

FRONTIER CENTER OF EXCELLENCE INTRO

Spock Workshop

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Noah Reddell
Manager, Frontier Center of Excellence

FRONTIER CENTER OF EXCELLENCE (COE)

What are we doing:

- Assisting in the **porting and tuning** of key DOE applications and libraries for *Frontier*.
- Helping to ensure the robustness of the *Frontier* **programming environment**.
- Advocating in the software-related **development activities** to ensure that the software environment supports end-user needs and priorities.
- Providing **training** through workshops, publications, and hackathons.

Staffing

- 11 staff from HPE's Performance Team, Programming Environment Group, CTO Office and **AMD**.
- Over two centuries collective experience in High Performance Computing, including:
 - expertise in physical sciences, computer science, electrical engineering and applied mathematics.
- Expertise in performance analysis, optimization, and scientific application development

ONGOING FRONTIER COE COLLABORATIONS

- **CAAR Teams** -- supporting preparations for exascale scientific simulations upon Frontier availability
 - Cholla, CoMet, GESTS, LBPM, LSMS, NAMD, NuCCOR, PIconGPU
- 27 ECP **Application Development (AD)** teams:
 - LatticeQCD, NWChemEx, GAMESS, EXAALT, ExaAM, QMCPACK, ExaWind, Combustion-Pele, ExaSMR, WDMApp, WarpX, ExaSky, EQSIM, Subsurface, E3SM-MMF, ExaSGD, CANDLE, ExaBiome, ExaFEL, Proxy Apps, Application Assessment, CODAR, CoPA, AMReX, CEED, ExaGraph, ExaLearn
- 25 ECP **Software Technologies (ST)**:
 - PMR SDK, Exascale MPI, Legion, UPC++ & GASNet, OMPI-X, RAJA/Kokkos, Argo, Exa-PAPI++, HPCToolkit, PROTEAS-TUNE, SOLLVE, xSDK, PETSc/Tao, STRUMPACK/FFTX, SUNDIALS/hypre, CLOVER, ALExa, ADIOS, VTK-m, VeloC-SZ, ALPINE, SW Ecosystem SDK, Packaging
- Supporting >300 users on HPE's *Poplar* and *Tulip* "COE Systems", and soon to add *Birch*.

SPOCK IS AN IMPORTANT STEP BEFORE FRONTIER ARRIVES

- Spock and Frontier are substantially similar
 - Same *HPE Cray software stack*
 - HPE Cray OS
 - HPE Cray Compiler
 - HPE Cray MPI
 - HPE Cray Performance and Correctness tools, Scientific Libraries, ML/DL etc.
 - AMD ROCm
 - Compute nodes with
 - AMD EPYC CPU
 - AMD Instinct GPU
 - AMD Infinity Fabric
- Spock vs Frontier Differences
 - A few orders of magnitude in total system computational power
 - Density: Spock is an air-cooled system and Frontier will be direct liquid-cooled
 - AMD EPYC CPU and AMD Instinct GPUs will be something yet to be released
 - Frontier compute nodes will have an HPE NIC direct-attached to each GPU
 - CPU-GPU link is AMD Infinity Fabric instead of PCIe
 - **A few additional months of software development and updates.**



SPOCK'S COUSIN AT HPE

- HPE's *Birch* system for the Frontier Center of Excellence
 - Same compute nodes and Spock and very similar system configuration
 - 12 compute nodes
 - Soon to be available to CAAR and ECP Teams
 - Existing users of Poplar and Tulip systems today will migrate to Birch (~300 accounts)
- The primary difference between Birch and Spock:
 - Pre-release development builds of HPE and AMD software regularly installed for early testing
- All of the training today is relevant to Birch
- *Current Poplar and Tulip users:* Watch for announcements on Frontier COE Confluence
 - The HPE Cray software stack and network is substantially different



REMEMBER: NO NDA TOPICS TODAY

- **Today is about Spock** – a released product from HPE with released tech. from AMD
- Today's training is open to a large audience and is not restricted to parties under NDA
- HPE and AMD are not able to share Confidential & Proprietary information, including
 - Any information about Frontier beyond what has been published publicly by ORNL, HPE, or AMD
 - Capabilities of future hardware
 - Future product names
 - Specific software development timelines and feature plans
- **Special Opportunity for follow-questions and discussion under NDA**
 - Available to current users of Tulip and Poplar, and others with access to Frontier COE Confluence
 - No agenda, just open opportunity to discuss interest items with the COE staff
 - See, “Watercooler Technical Sharing Series” details on Frontier COE Confluence (access restricted)
 - Tomorrow, May 21st, 2021 11a-12p ET



THANK YOU FOR YOUR INTEREST AND PARTICIPATION TODAY!

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Noah Reddell, noah.reddell@hpe.com

