E4S Overview and Demo

September 24, 2:30pm PT 2nd E4S Forum Workshop at EuroMPI/USA 2020 via Zoom

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https://e4s.io











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UNIVERSITY OF OREGON

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 As our software gets more complex, it is getting harder to install tools and libraries correctly in an integrated and interoperable software stack.



E4S: Extreme-scale Scientific Software Stack

- Curated, Spack based software distribution
- Spack binary build caches for bare-metal installs
 - x86_64, ppc64le (IBM Power 9), and aarch64 (ARM64)
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products
- Base images and full featured containers (GPU support)
- GitHub recipes for creating custom images from base images
- GitLab integration for building E4S images
- E4S validation test suite on GitHub
- E4S VirtualBox image with support for container runtimes
 - Docker
 - Singularity
 - Shifter
 - Charliecloud
- AWS and GCP images to deploy E4S

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Extreme-scale Scientific Software Stack (E4S)

- <u>E4S</u>: A Spack-based distribution of ECP ST and related and dependent software tested for interoperability and portability to multiple architectures
- Provides distinction between SDK usability / general quality / community and deployment / testing goals
- Will leverage and enhance SDK interoperability thrust
- Oct 2018: E4S 0.1 <u>24 full</u>, 24 partial release products
- Jan 2019: E4S 0.2 <u>37 full</u>, 10 partial release products
- Nov 2019: E4S 1.0 50 full, 5 partial release products
- Jan 2020: E4S 1.1 ppc64le and x86_64 release with 50 full (x86_64), 46 full (ppc64le) release products.



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Spack

- E4S uses the Spack package manager for software delivery
- Spack provides the ability to specify versions of software packages that are and are not interoperable.
- Spack is a build layer for not only E4S software, but also a large collection of software tools and libraries outside of ECP ST.
- Spack supports achieving and maintaining interoperability between ST software packages.
- https://spack.io



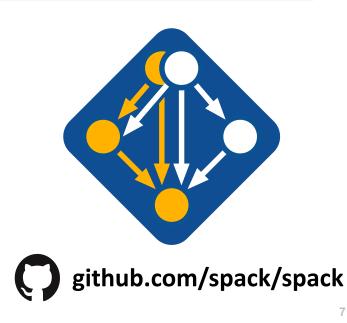
Spack enables software distribution for HPC

No installation required: clone and go

\$ git clone https://github.com/spack/spack \$ spack install tau

<pre>\$ spack install</pre>	tau	unconstrained
<pre>\$ spack install</pre>	tau@2.29.1	<pre>@ custom version</pre>
<pre>\$ spack install</pre>	tau@2.29.1 %gcc@7.3.0	% custom compiler
<pre>\$ spack install</pre>	<pre>tau@2.29.1 %gcc@7.3.0 +mpi+python+pthreads</pre>	+/- build option
<pre>\$ spack install</pre>	<pre>tau@2.29.1 %gcc@7.3.0 +mpi ^mvapich2@2.3~wrapperrpath</pre>	^ dependency information

- Each expression is a *spec* for a particular configuration
 - Each clause adds a constraint to the spec
 - Constraints are optional specify only what you need.
 - Customize install on the command line!
- Spec syntax is recursive
 - Full control over the combinatorial build space





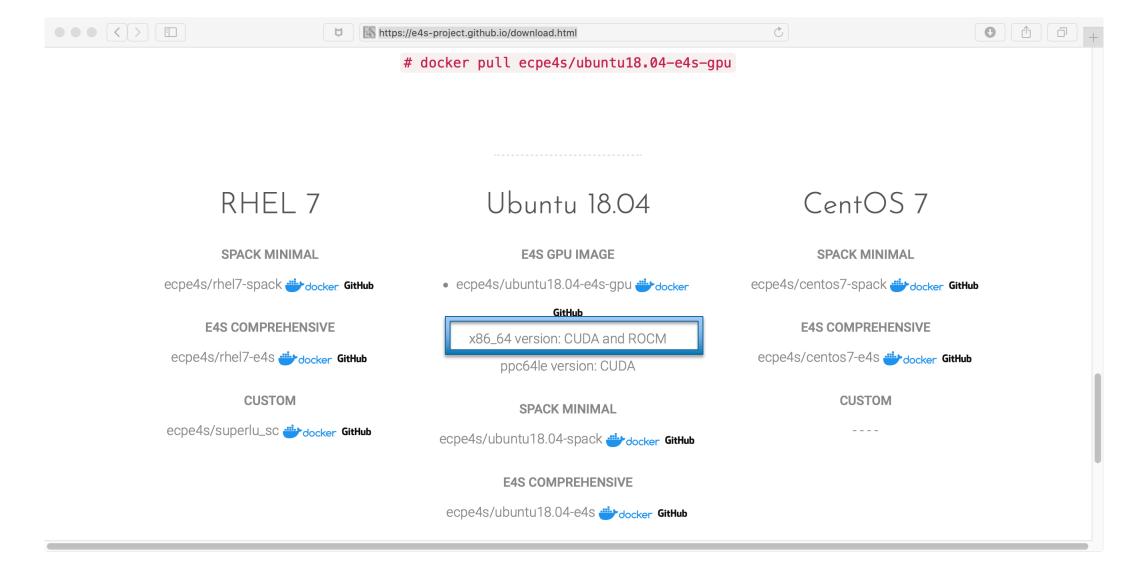
E4S Components

- E4S is a curated release of ECP ST products based on Spack [http://spack.io].
- E4S Spack cache to support bare-metal installs at facilities and custom container builds:
 - x86_64, ppc64le, and aarch64
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products.
- Base images and full featured containers with support for GPUs.
- GitHub recipes for creating custom images from base images.
- e4s-cl for container launch and for replacing MPI in application with system MPI libraries.
- Validation test suite on GitHub provides automated build and run tests.
- Automates build process via GitLab Continuous Integration to ensure packages can be built.
- E4S Doc Portal aggregates and summarizes documentation and metadata by raking product repos.
- E4S VirtualBox image with support for Docker, Shifter, Singularity, and Charliecloud runtimes.
- AWS image to deploy E4S on EC2.
- GCP image to deploy E4S.

https://e4s.io



Download E4S v1.1 GPU image





E4S v1.1 Release Available at DockerHub

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• 50 ECP ST Products

- Support for GPUs
 - AMD (ROCm 3.0)
 - NVIDIA (CUDA 10.1)
 - x86_64

% docker pull ecpe4s/ubuntu18.04-e4s-gpu



E4S v1.1 Release at DockerHub: GPU Support

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- 45+ ECP ST Products
- Support for GPUs
 - NVIDIA (CUDA 10.1.243)
 - ppc64le

% docker pull ecpe4s/ubuntu18.04-e4s-gpu

E4S v1.1.2 GPU Release for x86_64

EXASCALE

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• 50 ECP ST products

- Ubuntu v18.04 x86_64
- 5.3 GB compressed image
- AI/ML package support
 - TensorFlow
 - PyTorch
- Support for GPUs
 - AMD ROCm 3.1
 - NVIDIA CUDA 10.1.248

E4S v1.1 GPU Release for ppc64le

EXASCALE

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/spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/scr-1.2.2-5sepujyr7dp5eioymphnqva4atcjfc4e 35: strumpack /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/strumpack-3.1.1-jd7ytfdr4sagqdbxx3khjy2jamlfbru4 36: sundials /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/sundials-5.0.0-cjkp7zluit5jtm6ead74mavwko5thr2w /spack/opt/spack/linux-ubuntu18.04-ppc64le/acc-7.3.0/superlu-dist-6.1.1-6aklaz5snhaipunjjtirlo46za76zd2d 37: superlu-dist 38: sz /spack/opt/spack/linux-ubuntu18.04-ppc64le/acc-7.3.0/sz-1.4.12.3-7bnst7vnpuajazlaaxtot46oih4caoaa 39: tasmanian /spack/opt/spack/linux-ubuntu18.04-ppc64le/acc-7.3.0/tasmanian-7.0-e3r2dvv5nnpg7yafs5hzcocvkmxaf7pn 40: tau /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/tau-2.29-3eb5tlvcnukpkd2pls4z7ivhtc2ld7jm 41: trilinos /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/trilinos-12.14.1-jcikf6anps63huaohpymnm4xohgrrral 42: umpire /spack/opt/spack/linux-ubuntu18.04-ppc64le/qcc-7.3.0/umpire-0.3.3-bnxsv2cla4yc42mvfhvwlk7suylmbcou 43: unifyfs /spack/opt/spack/linux-ubuntu18.04-ppc64le/acc-7.3.0/unifyfs-develop-fazlm2dhtbnb2aegaadfcue2mkv74sco 44: upcxx /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/upcxx-2019.9.0-ndrgyemtolmjk7i3dduekjbt4i3uo2jz 45: veloc /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/veloc-1.1-h723o37b5mowzewdzgburtrawnb5ynhi 46: zfp /spack/opt/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/zfp-0.5.5-3r4a4s3gdegbdabvlwlswrgig62yc6yj

46 ECP ST products

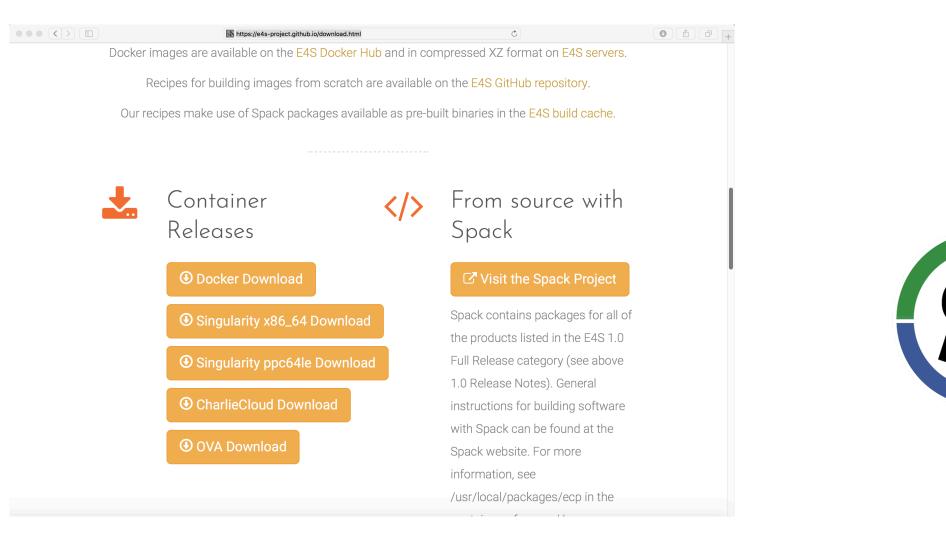
- Ubuntu v18.04 ppc64le
- AI/ML package support
 - TensorFlow
 - PyTorch
- Support for GPUs
 - NVIDIA CUDA 10.1

`spack find` shows what is installed

		5. roo	t@3b983c57f123: / (ssh)		
sameer@minotaur:~\$ doc	ker run -v \$HOME:/home/	sameer -it ecpe4s/ubuntu18.	04-ppc64le-e4s		
root@3b983c57f123:/# w		·			
/spack/bin/spack					
root@3b983c57f123:/# s	pack find				
==> 235 installed pack	ages				
linux-ubuntu18.04-p	pc64le / gcc@7.3.0				
adios@1.13.1	hdf5@1.10.5	lua-luafilesystem@1_7_0_2	py-async-generator@1.10	py-pexpect@4.6.0	raja@0.8.0
aml@0.1.0	hdf5@1.10.5	lua-luaposix@33.4.0	py-babel@2.7.0	py-pickleshare@0.7.4	rankstr@0.0.2
argobots@1.0rc1	hdf5@1.10.5	lwgrp@1.0.2	py-backcall@0.1.0	py-pillow@6.2.0	readline@8.0
autoconf@2.69	hpctoolkit@2019.08.14	lz4@1.9.2	py-blinker@1.4	py-prometheus-client@0.7.1	redset@0.0.3
automake@1.16.1	hwloc@1.11.11	lzo@2.10	py-certifi@2019.9.11	py-prompt-toolkit@2.0.9	rempi@1.1.0
axl@0.1.1	hypre@2.18.1	m4@1.4.18	py-certipy@0.1.3	py-ptyprocess@0.5.1	scr@1.2.2
binutils@2.32	intel-tbb@2019.4	margo@0.4.3	py-cffi@1.13.0	py-py@1.8.0	shuffile@0.0.3
bmi@develop	kokkos@2.7.00	matio@1.5.13	py-chardet@3.0.4	py-pycparser@2.19	snappy@1.1.7
boost@1.70.0	kokkos@2.9.00	mercury@1.0.1	py-cryptography@2.3.1	py-pygments@2.4.2	sqlite@3.30.1
boost@1.70.0	kokkos-kernels@2.7.00	mercury@1.0.1	py-cycler@0.10.0	py-pyjwt@1.7.1	strumpack@3.1.1
boost@1.70.0	kvtree@1.0.2	metis@5.1.0	py-cython@0.29.13	py-pyopenssl@19.0.0	suite-sparse@5.3.0
bzip2@1.0.8	leveldb@1.22	mfem@4.0.0	py-decorator@4.4.0	py-pyparsing@2.4.2	sundials@5.0.0
c-blosc@1.17.0	libarchive@3.3.2	mpich@3.2.1	py-entrypoints@0.3	py-python-dateutil@2.8.0	superlu@5.2.1
caliper@2.0.1	libbsd@0.9.1	mpifileutils@develop	py-idna@2.8	py-python-dateutil@2.8.0	superlu-dist@6.1.1
cmake@3.15.4	libcircle@0.2.1-rc.1	mumps@5.2.0	py-ipykernel@5.1.0	py-python-editor@1.0.4	sz@1.4.12.3
curl@7.63.0	libdwarf@20180129	nasm@2.14.02	py-ipython@7.3.0	py-python-oauth2@1.1.1	tar@1.32
darshan-runtime@3.1.7	libfabric@1.8.1	ncurses@6.1	py-ipython-genutils@0.2.0	py-pytz@2019.3	tasmanian@7.0
darshan-util@3.1.7	libffi@3.2.1	netcdf@4.7.1	py-jinja2@2.10.3	py-requests@2.22.0	tcl@8.6.8
diffutils@3.7	libiberty@2.31.1	netlib-scalapack@2.0.2	py-joblib@0.14.0	py-scikit-learn@0.21.3	texinfo@6.5
dtcmp@1.1.0	libiconv@1.16	nettle@3.4.1	py-jsonschema@2.6.0	py-scikit-optimize@0.5.2	trilinos@12.14.1
dyninst@10.1.0	libjpeg-turbo@2.0.3	ninja@1.9.0	py-jupyter-client@4.4.0	py-scipy@1.3.1	umpire@0.3.3
elfutils@0.177	libmonitor@2018.07.18	numactl@2.0.12	py-jupyter-console@5.2.0	py-setuptools@41.4.0	unifyfs@develop
emacs@26.2	libnrm@0.1.0	openblas@0.3.7	py-jupyter-core@4.4.0	py-setuptools@41.4.0	unzip@6.0
er@0.0.3	libpciaccess@0.13.5	openmpi@3.1.4	py-jupyter-notebook@4.2.3	py-simplegeneric@0.8.1	upcxx@2019.9.0
expat@2.2.9	libpfm4@4.10.1	openssl@1.1.1d	py-jupyterhub@1.0.0	py-six@1.12.0	util-macros@1.19.1
findutils@4.6.0	libpng@1.6.37	papi@5.7.0	py-kiwisolver@1.1.0	py-six@1.12.0	veloc@1.1
flatcc@0.5.3	libpthread-stubs@0.4	papyrus@develop	py-libensemble@0.5.2	py-sqlalchemy@1.3.9	xerces-c@3.2.2
flecsi@develop	libquo@1.3	parallel-netcdf@1.11.2	py-mako@1.0.4	py-tornado@6.0.3	xz@5.2.4
freetype@2.10.1	libsigsegv@2.12	parmetis@4.0.3	py-markupsafe@1.1.1	py-traitlets@4.3.3	zeromq@4.3.2
gdbm@1.18.1	libsodium@1.0.17	pcre@8.42	py-matplotlib@3.1.1	py-urllib3@1.25.6	zfp@0.5.5
gettext@0.20.1	libtool@2.4.6	pcre@8.42	py-mistune@0.7.1	py-vcversioner@2.16.0.0	zlib@1.2.11
git@2.21.0	libunwind@1.2.1	pdsh@2.31	py-mpi4py@3.0.1	py-wcwidth@0.1.7	zstd@1.4.3
glm@0.9.7.1	libunwind@2018.10.12	perl@5.30.0	py-nbconvert@4.2.0	py-ytopt@0.1.0	
globalarrays@5.7	libxml2@2.9.9	petsc@3.12.1	py-nbformat@4.4.0	py-zmq@17.1.2	
gmp@6.1.2	libyogrt@1.24	pkgconf@1.6.3	py-numpy@1.17.3	python@3.7.3	
gotcha@0.0.2	lmod@8.1.5	py-alembic@1.0.7	py-oauthlib@3.1.0	python@3.7.4	
gotcha@1.0.2	lua@5.3.5	py-asn1crypto@0.22.0	py-pamela@1.0.0	qthreads@1.14	

- All the versions coexist!
 - Multiple versions of same package are ok.
- Packages are installed to automatically find correct dependencies.
- Binaries work regardless of user's environment.
- Spack also generates module files.
 - Don't have to use them.

E4S Support for Singularity Container Runtime [Sylabs.io]



- wget http://oaciss.uoregon.edu/e4s/images/e4s_ubuntu1804_gpu_ppc64le_1.1.simg
- singularity exec --nv e4s_ubuntu1804_gpu_ppc64le_1.1.simg /bin/bash --rcfile /etc/bashrc
- spack find

E4S v1.1 GPU Support for ppc64le

fameer@cyclops:~ — ssh zorak — 137×51 Singularity> which python /usr/bin/python Singularity> python Python 3.6.10 |Anaconda, Inc.| (default, Jan 7 2020, 21:47:07) [GCC 7.3.0] on linux Type "help", "copyright", "credits" or "license" for more information. >>> import tensorflow >>> import torch >>> import cv2 >>> import pandas >>> import sklearn >>> import keras Using TensorFlow backend. >>> import matplotlib; import numpy; import scipy >>> torch.cuda.current device() 0 >>> tensorflow.test.is gpu available() 2020-02-20 19:46:00.714206: I tensorflow/core/common runtime/gpu/gpu device.cc:1433] Found device 0 with properties: name: Tesla V100-SXM2-32GB major: 7 minor: 0 memoryClockRate(GHz): 1.53 pciBusID: 0004:04:00.0 totalMemory: 31.72GiB freeMemory: 24.06GiB 2020-02-20 19:46:00.828521: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1433] Found device 1 with properties: name: Tesla V100-SXM2-32GB major: 7 minor: 0 memoryClockRate(GHz): 1.53 pciBusID: 0004:05:00.0 totalMemory: 31.72GiB freeMemory: 31.41GiB 2020-02-20 19:46:00.937000: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1433] Found device 2 with properties: name: Tesla V100-SXM2-32GB major: 7 minor: 0 memoryClockRate(GHz): 1.53 pciBusID: 0035:03:00.0 totalMemory: 31.72GiB freeMemory: 31.41GiB 2020-02-20 19:46:01.043356: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1433] Found device 3 with properties: name: Tesla V100-SXM2-32GB major: 7 minor: 0 memoryClockRate(GHz): 1.53 pciBusID: 0035:04:00.0 totalMemory: 31.72GiB freeMemory: 31.41GiB 2020-02-20 19:46:01.043434: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1512] Adding visible gpu devices: 0, 1, 2, 3 2020-02-20 19:46:09.555187: I tensorflow/core/common runtime/gpu/gpu device.cc:984] Device interconnect StreamExecutor with strength 1 ed ge matrix: 2020-02-20 19:46:09.555313: I tensorflow/core/common_runtime/gpu/gpu_device.cc:990] 0123 2020-02-20 19:46:09.555326: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1003] 0: N Y Y Y 2020-02-20 19:46:09.555334: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1003] 1: Y N Y Y 2020-02-20 19:46:09.555341: I tensorflow/core/common runtime/gpu/gpu device.cc:1003] 2: Y Y N Y 2020-02-20 19:46:09.555349: I tensorflow/core/common runtime/qpu/qpu device.cc:1003] 3: Y Y Y N 2020-02-20 19:46:09.555942: I tensorflow/core/common_runtime/qpu/qpu_device.cc:1115] Created TensorFlow device (/device:GPU:0 with 22986 MB memory) -> physical GPU (device: 0, name: Tesla V100-SXM2-32GB, pci bus id: 0004:04:00.0, compute capability: 7.0) 2020-02-20 19:46:09.556909: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1115] Created TensorFlow device (/device:GPU:1 with 30132 MB memory) -> physical GPU (device: 1, name: Tesla V100-SXM2-32GB, pci bus id: 0004:05:00.0, compute capability: 7.0) 2020-02-20 19:46:09.557139: I tensorflow/core/common_runtime/qpu/qpu_device.cc:1115] Created TensorFlow device (/device:GPU:2 with 30132 MB memory) -> physical GPU (device: 2, name: Tesla V100-SXM2-32GB, pci bus id: 0035:03:00.0, compute capability: 7.0) 2020-02-20 19:46:09.558067: I tensorflow/core/common runtime/apu/apu device.cc:1115] Created TensorFlow device (/device:GPU:3 with 30132 MB memory) -> physical GPU (device: 3, name: Tesla V100-SXM2-32GB, pci bus id: 0035:04:00.0, compute capability: 7.0) True >>>



E4S: ppc64le Base Container Images

EXASCALE COMPUTING

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	Try	the two-factor authenticatio	n beta. <u>L</u>	<u>.earn more ></u>			×
	Q Search for great content (e.g., mysql)	E;	kplore	Repositories	Organizations	Get Help 👻 exascale	eproject 🔻 🌍
ecpe4s	▼ Q ppc64le	×		Create	Repository +	Organizations	+
ecpe4s / ubuntu18(Updated 2 days ago	04_ppc64le_base		☆ 0	≟ 7	S PUBLIC		ng Project Super-conta
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ecpe4s / centos7_p Updated 2 days ago	pc64le_base		☆ 0	<u>↓</u> 10	S PUBLIC	Download Docker Desktop	
Tip: Not find	ling your repository? Try switching namespace via th	ne top left dropdown.					
						A P	Secure, rivate Repo Pricing

Hub.docker.comecpe4s

- Ubuntu 18.04
- RHEL/UBI 7.6
 Centos 7.6

E4S Spack Build Cache and Container Build Pipeline





Reproducible, Customizable Container Builds & Spack Mirrors

- E4S provides base images and recipes for building Docker containers based on SDKs
 - Git: <u>https://github.com/UO-OACISS/e4s</u>
 - E4S provides build caches for Spack for native bare-metal as well as container builds based installation of ST products
 - Build caches: <u>https://oaciss.uoregon.edu/e4s/inventory.html</u>
 - The build cache model can be extended to target platforms, and can be managed by facilities staff when appropriate.



E4S: Spack Build Cache at U. Oregon

Image: Second		
E4S Build Cache for Spack 0.15.4	ĺ.	
To use this build cache, just add it to your Spack spack mirror add E4S https://cache.e4s.io spack buildcache keys -it		
Click on one of the packages below to see a list of all available variants.		
• All Architectures OPPC64LE X86_64		
• All Operating Systems Centos 7 Centos 8 RHEL 7 RHEL 8 Ubuntu 18.04 Ubuntu 20.04	•	20,000+ binaries! S3 mirror
Last updated: 09-10-2020 08:45 PDT		No need to build
21905 Spack packages		from source code!
Search		
adiak@0.1.1 adios2@2.5.0 adios2@2.6.0 adios@1.13.1 adlbx@0.9.2 amg@1.2 aml@0.1.0 amrex@20.07 ant@1.10.0 ant@1.10.7		
argobots@1.0 argobots@1.0rc1 argobots@1.0rc2 arpack-ng@3.7.0 ascent@develop autoconf@2.69 automake@1.16.1 automake@1.16.2		
axl@0.1.1 axl@0.3.0 axom@0.3.3 bdftopcf@1.0.5 berkeley-db@18.1.40 berkeley-db@6.2.32 binutils@2.31.1 binutils@2.32 binutils@2.33.1		
binutils@2.34 bison@3.4.2 bmi@develop bolt@1.0 bolt@1.0rc2 bolt@1.0rc3 boost@1.70.0 boost@1.72.0 boost@1.73.0 boost@1.74.0		
butterflypack@1.1.0 butterflypack@1.2.0 bzip2@1.0.8 c-blosc@1.17.0 caliper@2.0.1 caliper@2.2.0 caliper@2.3.0 caliper@2.4.0		
camtimers@master catalyst@5.6.0 cinch@develop cinch@master cmake@3.13.4 cmake@3.14.5 cmake@3.14.7 cmake@3.15.4 cmake@3.16.2		

https://oaciss.uoregon.edu/e4s/inventory.html



WDMapp: Speeding up bare-metal installs using E4S build cache



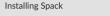
aoo Whole Device Model application



Applying for Access

WDMApp on Summit at OLCF

- □ WDMApp on Rhea at OLCF
- Setting up Spack



Cloning the WDMapp package repo

Rhea-Specific Setup

Adding the WDMapp package repo to Spack

Building WDMapp

Running the Cyclone Test Case Running the Cyclone Test Case -External Coupler

WDMapp on Longhorn at TACC

WDMApp on AiMOS at RPI

Setting up Spack

Building WDMAPP EFFIS

Read the Docs

Note

The E4S project has created a build cache for Rhea. This provides many packages as precompiled binaries, so will reduce the installation time. To use it:

\$ wget https://oaciss.uoregon.edu/e4s/e4s.pub \$ spack gpg trust e4s.pub \$ spack mirror add E4S https://cache.e4s.io/e4s

Building WDMapp

https://wdmapp.readthedocs.io/en/latest/machines/rhea.html

You should be able to just follow the generic instructions from Building WDMAPP.

Using E4S WDMapp docker container

Alternatively, the E4S project has created a docker image that mirrors the Rhea environment, which can be used for local development and debugging. To run this image, you need to have docker installed and then do the following:

\$ docker pull ecpe4s/ubi7.7_x86_64_base_wdm:1.0 \$ docker run -rm -it ecpe4s/ubi7.7_x86_64_base_wdm:1.0

In order for the image to get the access controlled components, you need to provide it with your private SSH key that provides access to the respective private github repos. In the image, do the following in the docker image:

cat > .ssh/id_rsa # Then copy&paste your private key # chmod 600 .ssh/id rsa

This provides an development environment with everything but the private codes preinstalled. All that's needed to complete building and installing them is:

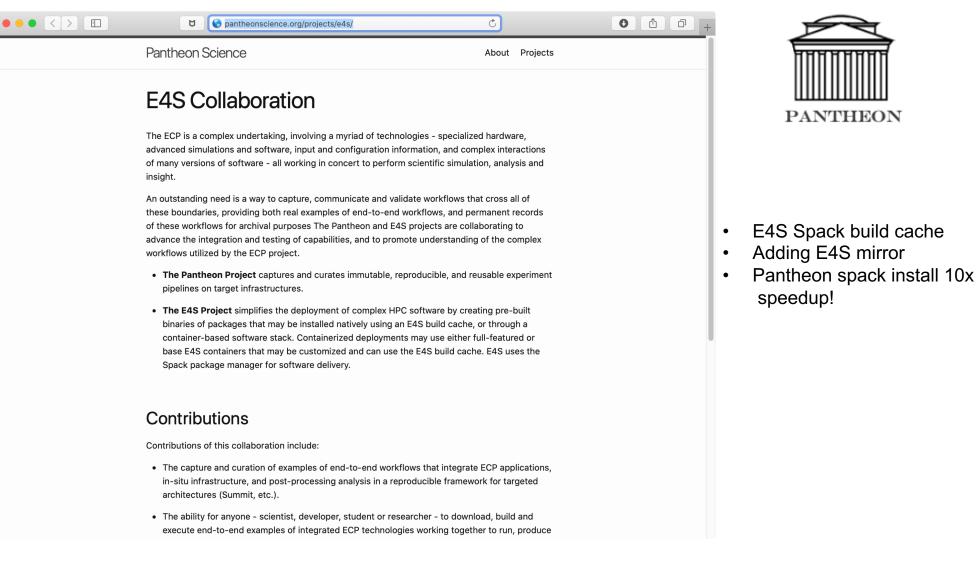
spack install wdmapp target=x86_64

- E4S Spack build cache
- Adding E4S mirror
- WDMapp install speeds up!



https://wdmapp.readthedocs.io/en/latest/machines/rhea.html

Pantheon Science at LANL



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https://pantheonscience.org/projects/e4s/

New E4S Spack Cache Website (under development)



● All ○ Ubuntu 18.04 ○ RHEL 7 ○ RHEL 8 ○ CentOS 7 ○ CentOS 8

● All ○ X86_64 ○ PPC64LE

Showing 306 packages representing 8607 binaries

adiak

Adiak collects metadata about HPC application runs and provides it to tools.

adios

The Adaptable IO System (ADIOS) provides a simple, flexible way for scientists to describe the data in their code that may need to be written, read, or processed outside of the running simulation.

adios2

The Adaptable Input Output System version 2, developed in the Exascale Computing Program

adlbx

aml

ADLB/X: Master-worker library + work stealing and data dependencies



E4S Spack Environment - Current Examples

- Building on **AWS Cloud** as part of Spack PR and Release Testing
 - CI Dashboard available @ https://cdash.spack.io
- Building at University of Oregon
 - ppc64le and x86/64 systems with mpich
- Building at OLCF Ascent
- Working on NERSC Cori and ALCF Theta currently
- See examples of how the environment is tailored for existing sites:
 - <u>https://github.com/UO-OACISS/e4s/tree/master/e4s-facility-environments</u>
- Binaries available in the E4S Build Cache
 - <u>https://oaciss.uoregon.edu/e4s/inventory.html</u>
 - Improved inventory page currently under development
- Google Cloud Platform (GCP) integration

E4S Dashboard for Spack Pull Request (PR) testing



R

[view timeline]

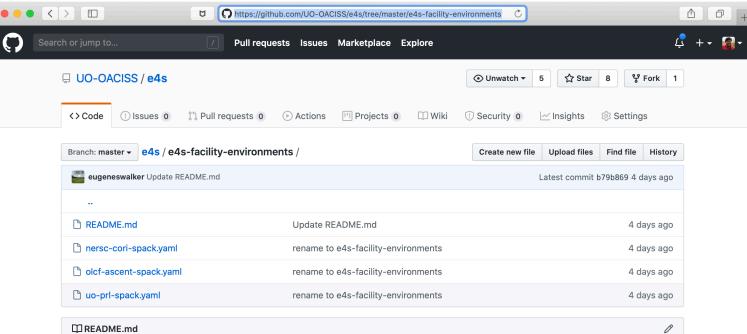
Latest PR Testing - E4S 237 builds

					Build		
Site	Build Name	Revision	Error	Warn ❤	Error	Warn ❤	Start Time 💙
Cloud Gitlab Infrastructure	Δ pdt@3.25.1%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	11f2d0	1	0	0	0	Aug 07, 2020 - 18:23 UTC
Cloud Gitlab Infrastructure	A globalarrays@5.7%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	84837c	0	26	0	0	12 hours ago
Cloud Gitlab Infrastructure	openmpi@3.1.6%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	84837c	0	20	0	14	12 hours ago
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Cloud Gitlab Infrastructure	∆ sundials@5.3.0%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	84837c	0	7	0	0	11 hours ago
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Cloud Gitlab Infrastructure	∆ libtool@2.4.2%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	11f2d0	0	6	0	0	Aug 07, 2020 - 18:50 UTC
Cloud Gitlab Infrastructure	A trilinos@12.18.1%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	84837c	0		0	49 ⁺⁴⁹ ₋₄₉	13 hours ago
Cloud Gitlab Infrastructure	Ibyogrt@1.24%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	33e7c8	0	4	0	0	10 minutes ago
Cloud Gitlab Infrastructure	∆ libquo@1.3.1%gcc@7.3.0 arch=linux-ubuntu18.04-x86_64 (PR Testing - E4S)	84837c	0	3	0	1	11 hours ago



https://cdash.spack.io

E4S Tailored to DOE Facility Environments



D README.md

E4S Spack Environments for Facility Builds

Here you will find E4S environment files designed to be used with Spack at the different facilities. Each environment file consists of mostly the same E4S Spack packages. Where the environments differ is in how external packages, compilers, and architecture targets are configured.

For general information on Spack Environments and External Packages, refer to the Official Spack documentation:

- Spack Tutorial on Environments https://spack-tutorial.readthedocs.io/en/latest/tutorial_environments.html
- Spack Environments Reference https://spack.readthedocs.io/en/latest/environments.html
- Spack External Packages https://spack.readthedocs.io/en/latest/build_settings.html



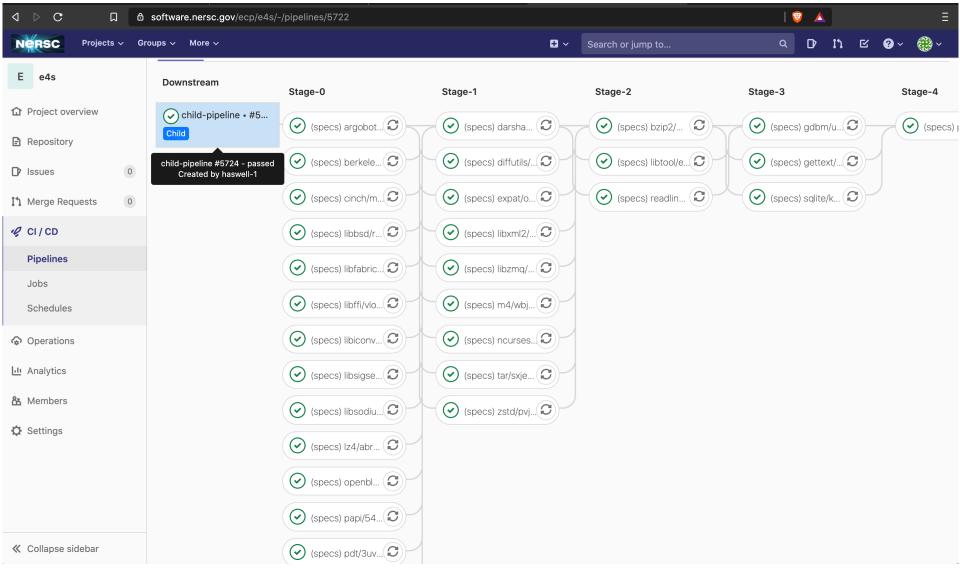
https://github.com/UO-OACISS/e4s/tree/master/e4s-facility-environments

E4S Build Pipeline Summary on Cori, NERSC

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Multi-stage E4S CI Build Pipeline on Cori, NERSC



E4S CI on Cori, NERSC

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E4S CI on Cori, NERSC

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E4S: Build Pipeline for Creating Spack Build Cache at U. Oregon

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- GitLabMulti-platform builds

ORNL GitLab Build Pipeline for E4S Spack Build Cache

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EXASCALE COMPUTING PROJECT			 Rep 	oroducible co	ntainer bui	lds

E4S VM Image for Google Cloud Project (GCP)

- VM Image for Google Compute Engine
 - Ubuntu 18.04
 - Intel Cascade Lake
- Spack v0.15.4
- Pre-configured to use E4S Cloud Build Cache
- 53 E4S Packages
 - SuperLU
 - Sundials
 - Trilinos
 - UPCXX
 - \circ ... and more



E4S GitLab via Google Kubernetes Engine

- E4S GitLab running via Google Kubernetes Engine (GKE)
 - GitLab Version 13.3.5 with updates deployed via Helm Chart
- GitLab Continuous Integration (CI)
 - Build E4S Spack packages using University of Oregon runners
- E4S package binaries automatically pushed to E4S Cloud Build Cache upon successful build
 - Spack mirror URL: <u>https://cache.e4s.io</u>
 - Spack mirror inventory: <u>https://oaciss.uoregon.edu/e4s/inventory.html</u>



E4S Container Images via gcr.io

- Pre-release container images deployed to Google Container Registry (gcr.io)
- Use of private registry eases collaboration burden during pre-release testing
- Shields end-users from potential bugs
- Image types:
 - Base layers
 - Base Spack images
 - GitLab CI Runner images
 - Full E4S images



E4S Repositories on GCP

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E4S VM Instances on GCP used by GitLab

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E4S Components





E4S DocPortal

- Provide a single online location for accurate product descriptions for ECP software products.
- Derived requirements:
 - Sustainable: Must be integrated into software team workflows.
 - Incremental: Must build on community approaches to providing this kind of information.
 - Extensible: Must be usable by any open source software team.
- Strategy:
 - Use the open source community approach of specially-name files in software repositories.
 - Adopt commonly used file names when available.
 - Identify new information items not already being requested.
 - Develop new special file names for information beyond what is already captured.
 - Create web-based raking tool to capture information from product repositories and present in summary form on a webpage.
 - Aggregates and summarizes documentation and metadata for E4S products
 - Regularly updates information directly from product repositories
 - Prototype: <u>https://e4s-project.github.io/DocPortal.html</u>

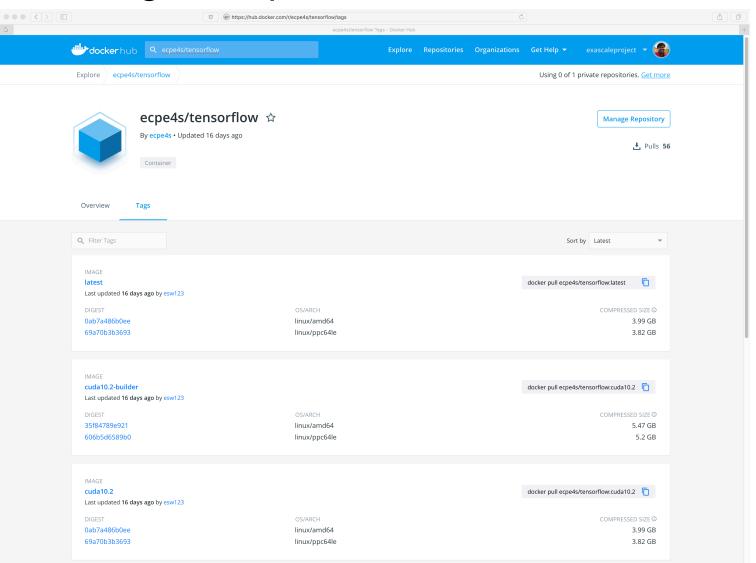
E4S DocPortal

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https://e4s-project.github.io/DocPortal.html

E4S: DockerHub Images: ecpe4s



- Dockerhub
- Tensorflow 2.2
- CUDA 10.2
- ppc64le



E4S: Multi-platform Reproducible Docker Recipes

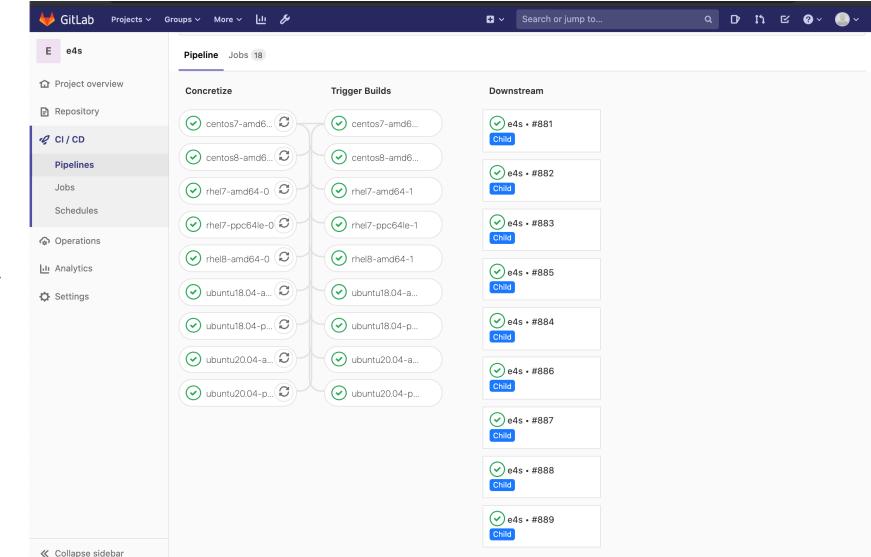
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spack.lock	use spack.lock in ubi7 ppc64le base recipe 18 hours ago	
spack.yaml	update ppc64le recipes to 1.3: use spack 0.13.1 + use base env + add 9 days ago	
E README.md	<i>i</i>	



University of Oregon GitLab CI

August 10, 2020 E4S Builds: •Ubuntu 18.04 •Ubuntu 20.04 •RHEL 7.6 •RHEL 8 •CentOS 7 •CentOS 8

Architectures: ppc64le and x86_64





E4S Validation Test Suite

0

- Provides automated build and run tests
- Validate container environments and products
- New LLVM validation test suite for DOE LLVM

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□ E4S	G-Project / testsuite	requests 0 🔹 Actions 🕅 Projects 0	O Unwatch → 8 ★ Star 2	
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• git clone https://github.com/E4S-Project/testsuite.git

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sameershende Adding a custom image for SC19 SuperLU tutorial.	a0b948d 10 days ago	Branch: master • e4s / docker / ubi7 / x86_64 / custom / superlu / Dockerfile Find file Copy path	
1 contributor		sameershende Adding a custom image for SC19 SuperLU tutorial. a869488 10 days ago 1 contributor	
35 lines (34 sloc) 579 Bytes	Raw Blame History 🖵 🖋 🛱	21 lines (13 sloc) 519 Bytes Raw Blame History 🖵 🖍 🍵	
<pre>spack: packages: all: compiler: [gcc@7.3.0] variants: +mpi providers: mpi: [mpich] buildable: true version: [] paths: {} modules: {} mpich: variants: ~wrapperpath buildable: true providers: {} modules: {} compiler: [] gcc: version: [7.3.0] buildable: true providers: {} compiler: [] gcc: specs: specs: specs: specs: specs: - superlu-dist - peths - mfem - strumpack - openblas view: false</pre>		 PMR SDK base image has Spack build cache GPG key installed. Base image has GCC and MPICH configured ABI level replacement (with system MPI). Customized container build using binaries fro Spack build cache for fast deployment. No need to rebuild packages from the source with Spack! 	for MPICI m E4S code.



E4S VirtualBox Image

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Home Trash Terminal	<pre>to load the AI/ML packages from E4S [https://e4s.io] natively, or: % runsi to run the Singularity E4S container. [livetau@localhost ~]\$ which docker /usr/bin/docker [livetau@localhost ~]\$ which singularity /usr/bin/singularity [livetau@localhost ~]\$ which shifter /usr/bin/shifter [livetau@localhost ~]\$ which ch-run /usr/local/packages/e4s/spack/opt/spack/linux-centos7-x86_64/gcc-7.3.0/charliecloud-0. 9.9-eap7xdowneblxvsjugkhga4z5dagkasf/bin/ch-run [livetau@localhost ~]\$ which spack /usr/local/packages/e4s/spack/bin/spack [livetau@localhost ~]\$ which spack /usr/local/packages/e4s/spack/bin/spack [livetau@localhost ~]\$ alias grep runsi alias runsi='singularity exec /home/livetau/ecp.simg /bin/bashrcfile /etc/bashrc' [livetau@localhost ~]\$ runsi Singularity> which spack /usr/local/packages/ecp/spack/bin/spack</pre>	ECP	Container RuntimesDockerShifterSingularityCharliecloud
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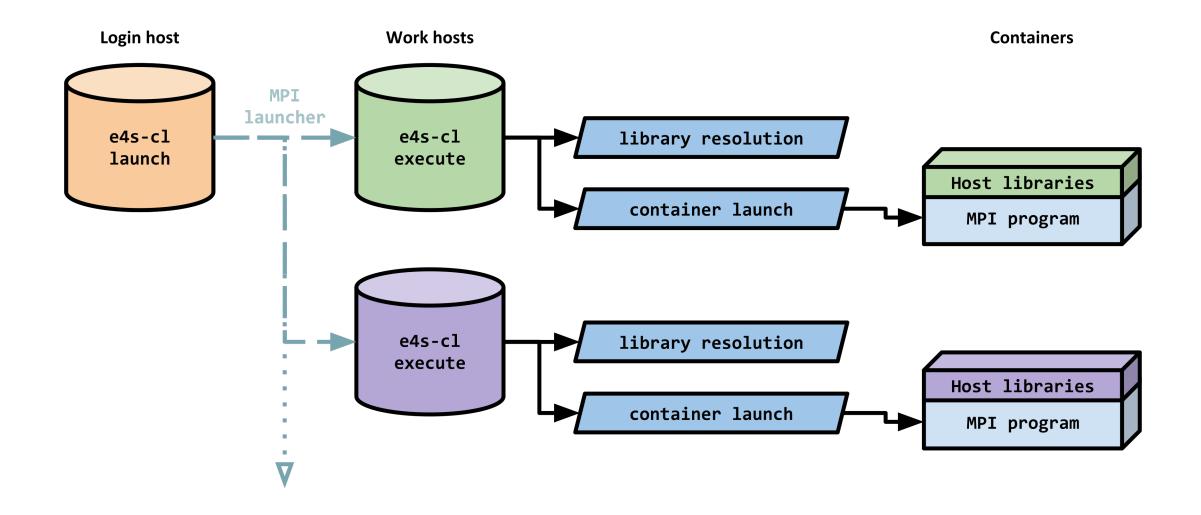


e4s-cl: A tool to simplify the launch of MPI jobs in E4S containers

- E4S containers support replacement of MPI libraries using MPICH ABI compatibility layer.
- Applications binaries built using E4S can be launched with Singularity using MPI library substitution for efficient inter-node communications.
- e4s-cl is a new tool that simplifies the launch and MPI replacement.
- Under development. Usage:
 - 1. e4s-cl profile detect -o <profile> <MPI executable>
 - 2. e4s-cl profile select <profile>
 - 3. e4s-c1 launch mpirun -np <> -hosts <> <command>



e4s-cl Container Launcher





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