

Award #: 1939486

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

PI: Sameer Shende Institution:University of Oregon

Background

Attendees

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

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

- AMD
- LBL
- LLNL
- NSF
- Nvidia

E4S Spack Build Cache

E4S Build Cache for Spack 0.13.3 o use this build cache, just add it to your Sp RHEL7 RHEL8 Ubuntu 18.04

cuda@10.1.243	3 curl@7.63.0	darshan-runtime@3.1.7	darshan-util@3.1.7	diffutils@3.7 doxygen@1.8.1	5 dtcmp@1.1.0		
dyninst@10.1.0)						
Click on the full spec link to find out more.							
Link	Arch	OS	Compiler	Created	Full Hash		
Full Spec	ppc64le	centos7	gcc@7.3.0	01-24-2020 19:04 PST	lqf23rj2bm25uisu7bhygaulsvfen3mp		
Full Spec	ppc64le	rhel7	gcc@7.3.0	01-24-2020 19:05 PST	gqv6ooysens76p2ecw7orxtlcfdruklh		
Full Spec	ppc64le	ubuntu18.04	gcc@7.3.0	01-24-2020 19:06 PST	g5spch6wlgjoonp6oca6clfyz3ggesyh		
Full Spec	x86_64	centos7	gcc@7.3.0	01-24-2020 19:04 PST	ymtprwfbjfg2f653sjudziqqrbdwkezo		
Full Spec	x86_64	centos8	gcc@7.3.0	01-24-2020 19:05 PST	qaric7cxnuiho2eb2e2bjxkyjstpbihu		
Full Spec	x86_64	rhel7	gcc@7.3.0	01-24-2020 19:05 PST	cj5rmqj5xtstrlc6wyvbkc33ih4c7zka		
Full Spec	x86_64	rhe18	gcc@7.3.0	01-24-2020 19:06 PST	dlkbcgrw7gpy3gpgrtymv3kyqiexkleo		
Full Spec	x86_64	ubuntu18.04	gcc@7.3.0	01-24-2020 19:07 PST	torjxbex4k4kguj66dge37dehjawl3fo		

Ifutils@0.177 emacs@26.2 environment-modules@4.3.1 er@0.0.3 exmcutils@0.5.7 expat@2.2.9 faodel@1.1906.1 findutils@4.6.0 flatcc@0.5.3 flecsi@develop flex@2.6.

Multi-platform Images

1 1 +

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.

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.

- Sandia
- SDSC
- TACC
- UCAR

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

••• < >	s-project.github.io/download.html	Ċ	
UBI 7	Ubuntu 18.04	CentOS 7	
BASE IMAGES	BASE IMAGES	BASE IMAGES	
ecpe4s/ubi7_x86_64_base	ecpe4s/ubuntu1804_x86_64_base	ecpe4s/centos7_x86_64_base	
🥗 docker GitHub 🕹	避 docker GitHub 🛨	👑 docker GitHub 🛓	
ecpe4s/ubi7_ppc64le_base	ecpe4s/ubuntu1804_ppc64le_base	ecpe4s/centos7_ppc64le_base	
docker GitHub 🛨	docker GitHub	👑 docker GitHub 🛓	
E4S COMPREHENSIVE IMAGE	ecpe4s/ubuntu1804_aarch64_base	E4S COMPREHENSIVE IMAGE	
ecpe4s/ubi7_x86_64_e4s		exascaleproject/e4s_x86_64	
docker GitHub 生	E4S COMPREHENSIVE IMAGE	🤠 docker GitHub 🛓	
CUSTOM IMAGES	ecpe4s/ubuntu1804_x86_64_e4s	CUSTOM IMAGES	
ecpe4s/superlu_sc 🖐 docker	011070141140070		
GitHub 📥	CUSTOM IMAGES		
	ecpe4s/ubuntu1804_aarch64_waggle		
	🤲 docker GitHub 🛨		

E4S Technology Products

•	•	45. tutorial⊛ip-172-31-1-143 (ssh)					
1:	adios	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/adios-1.13.1-v7jyzgyie7n542qppgoz2izthu6xeaj5					
2: aml /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/aml-0.1.0-ao2r76pzk5k6mdfvx3cixvqlyg7hzppt							
	argobots	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/argobots-1.0rc1-4kbgyfusscwopgzl76oaxpiglf6itptm					
	bolt	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/bolt-1.0b1-jenaxkneyprxga6abwaihlkuuoko4pwv					
	caliper	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/qcc-7.3.0/caliper-1.8.0-lrmti32xdayckyhk5vr5okrxtniv2pb5					
	darshan-runt						
	dyninst	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/qcc-7.3.0/dyninst-10.1.0-g3ogsuc2yztrb2agfgk4ga2ik7w6kg45					
	faodel	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/faodel-1.1906.1-gpadaotmehed2wejfxyeg7bxewtmsclc					
	flecsi	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/flecsi-develop-Zzth7esblvxalgdnvbxota6jfx2xzi3i					
	gasnet	/home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/ac-7.3.0/gasnet-1.30.0-hp4d5xsbhhq5qisbkmqodd6bkgmqrczo					
	geopm	/home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/geopm-0.4.0-ahho4xnuyymvurieuajfml4u42b7a3t6					
	globalarray						
	gotcha	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/aotcha-develop-dcaszr3n36z73pasm2d745rx5bzvr2ha					
	hdf5	/usr/local/packages/ccp/spack/pt/spack/linux-centos7-x86_64/acc-7.3.0/hdf5-1.10.5-ahv2hxb6f/aunew3a7pn41idazw474i					
		/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/hpctoolkit-2017.06-bogjp7bdarhaysswzp6p6w5skt5wa423					
	hypre	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/hypre-2.13.0-3kjyf17r23e76eojvojyfeacwd16ehb					
	kokkos	/home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/kokkos-2.03.00-a3ksyha6fflnlufs5sfanafwxeeeogey					
	legion	/home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/legion-17.10.0-cjomljrvcxzbhulznfc5luw6wiubnyr					
	libnrm	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/libnrm-0.1.0-ddwaupy5ag4dayahcpirzmxdaycdasrd					
	libquo	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/libquo-1.3-cdtpt/dmousmys5a4nvwsfyld3u3mc162					
	magma	/usr/local/packages/ecp/spack/opt/spack/linus-centos7-x86_64/gcc-4.8.5/magma-2.4.0-7cc275vlzmhypm5uuubj4krfsoqshhmr					
	mercury	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/mercury-1.0.1-rxg31qg5mratnsokdtqg676pqfs5md37					
	mfem	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/mfem=3.3.2-sdrntzuthtzaophdl63b3ujmzySytb4q					
	mpich	/home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/mpich-3.2.1-5j57f4j36vhcsxan2pwndouz27ge4ij4					
	mpifileutil						
	ninja	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/ninja-1.9.0-vwu3smyjyej50lkvhzsy4t4piilcgmql					
	openmpi	/home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/openmpi-3.0.1-hdjeffn2fs3iidk3whvv6smbrnmzqa2					
	papi	/home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/papi-5.5.1-abkudkdhzua3p4lnn7m6ssj3or45fjri					
	papyrus	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/papyrus-develop-77k6v4izzvjx222zbrpiexka7fmjsjar					
	parallel-ne						
	pdt	/home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/pdt-3.25-fjjddrbx7lx4hrqmqfwssq4oz46zvj5p					
	petsc	/home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/petsc-3.8.4-7naeokjkiniftmkecnapcn736bvnrdhl					
	athreads	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/gthreads-1.12-npkx43id5wewkrbsv6gpr76gisoozbpu					
	raja	/home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/raja-0.5.3-zrjr35xwjrfz6wacs4k36ilwc45m6aa6					
	rempi	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/rempi-1.1.0-rpzp7upbe4c3m2aug3l2we5rjxl62xd2					
	scr	/usr/local/packages/ecp/spack/pt/spack/linux-centos7-x86_64/acc-7.3.0/scr-1.2.2-fdqkeva2nf6yeda4qhwersf6ojwikxaz					
	strumpack	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/strumpack-3.1.1_q4wwcyff7lzrrbwc6np5jxezv6iix7ig					
	sundials	/home/packages/ecp/spack/opt/spack/linux-centos7-x86_64/acc-7.3.0/sundials-3.1.0-xrqsfvumk2jw7agidjsj7lva4w5kam3p					
	superlu-dis						
40: sz /usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/sz-1.4.12.3-dgykgp27gsnnyc2ktm6rnb6bfgxwg7vg							
	tasmanian	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/tasmanian-6.0-fv7z3ninw7agbvlw2jhau2hyx5ofyt4k					
	tau	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/tau-2.28-2zm23cf41u74wfp2ufrzo7bu22popu4x					
	trilinos	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/qcc-7.3.0/trilinos-12.12.1-kobl2zztgzcukmx5tktvmyradjt6qym7					
	turbine	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/turbine-1.0.0-6ct6q2xwav5n22xvf2exbmgpjwknkgho					
	umpire	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/umpire-master-4bditlkgpbuznpnnshpf3poxthmadefq					
	unifyfs	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/unifyfs-develop-s47fumyqwo7qxjdspwnadribvrkeppn5					
	upcxx	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/qcc-7.3.0/upcxx-2019.3.2-uezjtlwvssi5ztt6qltejmxzrv6etkh2					
	veloc	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/veloc-1.0-jmamhwdagwurlxa2ugn7gyugrdj4jz5p					
	vtkm	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/vtkm-master-g6zjyz5ja7olj7fbj2iga7ohfy4hx3f5					
	zfp	/usr/local/packages/ecp/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/zfp-0.5.4-kbmhpghxrfimhbhop6upwuj7herhm7pz					

- E4S containers.
- Hands-on exercises.

Web Resources

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

E4S Website: https://e4s.io

Acknowledgement

This work was supported by the NSF under award #1939486

Presenters

Packages in E4S Containers

Keynotes, talks and tutorials were presented by scientists and administrators from:

- University of Oregon
- NSF
- LBL
- LANL
- LLNL
- Sandia





