THE WORLD'S FIRST PETASCALE ARM SUPERCOMPUTER

Sandia National Laboratories

ASTRA

"Per aspera ad astra"

Experiences Scaling a Production Arm Supercomputer to Petaflops and Beyond

Kevin Pedretti for the Astra Team

POCs: Jim Laros (Platform), Kevin Pedretti (Software Stack), Si Hammond (Apps)
jhlaros@sandia.gov, ktpedre@sandia.gov, sdhammo@sandia.gov

U.S. DEPARTMENT OF ENERGY NNSA

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It Takes an Incredible Team…

- DOE Headquarters:
  - Thuc Hoang
  - Mark Anderson
- Sandia Procurement
- Sandia Facilities
- Incredible Sandia Team
- Colleagues at LLNL and LANL
  - Mike Lang
  - Rob Neely
  - Mike Collette
  - Alan Dayton
  - Trent D'Hooge
  - Todd Gamblin
  - Robin Goldstone
  - Anna Pietarila Graham
  - Sam Gutierrez
  - Steve Langer
  - Matt Leininger
  - Matt Legendre
  - Pat McCormick
  - David Nystrom
  - Howard Pritchard
  - Dave Rich
  - And loads more …

- HPE:
  - Mike V. and Nic Dube
  - Andy Warner
  - Erik Jacobson
  - John D'Arcy
  - Steve Cruso
  - Lori Gilbertson
  - Meredydd Evans
  - Cheng Liao
  - John Baron
  - Kevin Jameson
  - Tim Wilcox
  - Charles Hanna
  - Michael Craig
  - Patrick Raymond
  - And loads more …

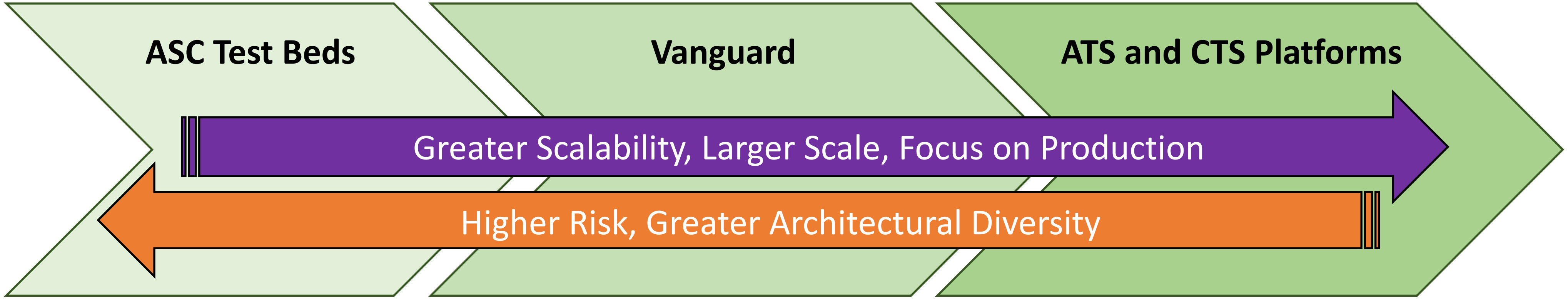
- Cavium/Marvel:
  - Giri Chukkapalli (now NVIDIA)
  - Todd Cunningham
  - Larry Wikelius
  - Raj Sharma Govindaiah
  - Kiet Tran
  - Joel James
  - And loads more…
- ARM:
  - ARM Research Team!
  - ARM Compiler Team!
  - ARM Math Libraries!
  - And loads more…

It Takes an Incredible Team…

Outline

- Astra Overview
- ATSE Software Stack
- Recent Application Results
- Conclusion – HPC on Arm, are we there yet?

Vanguard Program: Advanced Technology Prototype Systems



ASC Test Beds

Vanguard

ATS and CTS Platforms

Greater Scalability, Larger Scale, Focus on Production

Higher Risk, Greater Architectural Diversity

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, seek to increase technology and vendor choices
- **DOE/NNSA Tri-lab resource**

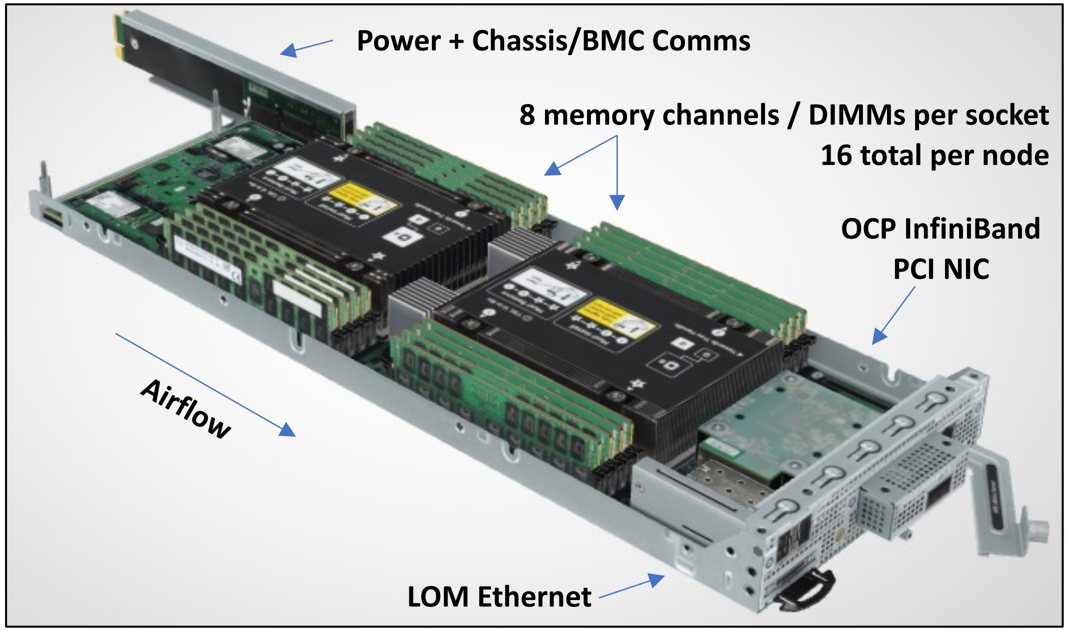
Production Platforms

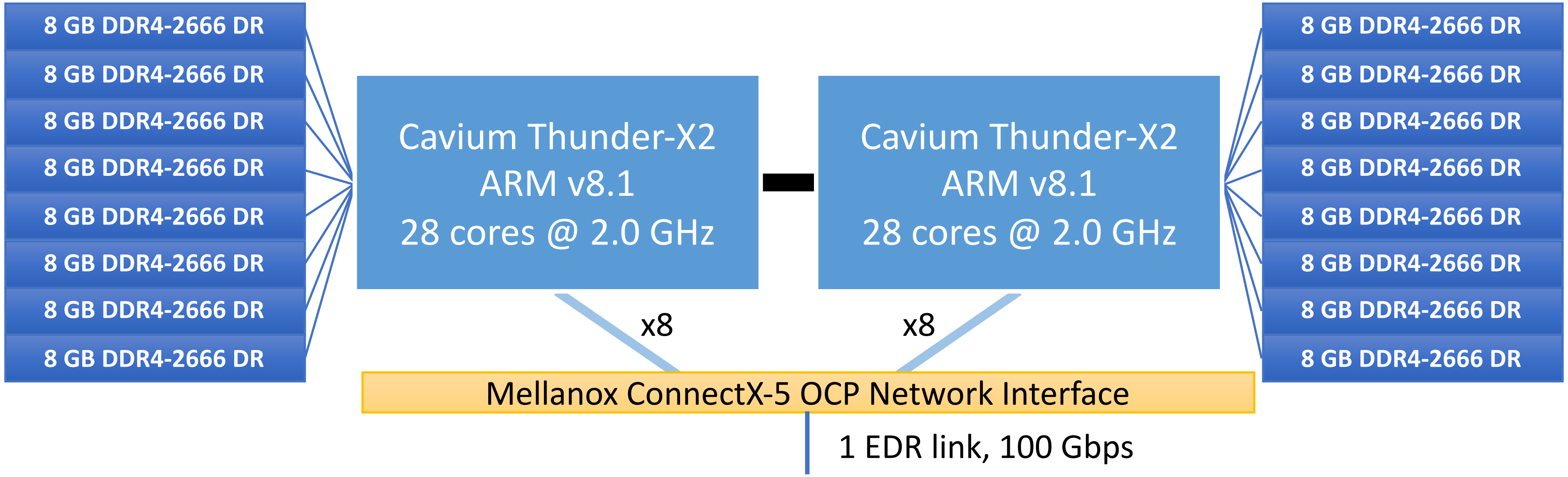
- Leadership-class systems (Petascale, Exascale, ...)
- Advanced technologies, sometimes first-of-kind
- Broad user-base
- Production use

Astra is the first Vanguard Platform

Astra Node Architecture

- **2,592** HPE Apollo 70 compute nodes
  - Cavium Thunder-X2 **Arm** SoC, 28 core, 2.0 GHz
  - 5,184 CPUs, 145,152 cores, 2.3 PFLOPs system peak
  - 128GB DDR Memory per node **(8 memory channels per socket)**
  - Aggregate capacity: 332 TB, Aggregate Bandwidth: 885 TB/s
- Mellanox IB EDR, ConnectX-5
- HPE Apollo 4520 All–flash storage, Lustre parallel file-system
  - Capacity: 990 TB (usable)
  - Bandwidth 244 GB/s


Power + Chassis/BMC Comms
8 memory channels / DIMMs per socket
16 total per node
OCP InfiniBand
PCI NIC
Airflow
LOM Ethernet



8 GB DDR4-2666 DR
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Cavium Thunder-X2
ARM v8.1
28 cores @ 2.0 GHz

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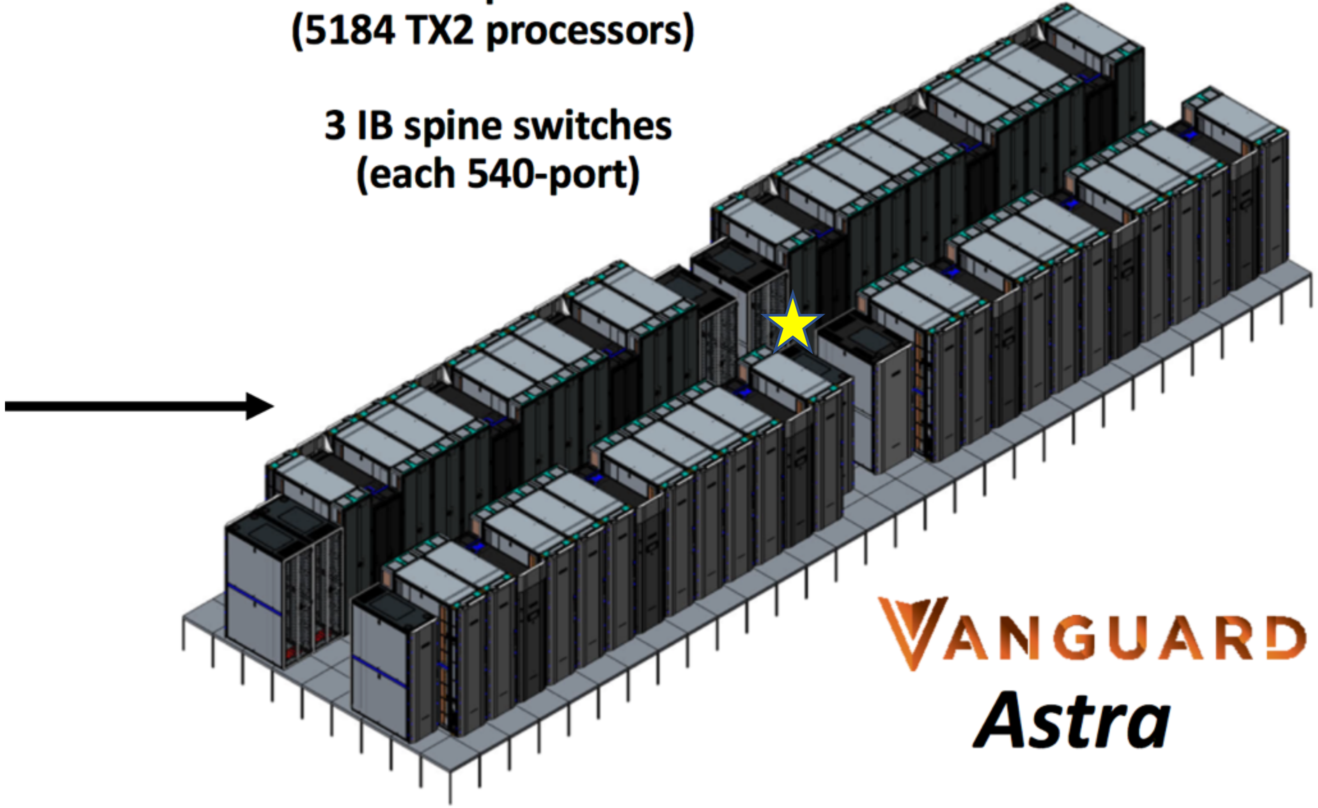
x8

x8

Mellanox ConnectX-5 OCP Network Interface

1 EDR link, 100 Gbps

Astra System Architecture



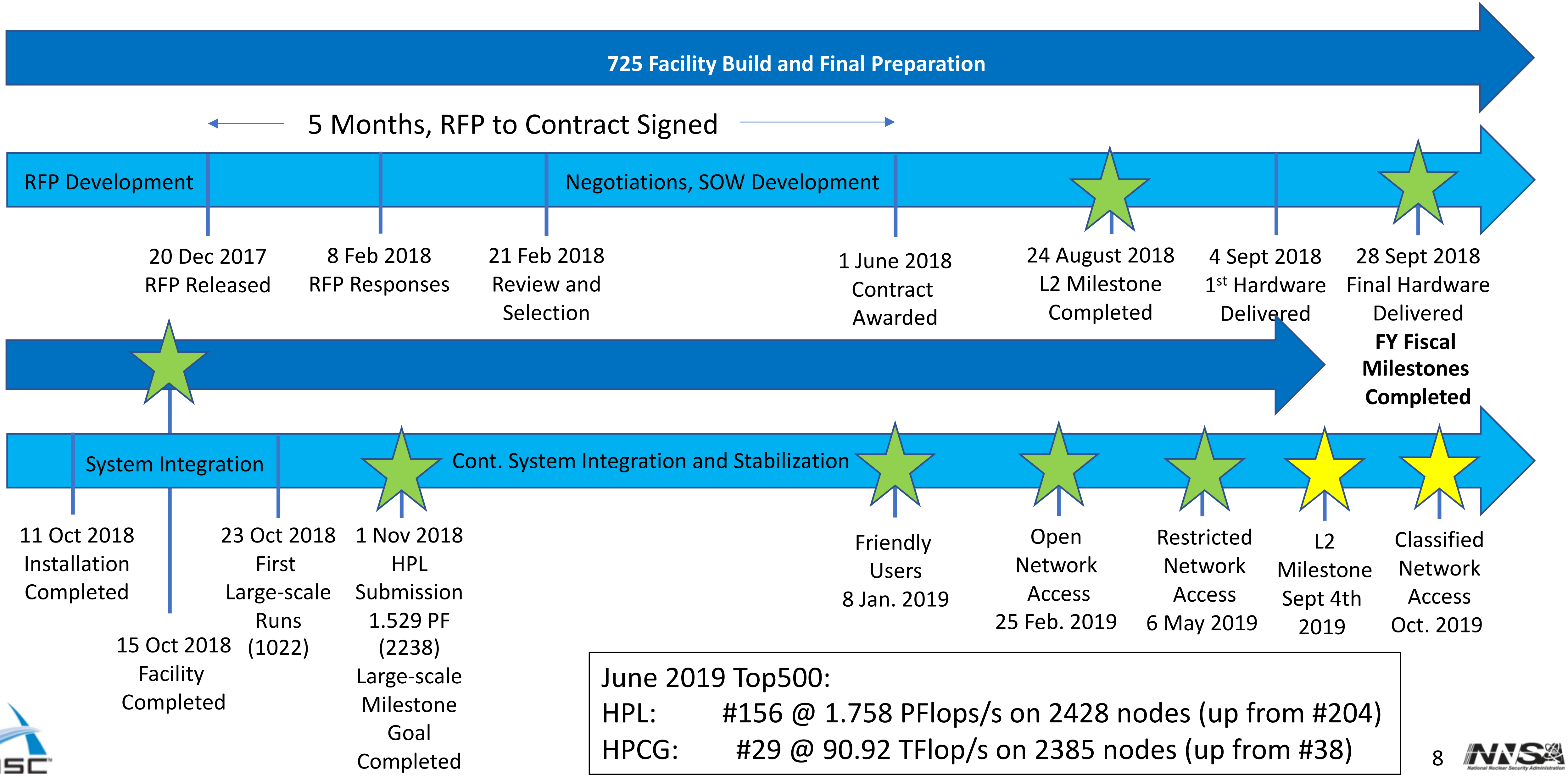
36 compute racks
(9 scalable units, each 4 racks)

2592 compute nodes
(5184 TX2 processors)

3 IB spine switches
(each 540-port)

VANGUARD
Astra

Vanguard-Astra: Timeline



725 Facility Build and Final Preparation

5 Months, RFP to Contract Signed

RFP Development

Negotiations, SOW Development

20 Dec 2017 RFP Released

8 Feb 2018 RFP Responses

21 Feb 2018 Review and Selection

1 June 2018 Contract Awarded

24 August 2018 L2 Milestone Completed

4 Sept 2018 1st Hardware Delivered

28 Sept 2018 Final Hardware Delivered

FY Fiscal Milestones Completed

System Integration

Cont. System Integration and Stabilization

11 Oct 2018 Installation Completed

15 Oct 2018 Facility Completed

23 Oct 2018 First Large-scale Runs (1022)

1 Nov 2018 HPL Submission 1.529 PF (2238) Large-scale Milestone Goal Completed

Friendly Users 8 Jan. 2019

Open Network Access 25 Feb. 2019

Restricted Network Access 6 May 2019

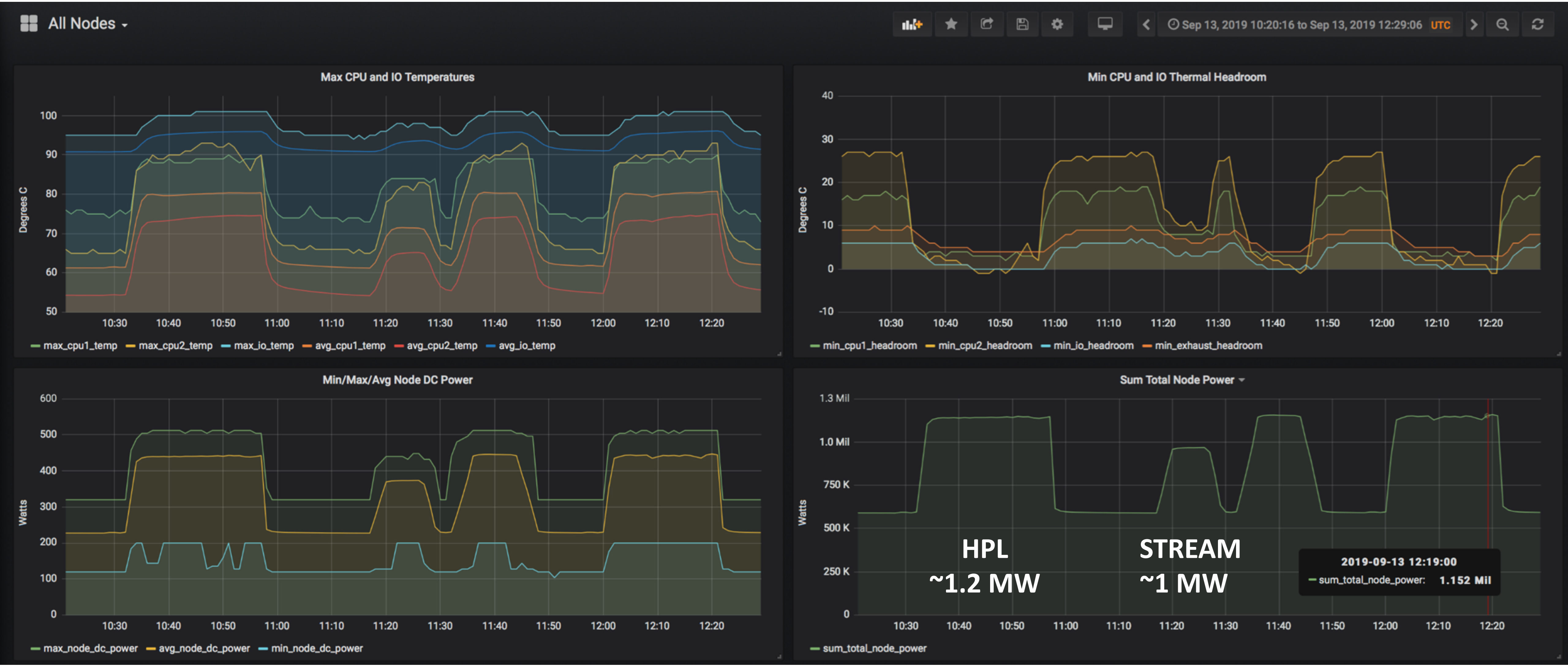
L2 Milestone Sept 4th 2019

Classified Network Access Oct. 2019

June 2019 Top500:
HPL: #156 @ 1.758 PFlops/s on 2428 nodes (up from #204)
HPCG: #29 @ 90.92 TFlop/s on 2385 nodes (up from #38)

Real-Time System Monitoring Has Been Key

- Tools: {BMC,PDU,Syslog,TX2MON} + TimescaleDB + Grafana



HPL
~1.2 MW

STREAM
~1 MW

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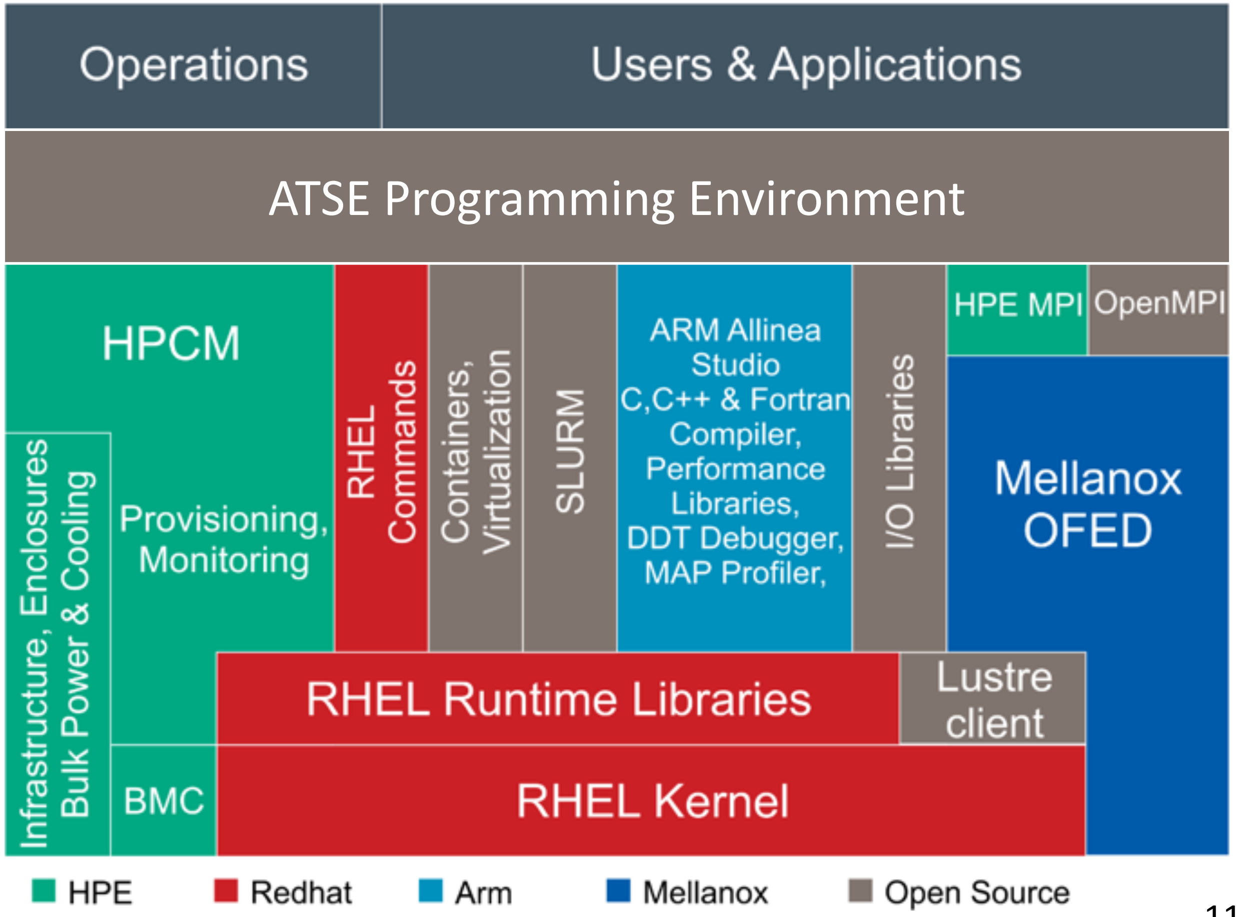
Astra Collaboration with HPE's HPC Software Stack

HPE's HPC Software Stack

- HPE:
  - HPE Cluster Manager
  - HPE MPI (+ XPMEM)
- Arm:
  - Arm HPC Compilers
  - Arm Math Libraries
  - Allinea Tools
- Mellanox-OFED & HPC-X
- RedHat 7.x for aarch64



Operations

Users & Applications

ATSE Programming Environment

HPCM

Infrastructure, Enclosures

Bulk Power & Cooling

Provisioning, Monitoring

BMC

RHEL Commands

Containers, Virtualization

SLURM

ARM Allinea Studio C,C++ & Fortran Compiler, Performance Libraries, DDT Debugger, MAP Profiler,

I/O Libraries

HPE MPI

OpenMPI

Mellanox OFED

RHEL Runtime Libraries

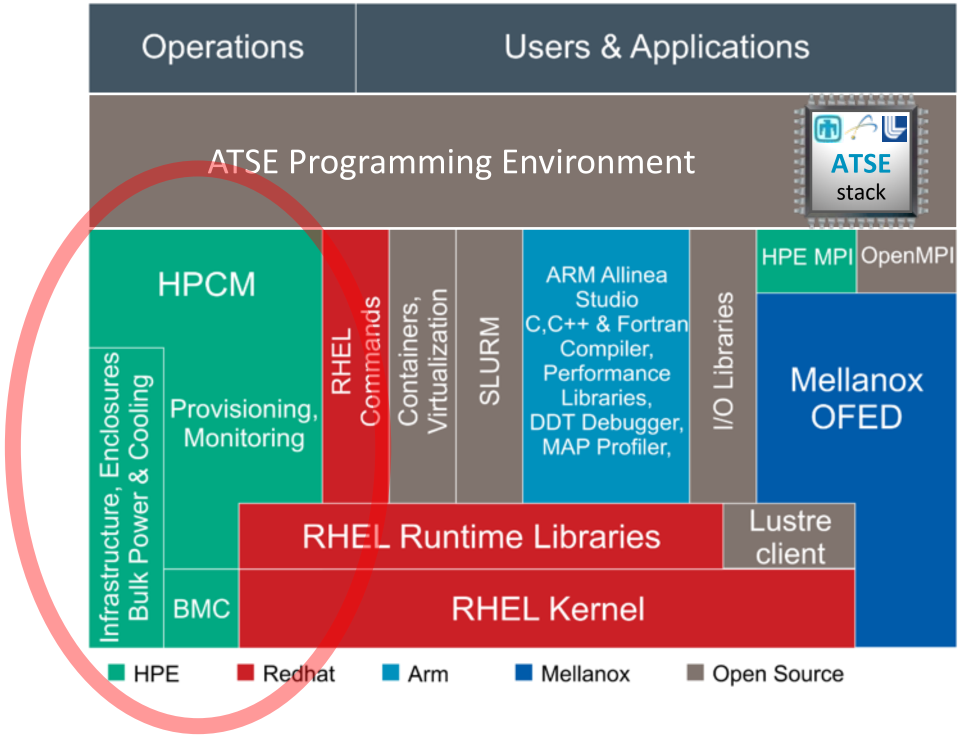
Lustre client

RHEL Kernel

🟩 HPE 🟥 Redhat 🟦 Arm 🟦 Mellanox 🟫 Open Source

HPCM Provides Scalable System Management for Astra

- HPCM: HPE Performance Cluster Manager
  - Merger of HPE CMU with SGI Icebox stack
  - New product at time of Astra deployment
- Collaboration resulted in new capabilities
  - Support for hierarchical leader nodes for non Icebox clusters (aka “Flat Clusters”)
    - **Demonstrated boot of 2592 nodes in < 10 min**
  - Resilient leader node failover
  - Scalable BIOS upgrades and configuration
  - Ability to deploy TOSS images (Tri-lab Operating System Stack)



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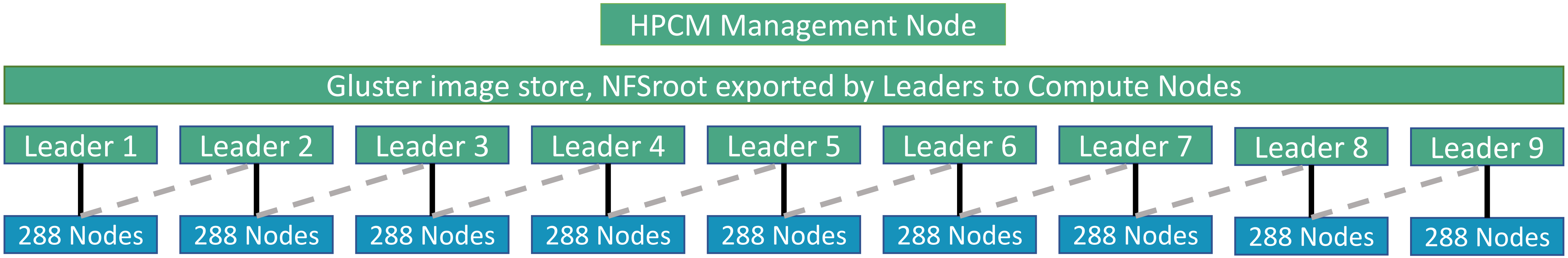


HPCM Management Node

Gluster image store, NFSroot exported by Leaders to Compute Nodes

Leader 1

Leader 2

Leader 3

Leader 4

Leader 5

Leader 6

Leader 7

Leader 8

Leader 9

288 Nodes

288 Nodes

288 Nodes

288 Nodes

288 Nodes

288 Nodes

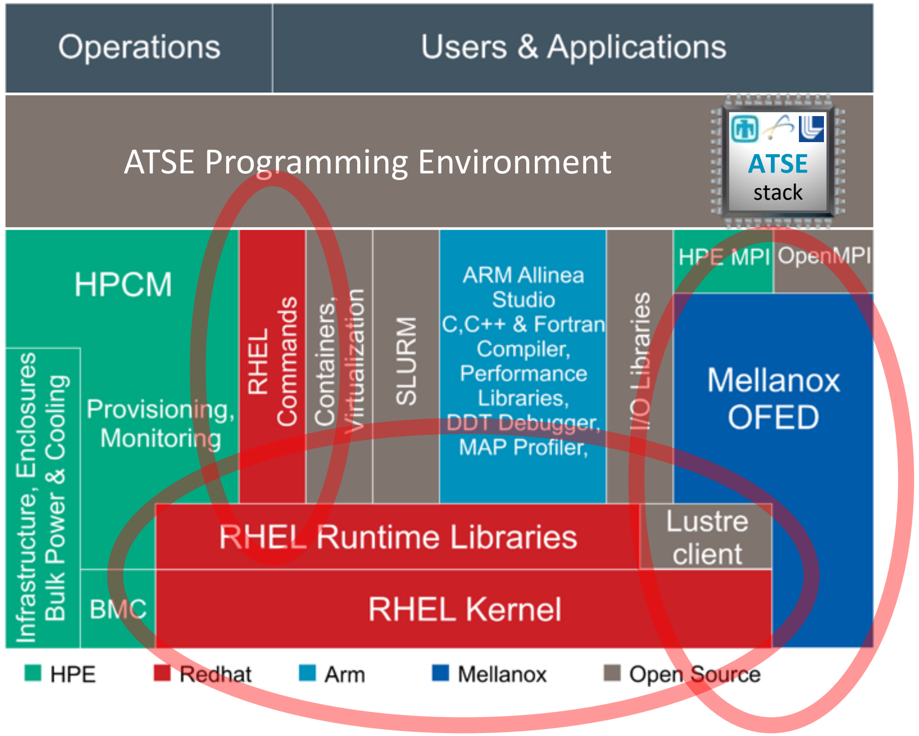
288 Nodes

288 Nodes

288 Nodes

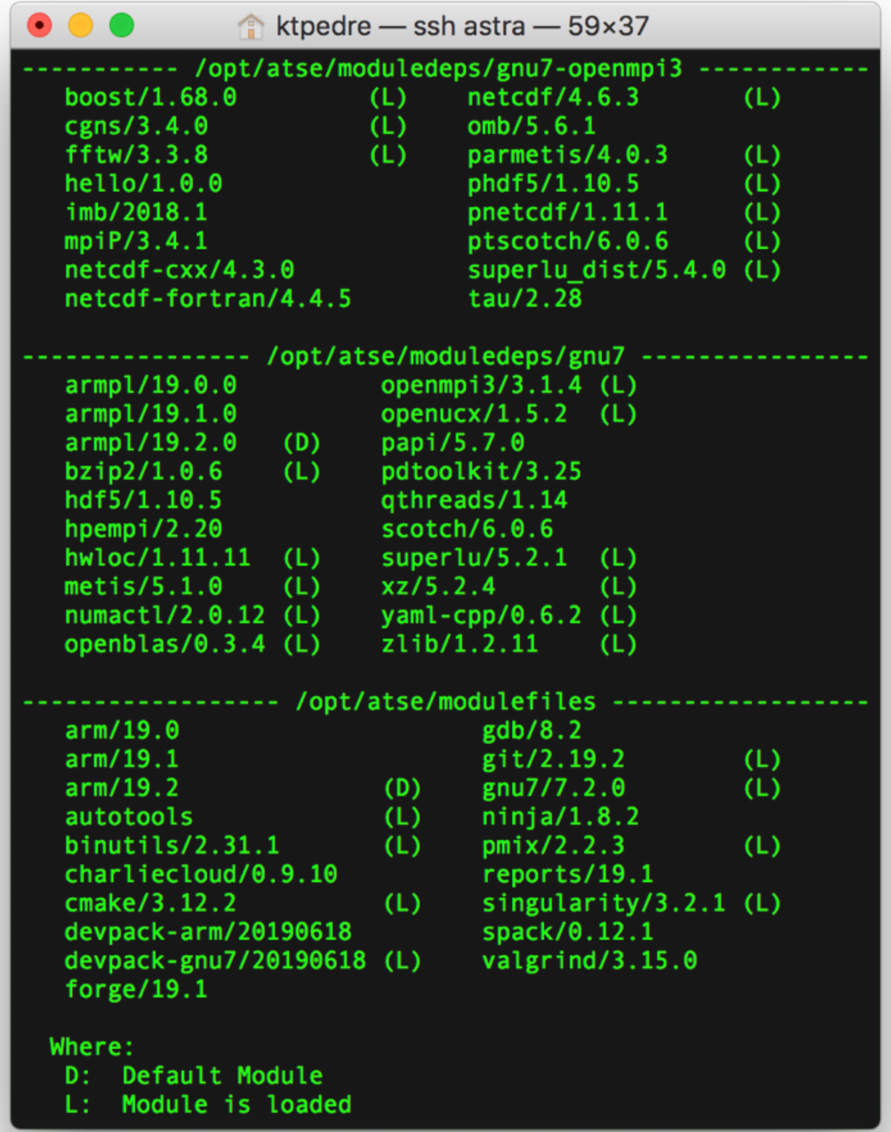
TOSS Provides Robust Base OS for Astra / ARM

- TOSS: Tri-lab Operating System Stack (Lead: LLNL, LANL, SNL)
  - Targets commodity technology systems (model: vendors provide HW, labs provide SW)
  - Red Hat 7 based; x86_64, ppc64le, and aarch64
  - ~4K packages on all archs, 200+ specific to TOSS
  - Partnership with RedHat with direct support
- Astra-related activities
  - Lustre enablement and bringup
  - Added support for Mellanox OFED InfiniBand stack, needed for advanced IB features
  - Debugged Linux Kernel issues on Arm, scale of Astra revealed bugs not previously seen
    - Kworker CPU hang – fix was in Linux upstream, but not in RedHat. Patch added to TOSS Linux kernel.
    - Sys_getdents64 oops – rare hang at job cleanup / exit.
      Actively debugging with RedHat + Marvell + HPE + Mellanox



ATSE is an Integrated Software Environment for ASC Workloads

- Advanced Tri-lab Software Environment
  - User-facing programming environment co-developed with Astra
  - Provides a common set of libraries and tools used by ASC codes
  - Integrates with TOSS and the vendor software stack
  - Derived from OpenHPC package recipes, similar look and feel **(add uarch optimizations, static libraries, -fPIC, add missing libs)**
- FY19 Accomplishments
  - Deployed TOSS + ATSE at transition to SRN (May'19)
  - Developed ATSE 1.2 with support for 2x compilers and 2x MPIs: {GNU7, ARM} x {OpenMPI3, HPE-MPI}
  - Built Trilinos and many ASC apps with ATSE
  - Packaged ATSE containers and tested up to 2048 nodes
- Future Directions
  - Migrate to Spack Stacks build
  - Add support for SNL adv. arch testbeds
  - Collaboration with RIKEN on McKernel



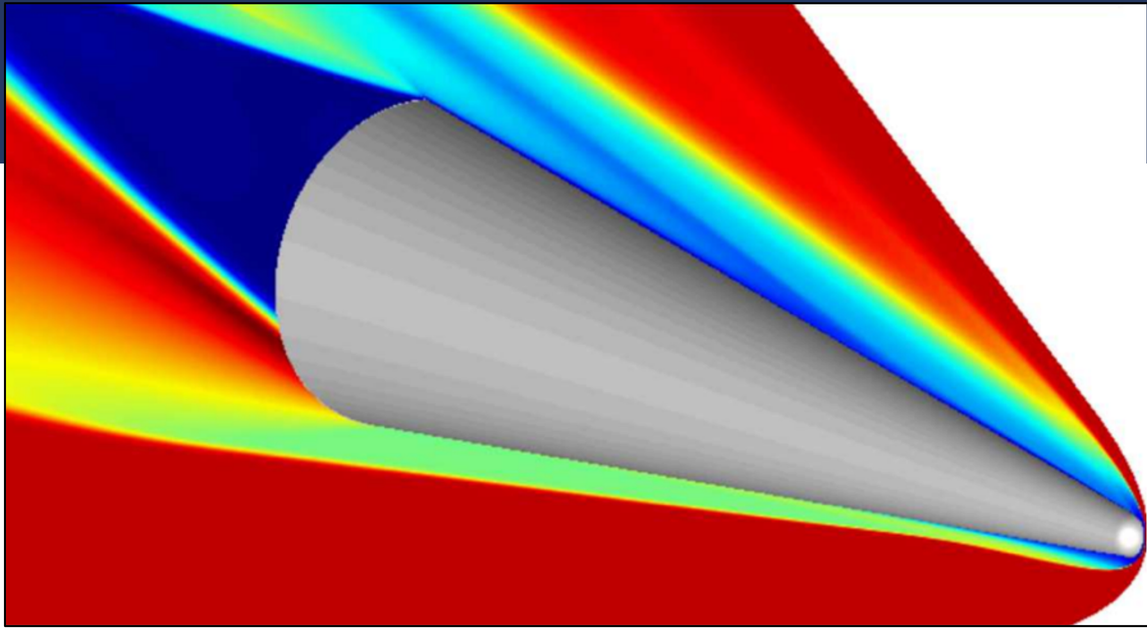
```
----------- /opt/atse/moduledeps/gnu7-openmpi3 ------------
   boost/1.68.0         (L)    netcdf/4.6.3       (L)
   cgns/3.4.0           (L)    omb/5.6.1
   fftw/3.3.8           (L)    parmetis/4.0.3     (L)
   hello/1.0.0                 phdf5/1.10.5       (L)
   imb/2018.1                  pnetcdf/1.11.1     (L)
   mpiP/3.4.1                  ptscotch/6.0.6     (L)
   netcdf-cxx/4.3.0            superlu_dist/5.4.0 (L)
   netcdf-fortran/4.4.5        tau/2.28

---------------- /opt/atse/moduledeps/gnu7 ----------------
   armpl/19.0.0          openmpi3/3.1.4 (L)
   armpl/19.1.0          openucx/1.5.2  (L)
   armpl/19.2.0   (D)    papi/5.7.0
   bzip2/1.0.6    (L)    pdtoolkit/3.25
   hdf5/1.10.5           qthreads/1.14
   hpempi/2.20           scotch/6.0.6
   hwloc/1.11.11  (L)    superlu/5.2.1  (L)
   metis/5.1.0    (L)    xz/5.2.4       (L)
   numactl/2.0.12 (L)    yaml-cpp/0.6.2 (L)
   openblas/0.3.4 (L)    zlib/1.2.11    (L)

------------------ /opt/atse/modulefiles ------------------
   arm/19.0                     gdb/8.2
   arm/19.1                     git/2.19.2         (L)
   arm/19.2                (D)  gnu7/7.2.0         (L)
   autotools               (L)  ninja/1.8.2
   binutils/2.31.1         (L)  pmix/2.2.3         (L)
   charliecloud/0.9.10          reports/19.1
   cmake/3.12.2            (L)  singularity/3.2.1 (L)
   devpack-arm/20190618         spack/0.12.1
   devpack-gnu7/20190618 (L)    valgrind/3.15.0
   forge/19.1

  Where:
   D:  Default Module
   L:  Module is loaded
```

Containerized SPARC HIFiRE-1 on Astra



In job script:

```
mpirun \
        --map-by core \
        --bind-to core \
        singularity exec atse-astra-1.2.1.simg
        container_startup.sh
```

container_startup.sh

```
#!/bin/bash
module purge
module load devpack-gnu7
./sparc
```

Early Results: SPARC on Astra, 56 MPI processes per node

Nodes	Trials	Native (seconds)	Container (seconds)	% Diff vs. Native
128	2	8164	8169	+ 0.1%
256	3	4473	4505	+ 0.7%
512	3	2634	2636	+ 0.1%
1024	1*	1827	1762	- 3.6%
2048	2	1412	1429	+ 1.2 %

Points:

- Supporting SPARC containerized build & deployment on Astra
- Enables easy test of new or old ATSE software stacks
- Near-native performance using a container
- Testing HIFiRE-1 Experiment (MacLean et al. 2008)

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Application Porting Summary

- **Applications ported during open and restricted phases:**
  - **SNL: SPARC, EMPIRE, SPARTA, Xyce, NALU, HOMME-X, LAMMPS, CTH, Zapotec**
  - **LANL: FLAG, PARTISN, VPIC**
  - **LLNL: ALE3D, Ares, PF3D**

- Utilized ATSE provided software stack and modules
  - Early work on ATSE using testbeds helped to iron out some initial issues
- Performance results vary, in some cases Trinity Haswell/CTS-1 are faster, others are slower
- Astra shows good scalability out to 2,048 nodes
- Early indications are that still room for improvement in compilers and math libraries (subject of continuing Astra projects)

Peak System Performance

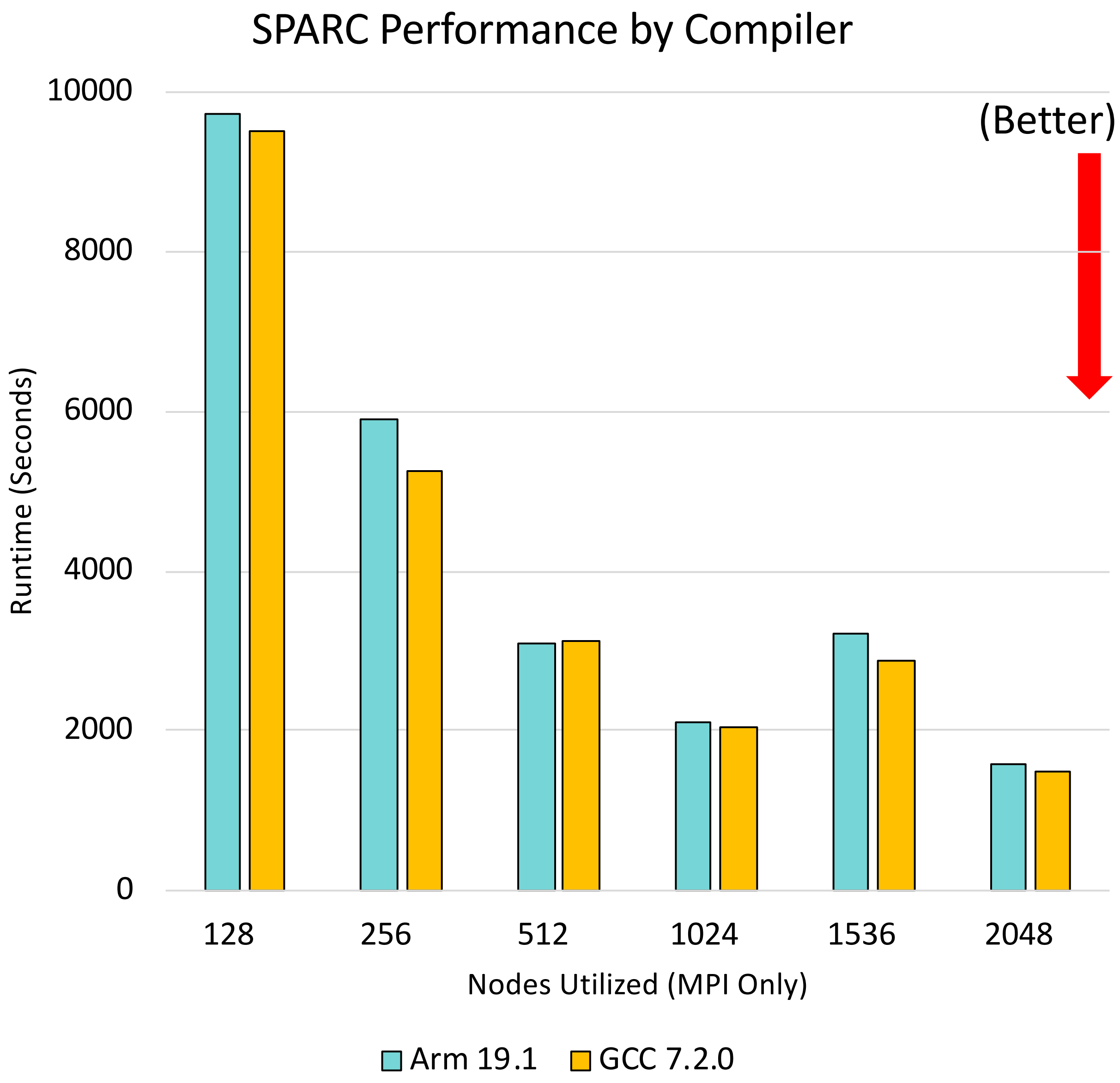
		CTS1	Trinity		Sierra		Astra
		Broadwell	Haswell	KNL	POWER9	V100 GPU	ThunderX2
LINPACK FLOP Rates (per Node)	Perf	1.09 TF/s	~0.86 TF/s	~2.06 TF/s	~1 TF/s	~21.91 TF/s	~0.71 TF/s
	Rel	1.00X	0.79X	1.89X	0.91X	20.01X	0.65X
Memory Bandwidth (STREAM) (per Node)	Perf	~136 GB/s	~120 GB/s	~90 GB/s / ~350 GB/s	~270GB/s	~850 GB/s x 4 = ~3.4 TB/s	~250 GB/s ★
	Rel	1.00X	0.88X	0.66X / 2.57X	1.99X	25.00X	1.84X
Power (Max TDP, per Node)	Watts	120W x 2 = 240W	135W x 2 = 270W	~250W	190W x 2 = 380W	~300W x 4 = 1.2kW	~180W x 2 = 360W
	Rel	1.00X	1.13X	1.04X	1.58X	5.00X	1.50X

Guidance figures, used peak values for benchmarks and TDP

GCC/Arm Compiler Comparison

SPARC CFD Simulation Code

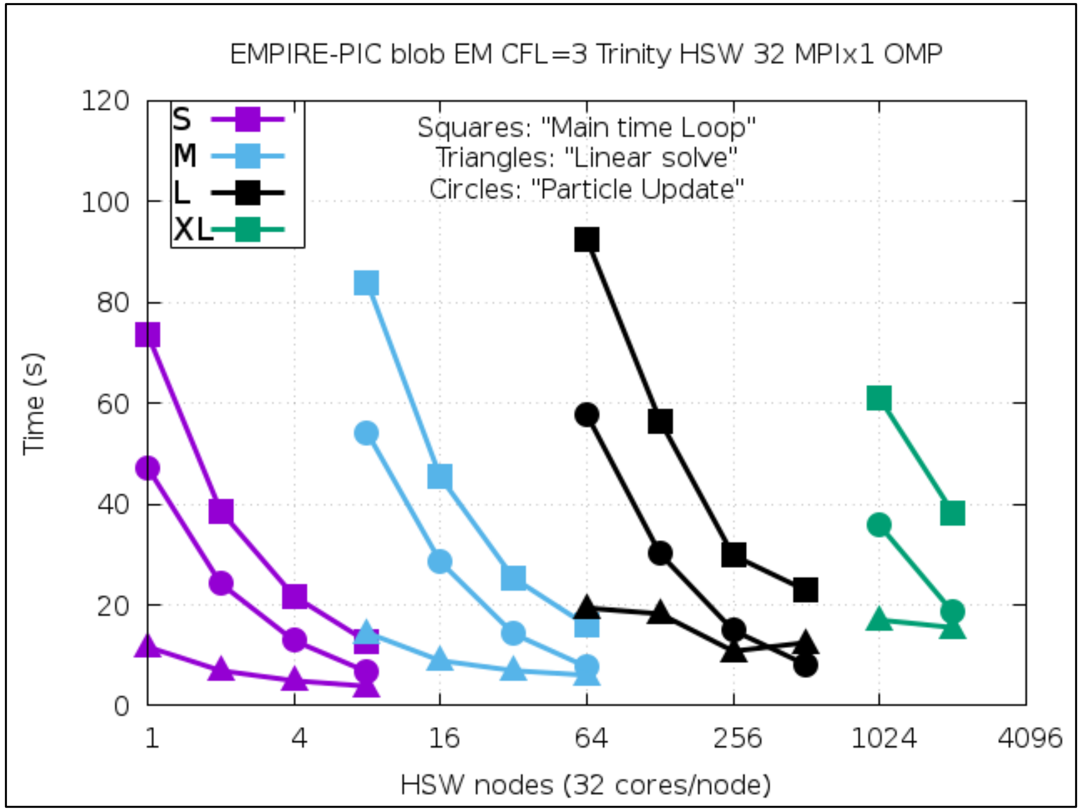
- SPARC is Sandia's latest CFD modeling code
  - Developed under NNSA ATDM Program
  - Written to be threaded and vectorized
  - Uses Kokkos programming abstractions
  - Approximately 2-3M lines of code for binary (including Trilinos packages, mostly C++, tiny bit of Fortran)
- Mixture of assembly and solve phases
- Successfully compiles with GCC and Arm HPC compilers on Astra
- Results show performance with Arm HPC compiler varies from 0.5% faster than GCC to 10% slower
  - This seems to be consistent across our code portfolio at present



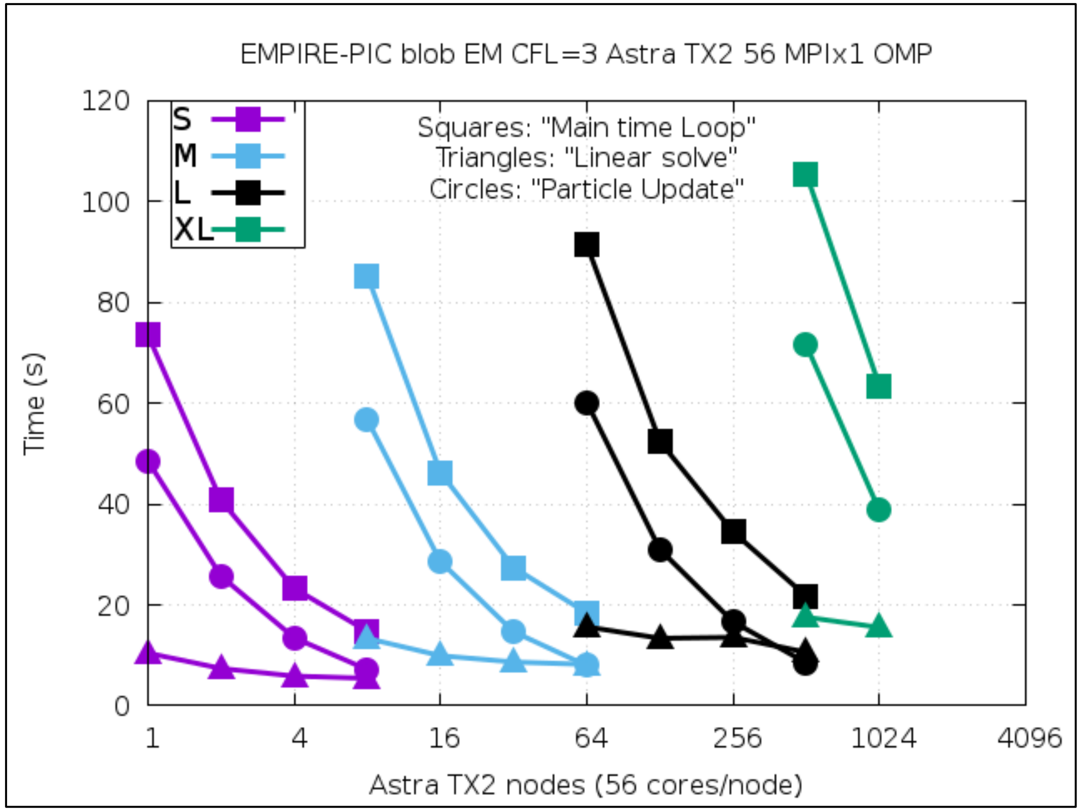
Similar Performance
TX2 vs. HSW

EMPIRE - PIC

(Better)



Trinity HSW 32 MPI x 1 OMP



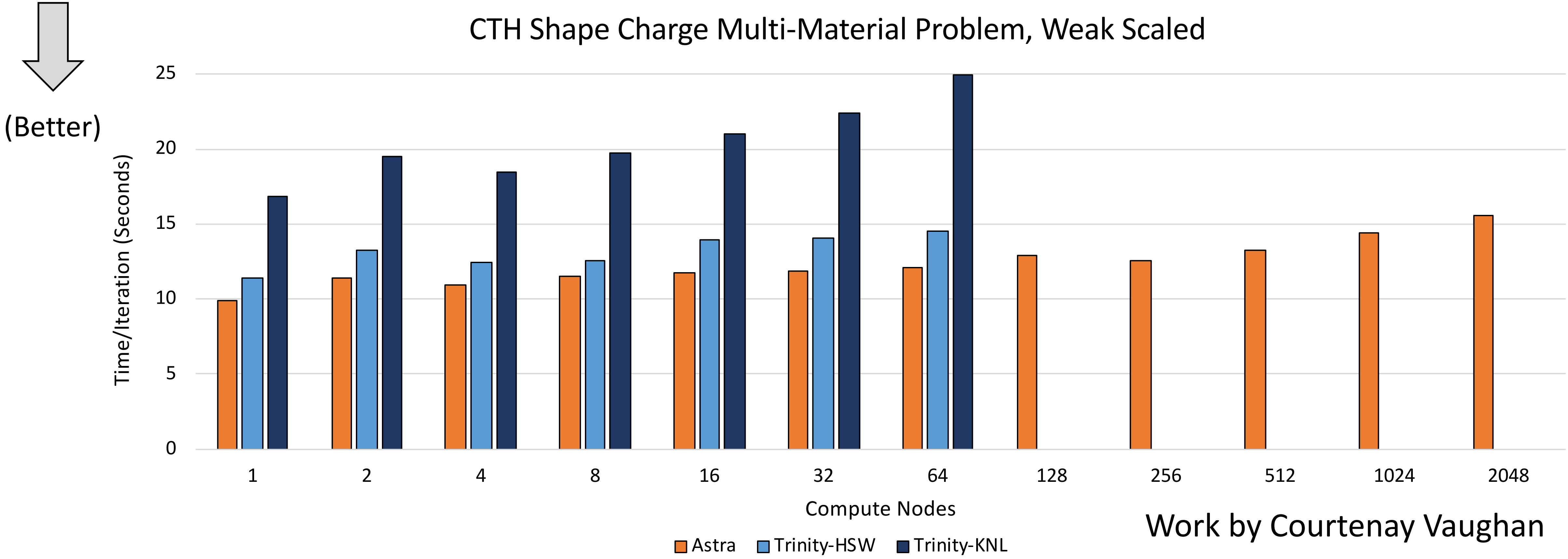
Astra TX2 56 MPI x 1 OMP

- Similar performance of Trinity-Haswell and Astra (MPI Only, performance is within 10% except for XL blob meshes which were run on fewer nodes for Astra)
- Similar scaling behavior between platforms

Work by Paul Lin and EMPIRE Team

Fortran Compiler Stress Test

CTH (Hydrodynamics, Fortran)

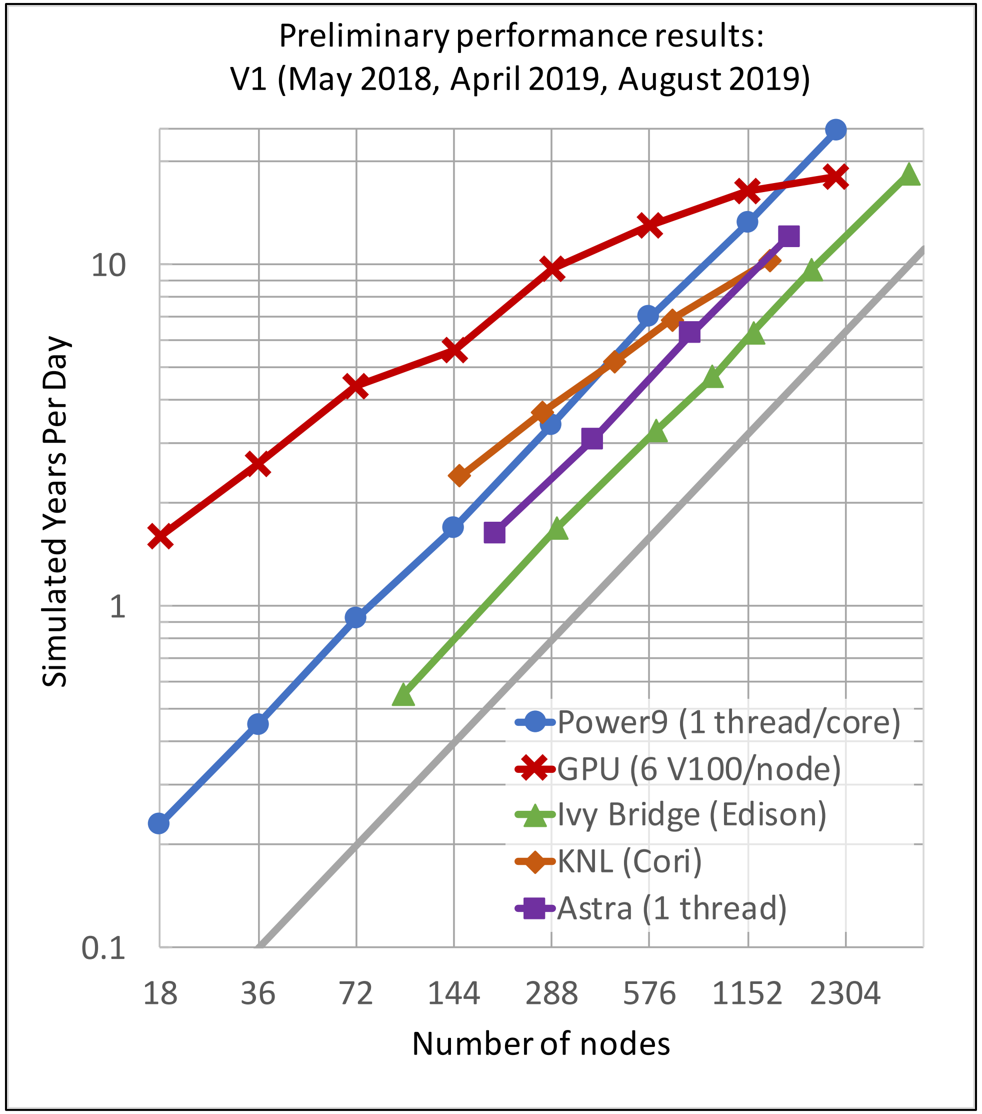


Work by Courtenay Vaughan

- CTH uses significant number of Fortran features (mixture from FORTRAN-IV to Fortran-90)
  - Large complex code which is extremely well trusted by analysts, known to be challenging with Fortran compilers on new platforms
- Successfully compiles with Arm Flang (used for these results) and ATSE-GCC installs

HOMME (Climate)

(Better)



Work by Oksana Guba and HOMME Team

- Climate modeling code which is partially developed at Sandia (ASCR)
  - Known to drive components and third parties libraries very hard (frequently the first to find issues during porting)
  - Strong driver for improvements in Trillinos solver libraries across DOE platforms
- Good scalability (want to see near straight lines if possible)
- Recent SMT-2 results are around 10% faster

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HPC on Arm, are we there yet? … Yes

- Basic HPC components supported and demonstrated @ scale
  - InfiniBand, UCX, MPI, Lustre, Linux, SLURM, …
- Compilers and math libraries work sufficiently well to get codes running
- Performance competitive with leading alternatives
- Offerings from a range of integrators

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- Compilers and math libraries work sufficiently well to get codes running
- Performance competitive with leading alternatives
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- SVE not proven yet, lack of accelerator options (changing)
- Performance not tuned in many packages / kernels yet
  - Need threaded and vectorized versions of kernels
- Still need work on profilers, debuggers, and memory correctness
- Lacking of standards for performance counters + power/energy

Questions?

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