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

SAND2018-2472C

VANGUARD

arm env

Sandia National Laboratories

Exceptional service in the national interest

SIAM PP18
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Kevin Pedretti
ktpedre@sandia.gov

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

CCR Center for Computing Research

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Outline

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

Vanguard: Prototype Systems for Advanced Architectures

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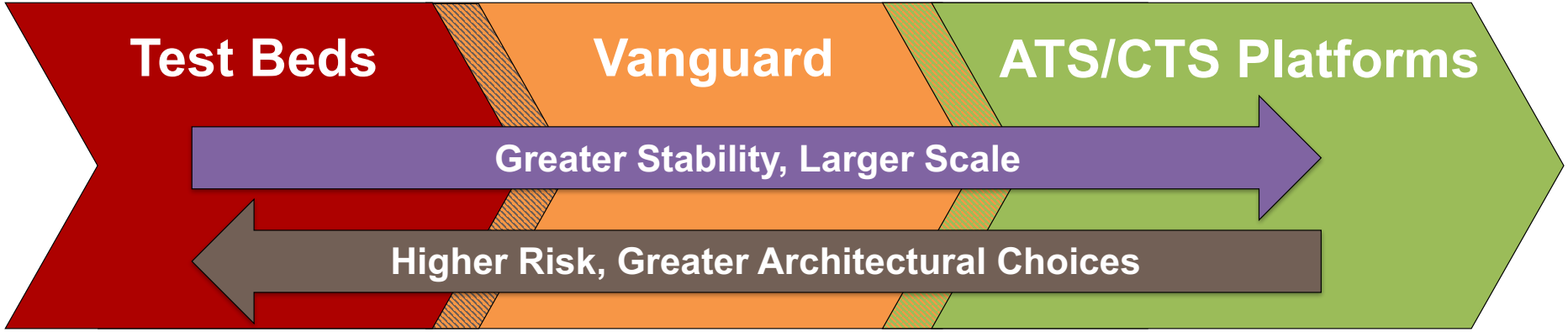
- Expand the HPC ecosystem by developing emerging, yet-to-be-proven, technologies
  - Is technology viable for future production platforms supporting ASC integrated codes?
  - Increase technology choices
- Address hardware and software technologies together
  - If hardware technology is new, gaps in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

Where Vanguard Fits



Test Beds

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

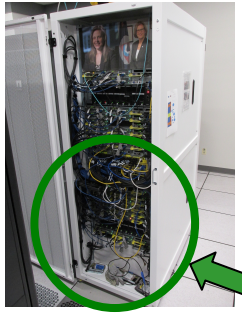
Vanguard

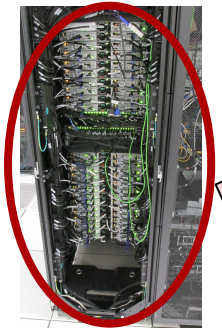
- Larger-scale experimental systems
- Focused efforts to mature new technologies
- Broader user-base
- **NOT PRODUCTION**
- Trilab resource but not formal campaign process

ATS/CTS Platforms

- Leadership-class systems (Petascale, Exascale, ...)
- Advanced technologies, sometimes first-of-kind
- Broad user-base
- **PRODUCTION USE**

Sandia's NNSA/ASC ARM Platforms





Sept 2011

APM/HPE
Xgene-1
ARM
Hammer

Applied Micro
X-Gene-1
47 nodes

Cavium/Penguin
ThunderX1
ARM
Sullivan

Cavium
ThunderX1
32 nodes

Cavium
HPE/Comanche
ThunderX2
ARM
Mayer

Pre-GA
Cavium
ThunderX2
47 nodes

TODAY

ARM
Next Gen
ARM
Vanguard
ARM

FY18
Vanguard-1
Petascale ARM
Platform

Future ASC
Platforms

= Retired

= 2015

= 2017

= 2018

Schedule – Past and Projected

- ✓ August 2017 Formed Tri-Lab software team (Sandia, Los Alamos, Livermore, NNSA HQ)
- ✓ September 22nd – 2nd Draft RFI released
- ✓ Week of September 25th – Prime F2F presentations
- ✓ December 2017 – ARM Tri-lab Software Environment (ATSE) draft
- ✓ RFP released December 20th, responses due February 8th
- ✓ January 11th – Vendor pre-proposal brief at Sandia NM CSRI
- ✓ RFP responses distributed to technical team members February 8th
- ▪ February-May 2018 – Technical review, source selection, SOW development, negotiation, and contract placement
- ▪ June 2018 – Initial ATSE stack release, ver. 2018.0, on early testbed
- ▪ 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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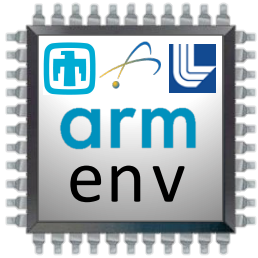
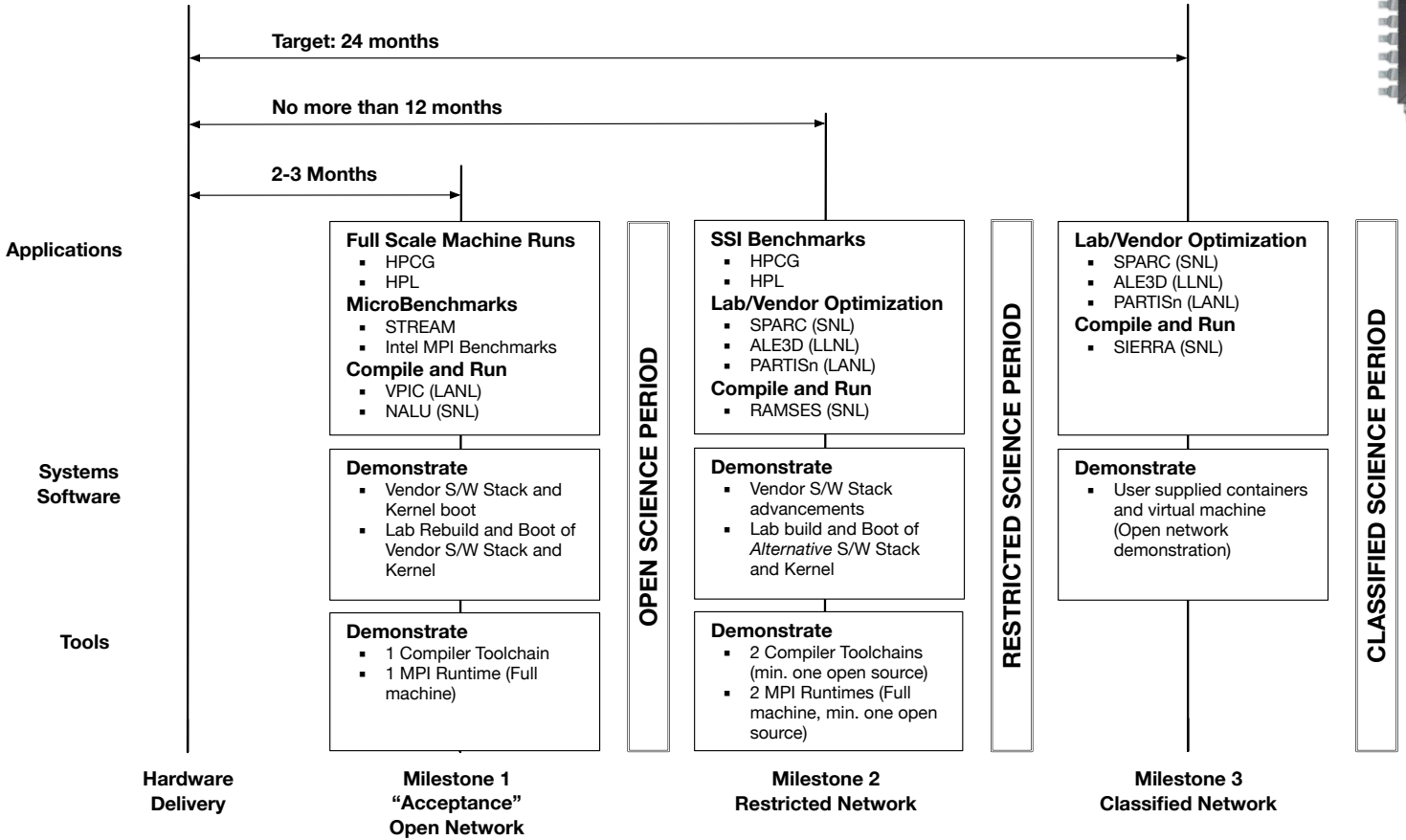
Vanguard Tri-Lab Software Effort



- 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

Acceptance Plan – Maturing the Stack

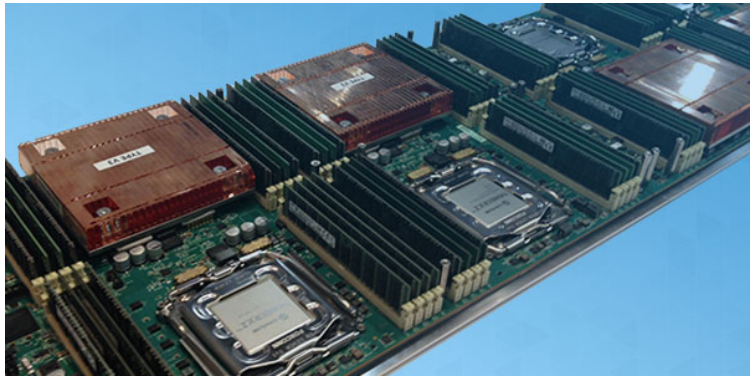


TOSS – Tri-lab Operating System Stack

- 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
  - Distribution of TOSS restricted due to licensing, vendors-only for lab use
  - Not focused on user-facing programming environment
  - Missing on ARM: Nvidia cudatoolkit & driver, AMD ROCm, security scanners, backup tools, firmware tools, third party software

Cray Programming Environment (PE)

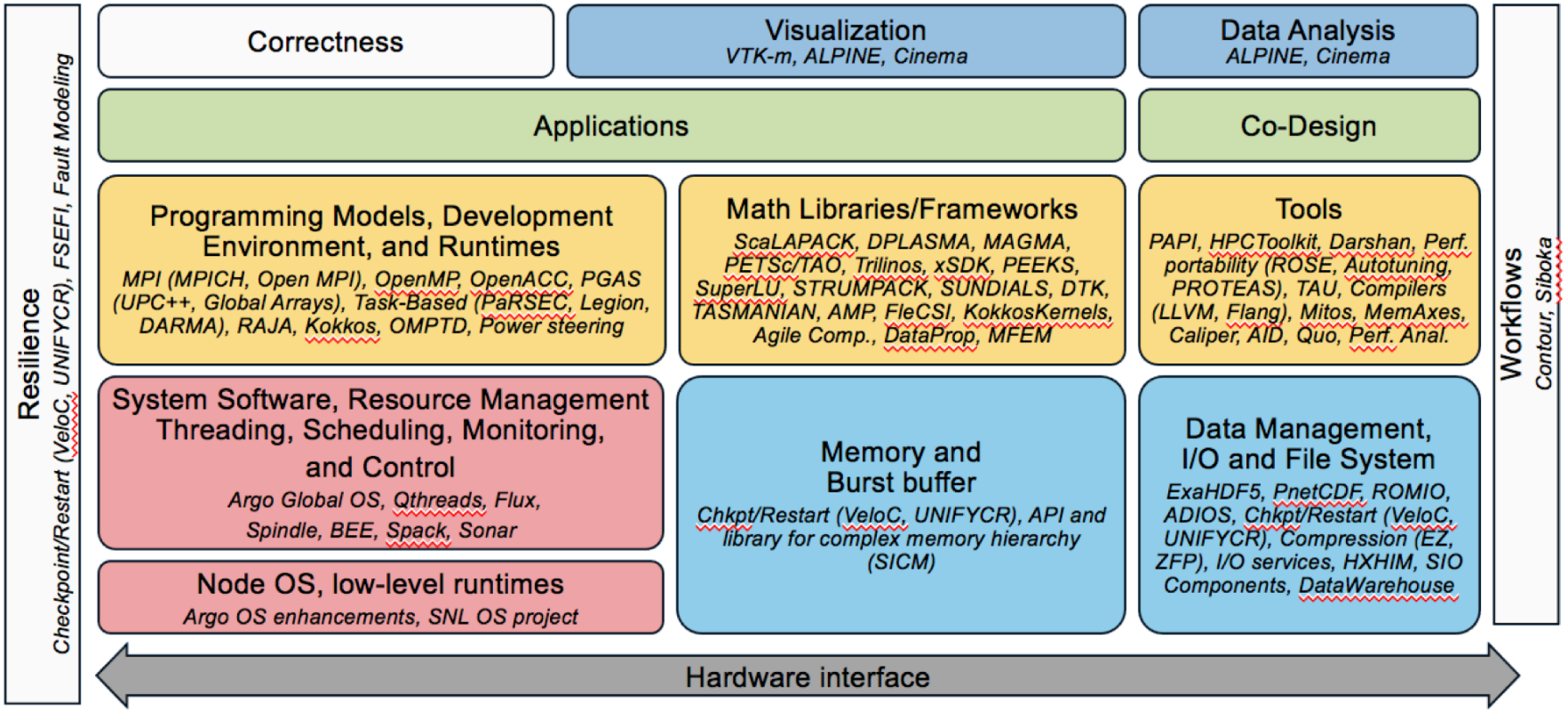
- Announced @ SC17
- Targets Cray XC50 systems, 2018H1
  - Cavium ThunderX2 64-bit ARMv8 CPUs
  - HPC tuned network stack, Aries Network
    - Cray Linux environment / SLES12-based
    - Cray programming environment
    - Cray compiling environment for ARM
  - Production-proven, same infrastructure as NNSA/ASC ATS-1 Trinity
- Concerns
  - Vendor-proprietary
  - Ability to get new software components added to Cray stack



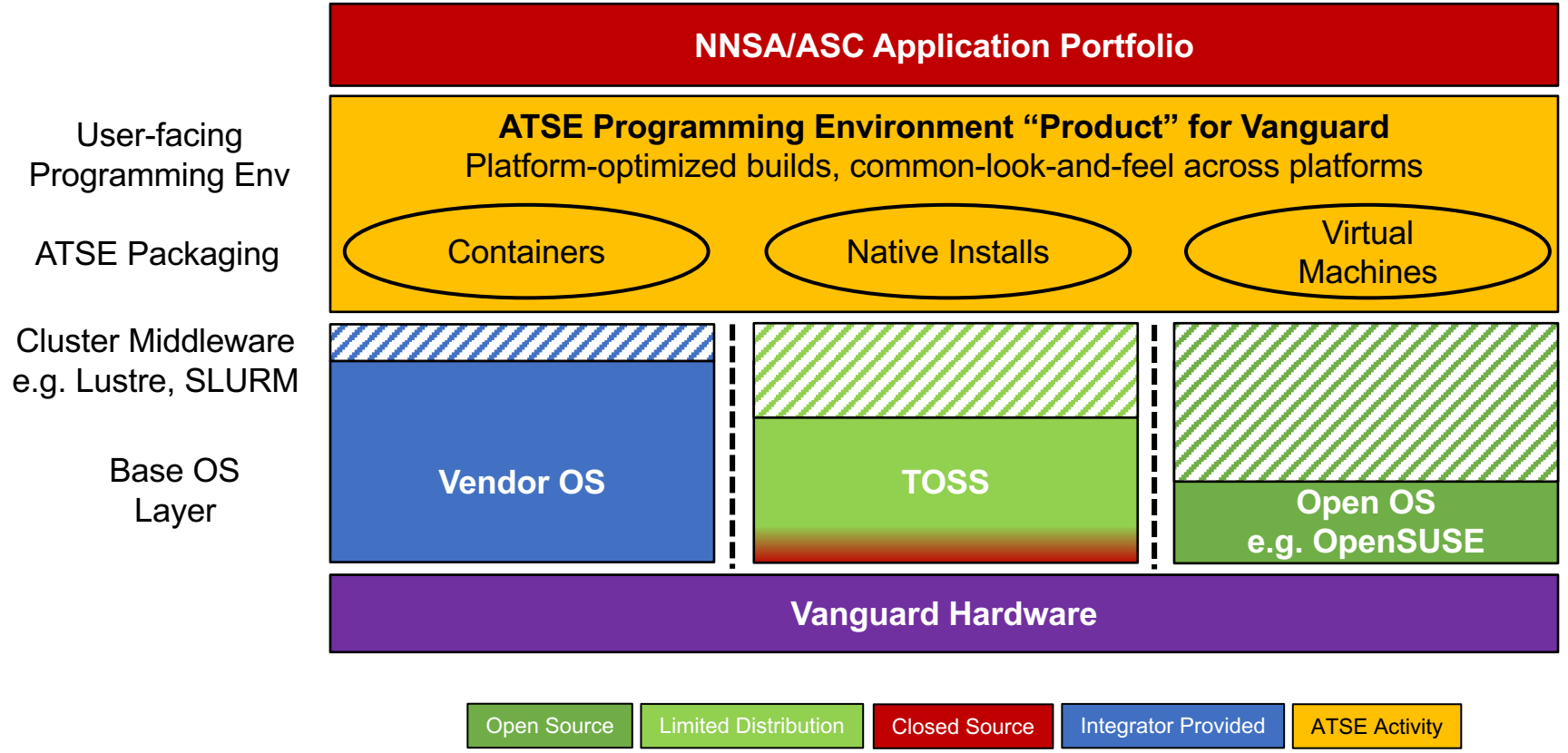
OpenHPC

- 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



ARM Tri-lab Software Environment (ATSE)



Integrate Components from Many Sources

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RHEL EPEL

TOSS

Vendor Software

ATSE Packages

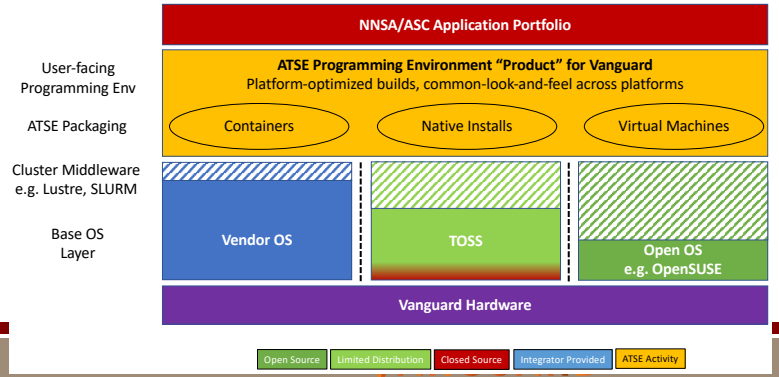
OpenHPC

Vendor Software

Koji Build Server

Open Build Server

ATSE Packager



Key:

- ATSE Activity
- Open Source
- Limited Distribution
- Closed Source
- Integrator Provided

Draft ATSE Timeline for 2018

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- March
  - Continue software stack explorations and gap analysis on testbeds
  - Setup OpenBuild server and replicate OHPC package builds for aarch64
- April – May
  - Develop ATSE Packager framework, ability to pull packages from TOSS, RHEL, OpenHPC OBS, vendor, and other sources
  - Identify initial component list
- June
  - Initial ATSE release 2018.0 on Mayer
    - Lab-distribution version: TOSS BaseOS + (ATSE-GCC | ATSE-ARM | ATSE-*)
    - Open-distribution version: OpenSUSE/CentOS BaseOS + ATSE-GCC
- July – August
  - Linux kernel optimization and HPC patches
  - Virtual machine support
- September – October
  - ATSE 2018.1 release
  - Initial upstream to OpenHPC push

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Compiler Dashboard

Early ThunderX2 Hardware, Single node

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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

Compiler Dashboard

Early ThunderX2 Hardware, Single node

Sandia National Laboratories

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STREAM			
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Results from Si Hammond @ Sandia

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
  - Support traditional HPC and emerging AI + ML workloads

Acknowledgments

- Sandia: Jim Laros, Si Hammond, Andrew Younge, Ruth Klundt, Jeff Ogden, Mike Aguilar, Ken Alvin, Rob Hoekstra, Jim Ang, Ron Brightwell
- Livermore: Rob Neely, Trent D'Hooge
- Los Alamos: Mike Lang, Pat McCormick
- DOE HQ: Thuc Hoang, Tina Macaluso, Emily Simpson

Example: Building an App

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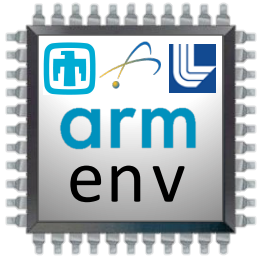
- Cmake, GNU autotools, other tools
- MPI (OpenMPI, MPICH2, rely on Vendor MPI)
- I/O libraries (HDF5, NetCDF)
- Mesh databases (Exodus, CGNS)
- Math libraries
- ParMetis, SuperLU
- Trilinos packages (Epetra, Tpetra, Belos, Aztec, Amesos, ...

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