, ...)
- Advanced technologies, sometimes first-of-kind
- Broad user-base
- Production use

Sandia's NNSA/ASC ARM Platforms



Exascale Platform

HPE Comanche

APM/HPE Xgene-1
ARM
Hammer

Cavium/Penguin ThunderX1
ARM
Sullivan

ARM Next Gen
ARM
Mayer

ARM Next Gen
ARM
Vanguard ARM

Sept 2011

47 nodes

Cavium ThunderX1
36 nodes

TODAY

Pre-GA Cavium ThunderX2
32 nodes

FY18 Phase 1 Petascale Platform

= Retired

= 2015

= 2017

= 2018

Schedule – Past and Projected

- ~~August 2017 Formed Tri-lab software team (Sandia, Los Alamos, Livermore, NNSA HQ)~~
- ~~September 22nd 2017 – 2nd Draft RFI released~~
  - Note: We are releasing the RFI via the procurement vehicle more frequently, possibly weekly, to maintain equality in the communication process.
- ~~Week of September 25th 2017 – Prime F2F presentations~~
- December 2017 – ARM Tri-lab Software Environment (ATSE) draft
- RFP release no later than January 12th
- RFP responses due no later than February 8th
- RFP responses distributed to technical team members February 9th
- February/March 2018 – Negotiations and SOW development
- March/April 2018 – SOW development and contract placement
- July/August 2018 – Phase 1 platform delivery begins

Construction

- Institutionally Funded
- Design/Build Contract Awarded
- All Permits Received – Site Preparation underway
- Groundbreaking Event 9/28/17
- 40% and 90% Design Reviews Completed
- 100% Design Review by 12/8/17
- Completion Data 7/15/18
- Will feature 90% liquid cooling 10% air cooling
- Thermosyphons & Air-Side Economization for Water/Energy Savings
- Solar Farm for LEED Certification
- Non-load-bearing, movable west wall for expansion (14,000 – 20,000sf)
- 7 MW power expandable to 15 MW

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Vanguard Tri-Lab Software Effort

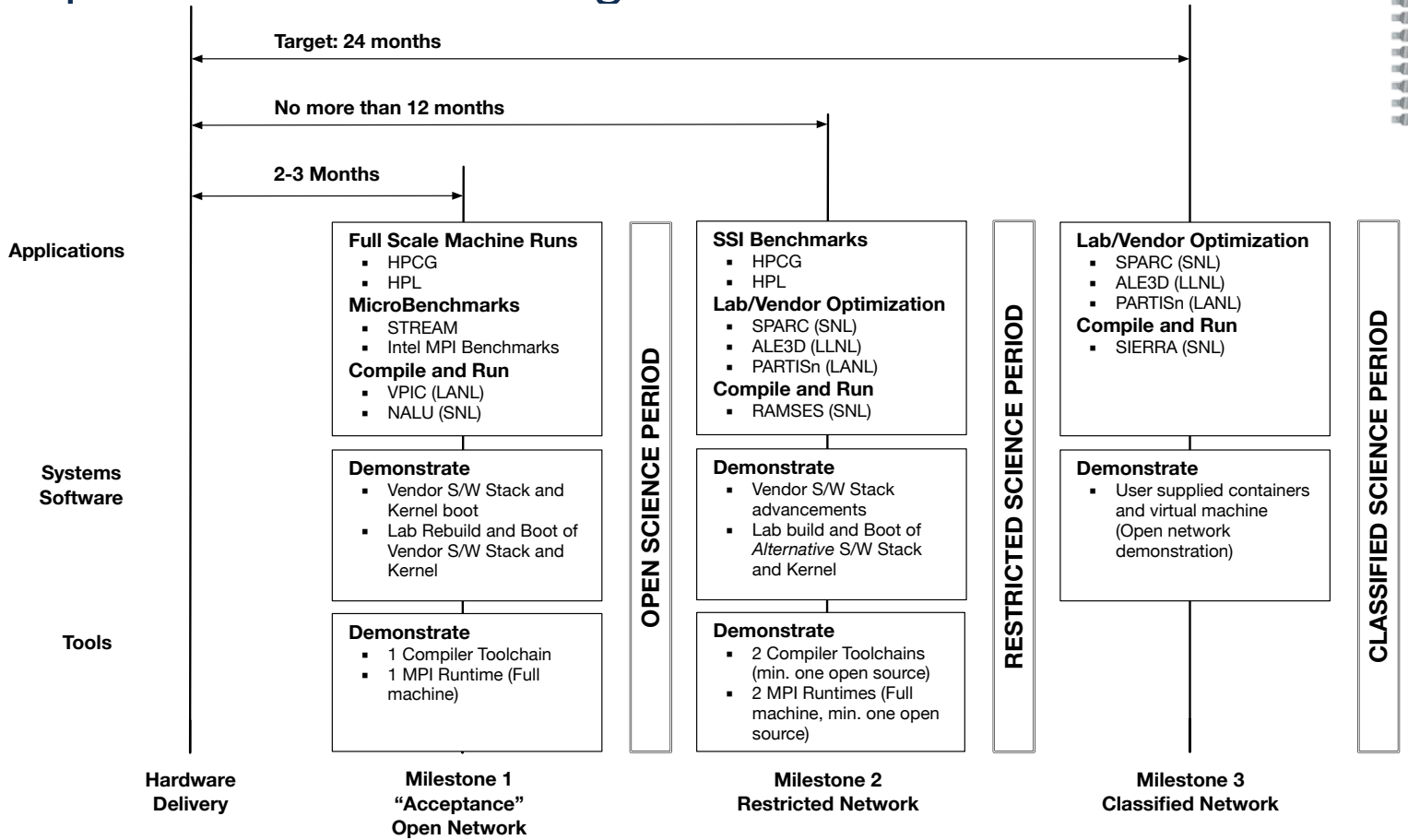
- Accelerate maturity of ARM ecosystem for ASC computing
  - Prove viability for NNSA integrated codes running at scale
  - Harden compilers, math libraries, tools, communication libraries
    - Heavily templated C++, Fortran 2003/2008, Gigabyte+ binaries, long compiles
  - Optimize performance, verify expected results
- Build integrated software stack
  - Programming env (compilers, math libs, tools, MPI, OMP, SHMEM, I/O, ...)
  - Low-level OS (optimized Linux, network, filesystems, containers/VMs, ...)
  - Job scheduling and management (WLM, app launcher, user tools, ...)
  - System management (boot, system monitoring, image management, ...)

Improve 0 to 60 time... ARM system arrival to useful work done

Software Stack Responsibilities

- Vendor
  - Deliver and support core elements of the software environment necessary for viable integrated system (called for in RFP)
  - Expect different levels of completeness depending on selected vendor
- Sandia and Tri-Lab team
  - Integrate system into our computing environment
  - Identify and resolve SW issues in collaboration with system vendor
  - Contribute tools and other capabilities to fill gaps
  - Regardless of selected vendor, ultimately use the Tri-lab developed SW stack to demonstrate applications

Acceptance Plan – Maturing the Stack

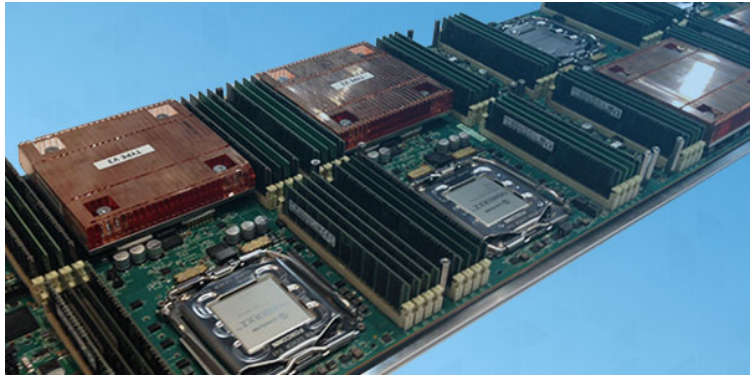


TOSS – Tri-lab Operating System Stack

- Targets commodity technology systems at NNSA Tri-labs (Lead: Livermore, Los Alamos, Sandia)
  - RHEL7 based, supports x86_64, ppc64le, and aarch64 from single source
  - ~4K packages on all archs, 200+ built for TOSS by LLNL (compilers, MPI, ...)
  - Baseline not optimized for particular system, labs optimize
  - Partnership with RHEL to add support for new hardware pre-GA
- Concerns
  - Missing on ARM: Nvidia cudatoolkit & driver, AMD ROCm, security scanners, backup tools, firmware tools, third party software
  - Only simple 2 node tests so far, larger scale testing soon on HPE Comanche
  - Distribution of TOSS restricted due to licensing, vendors-only for lab use

Cray Programming Environment (PE)

- Announced Monday Nov 13 @ SC17 (today)
- Targets Cray XC50 systems, 2018H1
  - Cavium ThunderX2 64-bit ARMv8 CPUs
  - HPC tuned network stack, Aries Network
    - Cray Linux environment / SLES12-based
    - Cray programming environment
    - Cray compiling environment for ARM
  - Production-proven, same infrastructure as NNSA/ASC ATS-1 Trinity

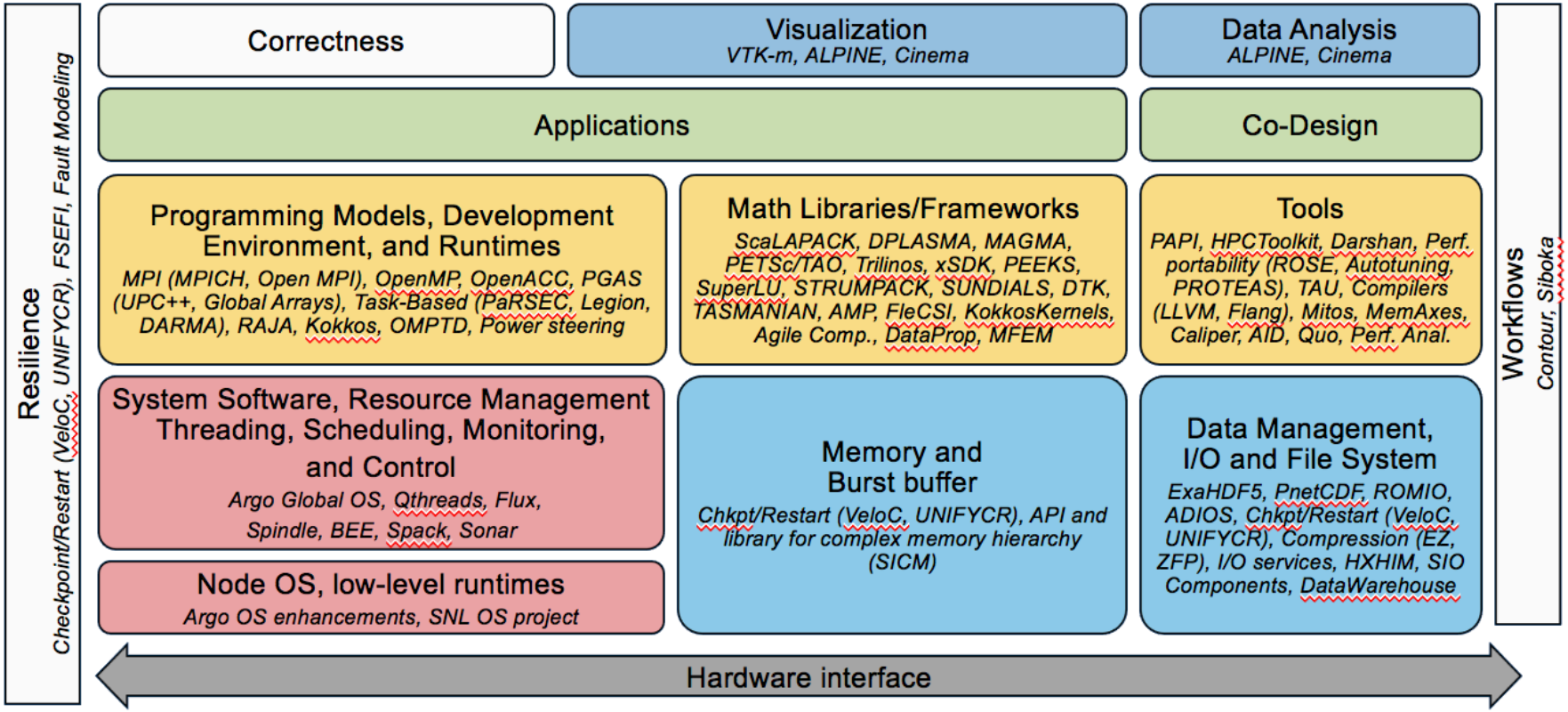


- Concerns
  - Vendor-proprietary
  - Ability to get new software components added to Cray stack

OpenHPC

- Targets HPC Linux clusters
  - Community effort
  - Common ingredients needed to deploy and manage an HPC cluster
  - Goal to enhance modularity and interchangeability of key components
  - Current release 1.3.3, builds on Centos 7.4 or SLES12, arm64 + x86_64
- Concerns
  - Lack of integration
  - Small cluster focused, lack of hierarchy needed for scalability
  - Ability to do optimized builds

Exascale Computing Project Software, Support on ARM



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Compiler Dashboard

Early ThunderX2 Hardware, Single node

Sandia National Laboratories

Workload	GCC 7.1	Vendor A	Vendor B
STREAM			
GUPS			
MiniFE			
Pennant			
Sweep3D			
LULESH			
OpenMPI 2.1.2			
Kokkos Kernels			
Trilinos			
NaluCFD			

Things are working surprisingly well

There are some issues, but being rapidly addressed and resolved

Performance is looking good.
Excellent on memory bandwidth, on par for compute. Should get significantly better with GA hardware and software tuning.

Key: Fastest | Middle | Slowest

Results from Si Hammond @ Sandia

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Conclusion

- Vanguard allows the DOE to take necessary risks to ensure a healthy HPC ecosystem for future production mission platforms
  - Increase technology choices
  - Prove ability to run multi-physics production applications at scale
- Vanguard Tri-lab software stack effort is maturing ARM for ASC computing
  - Harden compilers, math libs, and tools
  - Optimize performance, verify expected results
  - Increase modularity and openness of software stack

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