CSSI Elements: First Workshop on NSF and DOE High Performance Computing Tools

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Background

High Performance Computing (HPC) software has become increasingly complex to install. The complex inter-package dependencies can lead to significant loss of productivity.

Under the Exascale Computing Project (ECP) the Extreme Scale Scientific Software Stack (E4S) was developed to enable efficient, consistent access to the broad ecosystem of software essential to the scientific efforts of the DOE.

This SDK is available through a containerized distribution as well as Spack - an app store for supercomputers. Spack includes recipes for building packages from source code and is the primary means of deploying ECP software.

Web Resources

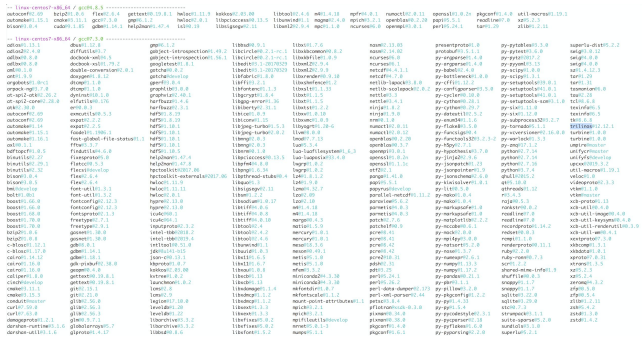
Workshop Website:
https://oaciss.uoregon.edu/NSFDOE19

E4S Website: https://e4s.io

Objective

The first NSF and DOE workshop on HPC tools brought together NSF resource providers and system administrators, NSF PIs and HPC application developers, and scientists and facilities administrators from the DOE national laboratories, and Industry. Participants in this two day program discussed and learned about ECP and E4S capabilities with an emphasis on HPC software packaging and deployment using Spack and containers.

Packages in E4S Containers



Topics

- Using Spack to install packages natively on Supercomputers.
- Developing new Spack recipes for integrating tools within the Spack environment.
- Deploying Spack based packages in an SDK.
- Using Spackstacks to build the software installation matrix based on different compilers and runtime libraries.
- Using source and binary builds of SDKs using Spack in E4S containers.
- Hands-on exercises.

Participants

The workshop was attended by 69 registered participants, including both on-site and online attendees, from institutions including:

- AMD
- LBL
- LLNL
- NSF
- Nvidia
- Sandia
- SDSC
- TACC
- UCAR
- University of Oregon

Keynotes, talks and tutorials were presented by scientists and administrators from institutions using and developing E4S technology.