HPC-BP Webinar: Extreme-scale Scientific Software Stack (E4S)

Wednesday, January 13th, 2021, 10am – 10:30am PT

ECP HPC-BP Webinar
https://exascaleproject.zoomgov.com/j/1616523770

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https://e4s.io
Challenges

• 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 (with 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

https://e4s.io
Extreme-scale Scientific Software Stack (E4S)

- **E4S**: 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 - 24 full, 24 partial release products
- Jan 2019: E4S 0.2 - 37 full, 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.
- Nov. 2020: E4S 1.2 – ppc64le and x86_64 release each with 67 full release products.

https://e4s.io
Spack is a flexible package manager for HPC

• How to install Spack (works out of the box):

```bash
$ git clone https://github.com/spack/spack
$ . spack/share/spack/setup-env.sh
```

• How to install a package:

```bash
$ spack install tau
```

• TAU and its dependencies are installed within the Spack directory.

• Unlike typical package managers, Spack can also install many variants of the same build.
  - Different compilers
  - Different MPI implementations
  - Different build options

Visit spack.io

@spackpm
github.com/spack/spack/spack
Spack provides the *spec* syntax to describe custom configurations

- 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

```bash
$ spack install tau
$ spack install tau@2.29
$ spack install tau@2.29 %gcc@7.3.0
$ spack install tau@2.29 %gcc@7.3.0 +mpi+python+pthreads
$ spack install tau@2.29 %gcc@7.3.0 +mpi ^mvapich2@2.3~wrapperrpath
```

unconstrained
@ custom version
% custom compiler
+/- build option
^ dependency information
`spack find` shows what is installed

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.
The Spack community is growing rapidly

- **Spack simplifies HPC software for:**
  - Users
  - Developers
  - Cluster installations
  - The largest HPC facilities

- **Spack is central to ECP’s software strategy**
  - Enable software reuse for developers and users
  - Allow the facilities to consume the entire ECP stack

- **The roadmap is packed with new features:**
  - Building the ECP software distribution
  - Better workflows for building containers
  - Stacks for facilities
  - Chains for rapid dev workflow
  - Optimized binaries
  - Better dependency resolution

Visit spack.io

github.com/spack/spack

@spackpm
Download E4S v1.2 GPU Container Image

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

---

**RHEL 7**

- SPACK MINIMAL
  - ecpe4s/rhel7-spac
- E4S COMPREHENSIVE
  - ecpe4s/rhel7-e4s
- CUSTOM
  - ecpe4s/superlu_sc

**Ubuntu 18.04**

- E4S GPU IMAGE
  - ecpe4s/ubuntu18.04-e4s-gpu
  - x86_64 version: CUDA and ROCM
  - ppc64le version: CUDA

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**CentOS 7**

- SPACK MINIMAL
  - ecpe4s/centos7-spac
- E4S COMPREHENSIVE
  - ecpe4s/centos7-e4s
- CUSTOM
  - ----

https://e4s.io
E4S v1.2 GPU Release for x86_64

- 67 ECP ST products
- Ubuntu v18.04 x86_64
- AI/ML package support
  - TensorFlow 2.3.5
  - PyTorch 1.8
  - Horovod
- Support for GPUs
  - AMD ROCm 3.8
  - NVIDIA CUDA 10.2, 11
- Kokkos with support for AMD GPUs!
E4S v1.2 GPU Release for x86_64

34: openpmd-api
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/openpmd-api-0.12.0-4myph6pbnjupgupxlvbvxqeqx6atyp
35: openmpi
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/openmpi-3.1.6-6yqtomy56as6xso2pdgkm4m4bcsouyfkf
36: papi
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/papi-6.0.0.1-gorrfrvrik575lldzgq46qmmu63kxl7x
37: papyrus
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/papyrus-develop-1u3dgpmwywykgy5mpw2dwcrol4wvbwai
38: parallel-netcdf
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/parallel-netcdf-1.12.1-tmmkzibn43rx7r7su6msxxusyrphdtn5
39: pfft
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/pfft-3.25.1-1kv5wuw5y72fypij13nqxvd7zpj6n1
40: petsc
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/petsc-3.13.4-ilg3u4rt5xrrqlim75tt73epxwux4fb
41: plasma
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/plasma-19.8.1-tjij7boj5ne5qj2jmwn5bqqt2fkmz23ke
42: precice
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/precice-2.1.0-ozdmba2h1ivcva3nklbeahlkgyuemw
43: pumi
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/pumi-2.2.2-52czzdbeq7pmjkd5nub5jgxzodcrph
44: py-jupyterhub
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/py-jupyterhub-1.0.0-1trw3cwlaij3kbbz6xm4mbvbkactsws3
45: py-libensemble
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/py-libensemble-0.7.0-mxvqxihiblqnmhlfepbxyboiskgyqyvev
46: qthreads
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/qthreads-1.14-neshscplhl7ttkebmd34rztalqihgdxh
47: raja
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/raja-0.11.0-w25bj2dys6cj7n7isgcjfyve3tuulev
48: rempi
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/rempi-1.11.0-sideqdbiik2ysehsh33lho5ictsb3t6
49: sctr
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/sctr-2.0.0-yc3chycq5guyyk6r4ujeiijy6egzq3rh3u
50: sstate
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/sstate-develop-jnysy2rh5xvwhua5ubtvq4bsd3py7d5
51: slepc
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/slepc-3.13.4-q3alqbpqsihvyjygrrnhb2qiisvifnp
52: strumpack
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/strumpack-4.0.0-rbtti5eq5cjfihsxv2uxey6m3f5ngg
53: sundials
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/sundials-5.3.0-3g52rh6ah6o4ucrgat5i4m6p16w6oj
54: superlu-dist
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/superlu-dist-6.3.1-o2hkon6dcoxn2rrbtlada2vcq35uin
55: stc
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/stc-0.8.3-oxxik7nsmugfoqy7xilzsgzt71it63eaj
56: swig
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/swig-4.0.1-htxmzjd5ced5yfiebw67jn5xc6p7g7x7g
57: tz /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/tz-2.1.0-tctuyiuzh6qqct cdrq2g3clil7xaq7vjtj
58: tasmanian
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/tasmanian-7.1-quo3grs5kb2xrvjufipi7vn6ccojnpfjadv
59: tau
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/tau-2.29-iuj2nbpmlfkt42ubwzg75a5ryru221kn
60: trilinos
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/trilinos-13.0.0-6xfnp44g5x7m7pn2en6gkwzfeckf3dx
61: turbine
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/turbine-1.2.3-4qjygvjxl3cbuyqu6zzrurbm4wfn6wkp
62: umap
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/umap-2.0.0-5tob3exrwmoidtu5spbow2dmsxnto
63: umpire
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/umpire-3.0.0-6w002uuvacucixkc6ad6g3ksus2yi
64: unifys
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/unifys-0.9.0-be7mqbngk7deewdvlvg1hdmdjkxnuiquil
65: upcxx
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/upcxx-2020.3.0-pshe62qymmrvsesq4p4k6bdq3fxuxcf
66: veloc
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/veloc-1.4-gk3iwfjhmkgk1awp7rmxf2e37rrqpm2
67: zfp
   /opt/spack/opt/spack/linux-ubuntu18.04-x86_64/gcc-7.5.0/zfp-0.5.5-6r6yaco7gga5wgbvuid3zt2iohrenej
E4S Support for Singularity Container Runtime [Sylabs.io]

- wget http://tau.uoregon.edu/ecp.simg
- singularity exec ecp.simg /bin/bash --rcfile /etc/bashrc
- spack find
E4S v1.2 Release: GPU, ppc64le for Docker Containers

- 67 ECP Products
- Support for GPUs
  - NVIDIA (CUDA 10.2)
  - ppc64le and x86_64

% docker pull ecpe4s/ubuntu18.04-e4s-gpu
E4S v1.2 GPU Release: 67 E4S Products (ppc64le)

- 67 ECP ST products
- Ubuntu v18.04 ppc64le
- Support for GPUs
- NVIDIA

Bash script examples:

1. adios2
   ```
   /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/adios2-2.6.0-veqgi5iqkx4kbbedhxorgyqvvqbtvos
   ```
2. aml
   ```
   /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/aml-0.1.0-fizigmywbeuuyzgg53ndzdhdyjx37op
   ```
3. amrex
   ```
   /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/amrex-20.10.4-2z5quivj3t3fbv5n6rrjv5bya7472em
   ```
4. arborx
   ```
   /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/arborx-0.9-beta-p7l7w7esbdrpqwhb7ispqphngq2tn4nt
   ```
5. ascent
   ```
   /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/ascent-develop-7ktzsmvlugv4dxoopp7hzjwvdyjxetn2ai
   ```
6. axom
   ```
   /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/axom-0.3.3-zfgq5s6aq6vxlodjnaeoffjyl26cmnp5
   ```
7. argobots
   ```
   /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/argobots-1.0-qra2gqxiusqqlbdrhmw5mvq2iga313l
   ```
8. bolt
   ```
   /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/bolt-1.0-ojy67kr47cbpbcvqaa64c7q7aysvndv
   ```
9. caliper
   ```
   /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/caliper-2.4.0-6xzehuuxs2updvlr2tdvcym3n6nf3y3l
   ```
10. darshan-runtime
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/darshan-runtime-3.2.1-6uzihv7v75yuv472jca4qpxqtdgtpnt2g
    ```
11. dyninst
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/dyninst-10.2.1-jvq4j3ehuh73pp67b4vdy4co3kivma5
    ```
12. faodel
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/faodel-1.1906.1-r7sasmsbb256mmn4trg59hnxce3e76uy
    ```
13. flecsi
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/flecsi-1.2kkxudrijvubmsabbmj3ums4yhrayk
    ```
14. flit
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/flit-2.1.0-tepztlt9kmefdfq4eoe2rbzwjaca56bmc
    ```
15. gasnet
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/gasnet-2020.3.0-uyuy6sitsczkffgbnm2xg0tgvme6b
    ```
16. ginkgo
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/ginkgo-1.3.0-dodvbixjpdg5icxrgomjegybobi331
    ```
17. globalarrays
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/globalarrays-5.7-32svrakwto5j54ca3l36rpvray25h
    ```
18. gotcha
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/gotcha-1.0.3-pvdjzcg3fqqpajcscorwidsllflmomzn
    ```
19. hdf5
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hdf5-1.10.6-arwhkmy4quglqntd7xraupvykgkprv70
    ```
20. hpctoolkit
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hpctoolkit-2020.08.03-qyayfprpr2aaleatxqz543cz5lcvviso7
    ```
21. hpx
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hpx-1.5.1-tzf5s3nklacexqjxfokigwqjzabybk
    ```
22. hypre
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/hypre-2.20.0-ewvm445dkzmj4up4grrreq7agpkcdgb
    ```
23. kokkos
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/kokkos-3.2.0-3qjzrzozl5qlqtq4atid3ylgkko3uk
    ```
24. kokkos-kernels
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/kokkos-kernels-3.2.0-0-ntrppubmexaqhdy4tjol6hnfnl5j4v6
    ```
25. legion
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/legion-20.03.0-xxtotheq7eqh7ccvq5qyfmmhimgtuic
    ```
26. librmm
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/librmm-0.1.0-q67khfsoflajb3ldjgg5e4aths5l5psf
    ```
27. libquco
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/libquco-1.3.1-sjyf6sc3adia34wlveacynrwhk7231u
    ```
28. magma
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/magma-2.5.4-fzeekdtrkybubo6i6nikiqczlwnt2jx
    ```
29. mercury
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mercury-1.0-ufxkkvb7osjwgbfvedhrtrouj6dfbz
    ```
30. mfem
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mfem-4.1.0-qgrepufdzopphysuyc6npp7k2tprd5w
    ```
31. mpich
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mpich-3.2.1-5m70fmmttnpv45duckrm3qy32dyheuny7
    ```
32. mpiutils
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/mpiutils-develop-605kx2pmx5yv0fdhkrbrvn2uy4k4uay
    ```
33. ninja
    ```
        /opt/spack/spack/linux-ubuntu18.04-ppc64le/gcc-7.3.0/ninja-1.10.1-cr2ada5fjgkvdtmxel4jz6venfiif5e
    ```
E4S v1.2 GPU Release: 67 E4S Products (ppc64le)
E4S Support for Singularity Container Runtime [Sylabs.io]

- wget http://oaciss.uoregon.edu/e4s/images/ubuntu18.04-e4s-gpu-ppc64le_1.2.simg
- singularity exec --nv ubuntu18.04-e4s-gpu-ppc64le_1.2.simg /bin/bash --rcfile /etc/bashrc
- spack find; module avail
E4S v1.2 GPU Support

```bash
alias runsi='singularity exec --nv /home/users/sameer/images/ubuntu18.04-e4s-gpu-ppc64le_1.2.simg /bin/bash --rcfile /etc/bashrc'
[sameer@gorgon ~]$ runsi
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 matplotlib
>>> import numpy

>>> tensorflow.test.is_gpu_available()
2020-11-05 17:09:35.705979: 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: 31.75GiB freeMemory: 12.35GiB
2020-11-05 17:09:35.778351: 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: 31.75GiB freeMemory: 31.44GiB
2020-11-05 17:09:35.907371: 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: 31.75GiB freeMemory: 883.50MiB
2020-11-05 17:09:35.989499: 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: 31.75GiB freeMemory: 31.44GiB
2020-11-05 17:09:35.989594: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1511] Adding visible gpu devices: 0, 1, 2, 3
2020-11-05 17:09:45.948104: I tensorflow/core/common_runtime/gpu/gpu_device.cc:984] Device interconnect StreamExecutor with strength 1 edge matrix:
2020-11-05 17:09:45.948182: I tensorflow/core/common_runtime/gpu/gpu_device.cc:990]  0 1 2 3
2020-11-05 17:09:45.948199: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1003] 0: N Y Y Y
2020-11-05 17:09:45.948210: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1003] 1: Y N Y Y
2020-11-05 17:09:45.948222: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1003] 2: Y Y Y N
2020-11-05 17:09:45.948232: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1003] 3: Y Y N N
2020-11-05 17:09:45.950552: I tensorflow/core/common_runtime/gpu/gpu_device.cc:1115] Created TensorFlow device (/device:GPU:0 with 11587 MB physical GPU (device: 0, name: Tesla V100-SXM2-32GB, pci bus id: 0004:04:00.0, compute capability: 7.0))
```
E4S: ppc64le Base Container Images

- Hub.docker.com
- ecpe4s

- Ubuntu 18.04
- RHEL/UBI 7.6
- Centos 7.6
### Multi-platform E4S Docker Recipes

#### 10 lines (6 sloc) | 178 Bytes

```bash
FROM ecpe4s/ubuntu18.04-spack-x86_64:0.14.1
WORKDIR /e4s-env
COPY /spack.yaml .
RUN spack install --cache-only
   && spack clean -a && rm -rf /tmp/root/spack-stage
WORKDIR /
```
E4S: Multi-platform Reproducible Docker Recipes

- x86_64
- ppc64le
- aarch64

https://e4s.io
E4S Spack environment spack.yaml

- Bare-metal install
  - `cat spack.yaml`
  - `spack -e . install`

- Docker build:
  - `docker build --no-cache -t ecpe4s/ubuntu18.04-e4s-x86_64:1.2`
E4S: Spack Build Cache at U. Oregon

- 27,000+ binaries
- S3 mirror
- No need to build from source code!

- [https://oaciss.uoregon.edu/e4s/inventory.html](https://oaciss.uoregon.edu/e4s/inventory.html)
WDMApp: Speeding up bare-metal installs using E4S build cache

- E4S Spack build cache
- Adding E4S mirror
- WDMApp install speeds up!
Pantheon and E4S build cache support end-to-end ECP examples

**Overview:** The Exascale Computing Project (ECP) is a complex undertaking, involving a myriad of technologies working together. An outstanding need is a way to capture, curate, communicate and validate workflows that cross all of these boundaries.

The Pantheon and E4S projects are collaborating to advance the integration and testing of capabilities, and to promote understanding of the complex workflows required by the ECP project. Utilizing a host of ECP technologies (spack, Ascent, Cinema, among others), this collaboration brings curated workflows to the fingertips of ECP researchers.

**Contributions**
- Curated end-to-end application/in-situ analysis examples can be run quickly by anyone on Summit. ([https://github.com/pantheonscience/ECP-E4S-Examples](https://github.com/pantheonscience/ECP-E4S-Examples))
- Pantheon/E4S integration speeds up build/setup times over source builds due to cached binaries (approx. 10x speed up).
E4S Validation Test Suite

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

```
git clone https://github.com/E4S-Project/testsuite.git
```

• git clone https://github.com/E4S-Project/testsuite.git
Reproducible Container Builds using E4S Base Images

- PMR SDK base image has Spack build cache mirror and GPG key installed.
- Base image has GCC and MPICH configured for MPICH ABI level replacement (with system MPI).
- Customized container build using binaries from E4S Spack build cache for fast deployment.
- No need to rebuild packages from the source code.
- Same recipe for container and native bare-metal builds with Spack!
E4S: GitLab Runner Images

- Dockerhub
- Bare-bones
- Multi-platform
- Build E4S
University of Oregon GitLab CI

E4S Builds:
- Ubuntu 18.04
- Ubuntu 20.04
- RHEL 7.6
- RHEL 8
- CentOS 7
- CentOS 8

Architectures:
- ppc64le and x86_64

• https://gitlab.e4s.io
Multi-stage E4S CI Build Pipeline on Cori, NERSC
ORNL GitLab Build Pipeline for E4S Spack Build Cache

- ppc64le (Ascent @ ORNL)
- Reproducible container builds
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: [https://e4s-project.github.io/DocPortal.html](https://e4s-project.github.io/DocPortal.html)
## E4S Products

<table>
<thead>
<tr>
<th>Name</th>
<th>Area</th>
<th>Description</th>
<th>Latest Update</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADIOS2</td>
<td>Data &amp; Viz</td>
<td>I/O and data management library for storage I/O, in-memory code coupling and online data analysis and visualization workflows.</td>
<td>2020-07-16 16:36:11</td>
</tr>
<tr>
<td>AML</td>
<td>PMR</td>
<td>Hierarchical memory management library from Argo.</td>
<td>2019-04-25 13:03:01</td>
</tr>
<tr>
<td>AMREX</td>
<td>PMR</td>
<td>A framework designed for building massively parallel block-structured adaptive mesh refinement applications.</td>
<td>2021-01-02 17:25:05</td>
</tr>
</tbody>
</table>

**Description:** AMReX is a publicly available software framework designed for building massively parallel block-structured adaptive mesh refinement (AMR) applications.

https://e4s-project.github.io/DocPortal.html
E4S VirtualBox Image

Container Runtimes
- Docker
- Shifter
- Singularity
- Charliecloud

https://e4s.io
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-cl launch mpirun -np <> -hosts <> <command>`

https://e4s.io
e4s-cl Container Launcher

Login host

```
e4s-cl launch
```

Work hosts

```
e4s-cl execute
```

Containers

```
library resolution
```

```
container launch
```

```
Host libraries
```

```
MPI program
```

```
library resolution
```

```
container launch
```

```
Host libraries
```

```
MPI program
```
## E4S Summary

### What E4S is not
- A closed system taking contributions only from DOE software development teams.
- A monolithic, take-it-or-leave-it software behemoth.
- A commercial product.
- A simple packaging of existing software.

### What E4S is
- Extensible, open architecture software ecosystem accepting contributions from US and international teams.
- Framework for collaborative open-source product integration.
- A full collection of compatible software capabilities and a manifest of a la carte selectable software capabilities.
- Vehicle for delivering high-quality reusable software products in collaboration with others.
- The conduit for future leading edge HPC software targeting scalable next-generation computing platforms.
  - A hierarchical software framework to enhance (via SDKs) software interoperability and quality expectations.
Future work, issues...

- Improved support for GPUs and visualization tools
- DOE LLVM
- Addition of CI testing
- Facility deployment
- Scalable startup with full-featured “Supercontainers”
- Improving the launch of MPI applications
- From-source builds assisted by a binary build cache or containers
- Docker and Singularity images are available for download
  - [https://e4s.io](https://e4s.io)
Performance Research Laboratory, University of Oregon, Eugene

www.uoregon.edu
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