Introduction to Spack in the ADMIRE Project

Usage of Spack in E4S in ECP

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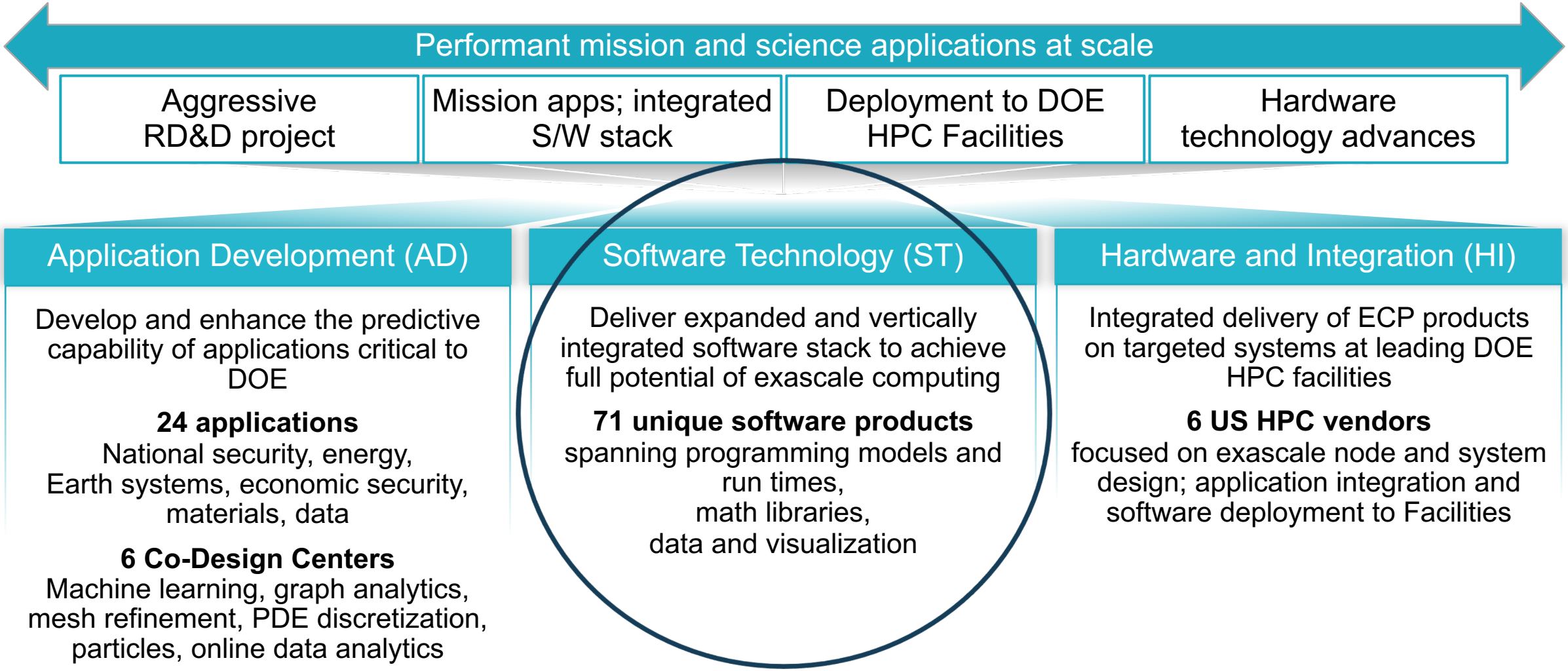
University of Oregon

ParaTools, Inc., ParaTools, SAS

ECP's holistic approach uses co-design and integration to achieve exascale computing



US DOE HPC Roadmap to Exascale Systems

2012-2020 | **2021-2023**

decommissioned

ORNL
Cray/AMD/NVIDIA

ANL
IBM BG/Q

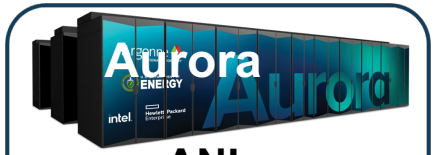
ANL
Cray/Intel KNL

LBNL
Cray/Intel Xeon/KNL

ORNL
IBM/NVIDIA

ORNL
HPE/AMD

Exascale Systems



ANL
Intel/HPE

LBNL
HPE/AMD/NVIDIA

LLNL
IBM BG/Q

LANL/SNL
Cray/Intel Xeon/KNL

LLNL
IBM/NVIDIA

LANL/SNL
HPE/Intel

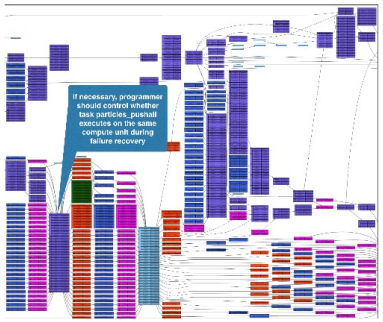
LLNL
HPE/AMD

ECP **Software Technology (ST)**

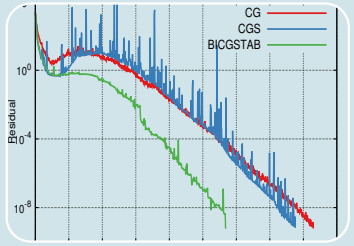
Goal

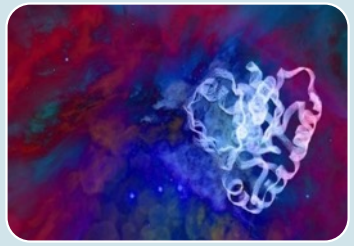
Build a comprehensive, coherent software stack that enables application developers to productively develop highly parallel applications that effectively target diverse exascale architectures

- Prepare SW stack for scalability with massive on-node parallelism
- Extend existing capabilities when possible, develop new when not
- Guide, and complement, and integrate with vendor efforts
- Develop and deliver high-quality and robust software products



ECP ST has six technical areas


Programming Models & Runtimes

- Enhance and get ready for exascale the widely used MPI and OpenMP programming models (hybrid programming models, deep memory copies)
- Development of performance portability tools (e.g. Kokkos and Raja)
- Support alternate models for potential benefits and risk mitigation: PGAS (UPC++/GASNet) ,task-based models (Legion, PaRSEC)
- Libraries for deep memory hierarchy and power management

Development Tools

- Continued, multifaceted capabilities in portable, open-source LLVM compiler ecosystem to support expected ECP architectures, including support for F18
- Performance analysis tools that accommodate new architectures, programming models, e.g., PAPI, Tau

Math Libraries

- Linear algebra, iterative linear solvers, direct linear solvers, integrators and nonlinear solvers, optimization, FFTs, etc
- Performance on new node architectures; extreme strong scalability
- Advanced algorithms for multi-physics, multiscale simulation and outer-loop analysis
- Increasing quality, interoperability, complementarity of math libraries

Data and Visualization

- I/O via the HDF5 API
- Insightful, memory-efficient in-situ visualization and analysis – Data reduction via scientific data compression
- Checkpoint restart

NNSA ST

- Open source NNSA Software projects
- Projects that have both mission role and open science role
- Major technical areas: New programming abstractions, math libraries, data and viz libraries
- Cover most ST technology areas
- Subject to the same planning, reporting and review processes

Software Ecosystem

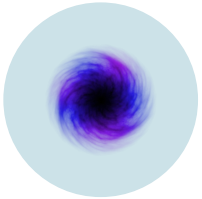
- Develop features in Spack necessary to support all ST products in E4S, and the AD projects that adopt it
- Development of Spack stacks for reproducible turnkey deployment of large collections of software
- Optimization and interoperability of containers on HPC systems
- Regular E4S releases of the ST software stack and SDKs with regular integration of new ST products

Extreme-scale Scientific Software Stack (E4S)

E4S: Better quality, documentation, testing, integration, delivery, building & use

Delivering HPC software to facilities, vendors, agencies, industry, international partners in a brand-new way

Quality Commitment
Community policies, improvement



DocPortal
Single portal to all E4S product info

Portfolio testing
Especially leadership platforms

Curated collection
The end of dependency hell

Quarterly releases
Release 22.11 – November

Build caches
10X build time improvement

Turnkey stack
A new user experience

https://e4s.io

E4S Strategy Group
US agencies, industry, international

E4S: Extreme-scale Scientific Software Stack

- E4S is a community effort to provide open-source software packages for developing, deploying and running scientific applications on HPC platforms.
- E4S has built a comprehensive, coherent software stack that enables application developers to productively develop highly parallel applications that effectively target diverse exascale architectures.
- E4S provides a curated, Spack based software distribution of 100+ HPC and AI/ML packages (e.g., TAU, TensorFlow, PyTorch).
- With E4S Spack binary build caches, E4S supports both bare-metal and containerized deployment for GPU based platforms.
  - X86_64, ppc64le (IBM Power 9), aarch64 (ARM64) with support for GPUs from NVIDIA, AMD, and Intel
  - HPC and AI/ML packages are optimized for GPUs and CPUs.
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products.
- Base images and full featured containers (with GPU support).
- Commercial support for E4S through ParaTools, Inc. for installation, maintaining an issue tracker, and ECP AD engagement.
  - https://dashboard.e4s.io https://e4s.io/talks/E4S_Support_Dec22.pdf
- E4S for commercial cloud platforms: AWS image supports multiple MPI implementations and containers with remote desktop (DCV).
  - Intel MPI, NVHPC, MVAPICH2, MPICH, OpenMPI with Fortran, C, C++ compilers
- e4s-cl container launch tool allows binary distribution of applications by substituting MPI in the containerized app with the system MPI.
- Quarterly releases: E4S 22.11 released on November 14, 2022: https://e4s.io/E4S_22.11.pdf

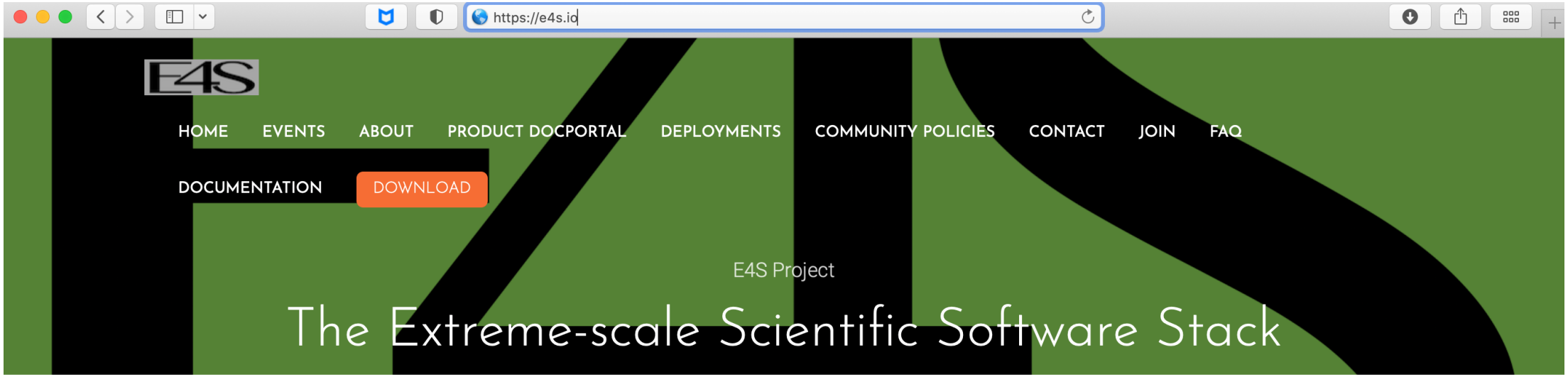
Extreme-scale Scientific Software Stack (E4S)

- E4S: HPC Software Ecosystem – a curated software portfolio
- A **Spack-based** distribution of software tested for interoperability and portability to multiple architectures with support for GPUs from NVIDIA, AMD, and Intel in a single distribution
- Available from **source**, **containers**, **cloud, binary caches**
- Leverages and enhances SDK interoperability thrust
- Not a commercial product – an open resource for all
- 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
- Feb 2020: E4S 1.1 - 61 full release products
- Nov 2020: E4S 1.2 (aka, 20.10) - 67 full release products
- Feb 2021: E4S 21.02 - 67 full release, 4 partial release
- May 2021: E4S 21.05 - 76 full release products
- Aug 2021: E4S 21.08 - 88 full release products
- Nov 2021: E4S 21.11 - 91 full release products
- Feb 2022: E4S 22.02 – 100 full release products
- May 2022: E4S 22.05 – 101 full release products
- August 2022: E4S 22.08 – 102 full release products
- November 2022: E4S 22.11 – 103 full release products

https://e4s.io

Also include other products .e.g.,
AI: PyTorch, TensorFlow (CUDA, ROCm)
Co-Design: AMReX, Cabana, MFEM

E4S Download from https://e4s.io



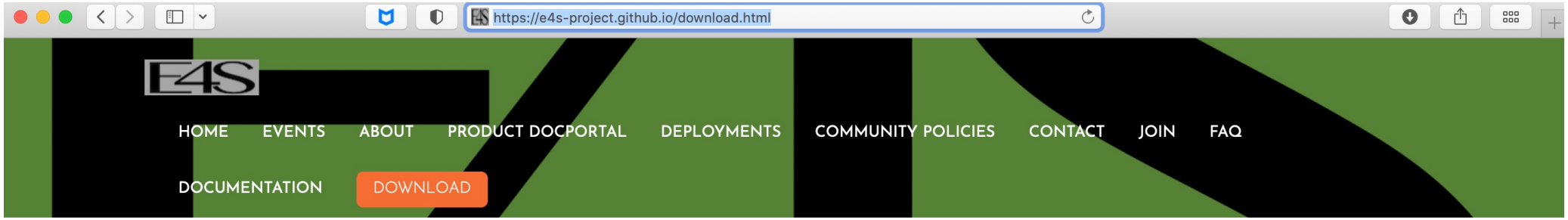
E4S 22.11 container images now available!

See Downloads for more information on E4S 22.11.

What is E4S?

The Extreme-scale Scientific Software Stack (E4S) is a community effort to provide open source software packages for developing, deploying and running scientific applications on high-performance computing (HPC) platforms. E4S provides from-source builds and containers of a broad collection of HPC software packages.

E4S Download from https://e4s.io



Acquiring E4S Containers

The current E4S container offerings include Docker images based on Red Hat Enterprise Linux 7, Red Hat Enterprise Linux 8, Ubuntu 18.04 (Bionic), and Ubuntu 20.04 (Focal Fossa) for Continuous Integration. Our images can run on X86_64, PPC64LE, and AARCH64 depending on the particular image. Our full E4S Release images (not for Continuous Integration) are based on Ubuntu 20.04 (x86_64, aarch64, ppc64le). In addition to offering a full E4S image containing a comprehensive selection of E4S software released on a quarterly cycle, we also offer a set of minimal base images suitable for use in Continuous Integration (CI) pipelines where Spack is used to build packages.

Docker images are available on the E4S Docker Hub.

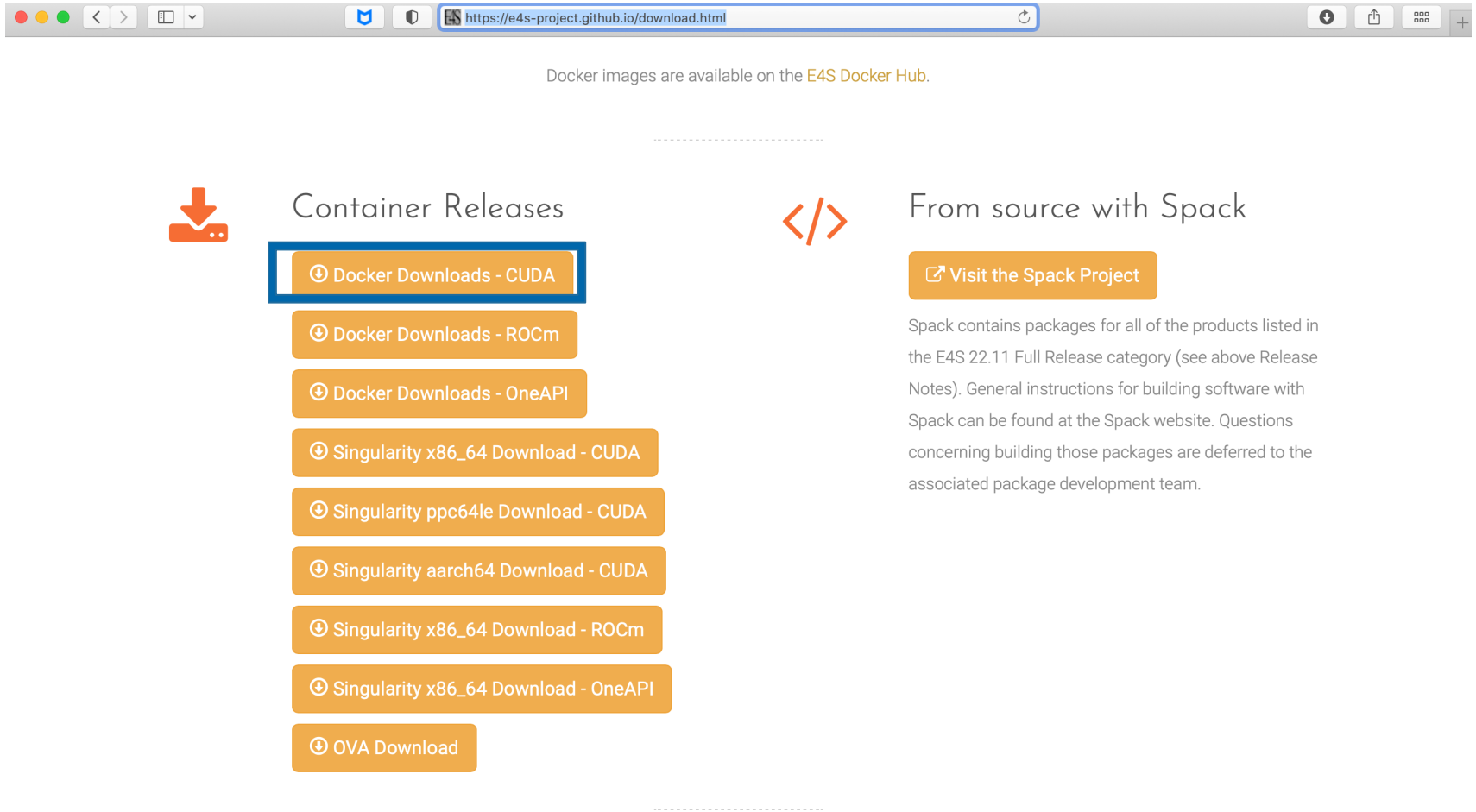
Container Releases

Docker Downloads - CUDA

From source with Spack

Visit the Spack Project

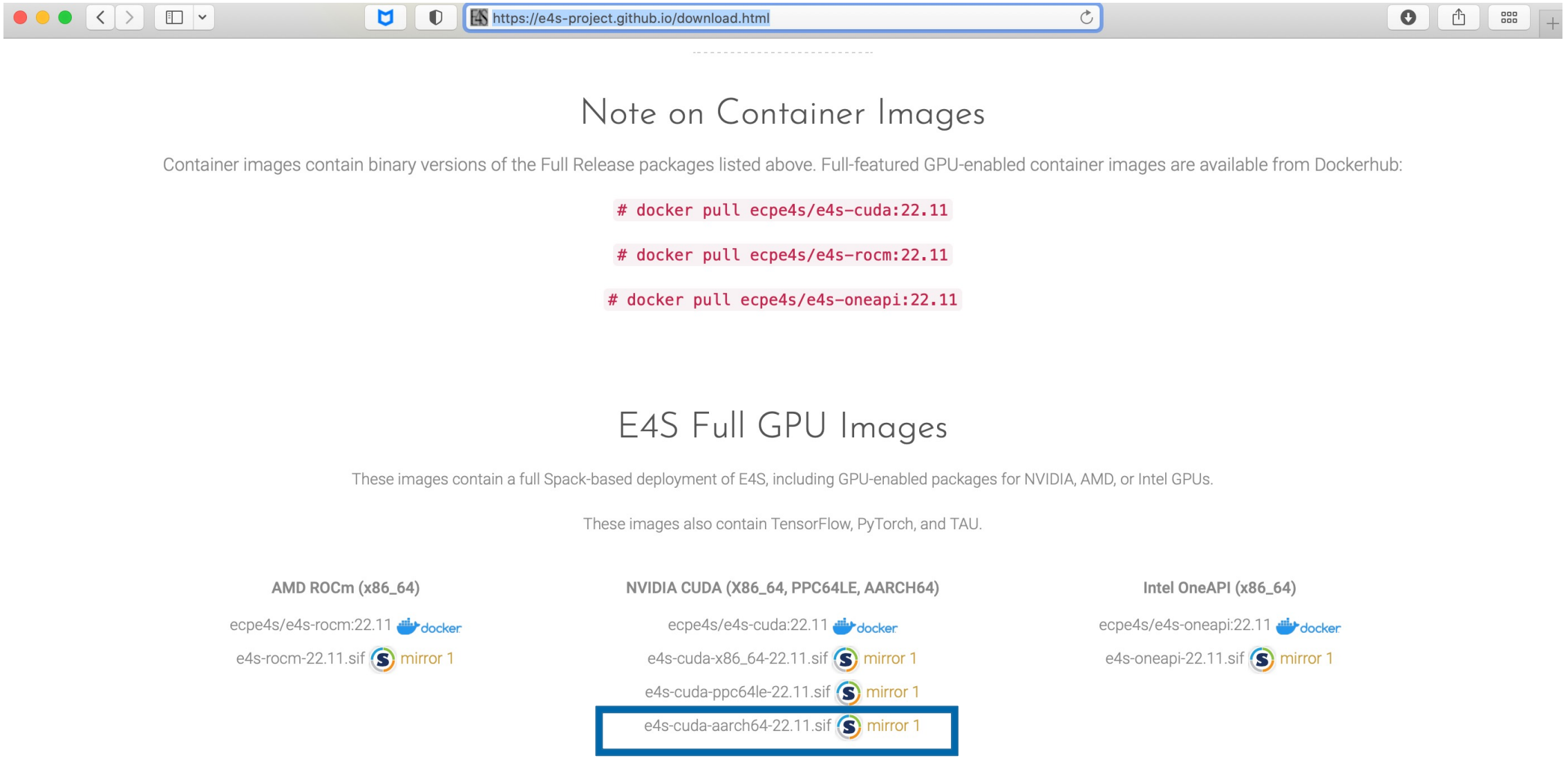
Download E4S 22.11 GPU Container Images: NVIDIA, AMD, Intel



- Separate full featured Singularity images for 3 GPU architectures
- GPU full featured images for
  - x86_64 (Intel, AMD, NVIDIA)
  - ppc64le (NVIDIA)
  - aarch64 (NVIDIA) NEW!
- Full featured images available on Dockerhub
- 100+ products on 3 architectures

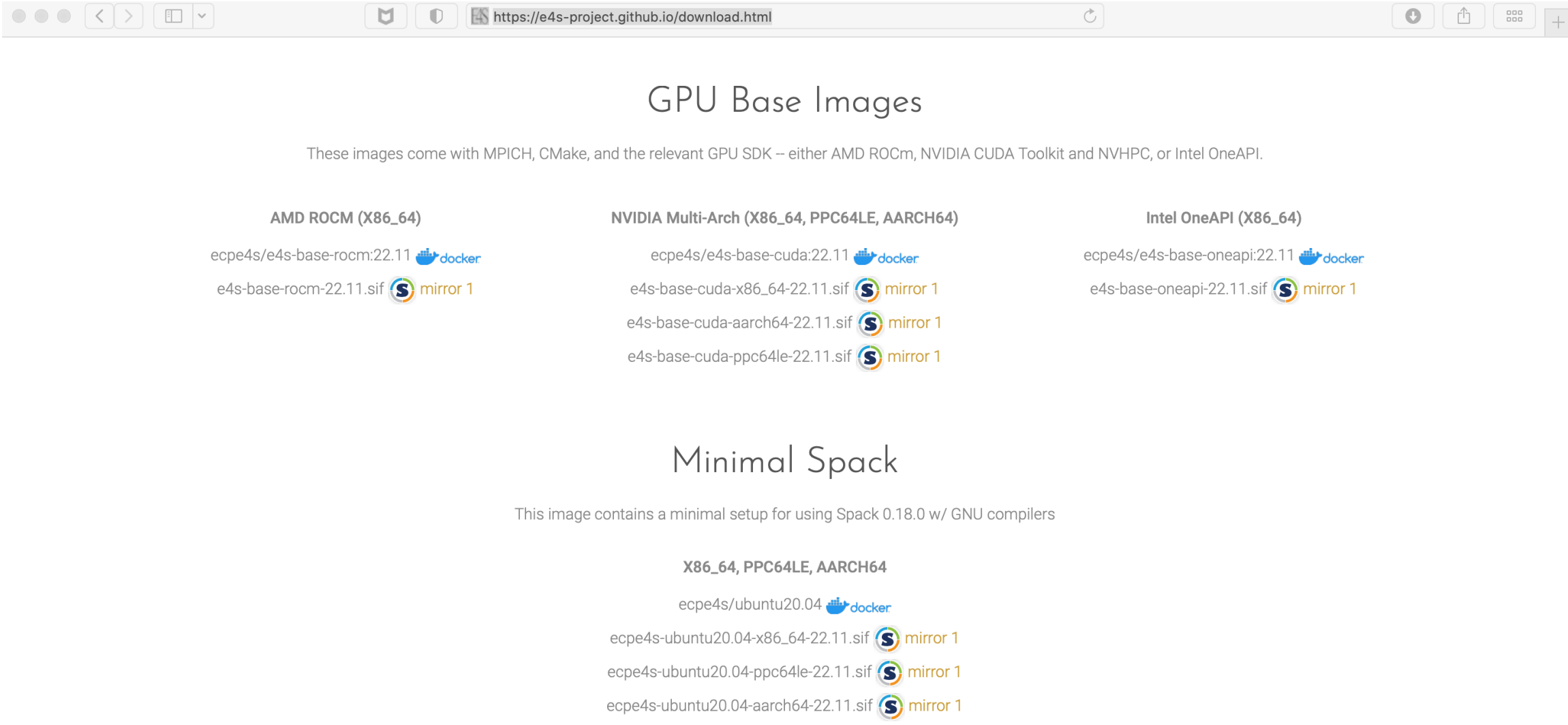
https://e4s.io

Download E4S 22.11 GPU Container Images: NVIDIA, AMD, Intel



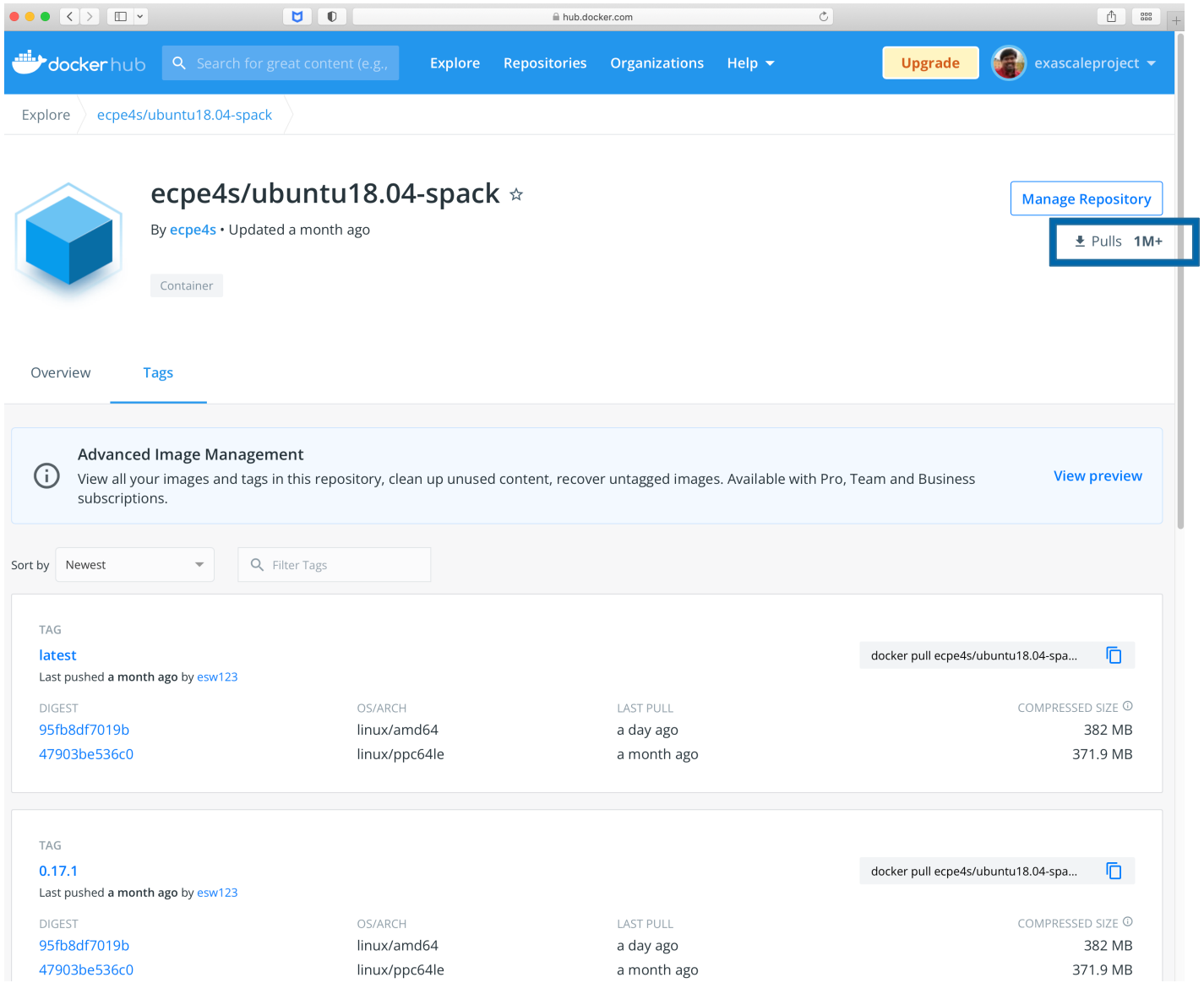
https://e4s.io

E4S 22.11 Base images and Minimal Spack images with MPI



https://e4s.io

Minimal Spack base image on Dockerhub



- Create custom container images
- 1M+ downloads!

22.11 Release: 100+ Official Products + dependencies (gcc, x86_64)

```
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```

GPU runtimes

- AMD (ROCm)
  - 5.2.0
- Intel (oneAPI)
  - 2022.1.0
- NVIDIA (CUDA)
  - 11.4.2
- NVHPC
  - 22.9

22.11 Release: 100 Official Products + dependencies (gcc, x86_64)

```
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  59:  openpmd-api       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openpmd-api-0.14.5-zhhv6pd2ubpohrnkbeyiuap7vlaqc7ne
  60:  papi              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/papi-6.0.0.1-7mdhp4vhvhv34zxjkd7fdxkmrb6w4atz
  61:  papyrus           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/papyrus-1.0.2-lmzmxzs23fhht6supkjicdkbyyudb35q
  62:  parallel-netcdf   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/parallel-netcdf-1.12.3-xbjo2gzly3df2k6ju2bqxypsgpj74av6
  63:  paraview          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/paraview-5.10.1-4h5qdhyzpcniaez2kuuvcdj6d4xhnys4
  64:  parsec            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/parsec-3.0.2209-7extkamumzt72g7vj63yteyplgftyz5e
  65:  pdt               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/pdt-3.25.1-lx67nrs24pkbnmnj7am3t75swtowtfc5
  66:  petsc             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/petsc-3.18.1-dedlz2pkohzwsnf25c76mw4m24ve3raa
  67:  phist             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/phist-1.11.2-o6oyojfq63ig32aprawafeemr5korrpm
  68:  plasma            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/plasma-22.9.29-lzl2zqixszecrubvztpjppftytfumjgq
  69:  plumed            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/plumed-2.8.0-epvuukmxngij4wbuvpad6tbx7mpredyf
  70:  precice           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/precice-2.5.0-y5ig3rxwfepuk7odzzsi5bbnqlbdeu25
  71:  pumi              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/pumi-2.2.7-vrzh5nche4gokubfuzmc46qz4mfqvcsg
  72:  py-cinemasci      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-cinemasci-1.3-jtx4it4i4a6auoaajeodp5pwst4lgghw
  73:  py-jupyterhub     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-jupyterhub-1.4.1-wi2zbgjgkigxwila5ok2pski2g7qzywl
  74:  py-libensemble    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-libensemble-0.9.3-exsvyi4ve2itudyzdolfdskyppuqegdj
  75:  py-parsl          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-parsl-1.1.0-rsijhwc7q4qlo7kh4furvo7muyouwdz6
  76:  py-radical-saga   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-radical-saga-1.16.0-bzyd6sofsz5cxlyuk2xrpugyuxflxtee
  77:  qthreads          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/qthreads-1.16-xjrlin56oafltc3ehvxdy74pz5zvcpkn
  78:  quantum-espresso  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/quantum-espresso-7.1-pf4cmxbnqmswwamoxnl2ihjgtz4p7kgp
  79:  raja              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/raja-2022.03.0-kf7ckzhggoh3iu3cshwonj5mafjkmgpl
  80:  scr               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/scr-3.0.1-47wtxqrwpia77oeyavpq5qkhdokgkuvu
  81:  slate             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/slate-2022.07.00-ofiigavw7kcyneulkfbazl3m45mufmvu
  82:  slepc             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/slepc-3.18.1-pi6plqtsnssyp37d2wlz3wfpylrrrcoh
  83:  stc               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/stc-0.9.0-wnlgngxsjzo4rg3yw2jtlzgnxvgr5nax
  84:  strumpack         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/strumpack-7.0.1-bcxv6bhle5e77wzvx3ambzaciqi4bb6h
  85:  sundials          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/sundials-6.4.1-nal5sibiqezc45fbz53cwrd34rxfcb4f
  86:  superlu-dist      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/superlu-dist-8.1.1-k7k4dihxflzall4wqz66rhs7agshu3bj
  87:  swig              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/swig-4.0.2-fortran-f6qkx5yz47aagowwl2rtbz4kucc6gh3j
  88:  sz                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/sz-2.1.12.2-2ilgy7ishmc2tbz2ghbtkaoasaltbiek
  89:  tasmanian         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/tasmanian-7.9-izwrkvlnjnevhtorhqesa6rkkmcf6t7x
  90:  tau               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/tau-2.32-qoombzmdp3qhettqxr4f4d44erxzjdx5
  91:  trilinos          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/trilinos-13.4.0-xnlfgmz4zeb7jdfdlx7bm5nnbc4qkr7l
  92:  turbine           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/turbine-1.3.0-mymxhgxtdpdowytnhsotcm3zvs2arpak
  93:  umap              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/umap-2.1.0-wpqbklc3pxmcyacmk6f3g5gxovaribg5
  94:  umpire            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/umpire-2022.03.1-2vs73ks3sglgqveks2awdrvuzbcx3quq
  95:  unifyfs           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/unifyfs-1.0-omawjudjfjow2xikcrzaqn3u3cvmjwzy
  96:  upcxx             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/upcxx-2022.9.0-nbwjd4sgirqplrgct4qamdivwskluxvy
  97:  variorum          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/variorum-0.6.0-azdafc4ozaosrpn5sfmbfsl5m4d4b3d7
  98:  veloc             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/veloc-1.5-rhta4y7xmuhj4sxsykgfyzbf3y4etenk
  99:  visit             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/visit-3.2.2-h7vjzfzlnfk2zbvz2ono4wokk3rutuy4
 100:  vtk-m             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/vtk-m-1.9.0-j52zqfh35h5qofzycu3uhndap3b4vlbx
 101:  wannier90         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/wannier90-3.1.0-npbjfugy4n64yzk2nitbjfm5z3li7dag
 102:  warpx             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/warpx-22.10-xcdmrukm6bkvf24npzxhk3ha5ydymmnh
 103:  zfp               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/zfp-0.5.5-dkanfr4t75fh3gwkpsdzhphs25h24nxp
```

Languages:

- Julia
- Python

AI products with GPU support

- Tensorflow
- Pytorch

3D Visualization

- Paraview
- VisIt
- TAU's paraprof …

E4S Support for CUDA variants on x86_64

```
Singularity> spack find +cuda cuda_arch=80
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
adios2@2.8.3        camp@2022.03.2  ginkgo@1.4.0   kokkos@3.7.00          omega-h@9.34.13   strumpack@7.0.1     umpire@2022.03.1
amrex@22.11         camp@2022.03.2  heffte@2.3.0   kokkos-kernels@3.7.00  petsc@3.18.1      sundials@6.4.1      vtk-m@1.9.0
arborx@1.3          chai@2022.03.0  hpx@1.8.1      lapackpp@2022.07.00    raja@2022.03.0    superlu-dist@8.1.1  zfp@0.5.5
blaspp@2022.07.00   dealii@9.4.0    hypre@2.26.0   magma@2.6.2            slate@2022.07.00  tasmanian@7.9
caliper@2.8.0       flecsi@2.1.0    kokkos@3.7.00  mfem@4.5.0             slepc@3.18.1      trilinos@13.4.0
==> 33 installed packages
Singularity> spack find +cuda cuda_arch=70
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
adios2@2.8.3        camp@2022.03.2  ginkgo@1.4.0   kokkos@3.7.00          omega-h@9.34.13   strumpack@7.0.1     umpire@2022.03.1
amrex@22.11         camp@2022.03.2  heffte@2.3.0   kokkos-kernels@3.7.00  petsc@3.18.1      sundials@6.4.1      vtk-m@1.9.0
arborx@1.3          chai@2022.03.0  hpx@1.8.1      lapackpp@2022.07.00    raja@2022.03.0    superlu-dist@8.1.1  zfp@0.5.5
blaspp@2022.07.00   dealii@9.4.0    hypre@2.26.0   magma@2.6.2            slate@2022.07.00  tasmanian@7.9
caliper@2.8.0       flecsi@2.1.0    kokkos@3.7.00  mfem@4.5.0             slepc@3.18.1      trilinos@13.4.0
==> 33 installed packages
Singularity>
```

E4S Support for ROCm variants for MI250X (gfx90a) on x86_64

```
Singularity> spack find +rocm amdgpu_target=gfx90a
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
amrex@22.11            gasnet@2022.9.0  lapackpp@2022.07.00  strumpack@7.0.1     upcxx@2022.9.0
arborx@1.3             ginkgo@1.4.0     magma@2.6.2          sundials@6.4.1      vtk-m@1.9.0
blaspp@2022.07.00      heffte@2.3.0     petsc@3.18.1         superlu-dist@8.1.1
camp@2022.03.2         hpx@1.8.1        raja@2022.03.0       tasmanian@7.9
chai@2022.03.0         hypre@2.26.0     slate@2022.07.00     trilinos@13.4.0
ecp-data-vis-sdk@1.0   kokkos@3.7.00    slepc@3.18.1         umpire@2022.03.1
==> 26 installed packages
Singularity>
```

22.11 Release: 100+ Official Products + dependencies (gcc, ppc64le)

```
 1:  adios2              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/adios2-2.8.3-xstw7pb2wnuauxru23yle4fwxftprwub
 2:  alquimia            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/alquimia-1.0.10-imnm7jcs2ouai2rxauuouvyckx7jgq66
 3:  aml                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/aml-0.2.0-zcs62l6fotx3x3qd5n6dw2yk6nq6p2lu
 4:  amrex               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/amrex-22.11-qkh4nkmrfvy3rsjuot4itoqkgs3ykbmh
 5:  arborx              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/arborx-1.3-sfc3s5436qqbeba3ifeuiphfnmby3c7s
 6:  archer              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/archer-2.0.0-256hr6lkxoiqfejxvgp5qrm23zjondko
 7:  argobots            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/argobots-main-6nktgpmhhyk4moukp5acd574r6tx645m
 8:  ascent              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ascent-0.8.0-ue6c6ykcj22v6cuhbbuwjxvheshdy7mq
 9:  axom                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/axom-0.7.0-tbaeg6h7snyrv2zaf5shhmmxx322ilq3
10:  bolt                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/bolt-2.0-qgdopshdcptzcnnda56mowvvvw2digyz
11:  butterflypack       /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/butterflypack-2.2.2-lrytvkbx54c64nw7sp4sgj7ju6zfpmzg
12:  cabana              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/cabana-0.5.0-dbnndtwheiqh23dhdzdirar6i6rygz7w
13:  caliper             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/caliper-2.8.0-ardfzvqrw5xx3eygslqy3wn3673fp4yv
14:  chai                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/chai-2022.03.0-y67sx56h67l3svnpgmyvwms2njk57uu7
15:  charliecloud        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/charliecloud-0.29-22lhik3wztz2lwgsp5ztaaxivczfnvts
16:  conduit             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/conduit-0.8.4-i2dirqo5kdnclzmo4z2g4py7wat2toil
17:  darshan-runtime     /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/darshan-runtime-3.4.0-6gwxbfzshgdkqlusyzriuuq7yvwil77f
18:  datatransferkit     /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/datatransferkit-3.1-rc3-yw7yb5352jm7ebuszgc7gxfmhjm2a6pz
19:  dyninst             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/dyninst-12.2.0-srymkrlxqo2uel246lxun4by46vcltax
20:  ecp-data-vis-sdk    /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ecp-data-vis-sdk-1.0-zx5zr5jbjurfk46l2rjmmznmotrn2rjj
21:  exaworks            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/exaworks-0.1.0-xwvmorfgk2pfzjuqja5qwuqsflb63ugu
22:  faodel              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/faodel-1.2108.1-fi5cqlv5vqkmjd6xdlm5cffq6gs7qa3c
23:  flecsi              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flecsi-2.1.0-ry6mptoqpps6zw5qp77oil2oepq5foai
24:  flit                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flit-2.1.0-3xcjxzekst34gvmawehi7ttpew6wbqim
25:  flux-sched          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/flux-sched-0.25.0-lsqmafqe4fxerkss5hcc5p3f6ifv44xu
26:  fortrilinos         /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/fortrilinos-2.1.0-ou6tjphmra6k4fjxeh3uasrtzcc6ftlm
27:  gasnet              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gasnet-2022.9.0-hcednfzbzdkoag6saykfup5dgz5f2ah2
28:  ginkgo              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/ginkgo-1.4.0-ihtmhzji6hamhvcaw45mzbsmyihmayvp
29:  globalarrays        /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/globalarrays-5.8-wcasxk7bjcsbjiathzocnfxdnx6pz5v5
30:  gotcha              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gotcha-1.0.4-pp3wx752o7eyg2bohct5nsh3j67ck7bs
31:  gptune              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/gptune-3.0.0-dxrelx4x3iptauno23qpscx76gvgbsag
32:  h5bench             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/h5bench-1.3-64tk47z26t3ier5oet3nck563ofpe6su
33:  hdf5                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-1.13.2-jtg6fulrjfl6tsvkkgcam2faconpjozz
34:  hdf5-vol-async      /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hdf5-vol-async-1.3-2idxkq4o4yf33sih3wh64ddj22sjhj34
35:  heffte              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/heffte-2.3.0-ybenwfs5whb623uwencjgdslhqnbyedc
36:  hpctoolkit          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpctoolkit-2022.10.01-3s4wo2fusrnfvteiqpjs5c4ainkmogzk
37:  hpx                 /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hpx-1.8.1-k4taf7ds4wjehmyvkz6ia7eceqdkpvh4
38:  hypre               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/hypre-2.26.0-xcdmzvzb5uv34kxzpugli72s24koebvx
39:  kokkos              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-3.7.00-ridq237k7wk7hnkosbkzjucnqg3avqwh
40:  kokkos-kernels      /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/kokkos-kernels-3.7.00-75g3c4e4vfl3p2bfkh3gna4ttju72eiu
41:  lammps              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/lammps-20220623-hqrhjr62kdzr35js3av7te6fz2bfibwc
42:  legion              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/legion-21.03.0-6lbyivddvseddjfujjwmvki56ipnk7cp
43:  libnrm              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libnrm-0.1.0-d7pfkkzjjrmrisboiqcl7yie4o6r4vxc
44:  libpressio          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libpressio-0.88.0-tu7zmnqrh7cnvq46m7r54spf7ofpw2ko
45:  libquo              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/libquo-1.3.1-gmno3vlx7vu25rtpshwyxkrbbpnyclqw
46:  magma               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/magma-2.6.2-rzszsgyer4k2bvbcv7367aumyeu4as54
47:  mercury             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mercury-2.1.0-6pfx2hulypvn5glao6nnfyyerojnq5sq
48:  metall              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/metall-0.21-7yh36oky4dmp5eujuzasx7vnncnucrow
49:  mfem                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mfem-4.5.0-i3ozodxminhapjxouwunz2huwla5v2qk
50:  mpark-variant       /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpark-variant-1.4.0-tkootg76dnc7lkamebzd4v63aadt2cow
51:  mpich               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpich-4.0.2-vuh7xcc7tiruyjeplretykmeui6jv52e
```

GPU runtimes for IBM Power

- CUDA 11.4
- NVHPC 22.9

Languages

- Julia
- Python

AI packages for NVIDIA GPU

- TensorFlow
- PyTorch

22.11 Release: 100+ Official Products + dependencies (gcc, ppc64le)

```
 52:  mpifileutils      /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/mpifileutils-0.11.1-shjxfjpjvnosjprrm2qzaqzbdpydp6yp
 53:  nccmp             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nccmp-1.9.0.1-7mveozgiw4pwfvx3jdmgf5re3liereqy
 54:  nco               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nco-5.0.1-cuqirm6youh4soh3m4jqyujd65lwrmh4
 55:  netcdf-c          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netcdf-c-4.9.0-k6yoh3wmoyjj6zkc56cof3ybadgkshvz
 56:  netlib-scalapack  /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/netlib-scalapack-2.2.0-ceqsztw3ftqckwgudwacd2dgtowj5y2r
 57:  nrm               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/nrm-0.1.0-jehz42dp6tq2cexmgxwiqfozxqfjkobw
 58:  omega-h           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/omega-h-9.34.13-m5bwhbsbeq2lcpwlaxhdrvad7dnljpyi
 59:  openmpi           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openmpi-4.1.4-se2ftqv5xsejkmzufpsdybmqwqblgkzr
 60:  openpmd-api       /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/openpmd-api-0.14.5-vynu7b5z3fbdx46raffz64dtvdtdejhx
 61:  papi              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papi-6.0.0.1-zsplngh5qplinhi4eegi5wzfw2qg6ru3
 62:  papyrus           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/papyrus-1.0.2-a6qveegb6k2ahymlzgglulee6ojoovqm
 63:  parallel-netcdf   /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parallel-netcdf-1.12.3-lw3glwqyttaalqt45k67owvfy5hqjnbp
 64:  parsec            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/parsec-3.0.2209-3xmklhbil6k2fpo4uveury3qdq3ae2um
 65:  pdt               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pdt-3.25.1-v4rjp5vwznt7s3d2cj4wawyhs2aagqye
 66:  petsc             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/petsc-3.18.1-td7n4vxji46oatcimj3zfhrf7g2o572b
 67:  phist             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/phist-1.11.2-rf7l2cixm47puybop3ayjxrra5plxdg3
 68:  plasma            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plasma-22.9.29-feh4vfflk4qck7vhtcw2fphq2dxq3rg
 69:  plumed            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/plumed-2.8.0-txmxzcerz46vn3j27rtwqpxxb3kpw5xs
 70:  precice           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/precice-2.5.0-iw2o7zwz7umgpssru3hoxqiigxrgdtul
 71:  pumi              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/pumi-2.2.7-qboyr63c55zh6rt6edw5drpgmky5bjpw
 72:  py-cinemasci      /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-cinemasci-1.7.0-p4rv2a3lrzfxr2jjdgwrxbi2zc4xxa6z
 73:  py-jupyterhub     /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-jupyterhub-1.4.1-cf3tays4l4k5drhetd6vuobfaoxke4rq
 74:  py-libensemble    /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-libensemble-0.9.3-3ohso23ip2jgcwxf67zkrszp2gkixa55
 75:  py-parsl          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-parsl-1.1.0-wuk64tyhzm3o3jw352ypu7uwjvqvvtwn
 76:  py-radical-pilot  /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-radical-pilot-1.16.0-dps7t7pvkves3wwrphxagoju6ghhzvub
 77:  py-radical-saga   /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/py-radical-saga-1.16.0-br3ptdqhlo5yzpe4qt662hb735wlkdgv
 78:  qthreads          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/qthreads-1.16-rtnk7rz6b3x5yileiufga2ipw55daiiq
 79:  quantum-espresso  /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/quantum-espresso-7.1-hpsqg56frlyptn6ebpfvqxx7zhl7boaw
 80:  raja              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/raja-2022.03.0-j5lmuroz6yj2ny37vcyucaws5dkqapmk
 81:  scr               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/scr-3.0.1-owoj4tln4vlw4rxym525alqrc2gykduy
 82:  slate             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slate-2022.07.00-gfetndk473optp5xbf7wjypkhvvicwv4
 83:  slepc             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/slepc-3.18.1-q7wi72flehxqkgpdft57gugcthrwxx34
 84:  stc               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/stc-0.9.0-myxazo2kbnkirwxwshrqqfgca4bo5tzd
 85:  strumpack         /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/strumpack-7.0.1-wsv5cgcffg2bh5rdpoab6odkv6ngtokn
 86:  sundials          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sundials-6.4.1-be5o3gu3lyz6chq477jnkbew2aoin24u
 87:  superlu-dist      /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/superlu-dist-8.1.1-xaslzn7y2pkysine4ukuly6fn5ib724g
 88:  swig              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/swig-4.0.2-fortran-ct3v7tcpfcx7gzyhgq7c47f2j6gj7oex
 89:  sz                /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/sz-2.1.12.2-djc27r3exk3ykrrx3dmku5f5vcw56d5d
 90:  tasmanian         /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tasmanian-7.9-xlbvfdtrbrea5ifsd3juqceyayrgyozd
 91:  tau               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/tau-2.32-bx7zr6szk652qsvgx24pqoq7br4xprgl
 92:  trilinos          /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/trilinos-13.4.0-3jyearqfpsvxc7j7eicaytfuzxr6hsny
 93:  turbine           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/turbine-1.3.0-ahvy6fjzi4pqgni4wv6zadaj4g26nsbj
 94:  umap              /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umap-2.1.0-fbkmjq3aseq4yn3xecmwlxz3i2f3logn
 95:  umpire            /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/umpire-2022.03.1-ngbjwhtklyap24fy7x2ixriflgzwdh26
 96:  unifyfs           /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/unifyfs-1.0-k4m4q726d6fqo4z27hy7g5y3l5zxmgvk
 97:  upcxx             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/upcxx-2022.9.0-xngkg2e35w3hxegp73jfuu4nm3hakkmc
 98:  veloc             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/veloc-1.5-2kisertu7gukltw3hgwt4a3fogipq5cp
 99:  vtk-m             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/vtk-m-1.9.0-xby4bbn4rsbs2o7tmshdrag5s4twtupk
100:  wannier90         /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/wannier90-3.1.0-7lbbjhbmvrm4tzvdvhlh3gcwxv6nfzii
101:  warpx             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/warpx-22.10-ciw2valpngmv7jmoq3eqcj552rrpbsy7
102:  yaksa             /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/yaksa-0.2-htchdndgcdknrsytcxm2rmeths3tdeca
103:  zfp               /spack/opt/spack/linux-ubuntu20.04-ppc64le/gcc-9.4.0/zfp-0.5.5-5ynyd5oyhsei32b3psgf32hv3b3cy4ub
```

GPU runtimes for IBM Power

- CUDA 11.4
- NVHPC 22.9

Languages

- Julia
- Python

AI packages for NVIDIA GPU

- TensorFlow
- PyTorch

E4S Support for CUDA variants on ppc64le

```
Singularity> spack find +cuda
-- linux-ubuntu20.04-ppc64le / gcc@9.4.0 ------------------------
adios2@2.8.3       caliper@2.8.0   ecp-data-vis-sdk@1.0   hpx@1.8.1             lapackpp@2022.07.00  petsc@3.18.1      sundials@6.4.1      umpire@2022.03.1
amrex@22.11        camp@0.2.3      flecsi@2.1.0           hwloc@2.8.0           magma@2.6.2          raja@0.14.0       superlu-dist@8.1.1  vtk-h@0.8.1
arborx@1.3         camp@2022.03.2  flux-core@0.44.0       hypre@2.26.0          mfem@4.5.0           raja@2022.03.0    tasmanian@7.9       vtk-m@1.7.1
ascent@0.8.0       camp@2022.03.2  ginkgo@1.4.0           kokkos@3.7.00         omega-h@9.34.13      slate@2022.07.00  tau@2.32            zfp@0.5.5
blaspp@2022.07.00  chai@2022.03.0  heffte@2.3.0           kokkos@3.7.00         papi@6.0.0.1         slepc@3.18.1      trilinos@13.4.0
cabana@0.5.0       dray@0.1.8      hpctoolkit@2022.10.01  kokkos-kernels@3.7.00 petsc@3.18.1         strumpack@7.0.1   umpire@6.0.0
==> 46 installed packages
Singularity> uname -a
Linux eagle 4.18.0-348.7.1.el8_5.ppc64le #1 SMP Wed Dec 8 21:26:34 EST 2021 ppc64le ppc64le ppc64le GNU/Linux
Singularity>
```

22.11 Release: 97 Official Products + dependencies (gcc, aarch64)

1:	adios2	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/adios2-2.8.3-tn6yp5hyy7pzu4dsbxe4btezwtu4tlre
2:	alquimia	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/alquimia-1.0.10-tdvinjiqt4e6eacmd6pnrrd3ue6k6i4j
3:	aml	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/aml-0.2.0-syvk6hnriqj77ncazqzqlmocbnkpclgu
4:	amrex	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/amrex-22.11-6ydr3w7ayovuh2yzvfsxoid2kgwnfpws
5:	arborx	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/arborx-1.3-jt7ve5rlwivzf5dzwyng26jam5fzjqci
6:	archer	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/archer-2.0.0-7f5pa6xnn5dv4jfvu7b4646ycqi6fzkc
7:	argobots	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/argobots-1.1-l74kgroqqhmojgtla6jc636nxy2dalfc
8:	axom	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/axom-0.7.0-t3kotm4x4z52ekeufo6jo4rr4vbze63w
9:	bolt	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/bolt-2.0-yvwovujhly33eswru7y5u7hrm5wrlvpb
10:	butterflypack	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/butterflypack-2.2.2-kpf7z2obladjl5oyh5vlirhnuurv3i3l
11:	cabana	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/cabana-0.5.0-vr5m5k2oaifqa5rf3avouo64goreqvxq
12:	caliper	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/caliper-2.8.0-jn2n6qmx4nr5wah2v74hobktmltdgl5y
13:	chai	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/chai-2022.03.0-5u6vclovphu7jujakax5hbcukh6qhymp
14:	charliecloud	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/charliecloud-0.29-ktfm7t2k7hpqtzrjmhcewcvgpi3grl5a
15:	conduit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/conduit-0.8.4-hvuikr4sv2kfcx4g35jfo6c2rj2zccmj
16:	dealii	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/dealii-9.4.0-falixullnfl4vjamcepzljuuscrwglzc
17:	datatransferkit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/datatransferkit-3.1-rc3-zisyujfjv4nttxhdnbncbdv6co75z5pv
18:	dyninst	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/dyninst-12.2.0-ypzolgjgzobolvpbgsi4jzfhcyk47vjq
19:	exaworks	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/exaworks-0.1.0-3m2ruyseumhukyekm2q4nt7rdvd7k4wg
20:	flecsi	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/flecsi-2.1.0-s6rs2yftyaxvxlnl7q7gp22gvekqa4y3
21:	flit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/flit-2.1.0-emd4kewqega7ex6b7fsoj7ks2jgfap2r
22:	flux-sched	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/flux-sched-0.25.0-lmqdl4srk3jhvioy5is6s63bhi3wss3l
23:	fortrilinos	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/fortrilinos-2.1.0-exjnwqhy36jgk3wzihytuxmhpu6ux37x
24:	gasnet	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/gasnet-2022.9.0-6bes46634npapndf4hjcntlbn5ivwrvp
25:	ginkgo	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/ginkgo-1.4.0-acxgljw53cythdethxhlzrhny4qsb5x2
26:	globalarrays	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/globalarrays-5.8-wzl7agux5xdxyyi4xngmd4xtgl5g3old
27:	gotcha	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/gotcha-1.0.4-gagcbny5lx6tabraefjzoiovbwbmdiiq
28:	gptune	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/gptune-3.0.0-4kplix3fdcstrt5dypqlrqaqrposgexi
29:	h5bench	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/h5bench-1.3-7lmvmdpwsk755x5wckemhryj64t6adku
30:	hdf5	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hdf5-1.12.2-asibqu6lil6f2khy4wz4jguvgdt6nasw
31:	heffte	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/heffte-2.3.0-52sxlh32xxlx7xqsu2hn67ituonhpetd
32:	hpctoolkit	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hpctoolkit-2022.10.01-bt53jfagmgfgympp6dcg3mma2xkj6z6j
33:	hypre	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/hypre-2.26.0-ohgawpjpqugg75igtu37gvh42akacask
34:	kokkos	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/kokkos-3.7.00-f7yk3y47vlms4qzwikqgktfxyc2w5w24
35:	kokkos-kernels	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/kokkos-kernels-3.7.00-atdbg7a5fyhnqwc2aiffor522mtaeswv
36:	lammps	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/lammps-20220623-erjtpwzq4kgfmmywp5ydvcdnltujb7fo
37:	legion	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/legion-21.03.0-o3f5hnenbldjwvb42quez4kajwxgm4xs
38:	libnrm	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/libnrm-0.1.0-xbrc2ijsh3z5yz7m5dqkzeblqtbc4dow
39:	libpressio	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/libpressio-0.88.0-ofdlcpilijgeket6wujc7s7clylphx2x
40:	libquo	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/libquo-1.3.1-yrjwwdkcw2syql7wqkladcc65bfj3z3n
41:	magma	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/magma-2.6.2-vlhdyh4rcsuyvn63s2g3kxooazucnzmn
42:	mercury	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mercury-2.1.0-32tqjycyhtonefmschzspb4t56hgqavs
43:	metall	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/metall-0.21-p62al2ga42ubtmfbbya4rvlrltoxmyyc
44:	metis	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/metis-5.1.0-zmoxqrtl3klpelmjeofnquikf2z3hktj
45:	mfem	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mfem-4.5.0-tf5sgtvrnsxhijo53nw6u53skhgis35j
46:	mpark-variant	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mpark-variant-1.4.0-ffmm7i4mnho7mpx6weaevaizygyccerb
47:	mpich	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mpich-4.0.2-4f7mm6hpijp7475nhxulp7nnffjbmwwu
48:	mpifileutils	/spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/mpifileutils-0.11.1-ptsvxdgt57g5ppuxfwzsaba6wwnicnth

GPU runtimes for aarch64

- CUDA 11.7.1
- NVHPC 22.9

Languages

- Julia
- Python

AI packages for NVIDIA GPU

- TensorFlow
- PyTorch

22.11 Release: 97 Official Products + dependencies (gcc, aarch64)

```
49:  netcdf-c            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/netcdf-c-4.9.0-2pfmvfxcyytym2mcbrv7wf5fz4lhyn5e
50:  netlib-scalapack    /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/netlib-scalapack-2.2.0-jibpglaalgul4vdvkthm2xffgsaqyk6x
51:  nccmp               /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/nccmp-1.9.0.1-bj5q4zadekltoplllmpwap55t6rhp7bn
52:  nco                 /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/nco-5.0.1-37anulj3jhpjq7uppvvaulv3rhiyfokp
53:  nrm                 /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/nrm-0.1.0-gaw4judk5h7leoarmnhglx7anwmot7ss
54:  omega-h             /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/omega-h-9.34.13-7akf22v6k6ez6zw3laipkgvodstcbs4x
55:  openmpi             /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/openmpi-4.1.4-tzwjiius6vahp7gqttpmj5dufkhuphnh
56:  openpmd-api         /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/openpmd-api-0.14.5-7n4dyx2hfvkaqlx42yczmptrbh6pjrww
57:  papi                /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/papi-6.0.0.1-whxzalkc552oguusqeoyhlud72dms63l
58:  papyrus             /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/papyrus-1.0.2-4izhlazxhbfgsu5wqr5mfph7nreryu7u
59:  parmetis            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/parmetis-4.0.3-uf2q6w2obb3ffd5saykavw64v4qxx77g
60:  parsec              /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/parsec-3.0.2209-kok6u7t4ktjs5hibskcui3ij5k273t4n
61:  pdt                 /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/pdt-3.25.1-tips7k5urkb4eo6gqs7h47dbtrr4w6x2
62:  petsc               /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/petsc-3.18.1-wa3y5fd6bpo6l2zcfs5aldzgqzn3lzgq
63:  plasma              /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/plasma-22.9.29-4flv33ga6ms6tk42s2wrxbglbtg5fmpu
64:  plumed              /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/plumed-2.8.0-a2mtftxdvwp4xui3h3o3hwj2cke3gsvq
65:  precice             /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/precice-2.5.0-3u3kp2fd3lxd4paqhcozknw362en4p4a
66:  pumi                /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/pumi-2.2.7-7pmitcrr6vf6b6e7tomboz6g6p2kke5l
67:  py-jupyterhub       /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-jupyterhub-1.4.1-xfqgddo75bxjnh7kdnikx53lwuo7gjfm
68:  py-libensemble      /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-libensemble-0.9.3-ekr7nmfgbbvrkar6mafzb3fzr42qigbz
69:  py-opentuner        /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-opentuner-0.8.7-ym2rlih2zrgsyamcxiol4udnxjwsw7qm
70:  py-parsl            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-parsl-1.1.0-m7wtbpe4nxq5mqdxirf22gwettjebvug
71:  py-radical-entk     /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-radical-entk-1.16.0-uspj343t5wdcgryqksrjabeqs3taa23x
72:  py-radical-pilot    /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-radical-pilot-1.16.0-gslzkf66ozxnl4wgl3njl3gnjuobczyx
73:  py-radical-saga     /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/py-radical-saga-1.16.0-wcz7tksshlxuahqyoyjojfpsyqzhlcc3
74:  qthreads            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/qthreads-1.16-c6uuprrtqcdkq75g5d3pur5iblvkutak
75:  quantum-espresso    /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/quantum-espresso-7.1-hw7oy3vjdllkjgaraslhbwetuxx72uxf
76:  raja                /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/raja-2022.03.0-6lmk4olb4ikhrg52wenkruy3o7oaeh4a
77:  scr                 /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/scr-3.0.1-byaglsu6i6bbenctnbibty42hv2jux7s
78:  slate               /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/slate-2022.07.00-je6innhafk7it6nh6pb472c6q4zc5jwx
79:  slepc               /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/slepc-3.18.1-yo2g4k4gimlkivptfwyz7zxc6qafrn2t
80:  stc                 /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/stc-0.9.0-66ur7lde4sehbiuhq725h4njmh67yn6t
81:  strumpack           /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/strumpack-7.0.1-6b43dyoqnfa5yge4u2ljmckfs4wjjgwa
82:  sundials            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/sundials-6.4.1-t2k7smta36vv4scpfvr72qvky37kzbvo
83:  superlu-dist        /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/superlu-dist-8.1.1-ul3qouwm24cvprbxaaevg7zrhyng55dv
84:  swig                /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/swig-4.0.2-fortran-wgukl4d4bbrvnln2dko27vmsbzm4vdoz
85:  sz                  /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/sz-2.1.12.2-6inw3xqodwku35vffczal7x7e32g6vzv
86:  tasmanian           /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/tasmanian-7.9-xehgodjpanihpukedfppvijv4kviffhl
87:  tau                 /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/tau-2.32-oi5yvfxkdx46hdjcwiwsatfnwapp2qga
88:  trilinos            /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/trilinos-13.4.0-7ig32xrxhx2wjyhga77bh4h3yraxgfwr
89:  turbine             /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/turbine-1.3.0-ttxgmsxu5juonlagdgr74ugifohitu65
90:  umap                /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/umap-2.1.0-kglnikj3dpcmeuwex3twovw7msjgkngb
91:  umpire              /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/umpire-2022.03.1-2aagqdhp5wysbf5wzanwjdpnf7mh7za4
92:  upcxx               /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/upcxx-2022.9.0-gaktmfdbhnugnhpwsrrnq3amjtlfffeg
93:  vtk-m               /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/vtk-m-1.9.0-mievxnqsq2ok6ysvl5lfrhraedcwvtfm
94:  wannier90           /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/wannier90-3.1.0-osqph5gscpas7ofgu5uedhlzacebeb5n
95:  warpx               /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/warpx-22.10-2uknrbmbuohzvolulhiqidwyc5unekkn
96:  yaksa               /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/yaksa-0.2-vpraougvigjq2c2wncmc7ebfgbwqon2d
97:  zfp                 /spack/opt/spack/linux-ubuntu20.04-aarch64/gcc-11.1.0/zfp-0.5.5-r4wxkyawwtixm3hpwh2pel5o2ihwzkip
```

GPU runtimes for aarch64

- CUDA 11.7.1
- NVHPC 22.9

Languages

- Julia
- Python

AI packages for NVIDIA GPU

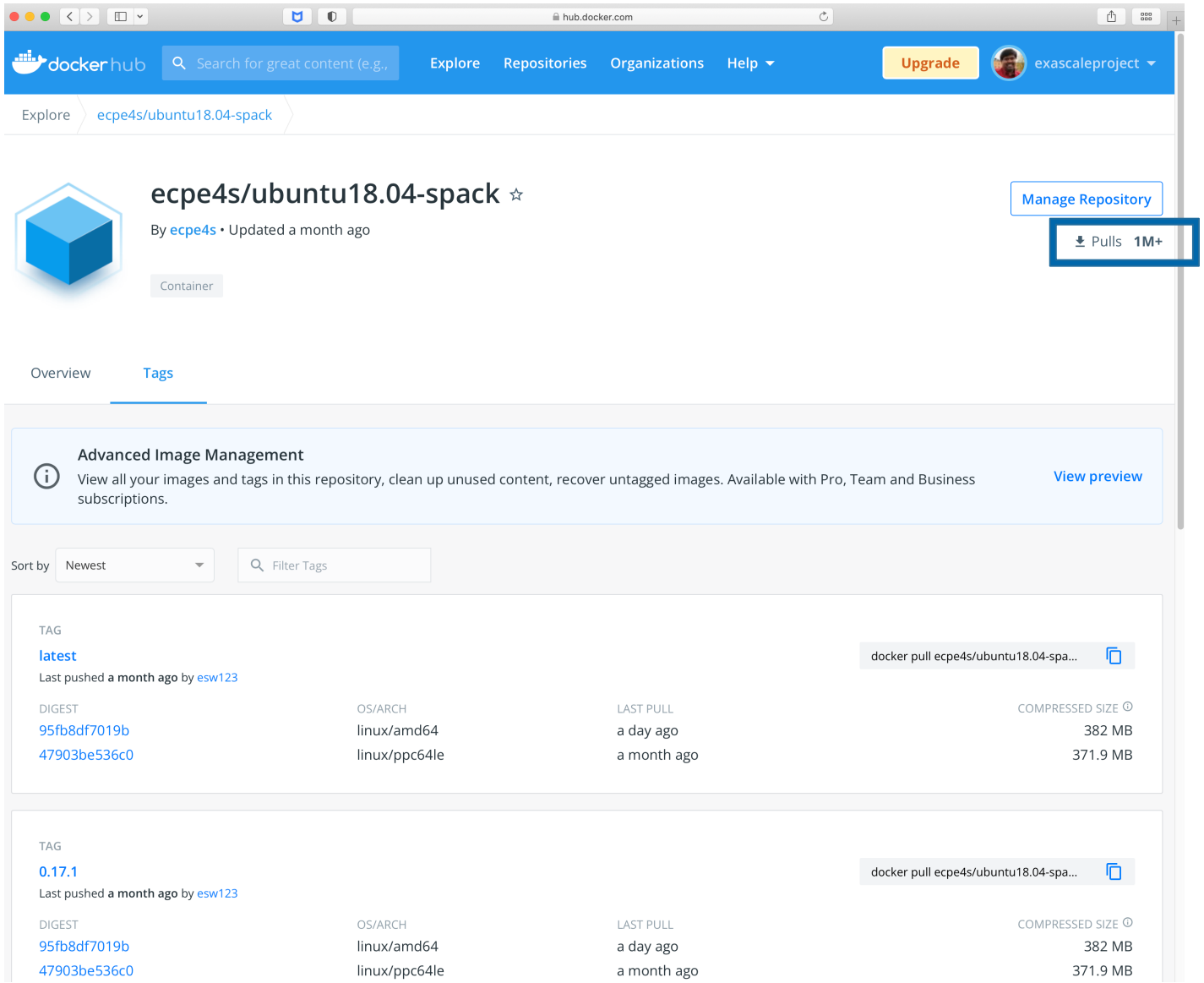
- TensorFlow
- PyTorch

E4S Support for CUDA variants on aarch64

```
Singularity> spack find +cuda  cuda_arch=80
-- linux-ubuntu20.04-aarch64 / gcc@11.1.0 ------------------------
adios2@2.8.3        camp@2022.03.2  ginkgo@1.4.0    kokkos-kernels@3.7.00  petsc@3.18.1       sundials@6.4.1      vtk-m@1.9.0
amrex@22.11         camp@2022.03.2  heffte@2.3.0    lapackpp@2022.07.00    raja@2022.03.0     superlu-dist@8.1.1  zfp@0.5.5
arborx@1.3          chai@2022.03.0  hypre@2.26.0    magma@2.6.2            slate@2022.07.00   tasmanian@7.9
blaspp@2022.07.00   dealii@9.4.0    kokkos@3.7.00   mfem@4.5.0             slepc@3.18.1       trilinos@13.4.0
caliper@2.8.0       flecsi@2.1.0    kokkos@3.7.00   omega-h@9.34.13        strumpack@7.0.1    umpire@2022.03.1
==> 32 installed packages
Singularity>
```

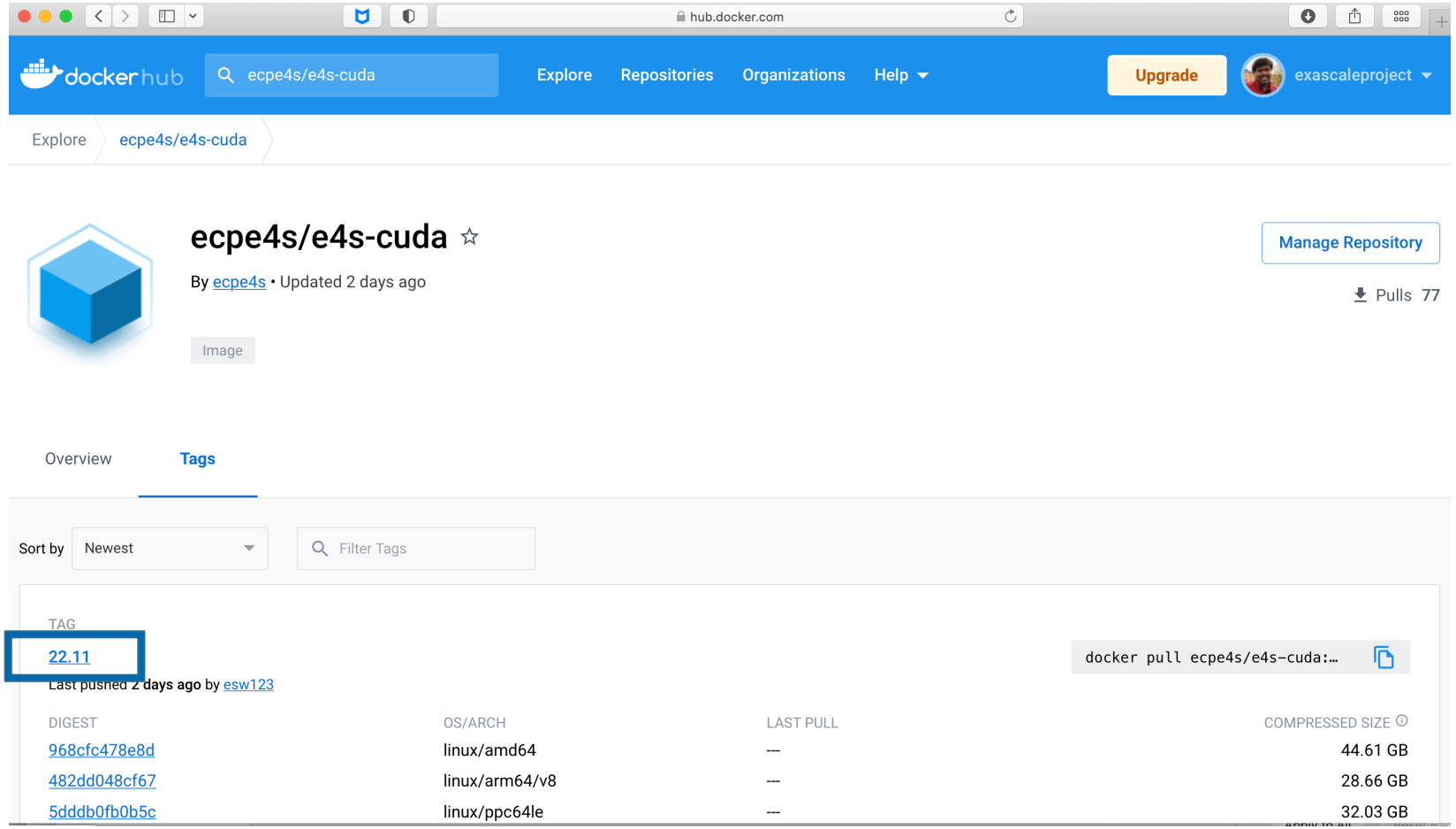
Support for A100 and T4 GPUs under aarch64

Minimal Spack base image on Dockerhub



- Create custom container images
- 1M+ downloads!

E4S 22.11 Release: GPU support for Docker Containers



- 100+ E4S Products
- Support for GPUs
  - x86_64
  - ppc64le
  - aarch64

% docker pull ecpe4s/e4s-cuda

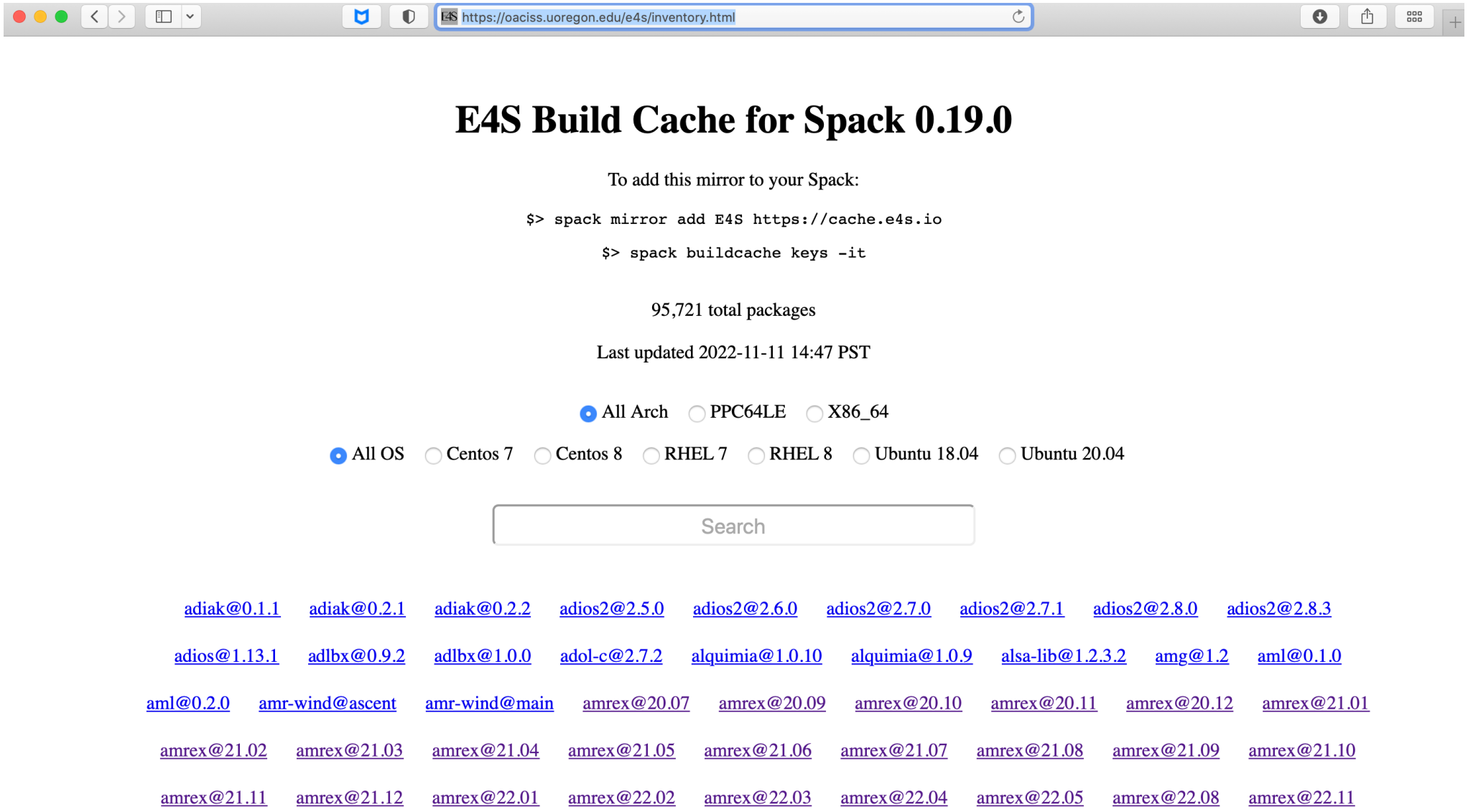
E4S bare-metal installation spack.yaml recipe

https://github.com/E4S-Project/e4s/blob/master/environments/21.11/spack-x86_64.yaml

```
30      elfutils:
31        variants: +bzip2 ~nls +xz
32      fftw:
33        variants: +openmp
34      hdf5:
35        variants: +fortran +hl +shared api=v18
36        version:
37        - 1.12.1
38      libfabric:
39        variants: fabrics=sockets,tcp,udp,rxm
40      libunwind:
41        variants: +pic +xz
42      mesa:
43        variants: ~llvm
44      mesa18:
45        variants: ~llvm
46      mpich:
47        variants: ~wrapperrpath
48      ncurses:
49        variants: +termlib
50      openblas:

52      trilinos:
53        variants: +amesos +amesos2 +anasazi +aztec +belos +boost +epetra +epetraext
54          +ifpack +ifpack2 +intrepid +intrepid2 +isorropia +kokkos +ml +minitensor +muelu
55          +nox +piro +phalanx +rol +rythmos +sacado +stk +shards +shylu +stokhos +stratimikos
56          +teko +tempus +tpetra +trilinoscouplings +zoltan +zoltan2 +superlu-dist gotype=long_long

58        variants: +pic
59
60    definitions:
61    - cuda_specs:
62      - amrex@21.11 +cuda cuda_arch=80
63      - caliper@2.7.0 +cuda cuda_arch=80
64      - chai@2.4.0 ~benchmarks ~tests +cuda cuda_arch=80 ^umpire ~shared
65      - flecsi@2.1.0 +cuda cuda_arch=80
66      - ginkgo@1.4.0 +cuda cuda_arch=80
67      - heffte@2.2.0 +cuda cuda_arch=80
68      - hpx@1.7.1 +cuda cuda_arch=80
69      - hypre@2.23.0 +cuda cuda_arch=80
70      - kokkos@3.4.01 +wrapper +cuda cuda_arch=80
71      - kokkos-kernels@3.4.01 +cuda cuda_arch=80 ^kokkos +wrapper +cuda cuda_arch=80
72      - magma@2.6.1 +cuda cuda_arch=80
73      - mfem@4.3.0 +cuda cuda_arch=80
74      - parsec@3.0.2012 +cuda cuda_arch=80
75      - petsc@3.16.1 +cuda cuda_arch=80
76      - raja@0.14.0 +cuda cuda_arch=80
77      - slate@2021.05.02 +cuda cuda_arch=80
78      - slepc@3.16.0 +cuda cuda_arch=80
79      - strumpack@6.1.0 ~slate +cuda cuda_arch=80
80      - sundials@5.8.0 +cuda cuda_arch=80
81      - superlu-dist@7.1.1 +cuda cuda_arch=80
82      - tasmanian@7.7 +cuda cuda_arch=80
83      - trilinos@13.2.0 +cuda cuda_arch=80
84      - umpire@6.0.0 ~shared +cuda cuda_arch=80
85      - upcxx@2021.9.0 +cuda
86      - vtk-m@1.6.0 +cuda cuda_arch=80
87      - zfp@0.5.5 +cuda cuda_arch=80
```

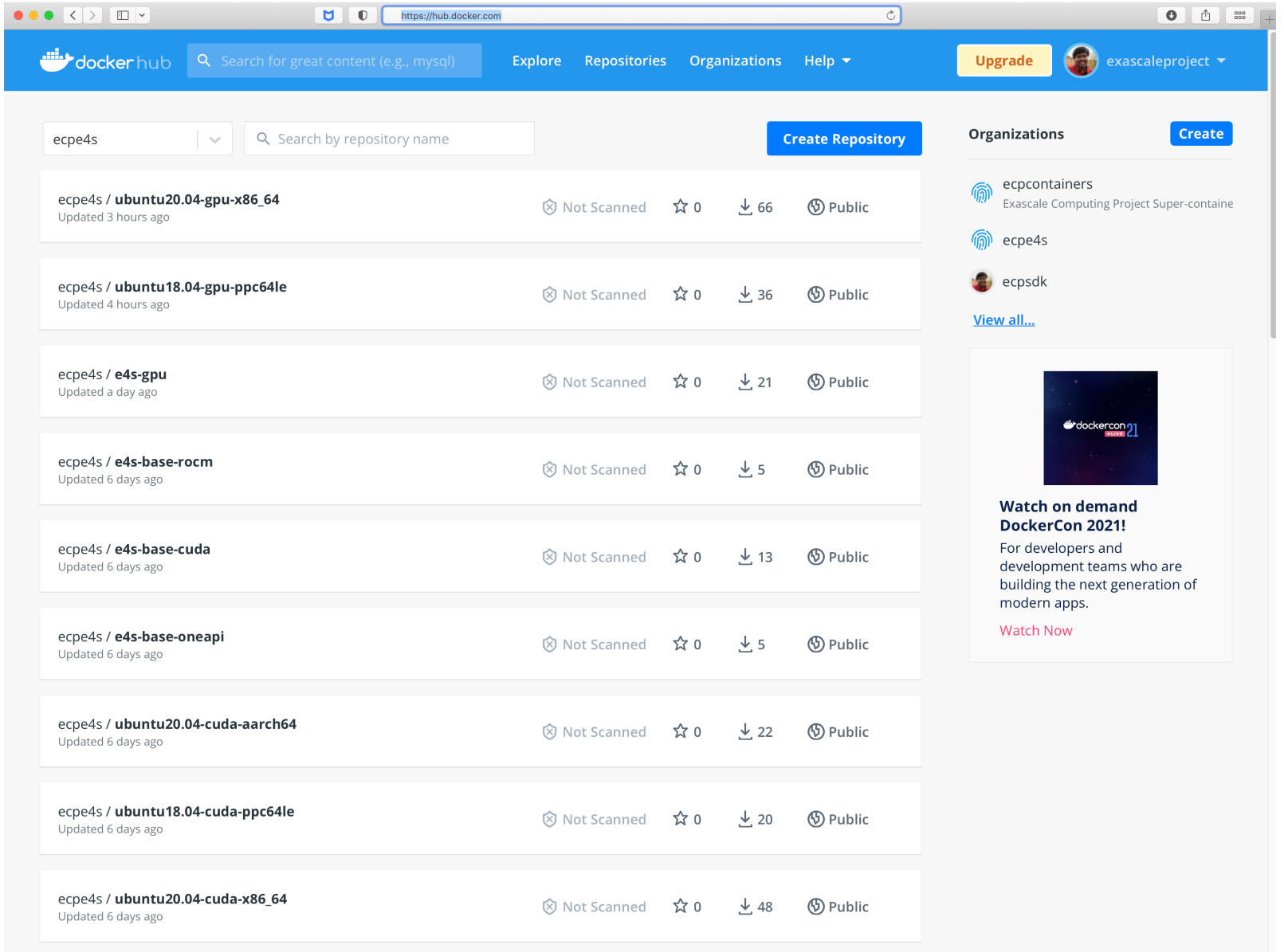
- Trilinos variants
- Built with CUDA

E4S Build Cache for Spack 0.19.0



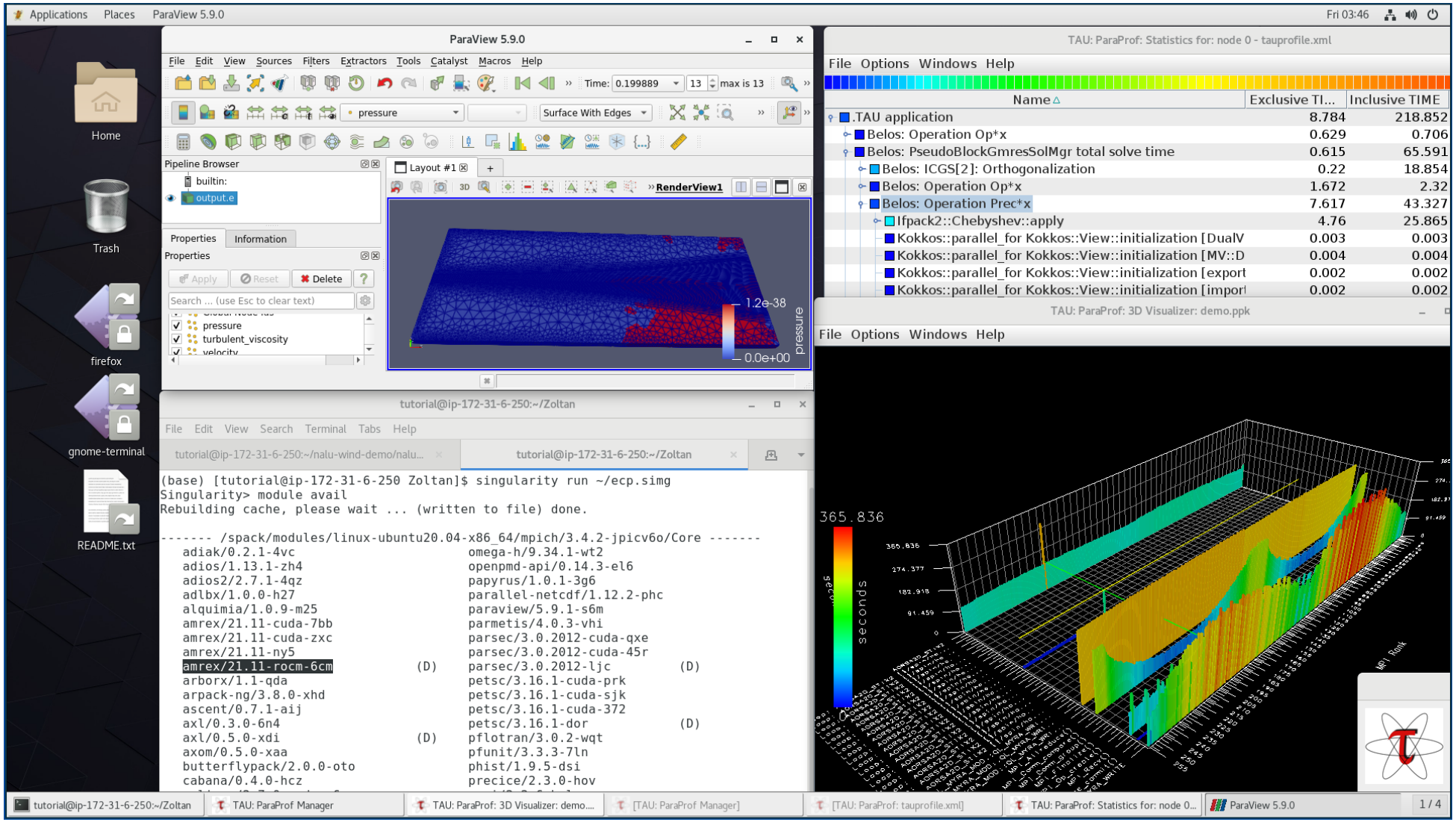
- Over 95,000 binaries!
- No need to recompile from source code.

E4S Base Container Images for x86_64, ppc64le, and aarch64



- Hub.docker.com
- ecpe4s
- Platforms:
  - x86_64
  - Ppc64le
  - aarch64
- GPU runtimes:
  - CUDA
  - ROCm
  - oneAPI

E4S 22.11 AWS image: US-West2 (OR)



E4S 22.11 AWS

- Intel oneAPI
- CUDA
- NVHPC
- ROCm
- AWS DCV
- Spack Build Cache
- ECP: Nalu-Wind
- Trilinos
- OpenFOAM
- ParaView
- TAU
- Docker
- Shifter
- Charliecloud
- E4S Singularity…

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 and Wi4MPI [CEA] for OpenMPI replacement.
- 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.
  - e4s-cl init --backend [singularity|shifter|docker] --image <file> --source <startup_cmds.sh>
  - e4s-cl mpirun -np <N> <command>
- Usage:

  . /opt/intel/oneapi/setvars.sh

  e4s-cl init --backend singularity --image ~/images/e4s-gpu-x86.sif --source ~/source.sh

  cat ~/source.sh

```
. /spack/share/spack/setup-env.sh
spack load trilinos+cuda cuda_arch=80
```

  e4s-cl mpirun -np 4 ./a.out

https://github.com/E4S-Project/e4s-cl

Spack Package Manager
https://spack.io

Slide credit: Todd Gamblin, LLNL

Spack enables Software distribution for HPC

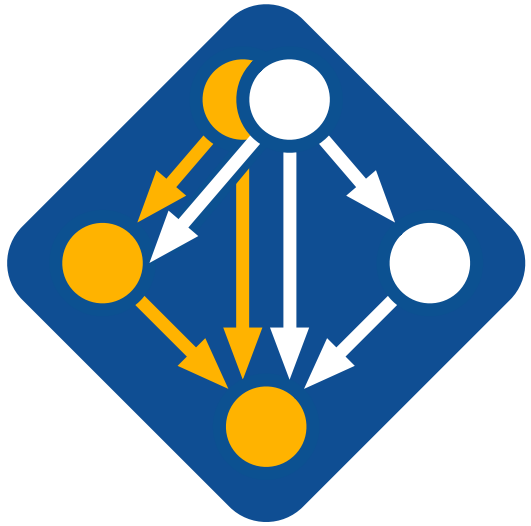
- Spack automates the build and installation of scientific software
- Packages are *parameterized,* so that users can easily tweak and tune configuration

No installation required: clone and go

```
$ git clone https://github.com/spack/spack
$ spack install hdf5
```

Simple syntax enables complex installs

```
$ spack install hdf5@1.10.5                  $ spack install hdf5@1.10.5 cppflags="-O3 -g3"
$ spack install hdf5@1.10.5 %clang@6.0       $ spack install hdf5@1.10.5 target=haswell
$ spack install hdf5@1.10.5 +threadssafe     $ spack install hdf5@1.10.5 +mpi ^mpich@3.2
```

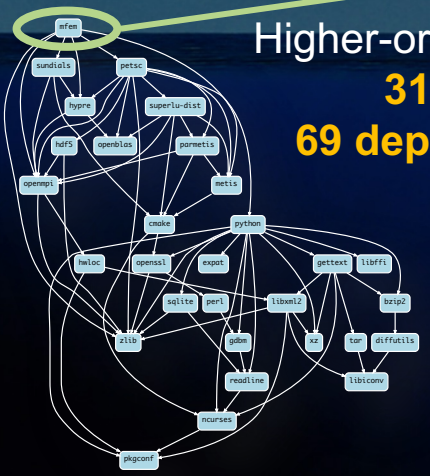


github.com/spack/spack

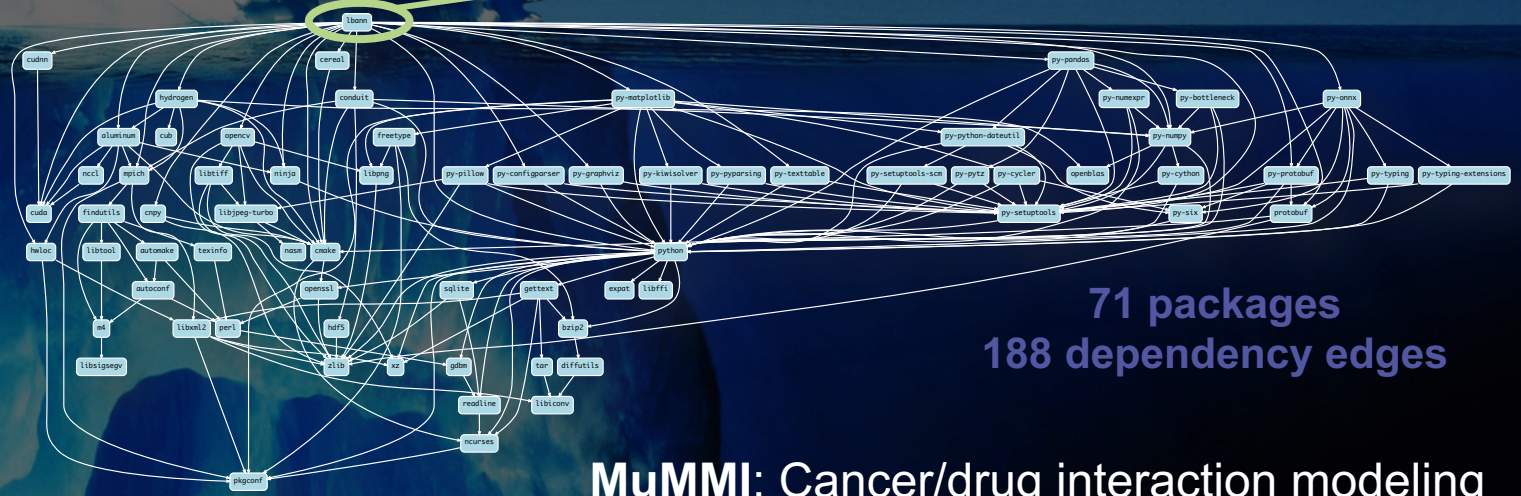
- Ease of use of mainstream tools, with flexibility needed for HPC
- In addition to CLI, Spack also:
  - Generates (but does **not** require) *modules*
  - Allows conda/virtualenv-like *environments*
  - Provides many devops features (CI, container generation, more)

HPC simulations rely on icebergs of dependency libraries

MFEM:
Higher-order finite elements
31 packages,
69 dependency edges

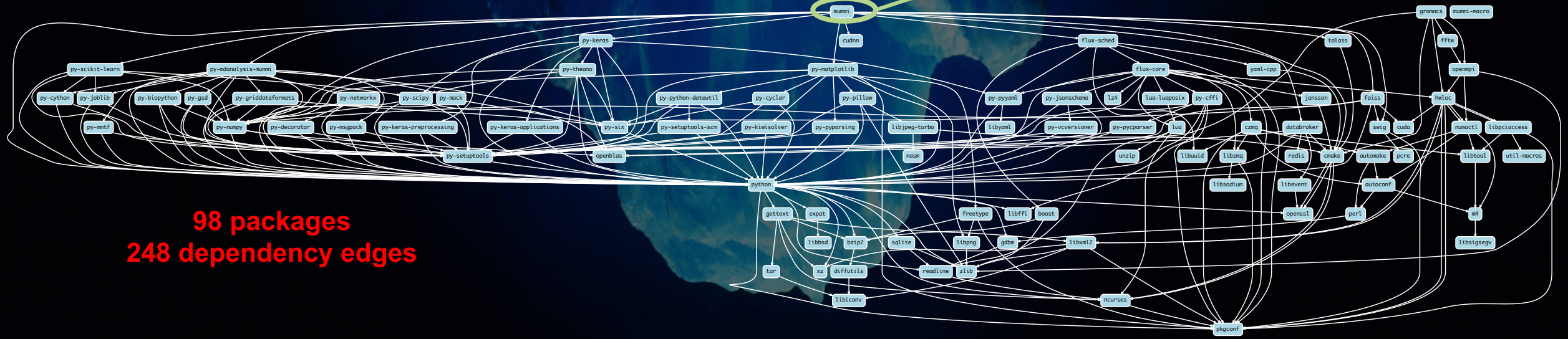


LBANN: Neural Nets for HPC



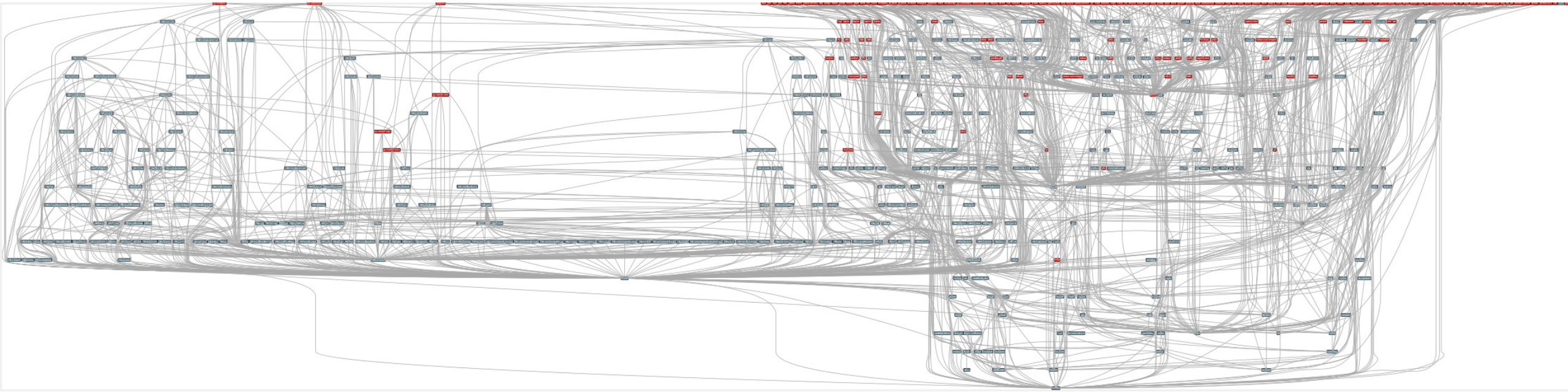
71 packages
188 dependency edges

MuMMI: Cancer/drug interaction modeling
Integrates MD , HPC scheduling, ML



98 packages
248 dependency edges

ECP's E4S stack is even larger than these codes



- Red boxes are the packages in it (about 100)
- Blue boxes are what *else* you need to build it (about 600)
- It's infeasible to build and integrate all of this manually

Some fairly common (but questionable) assumptions made by package managers (conda, pip, apt, etc.)

- **1:1 relationship between source code and binary (per platform)**
  - Good for reproducibility (e.g., Debian)
  - Bad for performance optimization
- **Binaries should be as portable as possible**
  - What most distributions do
  - Again, bad for performance
- **Toolchain is the same across the ecosystem**
  - One compiler, one set of runtime libraries
  - Or, no compiler (for interpreted languages)

Outside these boundaries, users are typically on their own

High Performance Computing (HPC) violates many of these assumptions

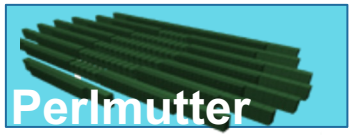
- **Code is typically distributed as source**
  - With exception of vendor libraries, compilers
- **Often build many variants of the same package**
  - Developers' builds may be very different
  - Many first-time builds when machines are new
- **Code is optimized for the processor and GPU**
  - Must make effective use of the hardware
  - Can make 10-100x perf difference
- **Rely heavily on system packages**
  - Need to use optimized libraries that come with machines
  - Need to use host GPU libraries and network
- **Multi-language**
  - C, C++, Fortran, Python, others all in the same ecosystem

Some Supercomputers

Current

Oak Ridge National Lab
Power9 / NVIDIA

RIKEN
Fujitsu/ARM a64fx



Lawrence Berkeley National Lab
AMD Zen / NVIDIA

Oak Ridge National Lab
AMD Zen / Radeon

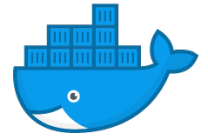
Upcoming

Argonne National Lab
Intel Xeon / Xe

Lawrence Livermore National Lab
AMD Zen / Radeon

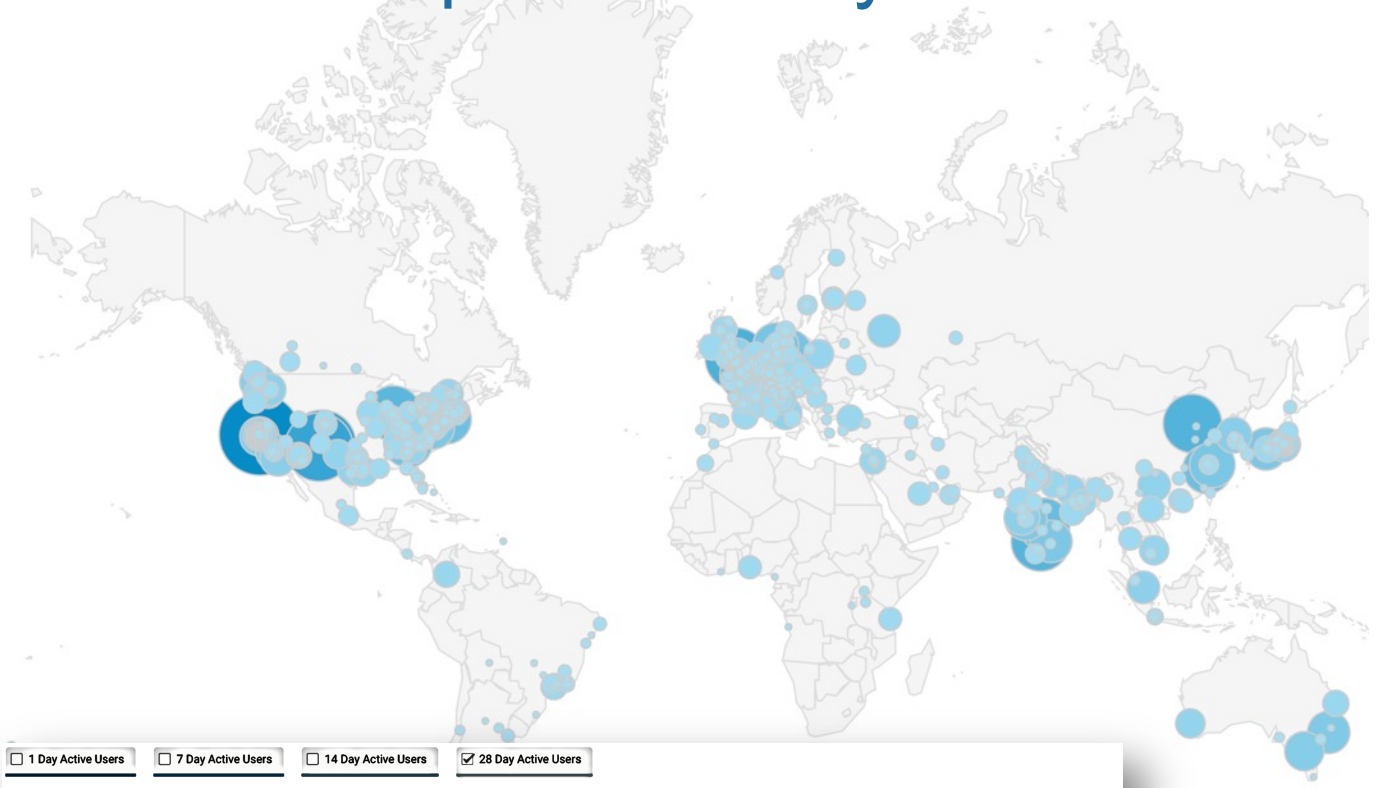
What about containers?

- **Containers provide a great way to reproduce and distribute an already-built software stack**
- **Someone needs to build the container!**
  - This isn't trivial
  - Containerized applications still have hundreds of dependencies
- **Using the OS package manager inside a container is insufficient**
  - Most binaries are built unoptimized
  - Generic binaries, not optimized for specific architectures
- **HPC containers may need to be *rebuilt* to support many different hosts, anyway.**
  - Not clear that we can ever build one container for all facilities
  - Containers likely won't solve the N-platforms problem in HPC

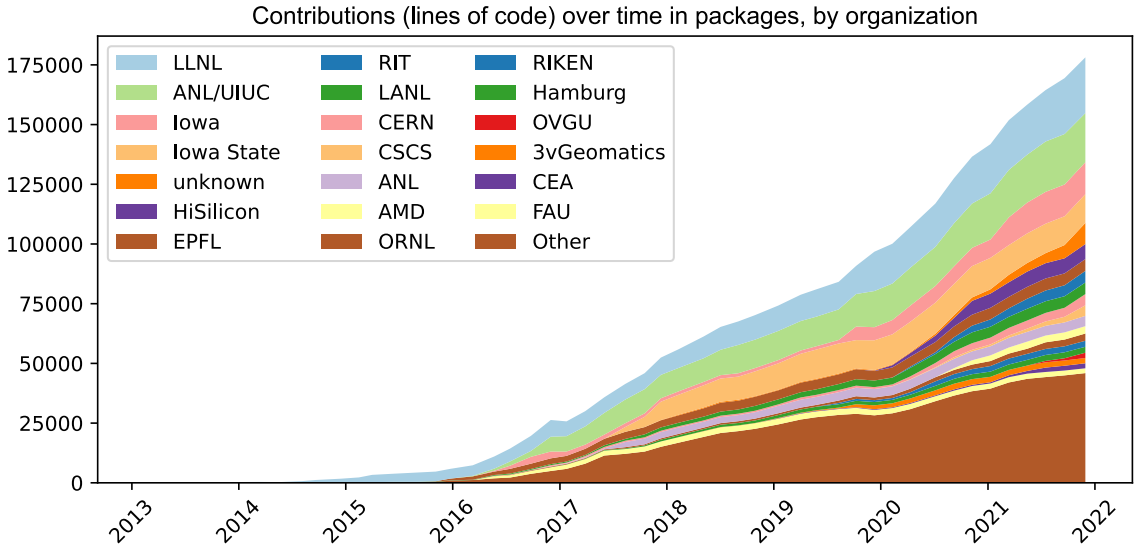


We need something more flexible to **build** the containers

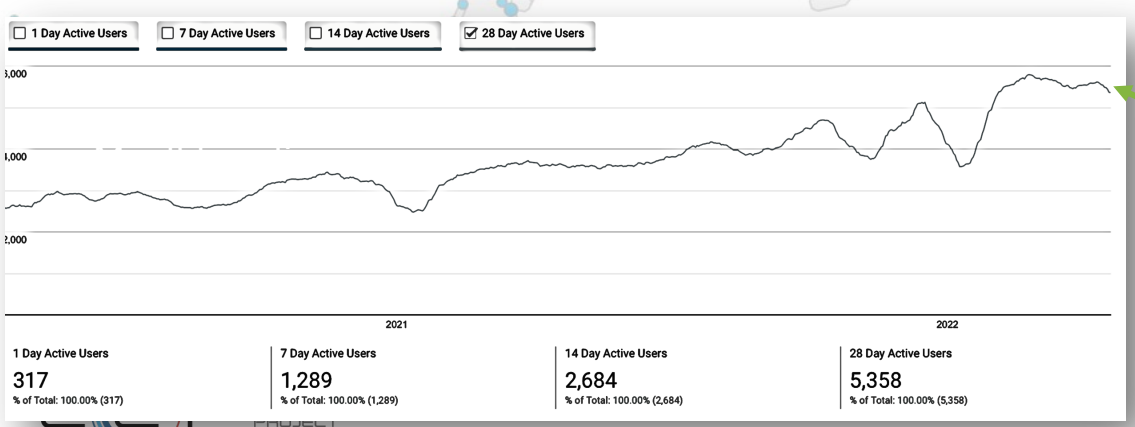
Spack sustains the HPC software ecosystem with the help of its many contributors



6,400+ software packages
Over 1,000 contributors



Most package contributions are ***not*** from DOE!



Nearly 6,000 monthly active users
(per documentation site)

Spack provides a *spec* syntax to describe customized installations

```
$ spack install mpileaks                      unconstrained
$ spack install mpileaks@3.3                  @ custom version
$ spack install mpileaks@3.3 %gcc@4.7.3       % custom compiler
$ spack install mpileaks@3.3 %gcc@4.7.3 +threads   +/- build option
$ spack install mpileaks@3.3 cppflags="-O3 -g3"    set compiler flags
$ spack install mpileaks@3.3 target=zen2      set target microarchitecture
$ spack install mpileaks@3.3 ^mpich@3.2 %gcc@4.9.3   ^ 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

Spack packages are *templates*
They use a simple Python DSL to define how to build

Not shown: patches, **resources**, **conflicts**, other directives.

```
from spack import *

class Kripke(CMakePackage):
    """Kripke is a simple, scalable, 3D Sn deterministic particle
       transport proxy/mini app.
    """

    homepage = "https://computation.llnl.gov/projects/co-design/kripke"
    url      = "https://computation.llnl.gov/projects/co-design/download/kripke-openmp-1.1.tar.gz"

    version('1.2.3', sha256='3f7f2eef0d1ba5825780d626741eb0b3f026a096048d7ec4794d2a7dfbe2b8a6')
    version('1.2.2', sha256='eaf9ddf562416974157b34d00c3a1c880fc5296fce2aa2efa039a86e0976f3a3')
    version('1.1', sha256='232d74072fc7b848fa2adc8a1bc839ae8fb5f96d50224186601f55554a25f64a')

    variant('mpi',    default=True, description='Build with MPI.')
    variant('openmp', default=True, description='Build with OpenMP enabled.')

    depends_on('mpi', when='+mpi')
    depends_on('cmake@3.0:', type='build')

    def cmake_args(self):
        return [
            '-DENABLE_OPENMP=%s' % ('+openmp' in self.spec),
            '-DENABLE_MPI=%s' % ('+mpi' in self.spec),
        ]

    def install(self, spec, prefix):
        # Kripke does not provide install target, so we have to copy
        # things into place.
        mkdirp(prefix.bin)
        install('../spack-build/kripke', prefix.bin)
```

Base package
(CMake support)

Metadata at the class level

Versions

Variants (build options)

Dependencies
(same spec syntax)

Install logic
in instance methods

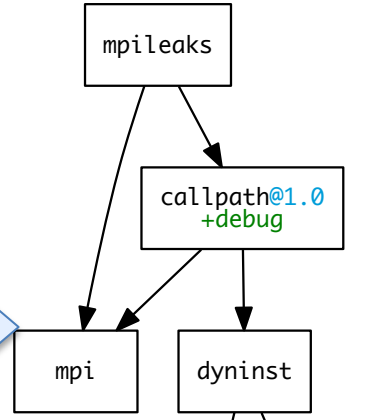
Don't typically need `install()` for `CMakePackage`, but we can work around codes that don't have it.

Concretization fills in missing configuration details when the user is not explicit.

```
mpileaks ^callpath@1.0+debug ^libelf@0.8.11
```

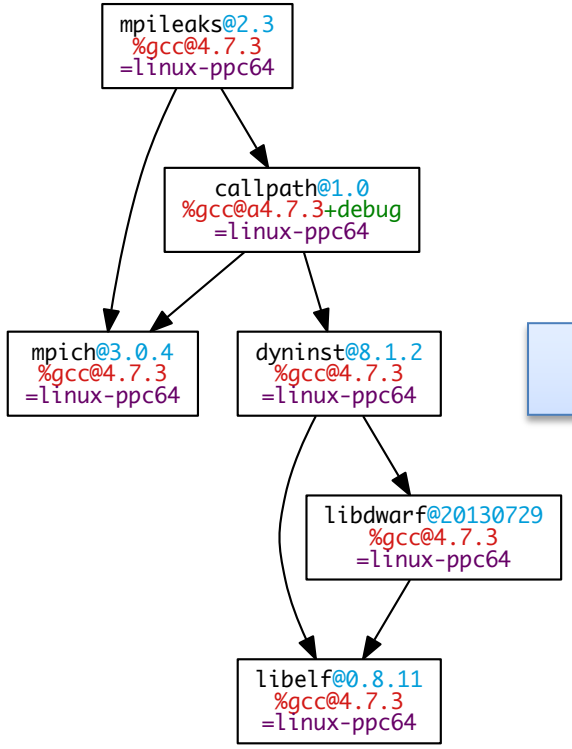
User input: *abstract* spec with some constraints

Normalize



Abstract, normalized spec with some dependencies

Concretize



Concrete spec is fully constrained and can be passed to install

Store

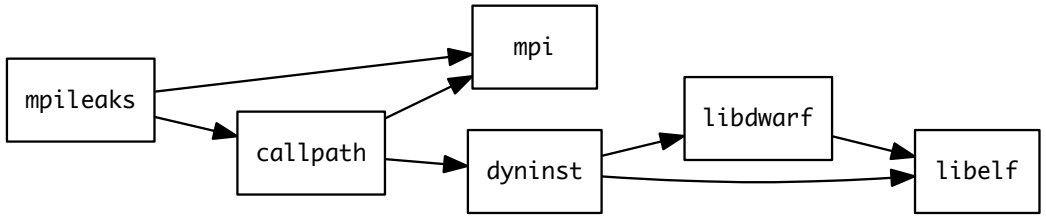
spec.yaml

```
spec:
- mpileaks:
    arch: linux-x86_64
    compiler:
      name: gcc
      version: 4.9.2
    dependencies:
      adept-utils: kszrtkpbzac3ss2ixcjkcorlaybnptp4
      callpath: bah5f4h4d2n47mgycej2mtrnrivvxy77
      mpich: aa4ar6ifj23yijqmdabeakpejcli72t3
    hash: 33hjjhxi7p6gyzn5ptgyes7sghyprujh
    variants: {}
    version: '1.0'
- adept-utils:
    arch: linux-x86_64
    compiler:
      name: gcc
      version: 4.9.2
    dependencies:
      boost: teesjv7ehpe5ksspjim5dk43a7qnowlq
      mpich: aa4ar6ifj23yijqmdabeakpejcli72t3
    hash: kszrtkpbzac3ss2ixcjkcorlaybnptp4
    variants: {}
    version: 1.0.1
- boost:
    arch: linux-x86_64
    compiler:
      name: gcc
      version: 4.9.2
    dependencies: {}
    hash: teesjv7ehpe5ksspjim5dk43a7qnowlq
    variants: {}
    version: 1.59.0
...
```

Detailed provenance stored with installed package

Spack handles combinatorial software complexity

Dependency DAG



Hash

Installation Layout

```
opt
└── spack
    ├── linux-rhel7-skylake
    |   └── gcc-8.3.0
    |       ├── mpileaks-1.0-hc4sm4vuzpm4znmvrfzri4ow2mkphe2e
    |       ├── callpath-1.0.4-daqqpssxb6qbfrztsezkmhus3xoflbsy
    |       ├── openmpi-4.1.4-u64v26igxvxyn23hysmklfums6tgjv5r
    |       ├── dyninst-12.1.0-u64v26igxvxyn23hysmklfums6tgjv5r
    |       ├── libdwarf-20180129-u5eawkvaoc7vonabe6nndkcfwuv233cj
    |       └── libelf-0.8.13-x46q4wm46ay4pltriijbgizxjrhbaka6
```

- Each unique dependency graph is a unique ***configuration***.
- Each configuration in a unique directory.
  - Multiple configurations of the same package can coexist.
- **Hash** of entire directed acyclic graph (DAG) is appended to each prefix.
- Installed packages automatically find dependencies
  - Spack embeds RPATHs in binaries.
  - No need to use modules or set LD_LIBRARY_PATH
  - Things work *the way you built them*

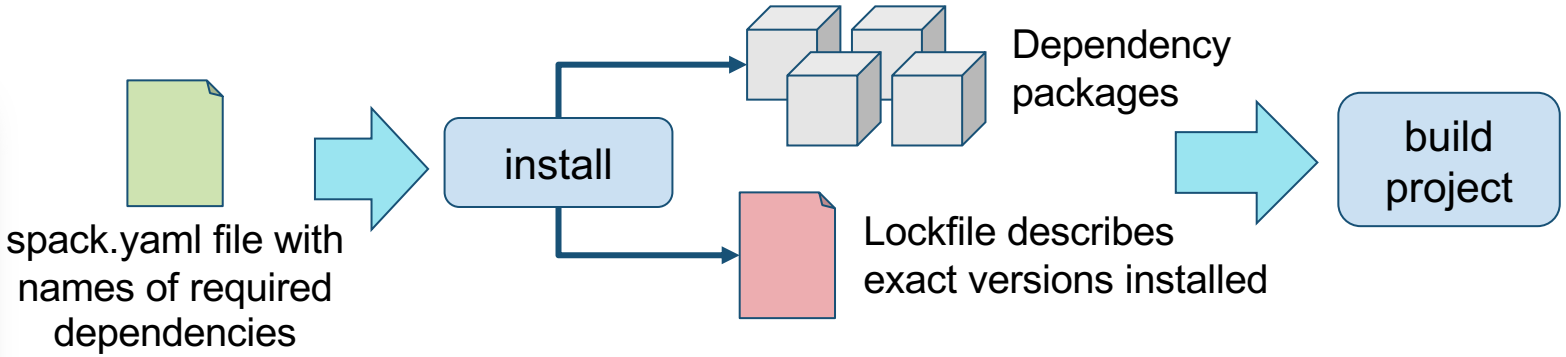
Spack environments enable users to build customized stacks from an abstract description

Simple spack.yaml file

```yaml
spack:
  # include external configuration
  include:
  - ../special-config-directory/
  - ./config-file.yaml

  # add package specs to the `specs` list
  specs:
  - hdf5
  - libelf
  - openmpi
```

Concrete spack.lock file (generated)

```
{
 "concrete_specs": {
   "6s63so2kstp3zyvjezglndmavy6l3nul": {
     "hdf5": {
         "version": "1.10.5",
         "arch": {
             "platform": "darwin",
             "platform_os": "mojave",
             "target": "x86_64"
         },
         "compiler": {
             "name": "clang",
             "version": "10.0.0-apple"
         },
         "namespace": "builtin",
         "parameters": {
             "cxx": false,
             "debug": false,
             "fortran": false,
             "hl": false,
             "mpi": true,
```

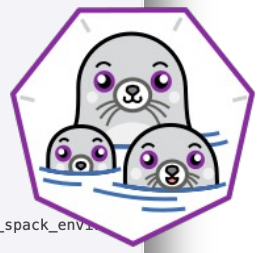


- spack.yaml describes project requirements
- spack.lock describes exactly what versions/configurations were installed, allows them to be reproduced.
- Can also be used to maintain configuration together with Spack packages.
  - E.g., versioning your own local software stack with consistent compilers/MPI implementations
  - Allows developers and site support engineers to easily version Spack configurations in a repository

Spack can generate multi-stage container build recipes

```
spack:
  specs:
  - gromacs+mpi
  - mpich

  container:
    # Select the format of the rec
    # singularity or anything else
    format: docker

    # Select from a valid list of
    base:
      image: "centos:7"
      spack: develop

    # Whether or not to strip bina
    strip: true

    # Additional system packages t
    os_packages:
    - libgomp

    # Extra instructions
    extra_instructions:
      final: |
RUN echo 'export PS1="\[$(tput bol

    # Labels for the image
    labels:
      app: "gromacs"
      mpi: "mpich"
```

```
# Build stage with Spack pre-installed and ready to be used
FROM spack/centos7:latest as builder

# What we want to install and how we want to install it
# is specified in a manifest file (spack.yaml)
RUN mkdir /opt/spack-environment \
&&  (echo "spack:" \
&&   echo "  specs:" \
&&   echo "  - gromacs+mpi" \
&&   echo "  - mpich" \
&&   echo "  concretization: together" \
&&   echo "  config:" \
&&   echo "    install_tree: /opt/software" \
&&   echo "  view: /opt/view") > /opt/spack-environment/spack.yaml

# Install the software, remove unecessary deps
RUN cd /opt/spack-environment && spack install && spack gc -y

# Strip all the binaries
RUN find -L /opt/view/* -type f -exec readlink -f '{}' \; | \
    xargs file -i | \
    grep 'charset=binary' | \
    grep 'x-executable\|x-archive\|x-sharedlib' | \
    awk -F: '{print $1}' | xargs strip -s

# Modifications to the environment that are necessary to run
RUN cd /opt/spack-environment && \
    spack env activate --sh -d . >> /etc/profile.d/z10_spack_environment.sh


# Bare OS image to run the installed executables
FROM centos:7

COPY --from=builder /opt/spack-environment /opt/spack-environment
COPY --from=builder /opt/software /opt/software
COPY --from=builder /opt/view /opt/view
COPY --from=builder /etc/profile.d/z10_spack_environment.sh /etc/profile.d/z10_spack_envi

e -y && yum install -y epel-release && yum update -y
l -y libgomp \
/cache/yum  && yum clean all

RUN echo 'export PS1="\[$(tput bold)\]\[$(tput setaf 1)\][gromacs]\[$(tput setaf 2)\]\u\[$(tput
```

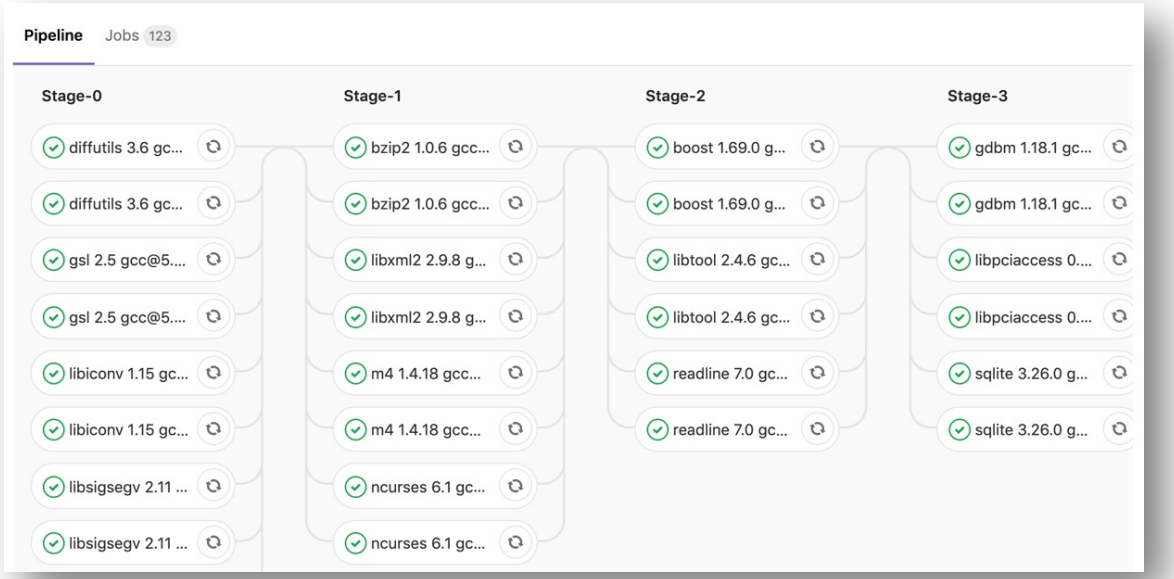


- Any Spack environment can be bundled into a container image
  - Optional container section allows finer-grained customization
- Generated Dockerfile uses multi-stage builds to minimize size of final image
  - Strips binaries
  - Removes unneeded build deps with `spack gc`
- Can also generate Singularity recipes

`spack containerize`

Spack has GitLab CI integration to automate package build pipelines

- Builds on Spack environments
  - Support auto-generating GitLab CI jobs
  - Can run in a Kube cluster or on bare metal runners at an HPC site
  - Sends progress to CDash




```yaml
spack:
  definitions:
  - pkgs:
    - readline@7.0
  - compilers:
    - '%gcc@5.5.0'
  - oses:
    - os=ubuntu18.04
    - os=centos7
  specs:
  - matrix:
    - [$pkgs]
    - [$compilers]
    - [$oses]
  mirrors:
    cloud_gitlab: https://mirror.spack.io
  gitlab-ci:
    mappings:
      - spack-cloud-ubuntu:
        match:
          - os=ubuntu18.04
        runner-attributes:
          tags:
            - spack-k8s
          image: spack/spack_builder_ubuntu_18.04
      - spack-cloud-centos:
        match:
          - os=centos7
        runner-attributes:
          tags:
            - spack-k8s
          image: spack/spack_builder_centos_7
  cdash:
    build-group: Release Testing
    url: https://cdash.spack.io
    project: Spack
    site: Spack AWS Gitlab Instance
```

spack test: write tests directly in Spack packages, so that they can evolve with the software

```
class Libsigsegv(AutotoolsPackage, GNUMirrorPackage):
    """GNU libsigsegv is a library for handling page faults in user mode."""

    # ... spack package contents ...

    extra_install_tests = ‘tests/.libs’

    def test(self):
        data_dir = self.test_suite.current_test_data_dir
        smoke_test_c = data_dir.join(‘smoke_test.c’)

        self.run_test(
            'cc’, [
                '-I%s' % self.prefix.include,
                '-L%s' % self.prefix.lib, '-lsigsegv’,
                smoke_test_c,
                '-o', 'smoke_test'
            ]
            purpose='check linking’)

        self.run_test(
            ‘smoke_test’, [], data_dir.join('smoke_test.out’),
            purpose=‘run built smoke test’)

        self.run_test('sigsegv1': ['Test passed’], purpose='check sigsegv1 output’)
        self.run_test('sigsegv2': ['Test passed’], purpose='check sigsegv2 output’)
```

Tests are part of a regular Spack recipe class

Easily save source code from the package

User just defines a `test()` method

Retrieve saved source.
Link a simple executable.

Spack ensures that `cc` is a compatible compiler

Run the built smoke test and verify output

Run programs installed with package

`spack external find` (new in v0.15, updated for 0.16)

```python
class Cmake(Package):
    executables = ['cmake']

    @classmethod
    def determine_spec_details(cls, prefix, exes_in_prefix):
        exe_to_path = dict(
            (os.path.basename(p), p) for p in exes_in_prefix
        )
        if 'cmake' not in exe_to_path:
            return None

        cmake = spack.util.executable.Executable(exe_to_path['cmake'])
        output = cmake('--version', output=str)
        if output:
            match = re.search(r'cmake.*version\s+(\S+)', output)
            if match:
                version_str = match.group(1)
                return Spec('cmake@{0}'.format(version_str))
```

Logic for finding external installations in `package.py`

```yaml
packages:
  cmake:
    externals:
      - spec: cmake@3.15.1
        prefix: /usr/local
```

`packages.yaml` configuration

- Spack has has had compiler detection for a while
  - Finds compilers in your PATH
  - Registers them for use
- We can find any package now
  - Package defines:
    - possible command names
    - how to query the command
  - Spack searches for known commands and adds them to configuration
- Easily enable rapid setup of tools in an environment

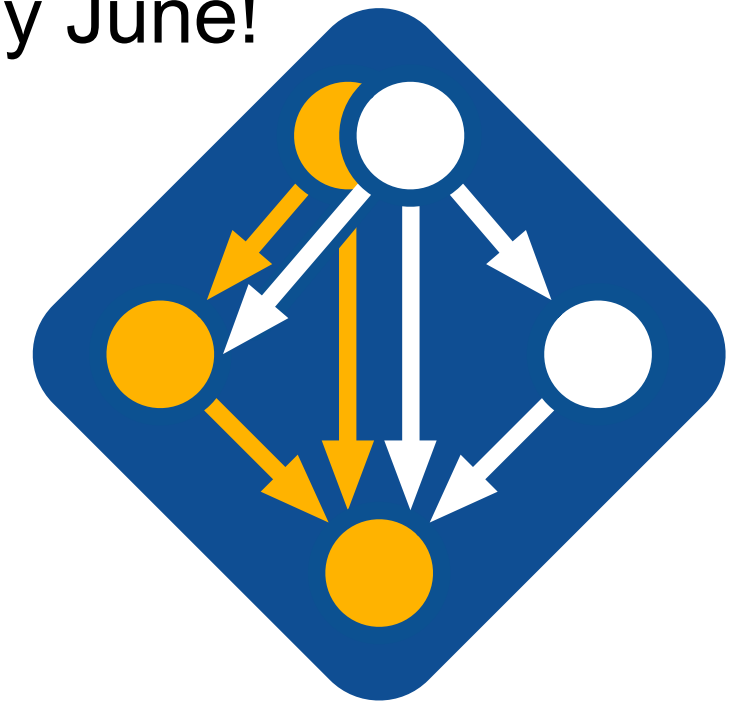
spack develop lets developers work on many packages at once

- Developer features so far have focused on single packages (`spack dev-build`, etc.)
- New spack develop feature enables development environments
  - Work on a code
  - Develop multiple packages from its dependencies
  - Easily rebuild with changes
- Builds on spack environments
  - Required changes to the installation model for dev packages
  - dev packages don't change paths with configuration changes
  - Allows devs to iterate on builds quickly

```
$ spack env activate .
$ spack add myapplication
$ spack develop axom@0.4.0
$ spack develop mfem@4.2.0



$ ls
spack.yaml    axom/    mfem/



$ cat spack.yaml
spack:
    specs:
        - myapplication    # depends on axom, mfem

    develop:
        - axom @0.4.0
        - mfem @develop
```

Spack v0.18.0 was released at ISC in early June!

- **Major new features:**
  1. `--reuse` enabled by default
     - Reuse installed packages and build caches
     - Use `spack install --fresh` to get the old behavior
  2. Finer-grained spec hash + provenance
  3. Better error messages
  4. Unify *when possible* in environments
  5. Cray manifest support
  6. Windows support
  7. New binary format + hardened package signing
  8. Bootstrap mirror generation (for air gaps)
  9. Makefile generation
  10. Conditional variant values and sticky variants



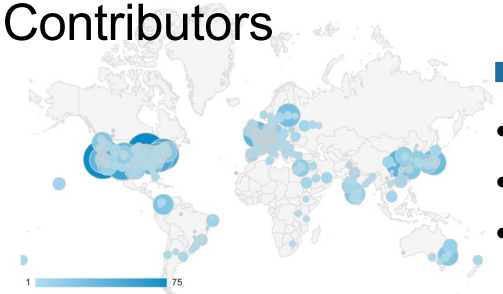
github.com/spack/spack

377 contributors to packages!
85 contributors to core!

Concretization is at the core of Spack!

This problem is NP-hard!

Contributors



- new versions
- new dependencies
- new constraints

package.py repository

concretizer

spack developers

yaml default config `packages.yaml`

admins, users

yaml local preferences config `packages.yaml`

users

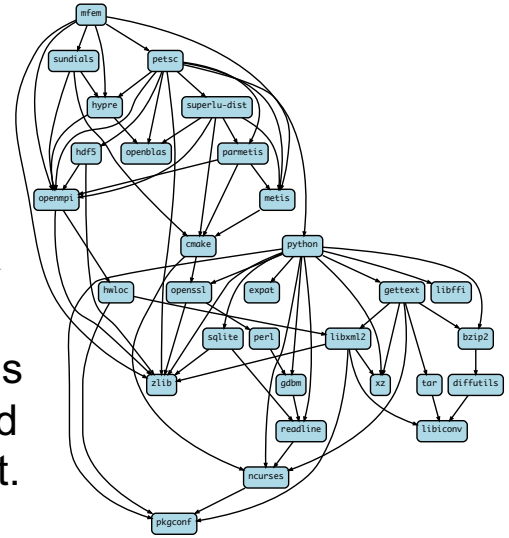
yaml environment config `spack.yaml`

users

Command line constraints

```
spack install hdf5@1.12.0 +debug
```

Concrete spec is fully constrained and can be built.



Crash course in ASP

- ASP syntax is derived from **Prolog**
- Basic piece of a program is a *term*
- Terms can easily represent any data structure, e.g. this is a graph with:
  - 2 nodes, one with a variant value
  - 1 dependency edge
- Terms followed by '.' are called *facts*
  - Facts say "this is true!"

```
enable_some_feature.

node("lammps").

node("cuda").

variant_value("lammps", "cuda", "False").

depends_on("lammps", "cuda", "link").
```

Crash course in ASP

- ASP programs also have ***rules***.
  - Rules can derive additional facts.
- **:-** can be read as **"if"**
  - The **head** (left side) is true
  - **If** the **body** (right side) is true
- **Comma** in the body is like "**and**"
  - Writing same head twice is like "or"
- Capital words are **variables**
  - Rules are instantiated with all possible substitutions for variables.

```
node(Dependency) :- node(Package), depends_on(Package, Dependency, Type).
```

```
node("cuda")
```

```
node("lammps").
depends_on("lammps", "cuda", "link").
```

Crash course in ASP

- ***Constraints*** say what ***cannot*** happen

```
path(A, B) :- depends_on(A, B).
path(A, C) :- path(A, B), depends_on(B, C).

:- path(A, B), path(B, A).       % this constraint says "no cycles"
```

- ***Choice rules*** give the solver freedom to choose from possible options:

```
% if a package is in the graph, solver must choose exactly one version
% out of that package's possible versions
1 { version(V) : possible_version(Package, V) } 1 :- node(Package).
```

ASP searches for *stable models* of the input program

- Stable models are also called ***answer sets***
- A ***stable model*** (loosely) is a set of true atoms that can be deduced from the inputs, where every rule is idempotent.
  - Similar to fixpoints
  - Put more simply: a set of atoms where all your rules are true!
- Unlike Prolog:
  - Stable models contain everything that can be derived (vs. just querying values)
  - ASP is guaranteed to complete!

Spack's concretizer is now implemented in ASP

- Used Clingo, the Potassco grounder/solver package
- ASP program has 2 parts:
  1. Large list of facts generated from package recipes (problem instance)
     - 60k+ facts is typical – includes dependencies, options, etc.
  2. Small logic program (~700 lines of ASP code)
- Algorithm (the part we write) is conceptually simpler:
  - Generate facts for all possible dependencies
  - Send facts and our logic program to the solver
  - Rebuild a DAG from the results

```
%-----------------------------------------------------------------------------
% Package: ucx
%-----------------------------------------------------------------------------
version_declared("ucx", "1.6.1", 0).
version_declared("ucx", "1.6.0", 1).
version_declared("ucx", "1.5.2", 2).
version_declared("ucx", "1.5.1", 3).
version_declared("ucx", "1.5.0", 4).
version_declared("ucx", "1.4.0", 5).
version_declared("ucx", "1.3.1", 6).
version_declared("ucx", "1.3.0", 7).
version_declared("ucx", "1.2.2", 8).
version_declared("ucx", "1.2.1", 9).
version_declared("ucx", "1.2.0", 10).

variant("ucx", "thread_multiple").
variant_single_value("ucx", "thread_multiple").
variant_default_value("ucx", "thread_multiple", "False").
variant_possible_value("ucx", "thread_multiple", "False").
variant_possible_value("ucx", "thread_multiple", "True").

declared_dependency("ucx", "numactl", "build").
declared_dependency("ucx", "numactl", "link").
node("numactl") :- depends_on("ucx", "numactl"), node("ucx").

declared_dependency("ucx", "rdma-core", "build").
declared_dependency("ucx", "rdma-core", "link").
node("rdma-core") :- depends_on("ucx", "rdma-core"), node("ucx").


%-----------------------------------------------------------------------------
% Package: util-linux
%-----------------------------------------------------------------------------
version_declared("util-linux", "2.29.2", 0).
version_declared("util-linux", "2.29.1", 1).
version_declared("util-linux", "2.25", 2).

variant("util-linux", "libuuid").
variant_single_value("util-linux", "libuuid").
variant_default_value("util-linux", "libuuid", "True").
variant_possible_value("util-linux", "libuuid", "False").
variant_possible_value("util-linux", "libuuid", "True").

declared_dependency("util-linux", "pkgconfig", "build").
declared_dependency("util-linux", "pkgconfig", "link").
node("pkgconfig") :- depends_on("util-linux", "pkgconfig"), node("util-linux").

declared_dependency("util-linux", "python", "build").
declared_dependency("util-linux", "python", "link").
node("python") :- depends_on("util-linux", "python"), node("util-linux").
```

Some facts for HDF5 package

Spack DSL allows *declarative* specification of complex constraints

CudaPackage: a mix-in for packages that use CUDA

```
class CudaPackage(PackageBase):
    variant('cuda', default=False,
            description='Build with CUDA')

    variant('cuda_arch',
            description='CUDA architecture',
            values=any_combination_of(cuda_arch_values),
            when='+cuda')

    depends_on('cuda', when='+cuda')

    depends_on('cuda@9.0:',     when='cuda_arch=70')
    depends_on('cuda@9.0:',     when='cuda_arch=72')
    depends_on('cuda@10.0:',    when='cuda_arch=75')

    conflicts('%gcc@9:', when='+cuda ^cuda@:10.2.89 target=x86_64:')
    conflicts('%gcc@9:', when='+cuda ^cuda@:10.1.243 target=ppc64le:')
```

There is a lot of expressivity in this DSL.

`cuda` is a variant (build option)

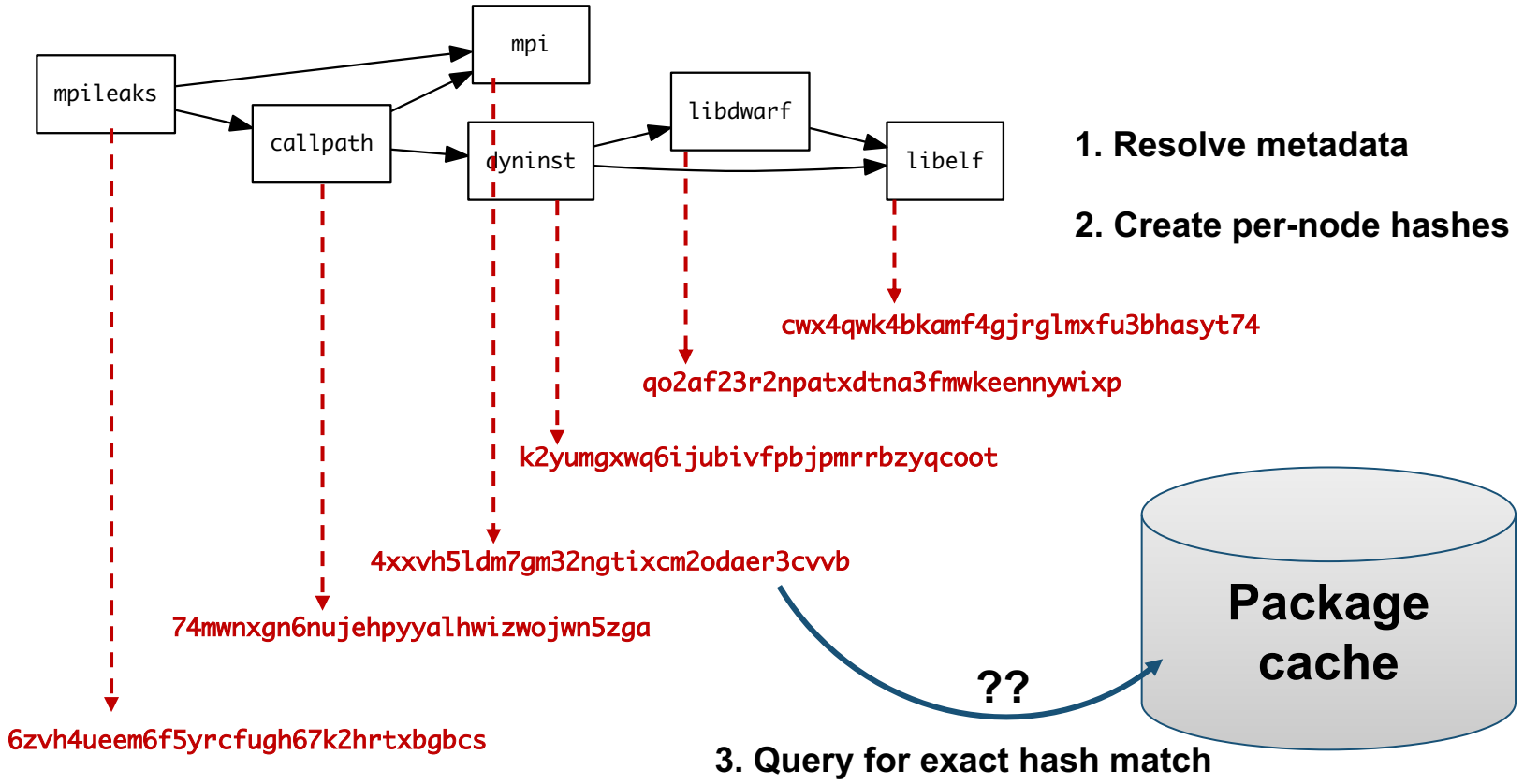
`cuda_arch` is only present if cuda is enabled

dependency on `cuda`, but only if `cuda` is enabled

constraints on `cuda` version

compiler support for x86_64 and `ppc64le`

Many packaging systems reuse builds via metadata hashes



- Hash matches are very sensitive to small changes
- In many cases, a satisfying cached or already installed spec can be missed
- Nix, Spack, Guix, Conan, and others reuse this way

We can be more aggressive about reusing packages.

- First, we need to tell the solver about all the installed packages!
- Add constraints for all installed packages, with their hash as the associated ID:

```
installed_hash("openssl","lwatuuysmwkhuahrncywvn77icdhs6mn").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node","openssl").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","version","openssl","1.1.1g").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node_platform_set","openssl","darwin").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node_os_set","openssl","catalina").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node_target_set","openssl","x86_64").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","variant_set","openssl","systemcerts","True").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node_compiler_set","openssl","apple-clang").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","node_compiler_version_set","openssl","apple-clang","12.0.0").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","concrete","openssl").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","depends_on","openssl","zlib","build").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","depends_on","openssl","zlib","link").
imposed_constraint("lwatuuysmwkhuahrncywvn77icdhs6mn","hash","zlib","x2anksgssxsxa7pcnhzg5k3dhgacglze").
```

Telling the solver to minimize builds is surprisingly simple: it's just the *impose* half of a generalized condition.

1. Allow the solver to *choose* a hash for any package:

```
{ hash(Package, Hash) : installed_hash(Package, Hash) } 1 :- node(Package).
```

2. Choosing a hash means we impose its constraints:

```
impose(Hash) :- hash(Package, Hash).
```

3. Define a build as something *without* a hash:

```
build(Package) :- not hash(Package, _), node(Package).
```

4. Minimize builds!

```
#minimize { 1@100,Package : build(Package) }.
```

With and without reuse optimization

Note the bifurcated optimization criteria

```
(spackle):solver> spack solve -Il hdf5
==> Best of 9 considered solutions.
==> Optimization Criteria:
  Priority  Criterion                                                Installed  ToBuild
  1         number of packages to build (vs. reuse)                          -       20
  2         deprecated versions used                                         0        0
  3         version weight                                                   0        0
  4         number of non-default variants (roots)                           0        0
  5         preferred providers for roots                                    0        0
  6         default values of variants not being used (roots)                0        0
  7         number of non-default variants (non-roots)                       0        0
  8         preferred providers (non-roots)                                  0        0
  9         compiler mismatches                                              0        0
  10        OS mismatches                                                    0        0
  11        non-preferred OS's                                               0        0
  12        version badness                                                  0        2
  13        default values of variants not being used (non-roots)            0        0
  14        non-preferred compilers                                          0        0
  15        target mismatches                                                0        0
  16        non-preferred targets                                            0        0

  -   zzngfs3  hdf5@1.10.7%apple-clang@13.0.0~cxx~fortran~hl~ipo~java+mpi+shared~szip~threadsafe+tools api=default b
  -   nsylovq      ^cmake@3.21.4%apple-clang@13.0.0~doc+ncurses+openssl+ownlibs~qt build_type=Release arch=darwin-bi
  -   xdbaqeo          ^ncurses@6.2%apple-clang@13.0.0~symlinks+termlib abi=none arch=darwin-bigsur-skylake
  -   kfureok              ^pkgconf@1.8.0%apple-clang@13.0.0 arch=darwin-bigsur-skylake
  -   5ekd4ap          ^openssl@1.1.1l%apple-clang@13.0.0~docs certs=system arch=darwin-bigsur-skylake
  -   xz6a265              ^perl@5.34.0%apple-clang@13.0.0+cpanm+shared+threads arch=darwin-bigsur-skylake
  -   xgt3tls                  ^berkeley-db@18.1.40%apple-clang@13.0.0+cxx~docs+stl patches=b231fcc4d5cff05e5c3a4814
  -   65edjf6                  ^bzip2@1.0.8%apple-clang@13.0.0~debug~pic+shared arch=darwin-bigsur-skylake
  -   662adoo                      ^diffutils@3.8%apple-clang@13.0.0 arch=darwin-bigsur-skylake
  -   fu7tfsr                          ^libiconv@1.16%apple-clang@13.0.0 libs=shared,static arch=darwin-bigsur-skyla
  -   vjg67nd                  ^gdbm@1.19%apple-clang@13.0.0 arch=darwin-bigsur-skylake
  -   tjceldr                      ^readline@8.1%apple-clang@13.0.0 arch=darwin-bigsur-skylake
  -   xevvljj                  ^zlib@1.2.11%apple-clang@13.0.0+optimize+pic+shared arch=darwin-bigsur-skylake
  -   xelfobh      ^openmpi@4.1.1%apple-clang@13.0.0~atomics~cuda~cxx~cxx_exceptions+gpfs~internal-hwloc~java~legacy
  -   zruns75          ^hwloc@2.6.0%apple-clang@13.0.0~cairo~cuda~gl~libudev+libxml2~netloc~nvml~opencl~pci~rocm+sha
  -   ib4fnkf              ^libxml2@2.9.12%apple-clang@13.0.0~python arch=darwin-bigsur-skylake
  -   dwiv2ys                  ^xz@5.2.5%apple-clang@13.0.0~pic libs=shared,static arch=darwin-bigsur-skylake
  -   blitnbl          ^libevent@2.1.12%apple-clang@13.0.0+openssl arch=darwin-bigsur-skylake
  -   h7jalyu          ^openssh@8.7p1%apple-clang@13.0.0 arch=darwin-bigsur-skylake
  -   7v7bqx2              ^libedit@3.1-20210216%apple-clang@13.0.0 arch=darwin-bigsur-skylake
```

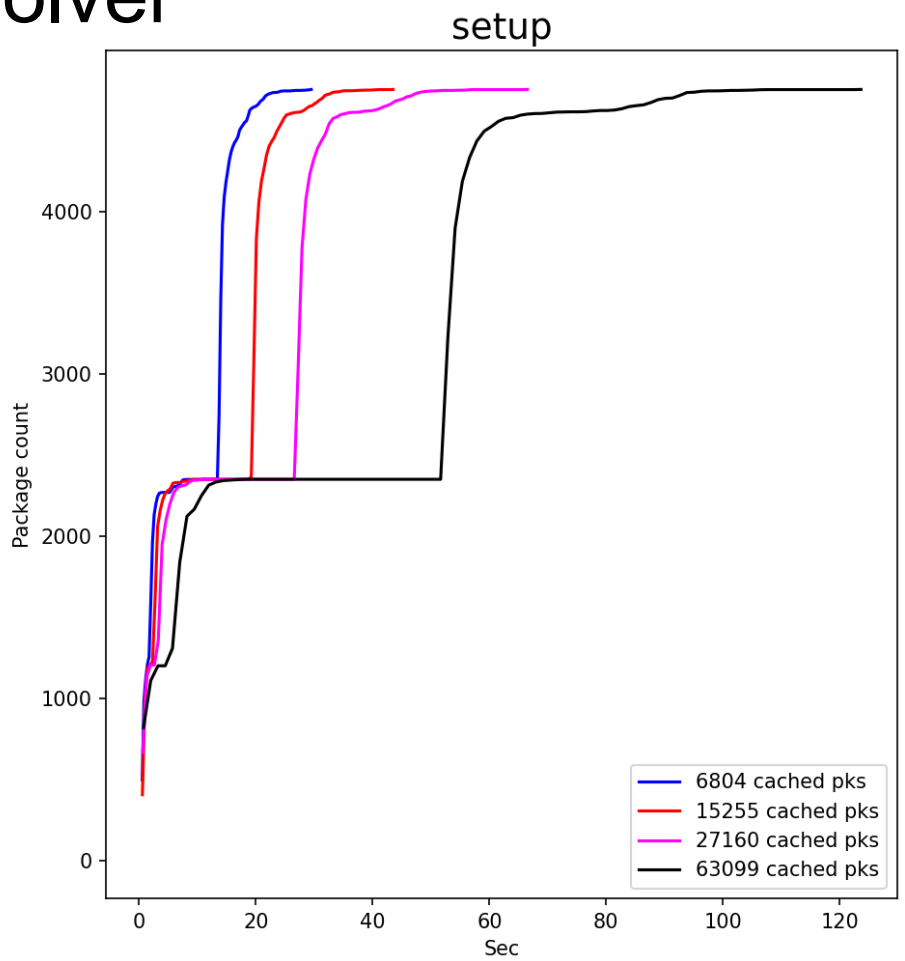
Pure hash-based reuse: all misses

```
(spackle):spack> spack solve --reuse -Il hdf5
==> Best of 10 considered solutions.
==> Optimization Criteria:
  Priority  Criterion                                                Installed  ToBuild
  1         number of packages to build (vs. reuse)                          -        4
  2         deprecated versions used                                         0        0
  3         version weight                                                   0        0
  4         number of non-default variants (roots)                           0        0
  5         preferred providers for roots                                    0        0
  6         default values of variants not being used (roots)                0        0
  7         number of non-default variants (non-roots)                       2        0
  8         preferred providers (non-roots)                                  0        0
  9         compiler mismatches                                              0        0
  10        OS mismatches                                                    0        0
  11        non-preferred OS's                                               0        0
  12        version badness                                                  6        0
  13        default values of variants not being used (non-roots)            1        0
  14        non-preferred compilers                                         15        4
  15        target mismatches                                                0        0
  16        non-preferred targets                                            0        0

  -   yfkfnsp  hdf5@1.10.7%apple-clang@12.0.5~cxx~fortran~hl~ipo~java+mpi+shared~szip~threadsafe+tools api=defaul
  [+] zd4m26e      ^cmake@3.21.1%apple-clang@12.0.5~doc+ncurses+openssl+ownlibs~qt build_type=Release arch=darwin
  [+] 53i52xr          ^ncurses@6.2%apple-clang@12.0.5~symlinks+termlib abi=none arch=darwin-bigsur-skylake
  [+] us36bwr          ^openssl@1.1.1l%apple-clang@12.0.5~docs+systemcerts arch=darwin-bigsur-skylake
  [+] 74mwnxg              ^zlib@1.2.11%apple-clang@12.0.5+optimize+pic+shared arch=darwin-bigsur-skylake
  -   3ijfnel      ^openmpi@4.1.1%apple-clang@12.0.5~atomics~cuda~cxx~cxx_exceptions+gpfs~internal-hwloc~java~leg
  -   jxexyb7          ^hwloc@2.6.0%apple-clang@12.0.5~cairo~cuda~gl~libudev+libxml2~netloc~nvml~opencl~pci~rocm+
  [+] ckdn5zf              ^libxml2@2.9.12%apple-clang@12.0.5~python arch=darwin-bigsur-skylake
  [+] k7auat3                  ^libiconv@1.16%apple-clang@12.0.5 libs=shared,static arch=darwin-bigsur-skylake
  [+] k2yumgx                  ^xz@5.2.5%apple-clang@12.0.5~pic libs=shared,static arch=darwin-bigsur-skylake
  [+] grgtlcd              ^pkgconf@1.8.0%apple-clang@12.0.5 arch=darwin-bigsur-skylake
  -   nnc66ug          ^libevent@2.1.12%apple-clang@12.0.5+openssl arch=darwin-bigsur-skylake
  [+] 63xbksk          ^openssh@8.6p1%apple-clang@12.0.5 arch=darwin-bigsur-skylake
  [+] snhgldt              ^libedit@3.1-20210216%apple-clang@12.0.5 arch=darwin-bigsur-skylake
  [+] qbkmtdd          ^perl@5.34.0%apple-clang@12.0.5+cpanm+shared+threads arch=darwin-bigsur-skylake
  [+] tnvkifs              ^berkeley-db@18.1.40%apple-clang@12.0.5+cxx~docs+stl patches=b231fcc4d5cff05e5c3a4814f
  [+] 7d5woqt              ^bzip2@1.0.8%apple-clang@12.0.5~debug~pic+shared arch=darwin-bigsur-skylake
  [+] vh6di3i              ^gdbm@1.19%apple-clang@12.0.5 arch=darwin-bigsur-skylake
  [+] qgy3v4l                  ^readline@8.1%apple-clang@12.0.5 arch=darwin-bigsur-skylake
```

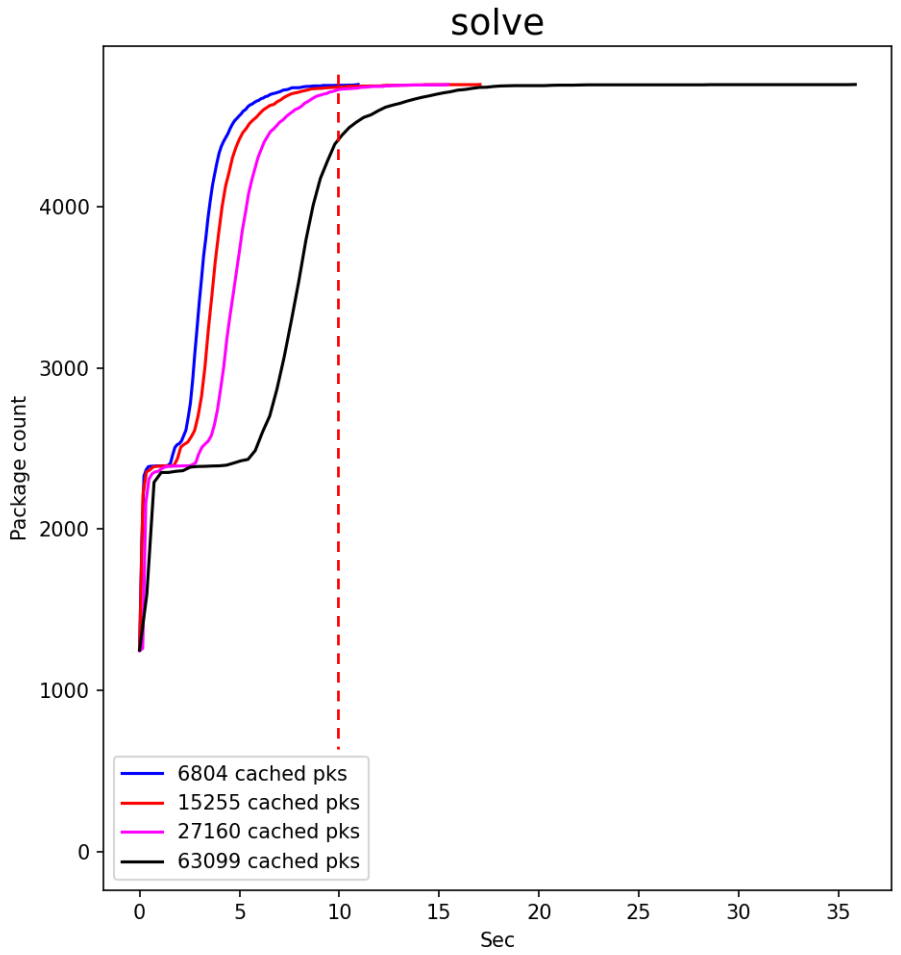
With --reuse: 16 packages were reusable

So far, it looks like we can handle very large problem sizes with the reusing solver

- Cumulative distribution of setup and solve times
- Hypothesis: we don't see big combinatorial blow-up b/c we're strict about dependency hashes
- Next: try mixed ABI, but *prefer* "pure" source-built dependencies

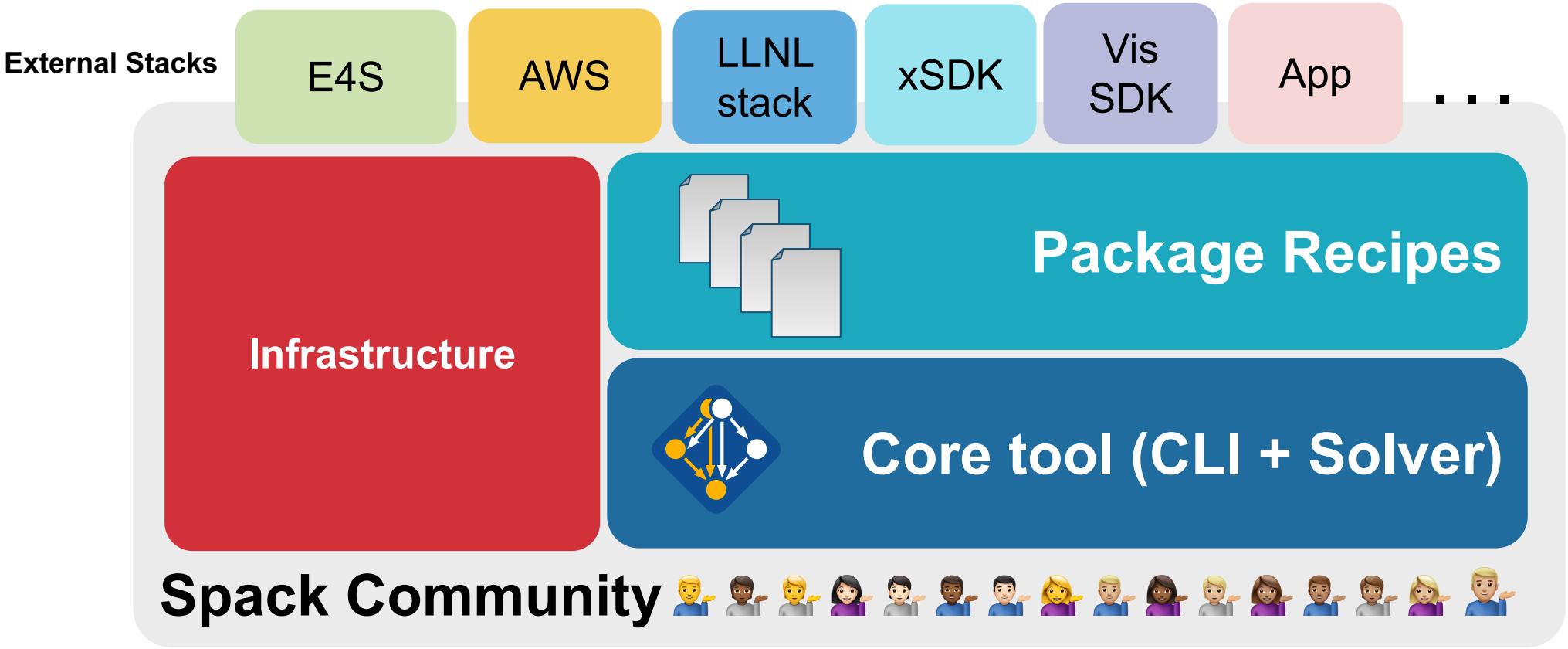


Most of the time is spent in setup (reading data in Python – can be sped up w/caching)



Even with 63k packages in a repo, nearly all package solves take < 10 sec

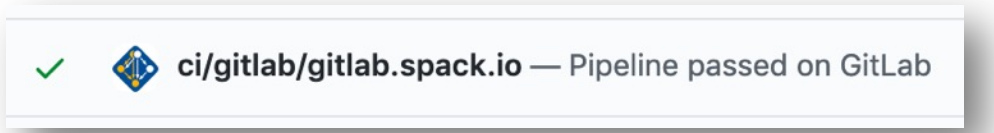
What does the Spack project look like?



CI has made Spack builds *much* more reliable!

Spack Contributions on GitHub

(over 1,000 contributors)

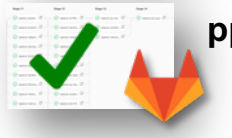


gitlab.spack.io

`spack.yaml` configurations (E4S, SDKs, AWS, others)

`spack ci`

x86_64 and **aarch64** pipelines in **AWS**



ppc64le, GPU pipelines at **U. Oregon**

Pipelines at **LLNL (Cray PE soon)**

GitLab CI builds (changed) packages
- On every pull request
- On every release branch

Do users really need to build from source?

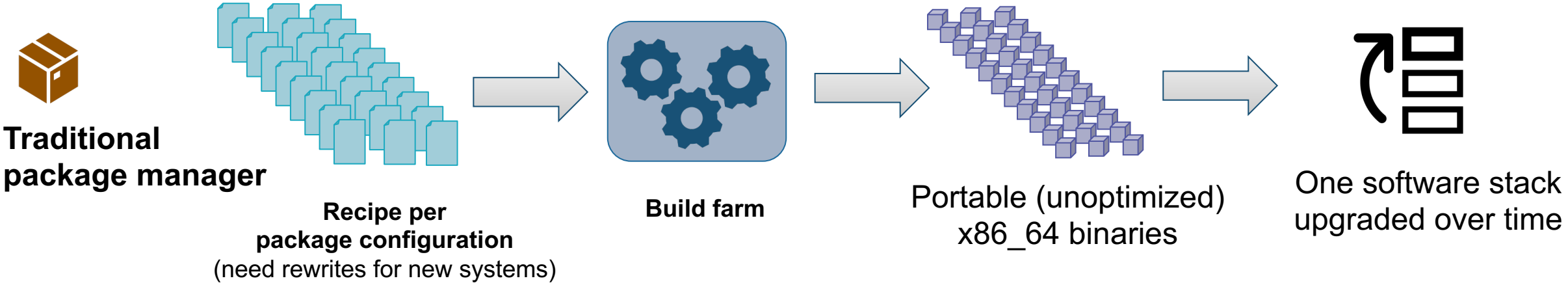
With v0.18, Spack has a public binary cache

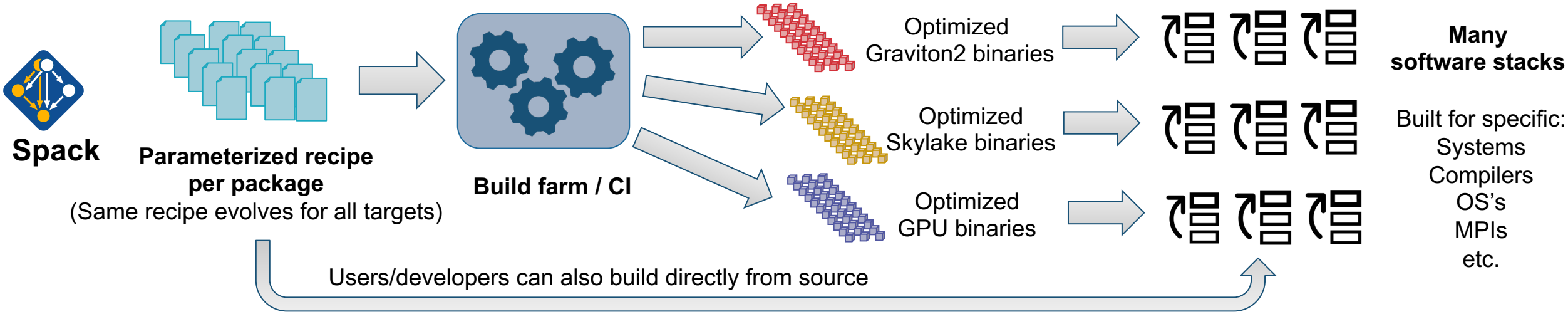
```
# latest v0.18.x release binaries
spack mirror add https://binaries.spack.io/releases/v0.18

# rolling release: bleeding edge binaries
spack mirror add https://binaries.spack.io/develop
```

- Over 3,000 builds in the cache so far:
  - Amazon Linux 2 x86_64_v4
  - Amazon Linux 2 aarch64
  - Amazon Linux 2 graviton2
  - Ubuntu 18.04 x86_64

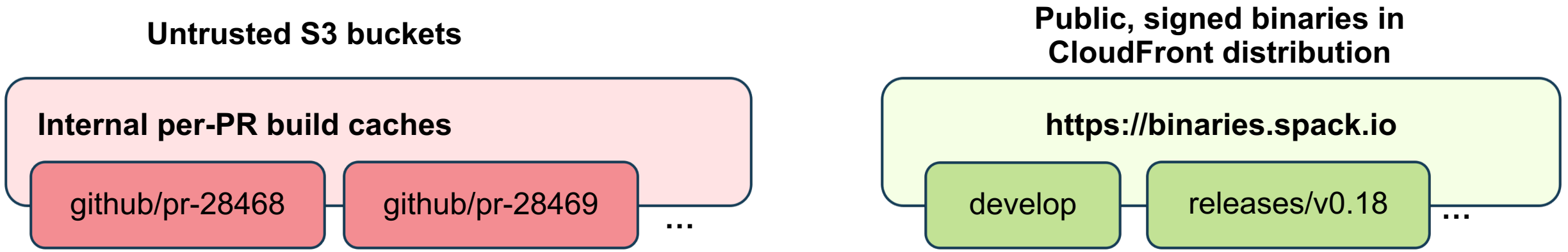
Do we trust binaries?

We aim to lower the burden of maintaining a binary distribution *and* make it easy to mix source builds with binaries.





Our infrastructure enables us to sustainably manage a binary distribution



Contributors submit package changes

- Iterate on builds in PR
- Caches prevent unnecessary rebuilds

Maintainers review PRs

- Verify PR build succeeded
- Review package code
- Merge to develop

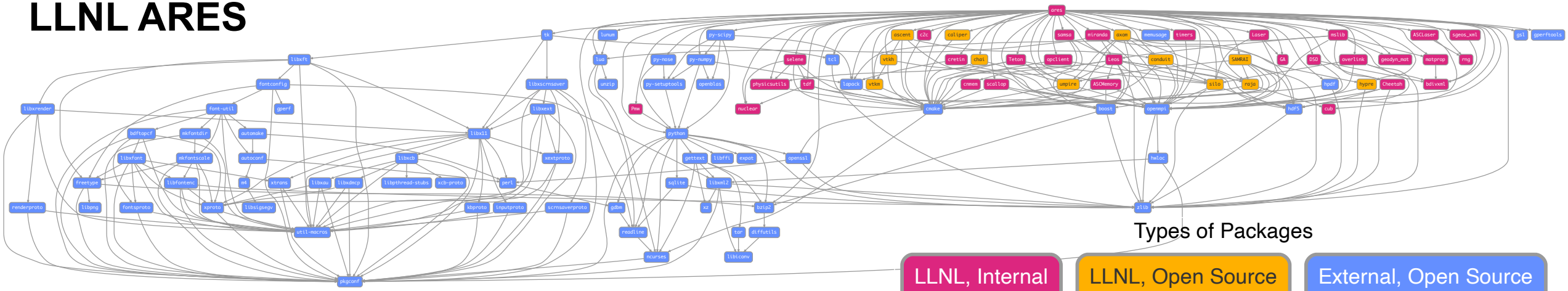
Rebuild and Sign

- Published binaries built ONLY from approved code
- Protected signing runners
- Ephemeral keys

- Moves bulk of binary maintenance upstream, onto PRs
  - Production binaries never reuse binaries from untrusted environment

Why should we care about this for our HPC codes?

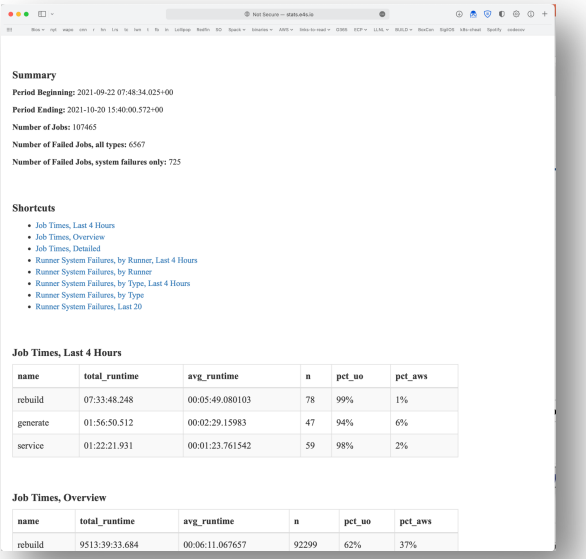
LLNL ARES



- Our codes use a lot of external software
  - *Most* packages are external open source
  - Many LLNL packages are also open source and developed in the open
- We *cannot* replace all these OSS components with our own
  - How do we vet all these components?
- **Key question:** Who/what do you trust to validate the components?
  - Current processes are not scalable and not automated!

We will continue scaling this infrastructure out!

- We are doing 40k builds per week!
  - There are lots of optimizations left to do on the build pipelines
  - We think we can eventually scale to all 6,400 Spack packages
- Goal: make source builds unnecessary for most users
  - Source builds are optimized for x86_64_v4 (avx512), graviton, etc.
  - Source builds will still be seamless – key for reproducibility
  - Use `spack develop` to tweak (almost) any binary you can install
- We will keep scaling OS, compiler, and arch support
  - Current crop of compilers and OS's is a bit old – expect a refresh
  - Cray PE build coming soon!
- Amazon Linux 2 builds work on AWS ParallelCluster NOW!



Summary

Period Beginning: 2021-09-22 07:48:34.025+00

Period Ending: 2021-10-20 15:40:00.572+00

Number of Jobs: 107465

Number of Failed Jobs, all types: 6567

Number of Failed Jobs, system failures only: 725

Shortcuts

- Job Times, Last 4 Hours
- Job Times, Overview
- Job Times, Detailed
- Runner System Failures, by Runner, Last 4 Hours
- Runner System Failures, by Runner
- Runner System Failures, by Type, Last 4 Hours
- Runner System Failures, by Type
- Runner System Failures, Last 20

Job Times, Last 4 Hours

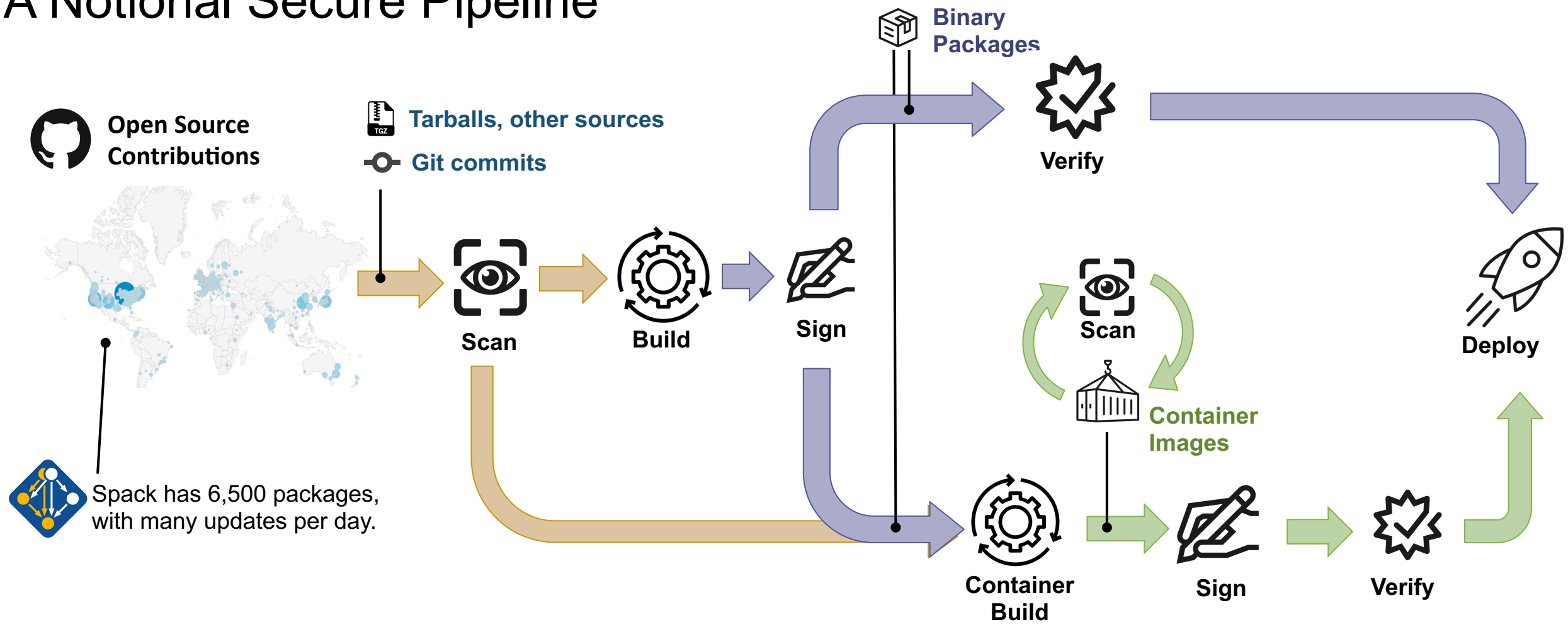
name	total_runtime	avg_runtime	n	pct_uo	pct_aws
rebuild	07:33:48.248	00:05:49.080103	78	99%	1%
generate	01:56:50.512	00:02:29.15983	47	94%	6%
service	01:22:21.931	00:01:23.761542	59	98%	2%

Job Times, Overview

name	total_runtime	avg_runtime	n	pct_uo	pct_aws
rebuild	9513:39:33.684	00:06:11.067657	92299	62%	37%

Build stats at https://stats.e4s.io

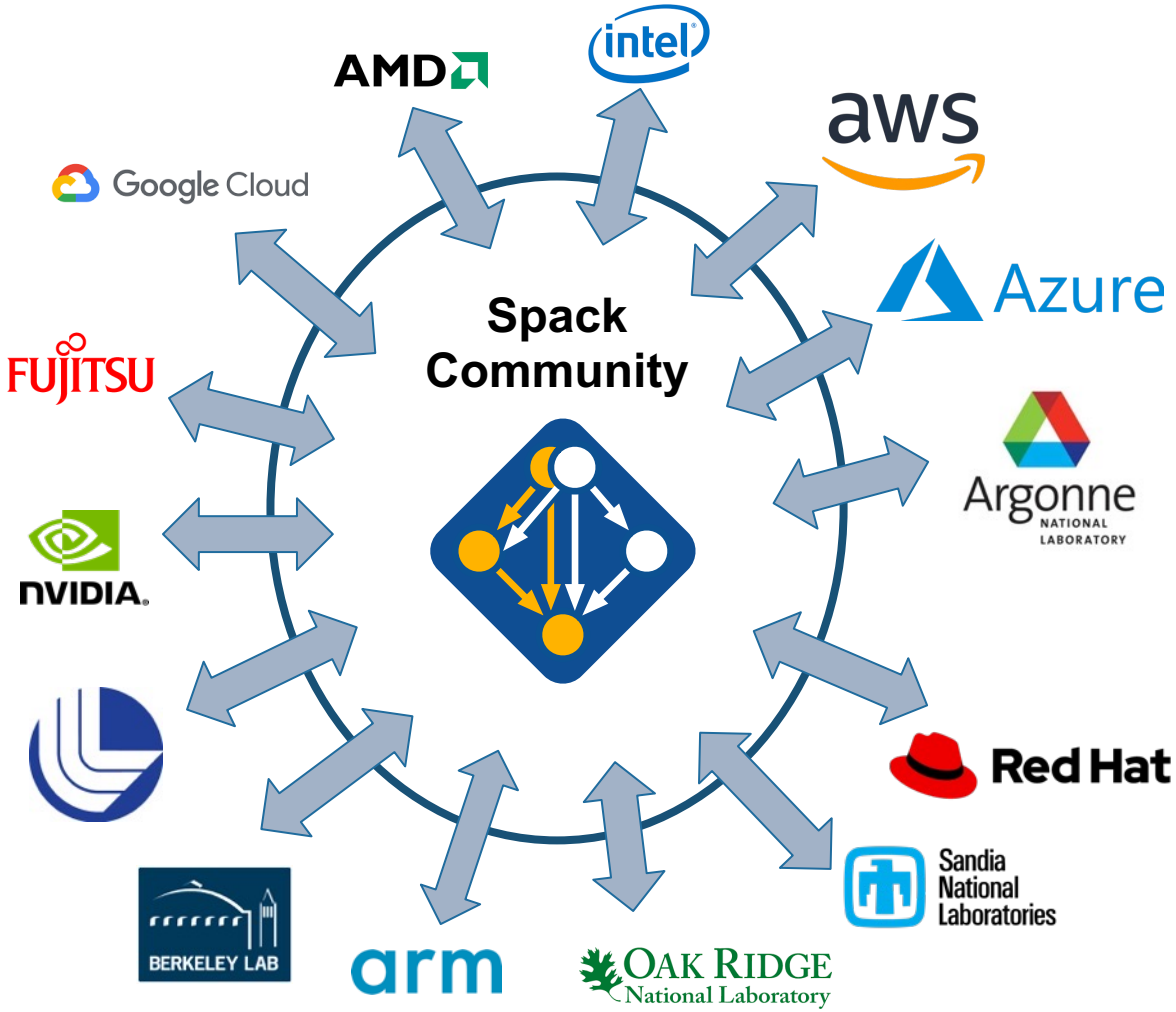
A Notional Secure Pipeline



- We are working to establish a set of guidelines for supply chain integrity
  - Labs are trending towards GitLab, Spack for HPC
  - Standard container formats can help with scanning
  - Standard Software Bill of Materials (SBOM) format could help sites cross-validate codes
- Spack can help to standardize some of this.

Spack's long-term strategy is based around broad adoption and collaboration

- **Not sustainable without a community**
  - Broad adoption incentivizes contributors
  - Cloud resources and automation absolutely necessary
- **Preserves build knowledge in a cross-platform, reusable way**
  - Minimize rewriting recipes when porting
- **CI ensures builds continue to work as packages evolve**
  - Keep packages flexible but verify key configurations
- **Growing contributor base and automation are the top priorities**
  - **377 contributors to 0.18 release!**



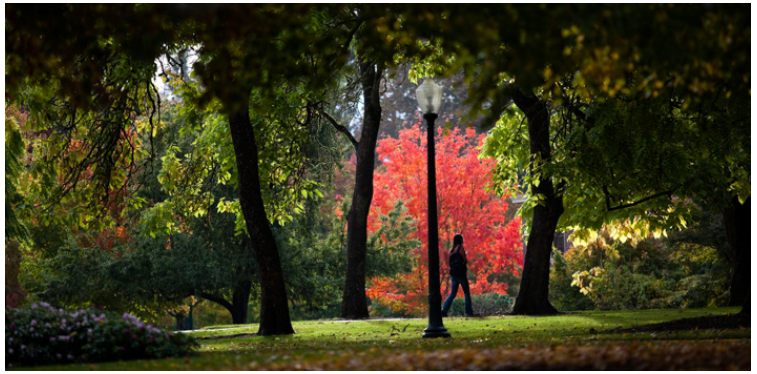
E4S Summary

What E4S is not	• What E4S is
A closed system taking contributions only from DOE software development teams.	Extensible, open architecture software ecosystem accepting contributions from US and international teams. Framework for collaborative open-source product integration.
A monolithic, take-it-or-leave-it software behemoth.	A full collection of compatible software capabilities **and** A manifest of a la carte selectable software capabilities.
A commercial product.	Vehicle for delivering high-quality reusable software products in collaboration with others.
A simple packaging of existing software.	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.

Vision for E4S Now and in the Future

- E4S has emerged as a new top-level component in the DOE HPC community, enabling fundamentally new relationships
- E4S has similar potential for new interactions with other US agencies, US industry and international collaborators. NSF and UK are examples
- The E4S portfolio can expand to include new domains (ML/AI), lower—level components (OS), and more.
- E4S can provide better (increased quality), faster (timely delivery of leading-edge capabilities) and cheaper (assisting product teams)

Performance Research Laboratory, University of Oregon, Eugene



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- Department of Defense (DoD)
  - PETTT, HPCMP
- National Science Foundation (NSF)
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- NASA
- CEA, France
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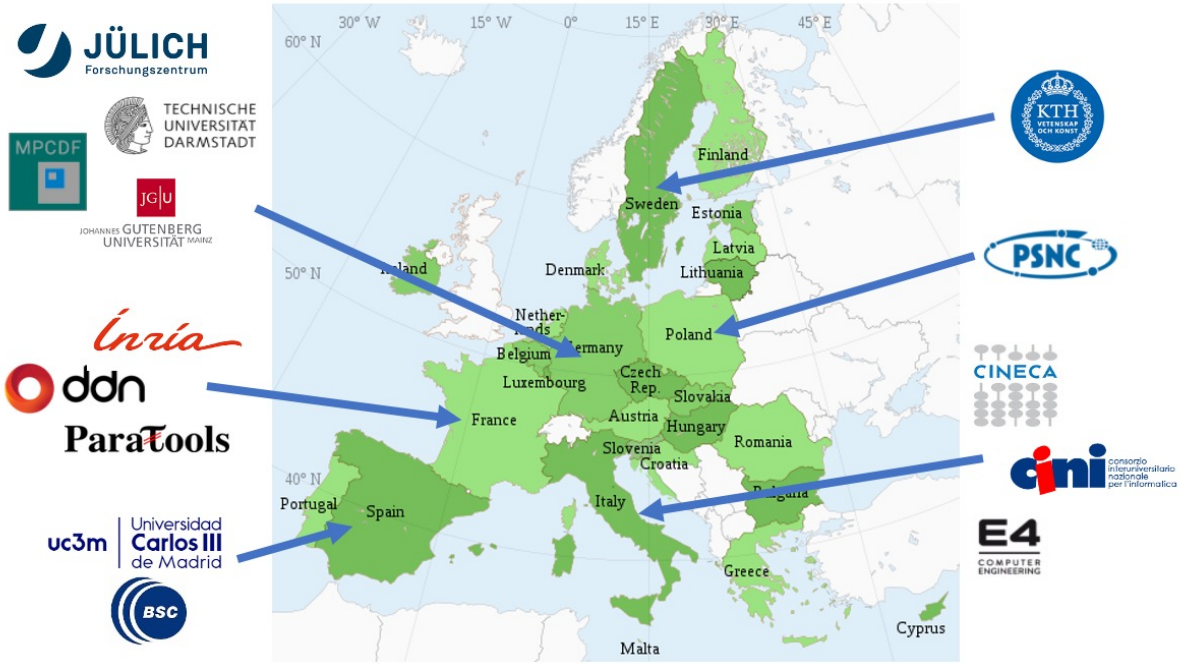
  - The Ohio State University
  - ParaTools, Inc.
  - University of Tennessee, Knoxville
  - T.U. Dresden, GWT
  - Jülich Supercomputing Center

Thank you: ADMIRE

https://admire-eurohpc.eu



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Thank you

https://www.exascaleproject.org

This research was supported by the Exascale Computing Project (17-SC-20-SC), a joint project of the U.S. Department of Energy's Office of Science and National Nuclear Security Administration, responsible for delivering a capable exascale ecosystem, including software, applications, and hardware technology, to support the nation's exascale computing imperative.

Thank you to all collaborators in the ECP and broader computational science communities. The work discussed in this presentation represents creative contributions of many people who are passionately working toward next-generation computational science.

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