# E4S: Extreme-scale Scientific Software Stack

High Throughput Computing (HTC23)
https://agenda.hep.wisc.edu/event/2014/contributions/28449/
July 14, 2023, 11:15am CT  - 11:45am CT
Howard Auditorium
Fluno Center on the University of Wisconsin-Madison Campus

**Prof. Sameer Shende**
Research Professor and Director,
Performance Research Laboratory, OACISS, University of Oregon
President and Director, ParaTools, Inc.
https://e4s.io/talks/E4S_HTC23.pdf

# Challenges

- As our software gets more complex, it is getting harder to install our tools and libraries correctly in an integrated and interoperable software stack to deploy our applications to the high throughput computing (HTC) platforms!

- E4S is a containerized platform that features a capable HTC software stack with support for GPUs

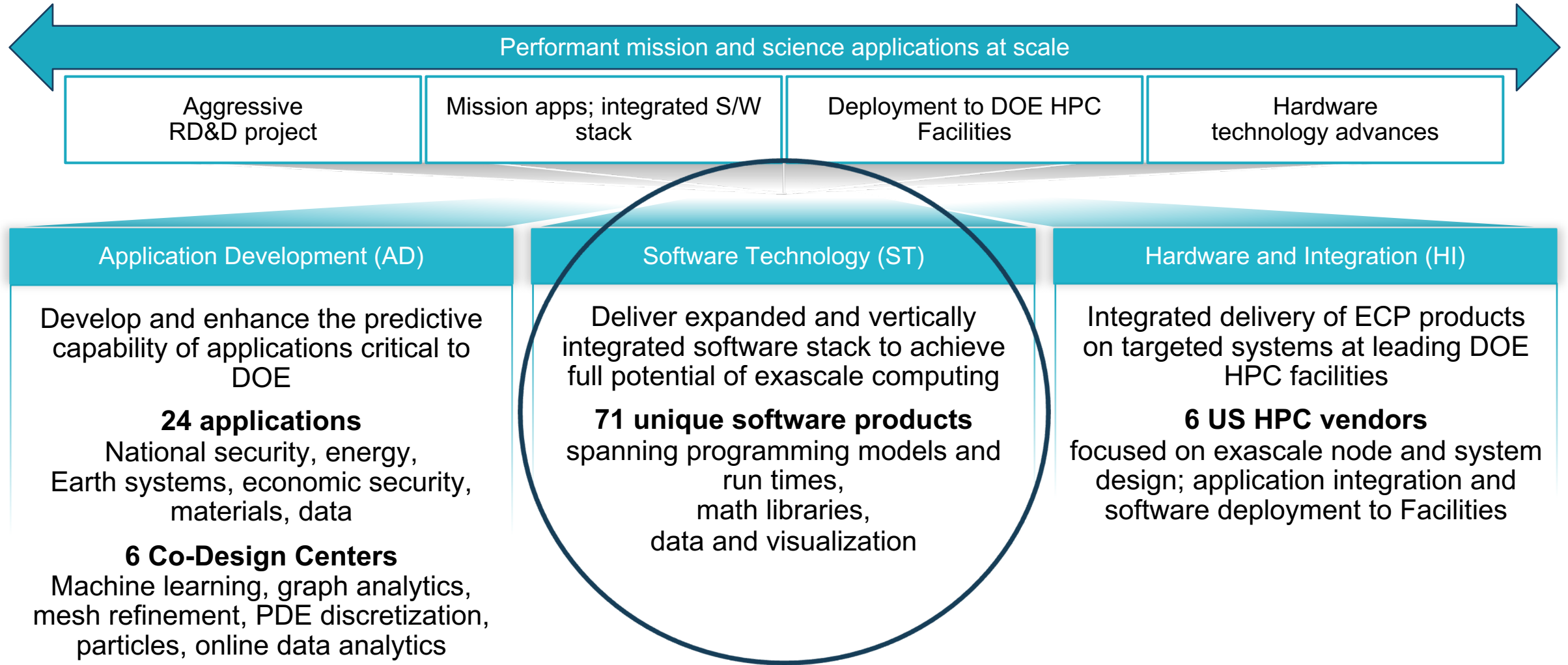# Extreme-scale Scientific Software Stack (E4S)
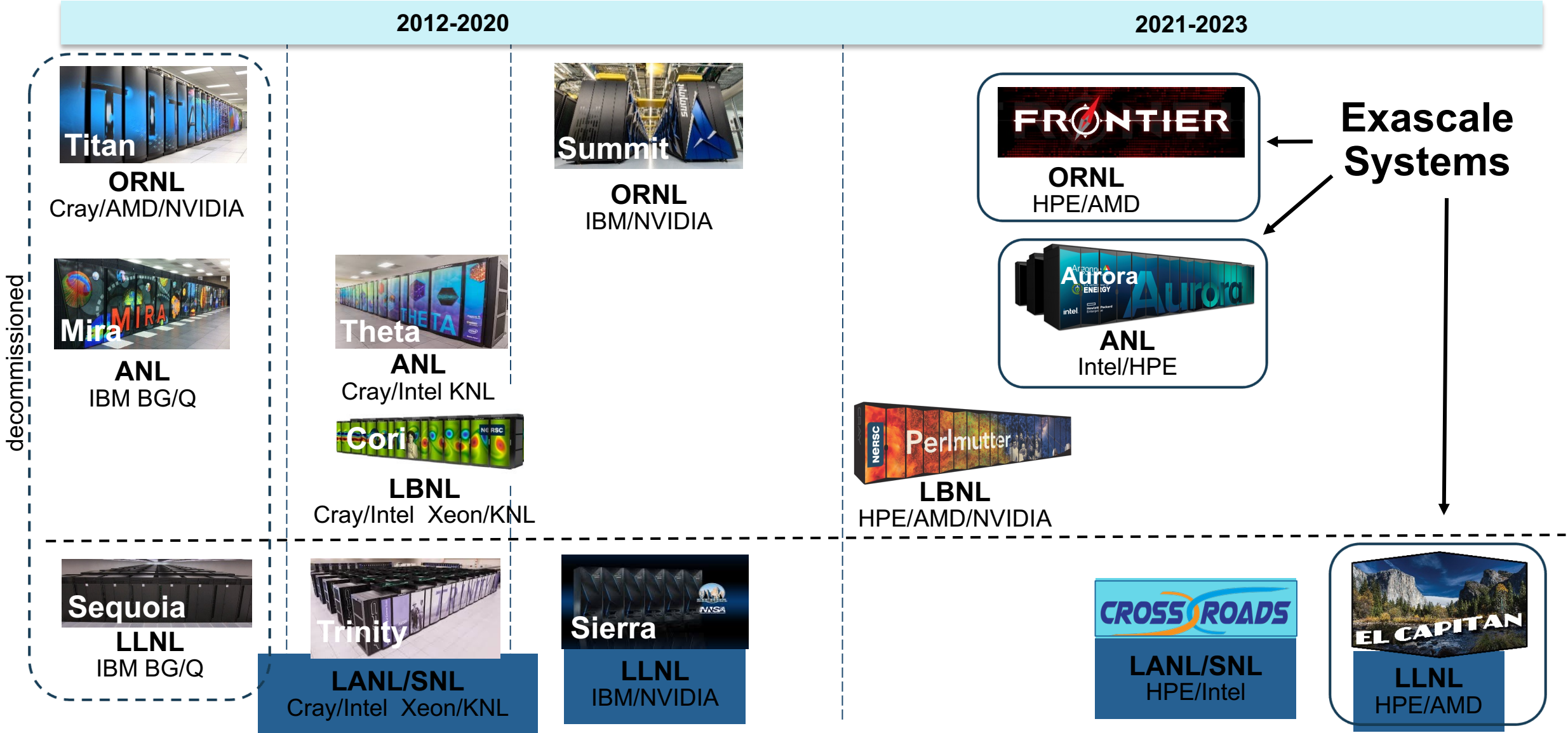
# Exascale Computing Project (ECP)



https://exascaleproject.org

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

**Performant mission and science applications at scale**

| Aggressive RD&D project | Mission apps; integrated S/W stack | Deployment to DOE HPC Facilities | Hardware technology advances |
|---|---|---|---|

## Application Development (AD)

Develop and enhance the predictive capability of applications critical to DOE

**24 applications**
National security, energy, Earth systems, economic security, materials, data

**6 Co-Design Centers**
Machine learning, graph analytics, mesh refinement, PDE discretization, particles, online data analytics

## Software Technology (ST)

Deliver expanded and vertically integrated software stack to achieve full potential of exascale computing

**71 unique software products**
spanning programming models and run times,
math libraries,
data and visualization

## Hardware and Integration (HI)

Integrated delivery of ECP products on targeted systems at leading DOE HPC facilities

**6 US HPC vendors**
focused on exascale node and system design; application integration and software deployment to Facilities

# US DOE HPC Roadmap to Exascale Systems

| 2012-2020 | 2021-2023 |
|---|---|

decommissioned

**Titan**
**ORNL**
Cray/AMD/NVIDIA

**Mira**
**ANL**
IBM BG/Q

**Theta**
**ANL**
Cray/Intel KNL

**Cori**
**LBNL**
Cray/Intel Xeon/KNL

**Summit**
**ORNL**
IBM/NVIDIA

**FRONTIER**
**ORNL**
HPE/AMD

← **Exascale Systems**

**Aurora**
**ANL**
Intel/HPE

**Perlmutter**
**LBNL**
HPE/AMD/NVIDIA

**Sequoia**
**LLNL**
IBM BG/Q

**Trinity**
**LANL/SNL**
Cray/Intel Xeon/KNL

**Sierra**
**LLNL**
IBM/NVIDIA

**CROSSROADS**
**LANL/SNL**
HPE/Intel

**EL CAPITAN**
**LLNL**
HPE/AMD

ECP EXASCALE COMPUTING PROJECT

# 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
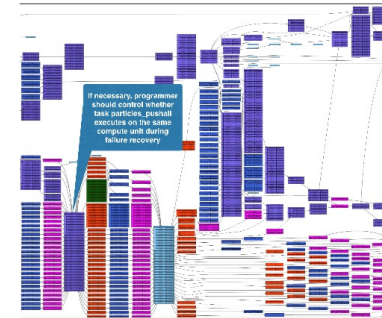
# Extreme-scale Scientific Software Stack (E4S)

- <u>E4S</u>: 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 each release

- 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

- February 2023: E4S 23.02 – 106 full release products

- May 2023: E4S 23.05 – 109 full release products

**Spack**

**E4S**

https://e4s.io

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

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# 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, 50+ EDA (e.g., Xyce), and AI/ML packages (e.g., 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_June23.pdf
- e4s-cl container launch tool allows binary distribution of applications by substituting MPI in the containerized app with the system MPI. e4s-alc is a tool to create custom container images from base images
- Quarterly releases: E4S 23.05 released on May 31, 2023: https://e4s.io/talks/E4S_23.05.pdf
- E4S for commercial cloud platforms: AWS image supports MPI implementations and containers with remote desktop (DCV).
    - Intel MPI, NVHPC, MVAPICH2, MPICH, MPC, OpenMPI

# Getting started with E4S on OSG-HTC

```
[sameer@ap20 example]$ ls /cvmfs/singularity.opensciencegrid.org/ecpe4s/
e4s-cuda:22.11   e4s-cuda:23.05   e4s-oneapi:22.11   e4s-oneapi:23.05   e4s-rocm:22.11   e4s-rocm:23.052

[sameer@ap20 example]$ cat workload.submit

+SingularityImage = "/cvmfs/singularity.opensciencegrid.org/ecpe4s/e4s-cuda:23.05"

requirements = GPUs_Capability >= 8.0

executable   = test.sh
arguments    =
input        =
output       = $(Cluster).$(Process).out
error        = $(Cluster).$(Process).err
log          = $(Cluster).$(Process).log

request_cpus = 1
request_gpus = 1
request_memory = 8GB

queue 1


[sameer@ap20 example]$ cat test.sh
#!/bin/bash

set -e

echo "I'm running on "`hostname -f`
echo "OSG site: $OSG_SITE_NAME"

echo

export CUDA_VISIBLE_DEVICES=0
cd /opt/demo/python_tests
./run.sh

echo "Arch list:"
python -c "import torch; print(torch.cuda.get_arch_list())"

nvidia-smi
lscpu

[sameer@ap20 example]$ condor_submit workload.submit
```

cd /cvmfs/singularity.opensciencegrid.org/ecpe4s

# Getting started with E4S on OSG-HTC

```
I'm running on gpu10.cluster
OSG site: PDX-Coeus-CE1
...
f6.py:
PyTorch DeviceName: NVIDIA RTX A5000
99 851.0418701171875
199 14.9901114212036133
299 0.35536718368530273
399 0.0092444419634342194
499 0.0004737153649330139
Arch list:
['sm_35', 'sm_70', 'sm_75', 'sm_80', 'sm_90']
Sat Jul  8 09:36:17 2023
+-----------------------------------------------------------------------------------------+
| NVIDIA-SMI 530.30.02              Driver Version: 530.30.02      CUDA Version: 12.1      |
|-----------------------------------------+----------------------+----------------------+
| GPU  Name                 Persistence-M | Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf            Pwr:Usage/Cap |          Memory-Usage | GPU-Util  Compute M. |
|                                          |                       |               MIG M. |
|=========================================+======================+======================|
|   0  NVIDIA RTX A5000             On | 00000000:01:00.0 Off |                  Off |
| 30%   31C    P8              26W / 230W|       3MiB / 24564MiB |      0%      Default |
|                                          |                       |                  N/A |
+-----------------------------------------+----------------------+----------------------+
|   1  NVIDIA RTX A5000             On | 00000000:41:00.0 Off |                  Off |
| 30%   24C    P8              16W / 230W|       3MiB / 24564MiB |      0%      Default |
|                                          |                       |                  N/A |
+-----------------------------------------+----------------------+----------------------+
|   2  NVIDIA RTX A5000             On | 00000000:81:00.0 Off |                  Off |
| 30%   24C    P8              16W / 230W|       3MiB / 24564MiB |      0%      Default |
|                                          |                       |                  N/A |
+-----------------------------------------+----------------------+----------------------+
|   3  NVIDIA RTX A5000             On | 00000000:C1:00.0 Off |                  Off |
| 30%   24C    P8              24W / 230W|       3MiB / 24564MiB |      0%      Default |
|                                          |                       |                  N/A |
+-----------------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------------------+
| Processes:                                                                              |
|  GPU   GI   CI        PID   Type   Process name                          GPU Memory |
|        ID   ID                                                           Usage      |
|=========================================================================================|
|  No running processes found                                                            |
+-----------------------------------------------------------------------------------------+
Architecture:                    x86_64
CPU op-mode(s):                  32-bit, 64-bit
Byte Order:                      Little Endian
Address sizes:                   43 bits physical, 48 bits virtual
CPU(s):                          64
On-line CPU(s) list:             0-63
```

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# E4S Support for AI/ML frameworks with V100, A100, and H100 GPUs

```
Singularity> python
Python 3.8.10 (default, Nov 14 2022, 12:59:47)
[GCC 9.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import numpy
>>> import scipy
>>> import matplotlib
>>> import tensorflow
>>> tensorflow.__version__
'2.12.0'
>>> import torch
>>> torch.__version__
'2.0.0'
>>> torch.cuda.get_device_name(torch.cuda.current_device())
'NVIDIA H100 PCIe'
>>>
```

E4S 23.05 supports NVIDIA H100 GPUs with TensorFlow 2.12.0 and PyTorch 2.0.0

# Python tools in E4S 23.05 on Expanse at SDSC

```
[sshende@login02 ~]$ srun --gpus=1 --partition=gpu-debug --wait=0 --pty --account=DDP408 --time=0:10:00 --nodes=1 --ntasks-per-node=4 --mem=8G --export=ALL /bin/bash
srun: job 24032821 queued and waiting for resources
srun: job 24032821 has been allocated resources
[sshende@exp-7-59 ~]$ cd /cm/shared/apps/containers/singularity/e4s/v23.05
[sshende@exp-7-59 v23.05]$ module load singularitypro
[sshende@exp-7-59 v23.05]$ singularity run -e --nv e4s-cuda80-x86_64-23.05.sif
Singularity> ls /usr/local/lib/python3.8/dist-packages/
```

| | | | | |
|---|---|---|---|---|
| absl | gnureadline-8.1.2.dist-info | matplotlib-3.7.1.dist-info | pyasn1_modules | tensorboard_data_server-0.7.0.dist-info |
| absl_py-1.4.0.dist-info | gnureadline.cpython-38-x86_64-linux-gnu.so | matplotlib-3.7.1-py3.8-nspkg.pth | pyasn1_modules-0.3.0.dist-info | tensorflow |
| astunparse | gnureadline.libs | minio | __pycache__ | tensorflow-2.12.0.dist-info |
| astunparse-1.6.3.dist-info | google | minio-7.1.12.dist-info | pycparser | tensorflow_estimator |
| boto3 | google_auth-2.18.1.dist-info | ml_dtypes | pycparser-2.21.dist-info | tensorflow_estimator-2.12.0.dist-info |
| boto3-1.20.35.dist-info | google_auth-2.18.1-py3.9-nspkg.pth | ml_dtypes-0.1.0.dist-info | pylab.py | tensorflow_io_gcs_filesystem |
| botocore | google_auth_oauthlib | mpl_toolkits | pyparsing | tensorflow_io_gcs_filesystem-0.32.0.dist-info |
| botocore-1.23.42.dist-info | google_auth_oauthlib-1.0.0.dist-info | mpmath | pyparsing-3.0.9.dist-info | termcolor |
| cachetools | google_pasta-0.2.0.dist-info | mpmath-1.3.0.dist-info | py.py | termcolor-2.3.0.dist-info |
| cachetools-5.3.0.dist-info | grpc | networkx | _pytest | tokenizers |
| certifi | grpcio-1.54.2.dist-info | networkx-3.1.dist-info | pytest | tokenizers-0.13.3.dist-info |
| certifi-2022.12.7.dist-info | h5py | numpy | pytest-7.3.1.dist-info | tokenizers.libs |
| cffi | h5py-3.8.0.dist-info | numpy-1.23.5.dist-info | python_dateutil-2.8.2.dist-info | tomli |
| cffi-1.15.1.dist-info | h5py.libs | numpy.libs | pytz | tomli-2.0.1.dist-info |
| _cffi_backend.cpython-38-x86_64-linux-gnu.so | huggingface_hub | nvfuser | pytz-2022.7.dist-info | torch |
| charset_normalizer | huggingface_hub-0.14.1.dist-info | oauthlib | pywaggle-0.55.1.dist-info | torch-2.0.0.dist-info |
| charset_normalizer-2.1.1.dist-info | idna | oauthlib-3.2.2.dist-info | pywagglemsg-0.4.0.dist-info | torchaudio |
| clang | idna-3.4.dist-info | opencv_python-4.7.0.72.dist-info | PyYAML-6.0.dist-info | torchaudio-2.0.1+3b40834.dist-info |
| clingo | importlib_metadata | opencv_python.libs | readline.py | torchgen |
| clingo-5.6.2.dist-info | importlib_metadata-6.6.0.dist-info | opt_einsum | regex | torchvision |
| contourpy | importlib_resources | opt_einsum-3.3.0.dist-info | regex-2023.5.5.dist-info | torchvision-0.15.1a0+42759b1.dist-info |
| contourpy-1.0.7.dist-info | importlib_resources-5.12.0.dist-info | packaging | requests | tqdm |
| cv2 | iniconfig | packaging-23.1.dist-info | requests-2.28.1.dist-info | tqdm-4.65.0.dist-info |
| cycler-0.11.0.dist-info | iniconfig-2.0.0.dist-info | pasta | requests_oauthlib | transformers |
| cycler.py | isympy.py | pika | requests_oauthlib-1.3.1.dist-info | transformers-4.29.2.dist-info |
| dateutil | jax | pika-1.3.2.dist-info | rsa | typing_extensions-4.6.0.dist-info |
| _distutils_hack | jax-0.4.10.dist-info | PIL | rsa-4.9.dist-info | typing_extensions.py |
| distutils-precedence.pth | jinja2 | Pillow-9.5.0.dist-info | s3transfer | urllib3 |
| exceptiongroup | Jinja2-3.1.2.dist-info | Pillow.libs | s3transfer-0.5.2.dist-info | urllib3-1.26.13.dist-info |
| exceptiongroup-1.1.1.dist-info | jmespath | pip | scipy | waggle |
| filelock | jmespath-0.10.0.dist-info | pip-23.1.2.dist-info | scipy-1.10.1.dist-info | wagglemsg |
| filelock-3.12.0.dist-info | keras | pkg_resources | scipy.libs | werkzeug |
| flatbuffers | keras-2.12.0.dist-info | platformdirs | setuptools | Werkzeug-2.3.4.dist-info |
| flatbuffers-23.5.9.dist-info | kiwisolver | platformdirs-3.5.1.dist-info | setuptools-65.6.3.dist-info | wheel |
| fontTools | kiwisolver-1.4.4.dist-info | pluggy | six-1.16.0.dist-info | wheel-0.38.4.dist-info |
| fonttools-4.39.4.dist-info | libclang-16.0.0.dist-info | pluggy-1.0.0.dist-info | six.py | wrapt |
| fsspec | markdown | pooch | sympy | wrapt-1.14.1.dist-info |
| fsspec-2023.5.0.dist-info | Markdown-3.4.3.dist-info | pooch-1.7.0.dist-info | sympy-1.12.dist-info | _yaml |
| functorch | markupsafe | protobuf-4.23.1.dist-info | tensorboard | yaml |
| gast | MarkupSafe-2.1.2.dist-info | pyasn1 | tensorboard-2.12.3.dist-info | zipp |
| gast-0.4.0.dist-info | matplotlib | pyasn1-0.5.0.dist-info | tensorboard_data_server | zipp-3.15.0.dist-info |

```
Singularity> python
Python 3.8.10 (default, Nov 14 2022, 12:59:47)
[GCC 9.4.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import torch
>>> import tensorflow
>>> import scipy
>>> import numpy
>>> import matplotlib
>>> import keras
>>>
```

**cd /cm/shared/apps/containers/singularity/e4s/v23.05**

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# E4S includes Julia with support for CUDA and MPI

```
Singularity> which julia
/usr/local/julia/1.9.0/bin/julia
Singularity> cd /opt/demo/Julia/
GrayScott.jl/  Mandelbrot/    MPI_example/
Singularity> cd /opt/demo/Julia/MPI_example/
Singularity> ls
foo.jl  run.sh
Singularity> cat foo.jl
# examples/01-hello.jl
using MPI
MPI.Init()

comm = MPI.COMM_WORLD
println("Hello world, I am $(MPI.Comm_rank(comm)) of $(MPI.Comm_size(comm))")
MPI.Barrier(comm)

# From: https://juliaparallel.org/MPI.jl/stable/usage/
Singularity> cat ./run.sh
#!/bin/bash
mpirun -np 4 julia --project ./foo.jl
Singularity> ./run.sh
Hello world, I am 0 of 4Hello world, I am 1 of 4Hello world, I am 2 of 4Hello world, I am 3 of 4


Singularity> ▊
```

# Considerations while deploying HPC/AI workloads to the cloud

- Which cloud provider?
  - AWS, OCI, GCP, Azure, …
  - Why not all?

- HPC and AI/ML workloads need low latency, high bandwidth
  - Which MPI?

- Which image?
  - Base Ubuntu without HPC tools or libraries? Too steep a learning curve

- Provisioning and building the image on different cloud providers
  - Command line interfaces can be cumbersome to use

- Bursting to the cloud from on-prem clusters using batch submission scripts?

# Key considerations for cloud-based deployment for E4S

- MPI - the core inter-node communication library has several implementations
  - Intel MPI, MVAPICH2-X, OpenMPI
  - Interfacing MPI with the job scheduling package (MOAB, Torque, SLURM)

- Cloud providers have different inter-node network adapters:
  - Elastic Fabric Adapter (EFA) on AWS
  - Infiniband on Azure
  - Mellanox Connect-X 5 Ethernet (ROCE) on Oracle Cloud Infrastructure (OCI)

- Intra-node communication with XPMEM (driver and kernel module support is critical)

- GPU Direct Async (GDR) support for communication between GPUs in MVPICH-Plus release

- ParaTools, Inc. building E4S optimized with MVAPICH-Plus for AWS, OCI, GCP, and Azure

- Using Adaptive Computing's ODDC interface to launch E4S jobs on multiple cloud providers!

# Adaptive Computing's ODDC interface for E4S
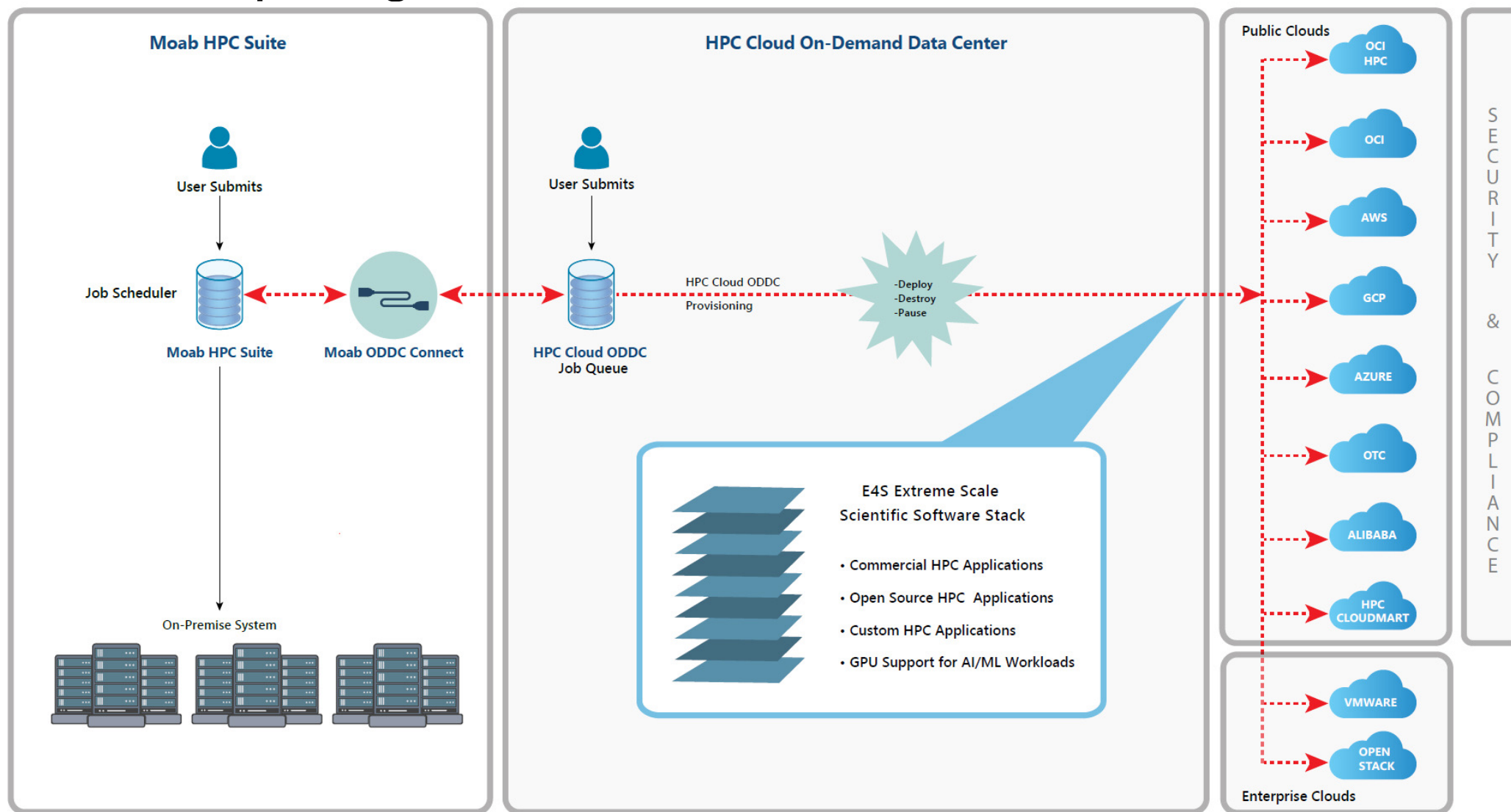
# E4S 23.05 AWS image: US-West2 (OR)



E4S 23.05 AWS
- Intel oneAPI
- CUDA
- NVHPC
- ROCm
- AWS DCV
- Spack Build Cache
- ECP: Nalu-Wind
- Trilinos 13.4.0
- OpenFOAM
- ParaView
- TAU
- Docker
- Shifter
- Charliecloud
- E4S Singularity
- EDA tools…

# E4S for Commercial Cloud Platforms for EDA on AWS

- <u>E4S</u>: HPC Software Ecosystem – a curated software portfolio for Electronic Design Automation



## E4S EDA on AWS

- Magic
- ACT
- Klayout
- Qflow
- Xschem
- Xcircuit
- Yosys
- Volator
- OpenROAD
- OpenLane
- OpenFASOC
- iVerilog
- Gtkwave
- Irsim
- Qrouter
- Fault
- GDS3D
- Rggen
- Python tools
  - Cocotb
  - Amaranth
  - Edalize
  - Gdsfactory
  - Gdspy
  - OpenRAM
  - Gdstk
  - Silicon compiler
  - Volare …
- PDKs
  - GF
  - Skywater

## https://e4s.io/eda

# E4S for Commercial Cloud Platforms for EDA on AWS

- **E4S**: HPC Software Ecosystem – a curated software portfolio for Electronic Design Automation

- OpenROAD
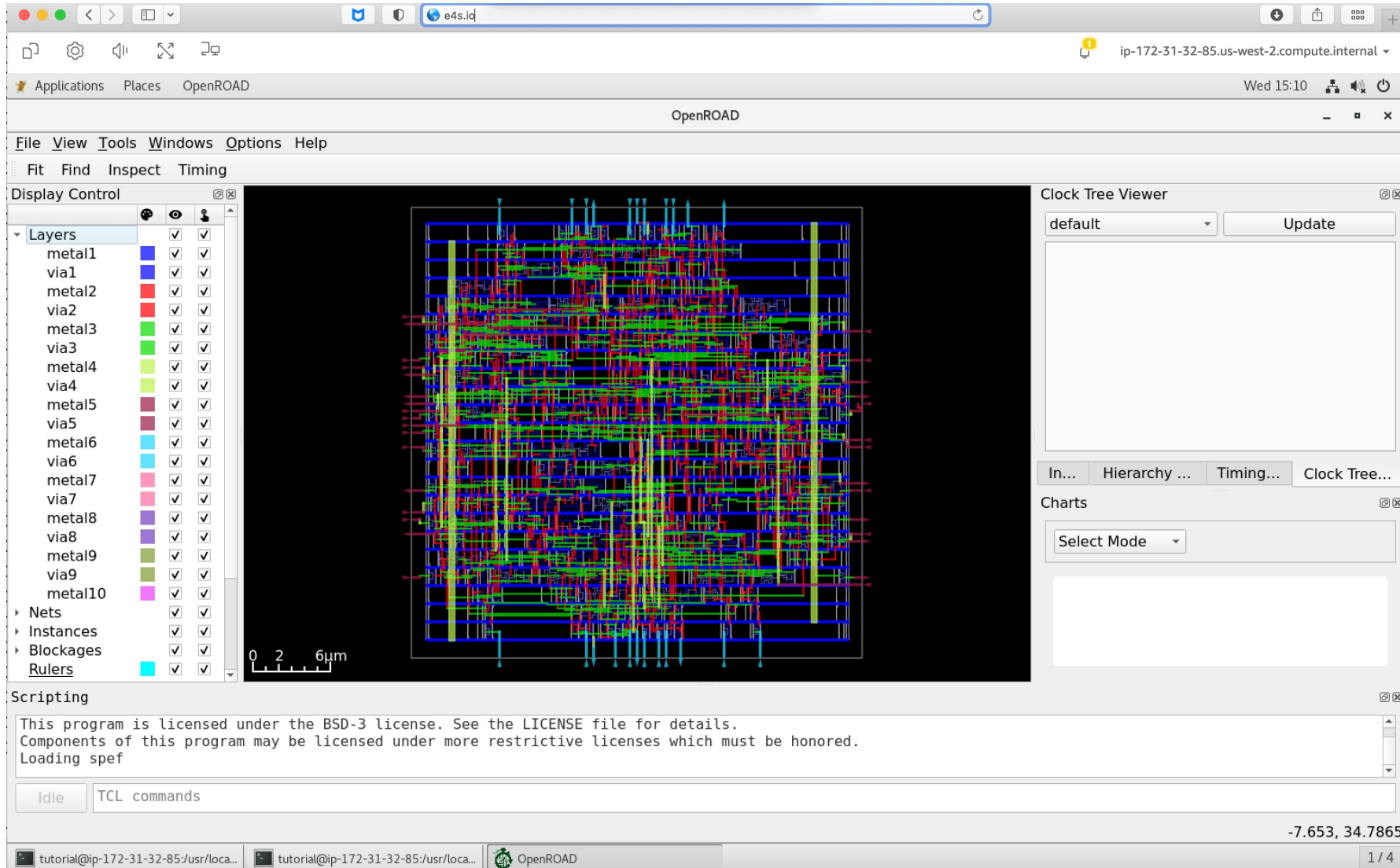


**E4S EDA on AWS**
- Magic
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- Fault
- GDS3D
- Rggen
- Python tools
  - Cocotb
  - Amaranth
  - Edalize
  - Gdsfactory
  - Gdspy
  - OpenRAM
  - Gdstk
  - Silicon compiler
  - Volare …
- PDKs
  - GF
  - Skywater

# E4S for Commercial Cloud Platforms for EDA on AWS

- **E4S**: HPC Software Ecosystem – a curated software portfolio for Electronic Design Automation

| # | Packages currently in E4S | URL |
|---|---|---|
| 1 | Magic | http://opencircuitdesign.com/magic/ |
| 2 | Xyce | https://xyce.sandia.gov |
| 3 | NGSPICE | https://ngspice.sourceforge.io |
| 4 | KLayout | https://www.klayout.de |
| 5 | Qflow | http://opencircuitdesign.com/qflow |
| 6 | OR-Tools | https://developers.google.com/optimization |
| 7 | IRSIM | http://opencircuitdesign.com/irsim/ |
| 8 | OpenROAD | https://github.com/The-OpenROAD-Project/OpenROAD |
| 9 | OpenLane | https://openlane.readthedocs.io/ |
| 10 | OpenFASOC | https://openfasoc.readthedocs.io/ |
| 11 | Open_PDKs | http://opencircuitdesign.com/open_pdks/ |
| 12 | Netgen | http://opencircuitdesign.com/netgen/ |

| # | Packages currently in E4S | URL |
|---|---|---|
| 13 | Yosys | https://github.com/YosysHQ/yosys |
| 14 | Xcircuit | http://opencircuitdesign.com/xcircuit/ |
| 15 | Graywolf | https://github.com/rubund/graywolf |
| 16 | OpenSTA | https://github.com/The-OpenROAD-Project/OpenSTA |
| 17 | OpenTimer | https://github.com/OpenTimer/OpenTimer |
| 18 | Qrouter | http://opencircuitdesign.com/qrouter/ |
| 19 | Xscheme | https://github.com/silicon-vlsi-org/eda-xschem |
| 20 | RISC-V GNU Toolchain | https://github.com/riscv-collab/riscv-gnu-toolchain |
| 21 | Fault: Design for Test | https://github.com/AUCOHL/Fault |
| 22 | NVC | https://github.com/nickg/nvc |
| 23 | Amaranth | https://github.com/amaranth-lang/amaranth |
| 24 | Cocotb | https://github.com/cocotb/cocotb |

## https://e4s.io/eda

# E4S for Commercial Cloud Platforms for EDA on AWS

- <u>E4S</u>: HPC Software Ecosystem – a curated software portfolio for Electronic Design Automation

| # | Packages currently in E4S | URL |
|---|---|---|
| 25 | Covered | https://github.com/hpretl/verilog-covered |
| 26 | Edalize | https://github.com/olofk/edalize |
| 27 | Gaw3-xschem | https://github.com/StefanSchippers/xschem-gaw.git |
| 28 | GDSFactory | https://github.com/gdsfactory/gdsfactory |
| 29 | GDSPy | https://github.com/heitzmann/gdspy |
| 30 | GDS3D | https://github.com/trilomix/GDS3D |
| 31 | Ghdl | https://github.com/ghdl/ghdl |
| 32 | Gtkwave | https://github.com/gtkwave/gtkwave |
| 33 | iic-osic | https://github.com/hpretl/iic-osic.git |
| 34 | Iverilog | https://github.com/steveicarus/iverilog.git |
| 35 | Netlistsvg | https://github.com/nturley/netlistsvg |
| 36 | Ngspyce | https://github.com/ignamv/ngspyce |

| # | Packages currently in E4S | URL |
|---|---|---|
| 37 | Padring | https://github.com/donn/padring |
| 38 | Pyverilog | https://github.com/PyHDI/Pyverilog |
| 39 | OpenRAM | https://github.com/VLSIDA/OpenRAM |
| 40 | Rggen | https://github.com/rggen/rggen |
| 41 | Spyci | https://github.com/gmagno/spyci |
| 42 | Volare | https://github.com/efabless/volare |
| 43 | Siliconcompiler | https://github.com/siliconcompiler/siliconcompiler |
| 44 | Verilator | https://github.com/verilator/verilator |
| 45 | Sky130 | SkyWater Technologies 130nm CMOS PDK |
| 46 | Actflow | https://github.com/asyncvlsi/actflow.git |
| 47 | Qucs-s | https://github.com/Qucs |
| 48 | ADMS | https://github.com/Qucs/ADMS.git |
| 49 | Gdstk | https://heitzmann.github.io/gdstk/ |
| 50 | xcell | https://github.com/asyncvlsi/xcell.git |

# https://e4s.io/eda

EXASCALE COMPUTING PROJECT

# Spack

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

# Spack is a flexible package manager for HPC

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

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

- How to install a package:

```
$ spack install tau
```

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

- Unlike typical package managers, Spack can also install many variants of the same build.

  - Different compilers
  - Different MPI implementations
  - Different build options
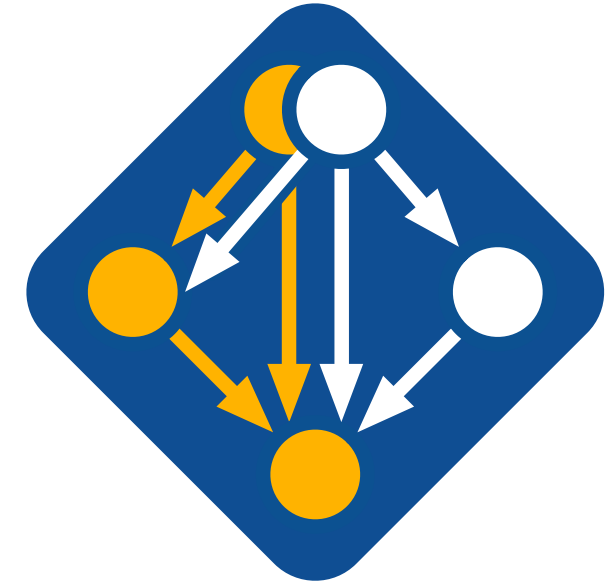
**Visit spack.io**

**github.com/spack/spack**

**@spackpm**

# Spack provides the *spec* syntax to describe custom configurations

```
$ git clone https://github.com/spack/spack
$ . spack/share/spack/setup-env.sh
$ spack compiler find                                          # set up compilers
$ spack external find                                          # set up external packages
```

```
$ spack install tau                                            unconstrained
$ spack install tau@2.32                                       @ custom version
$ spack install tau@2.32 %gcc@9.3.0                            % custom compiler
$ spack install tau@2.32 %gcc@9.3.0 +rocm                      +/- build option
$ spack install tau@2.32 %gcc@9.3.0 +mpi ^mvapich2@2.3~wrapperrpath   ^ 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

# The Spack community is growing rapidly

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

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

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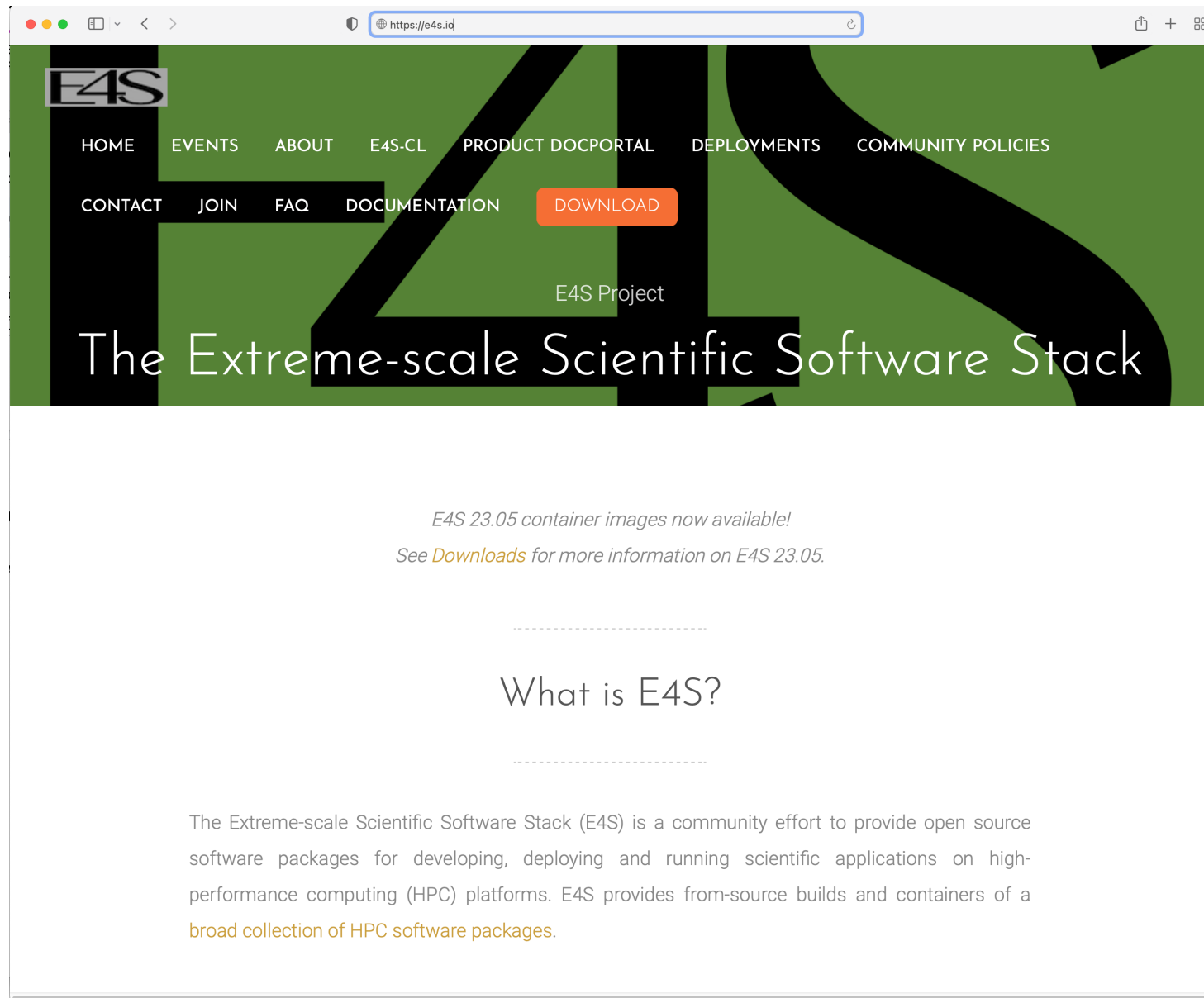  - Optimized binaries
  - Better dependency resolution
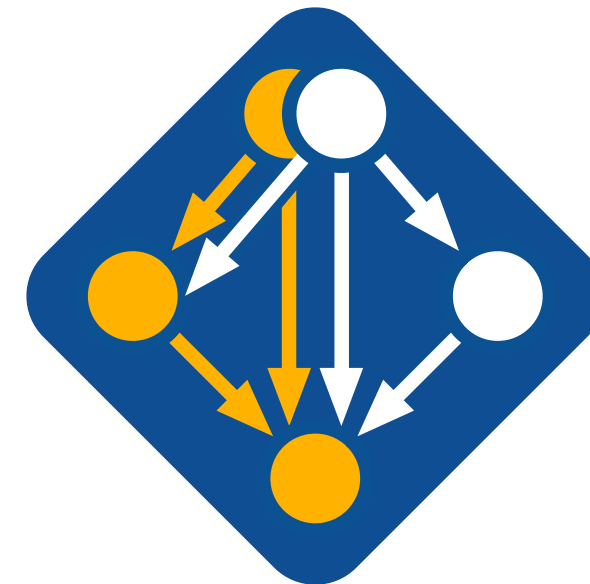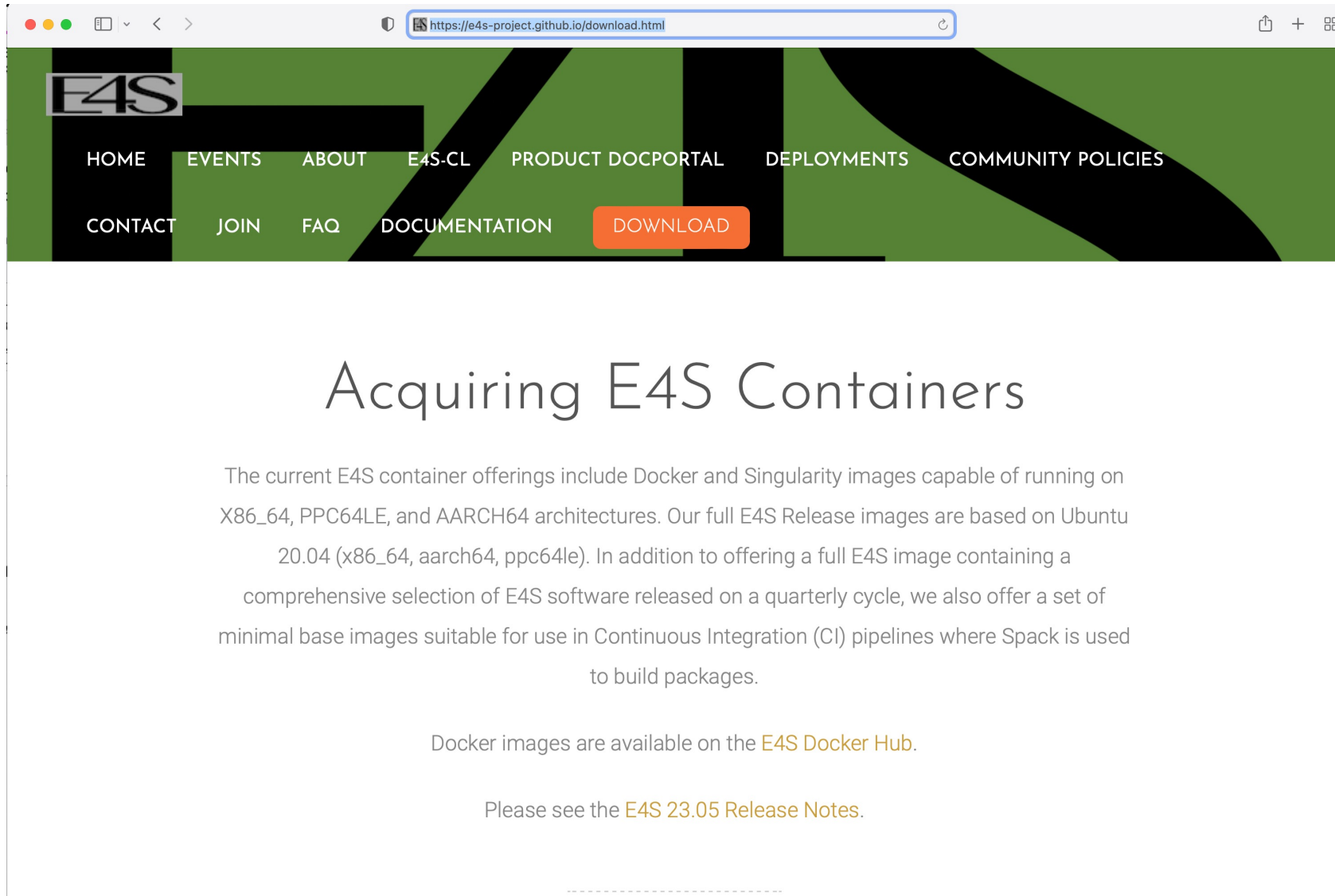
**Visit spack.io**

**github.com/spack/spack**

**@spackpm**

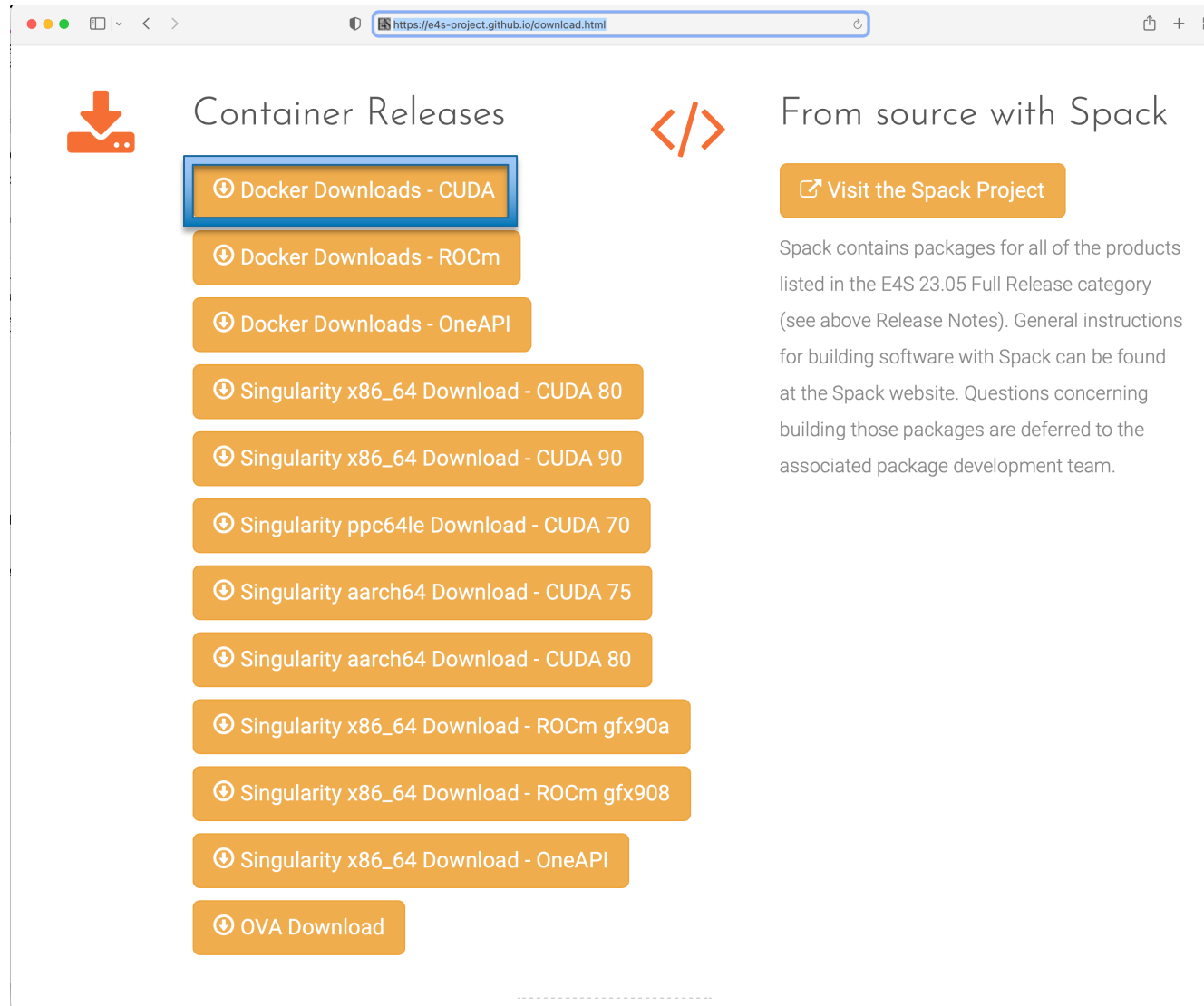# E4S Download from https://e4s.io

# E4S Container Download from https://e4s.io



Acquiring E4S Containers

The current E4S container offerings include Docker and Singularity images capable of running on X86_64, PPC64LE, and AARCH64 architectures. Our full E4S Release images 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.

Please see the E4S 23.05 Release Notes.

# Download E4S 23.05 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)
- Full featured images available on Dockerhub
- 100+ products on 3 architectures

https://e4s.io

# Download E4S 23.05 GPU Container Images: AMD, Intel, and NVIDIA



https://e4s.io

# Intel Compilers and MPI Libraries Now Accessible in E4S Containers: A Breakthrough Collaboration Driving Productivity and Sustainability

- Background:
  - E4S provides a unified software stack of libraries and tools for portable performance on HPC systems, especially GPU-based systems.
  - E4S promises seamless portability for onsite and cloud-based workflows through its container-based approach.
  - Intel compilers and libraries available in E4S accelerates preparations for Aurora and future Intel-based GPU systems.
  - E4S eliminates the need for separate management of access to Intel compilers and libraries, benefiting users
  - Many important workflows, especially regression testing and turnkey usage for Intel platforms become feasible and easier

- The E4S-Intel agreement makes Intel compilers and MPI libraries available via E4S containers:
  - Enables full testing and execution of HPC libraries and tools on Intel platforms via E4S, including Aurora early access systems
  - Represents a win-win for DOE, Intel, and the broader E4S user community that is developing at other US agencies and industry

- The Intel agreement brings Intel in line with E4S  builds that include AMD and NVIDIA tools.

- The E4S-Intel agreement is possible through the partnership of ECP and the E4S commercial provider, ParaTools, Inc.

# E4S base container images allow users to customize their containers



- Intel oneAPI
- AMD ROCm
- NVIDIA NVHPC and CUDA

https://e4s.io

# e4s-alc: a new tool to customize container images



Add to a base image:

- Spack packages
- OS packages
- Tarballs

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

# e4s-alc: E4S à la carte – a tool to customize container images

README.md

```
$ e4s-alc init
```

Create image

```
$ e4s-alc create \
      --image centos:8 \
      --name my-centos-image \
      -p py-numpy \
      -p autodiff
```

or

```
$ e4s-alc create \
      --image ubuntu:22.04 \
      --name my-ubuntu-image \
      --no-spack
```

or

```
$ cat test.json

{
      "image": "ubuntu:22.04",
      "name": "test-file-kokkos-raja",
      "spack": true,
      "spack-packages": [
            "kokkos",
            "raja"
      ],
      "os-packages": [
            "neovim",
            "valgrind"
      ]
}

$ e4s-alc create -f test.json
```

Add packages to a container image:
- Spack packages
- OS packages (yum/apt/zypper)
- Add a tarball to a location
- Create a new container image
- Works for Docker & Singularity!

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

EXASCALE
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# E4S 23.05 DOE LLVM and CI images



https://e4s.io

# E4S 23.05 Detailed Documentation for Bare-metal Installation



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

E4S

HOME    EVENTS    ABOUT    E4S-CL    PRODUCT DOCPORTAL    DEPLOYMENTS    COMMUNITY POLICIES    CONTACT    JOIN    FAQ

DOCUMENTATION    DOWNLOAD

## Extreme-scale Scientific Software Stack (E4S)
## version 23.05

Exascale Computing Project (ECP) Software Technologies (ST) software, Extreme-scale Scientific Software Stack (E4S) v23.05, includes a subset of ECP ST software products, and demonstrates the target approach for future delivery of the full ECP ST software stack. Also available are a number of ECP ST software products that support a Spack package, but are not yet fully interoperable. As the primary purpose of the v23.05 is demonstrating the ST software stack release approach, not all ECP ST software products were targeted for this release. Software products were targeted primarily based on existing Spack package maturity, location within the scientific software stack, and ECP SDK developer experience with the software. Each release will include additional software products, with the ultimate goal of including all ECP ST software products.

**E4S ReadTheDocs: Full Documentation.**

**E4S ReadTheDocs: Support Guide.**

E4S Deployment Dashboard.

E4S v23.05 Release Notes PDF.

E4S v23.05 Spack Environment Notes.
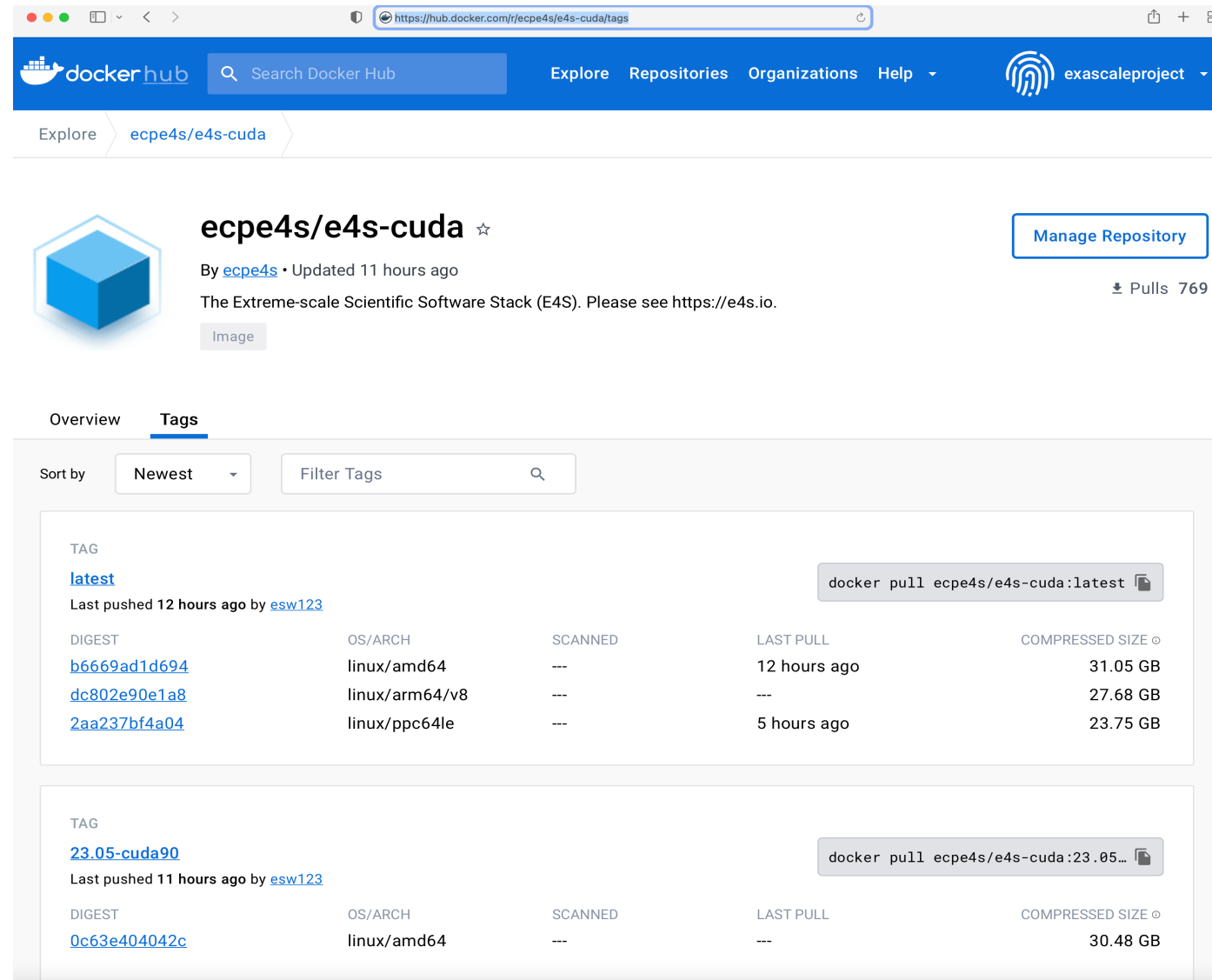
E4S Manual Installation Instructions.

E4S Container Installation Instructions.

Recipes for building E4S images from scratch.

Prebuilt binaries used in E4S images are stored in the E4S Build Cache.

ECP EXASCALE COMPUTING PROJECT

# E4S 23.05 full featured container release on Dockerhub



Architectures:
- x86_64
- aarch64
- ppc64le

Software:
- CUDA 12.0
- NVHPC 23.3
- oneAPI 2023.1

docker pull ecpe4s/e4s-cuda:23.05

# E4S 23.05 base container release on DockerHub



Architectures:
- x86_64
- aarch64
- ppc64le

Software:
- CUDA 12.0
- NVHPC 23.3
- oneAPI 2023.1

docker pull ecpe4s/e4s-base-cuda

# Minimal Spack base image on Dockerhub



- Create custom container images
- 1M+ downloads!

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

```
 1:  adios2             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/adios2-2.9.0-wr34ihoz2sk6iarctnuyxfhsctxwkvq4
 2:  alquimia           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/alquimia-1.0.10-gba5ayv4ps6ilmh5hc7krkoa4h3ksbvz
 3:  aml                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/aml-0.2.0-goqtywxxw2lwciznqkc44paexlucn33v
 4:  amrex              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/amrex-23.05-2syxxbx3xwppc4ut7mbrmlev4ycty4ep
 5:  arborx             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/arborx-1.3-cvlmzk4kzetidsscc4nd4oprdyvcsp3l
 6:  archer             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/archer-2.0.0-vl5rv2ygrh4znug7rdk6jhh6t4nemk5l
 7:  argobots           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/argobots-1.1-f6b6was4pd7d2u2fwvpxdoqffdbate2o
 8:  axom               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/axom-0.7.0-epaxouqc4ul2kppggnhtvnjl6fr3goik
 9:  bolt               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/bolt-2.0-zb4pgmqyozhf3ofvhdo26gpj2hibbc2t
10:  bricks             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/bricks-r0.1-ymuymne4nwfwytzckstwl6macyp6kkk2
11:  butterflypack      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/butterflypack-2.2.2-kzdbd4fzvqfjn575hojafxlen2gzwx2n
12:  cabana             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/cabana-0.5.0-hit7qxj2pwnvgmd5kkaeglbnvqsdgf7n
13:  caliper            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/caliper-2.9.0-cthblsk6ogn43qnufgbxczjvcrawqzab
14:  chai               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/chai-2022.03.0-6gi2vpoxdvy25sat6cdubunutp24i5sk
15:  charliecloud       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/charliecloud-0.32-bmfm6chwp4g6mgnhjgcrh356gusbrzes
16:  conduit            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/conduit-0.8.7-mfdfackt6xuqmyfqdwtiwszivxtrwho2
17:  darshan-runtime    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/darshan-runtime-3.4.2-nfblomjg6ejmigmmhu3dux6v7iojxnpf
18:  datatransferkit    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/datatransferkit-3.1-rc3-enk32naiegjk42bex5mvuk3y3mefdef6
19:  dyninst            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/dyninst-12.3.0-k3myl3szf7v3e2jcqoqwwglwyig4444o
20:  ecp-data-vis-sdk   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/ecp-data-vis-sdk-1.0-s4ya3uqeb2ecyextvb42yprv5zy5l2qk
21:  exaworks           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/exaworks-0.1.0-lxqwv3cswo6pglbycqcacwatuhf6iln2
22:  faodel             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/faodel-1.2108.1-gxc7m6ajdyb2jupcvx5qrvppe4jlcqt6
23:  flecsi             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flecsi-2.1.0-mfszzzew3vlkejgw43xuakoftuxrqnhm
24:  flit               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flit-2.1.0-3ptdgvs22o5ng3euhs6eci5nhaq4jctb
25:  flux-sched         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/flux-sched-0.27.0-snqo4rzjtvrmjkdvlkcixuw4vyt4ypie
26:  fortrilinos        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/fortrilinos-2.2.0-dlxz63fh2tljmw2rje5srgfgdbx64adv
27:  gasnet             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gasnet-2023.3.0-aufps4j5ilwaosagcfyhwe4anrv6uknz
28:  ginkgo             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/ginkgo-1.5.0-4gsh6pioh6qab3d67j7wtfk5qbfz7lnb
29:  globalarrays       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/globalarrays-5.8.2-nzag4ztsjddm67gdurpwtirprgb3rkgz
30:  gotcha             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gotcha-1.0.4-3rwc6g46qxsit3vswvzi6icv67li57wi
31:  gptune             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/gptune-4.0.0-dyxc7tkwnenjgl2edjqhvyg7eld643xx
32:  h5bench            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/h5bench-1.3-34odudjnlnjbfxl7a44e32gwmuoe6wn6
33:  hdf5               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hdf5-1.14.1-2-2naucnnhfn57lxmb3dcfls42m4hwdkeg
34:  hdf5-vol-async     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hdf5-vol-async-1.5-nwt25ouh2i5vtwvwsaijpnklgowag7ku
35:  heffte             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/heffte-2.3.0-rib3o742d45ng7ukq4qq4vh3lst5dccc
36:  hpctoolkit         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hpctoolkit-2023.03.01-sbctldelht4ntvzahpd6q5rj23fs25ar
37:  hpx                /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hpx-1.9.0-374gqtjzm47p6ea3xsuahpagrq2ogwvy
```

GPU runtimes
- AMD (ROCm)
  - 5.4.3
- NVIDIA (CUDA)
  - 12.0
- NVHPC
  - 23.3
- Intel oneAPI
  - 2023.1

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

```
38:  hypre            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/hypre-2.28.0-mozopbseodwvy7r7xklin7jnsuh5s7yi
39:  kokkos           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/kokkos-4.0.01-tgv5irdj4skczex6c2rvfty274vwuyk7
40:  kokkos-kernels   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/kokkos-kernels-3.7.00-2whrnbzjyni42dytgehkubhke2zgaj5u
41:  lammps           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/lammps-20220623.3-cso7xzxuaz5jyld3n6seug2cexxbfnpc
42:  lbann            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/lbann-0.102-hf442maq5bbf5nndr4fqlyhxakdndm23
43:  legion           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/legion-23.03.0-ksb4tvggo6sfcfjiicnszyr5appehqxn
44:  libnrm           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libnrm-0.1.0-h5ggd2cgai43porp2s2berqrsnki2j6c
45:  libpressio       /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libpressio-0.95.1-h54uerfc7gttwaokywa5cwntylrnklen
46:  libquo           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/libquo-1.3.1-e6ulmqqbtpfcjjypvdqrbpkb4brzkgpf
47:  loki             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/loki-0.1.7-a4etdi45t2fbweddhjur5t5p56tiu2ca
48:  magma            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/magma-2.7.1-dapbrjq25hsqg2cztteuusqkismcpnbu
49:  mercury          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mercury-2.2.0-iap2sil3mo6g6aljjvg34vtnxh2sglof
50:  metall           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/metall-0.25-2xic6pnhpbolhaknalu2qpjnw4bkvemi
51:  mfem             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mfem-4.5.2-2f3kkx62ogbv6bw6sdcybkawubvcyg2n
52:  mgard            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mgard-2023-03-31-4maqkp6n3e2xshtu2y3tnve5ch7jdb43
53:  mpark-variant    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpark-variant-1.4.0-6f25xadnfdzmpweuit4yvpl34katnt4s
54:  mpich            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpich-4.1.1-4cbi7qhusseuuh6bcs6lokwgwh6s3itl
55:  mpifileutils     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/mpifileutils-0.11.1-tuy2ycdld67kuv3ppp3diqy4o2bmvhok
56:  nccmp            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nccmp-1.9.0.1-qmoiwfcpcnknojwspffuvgrw3n3mphzb
57:  nco              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nco-5.1.5-wwe7fm6df3zhc6d6qckvbcyxo5dqawpf
58:  netlib-scalapack /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/netlib-scalapack-2.2.0-3zhwrxw6f2ohmbnpeec34ksb4h7svs65
59:  nrm              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/nrm-0.1.0-47ydygda2r3njdpkxyj4wrfpgfdt2zzl
60:  omega-h          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/omega-h-9.34.13-m2wmv5mmoxpoy622e6tbk7jzey2ufdvi
61:  openfoam         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openfoam-2206-zftm6f5mhvnhxben2nzeqantgg4lll5d
62:  openmpi          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openmpi-4.1.5-ed5u3cdcbks6dcve6ftb336v5uhwj4by
63:  openpmd-api      /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/openpmd-api-0.15.1-uzamcamznyauzeem57j72gx2ascjpmju
64:  papi             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/papi-6.0.0.1-j7dmzprtcei2ifgjykb7rmkbf3gydfk7
65:  papyrus          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/papyrus-1.0.2-kuro7vtc7kh6fot5xmah6awfwgi5chm2
66:  parallel-netcdf  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/parallel-netcdf-1.12.3-mldyjplnyhw7qiljd327wda7exvpcvtf
67:  paraview         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/paraview-5.11.1-x4aqroj67nfq7gpk7w3pwlxhpfhjyrno
68:  parsec           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/parsec-3.0.2209-wvchc4psqj3uotxff24xyc24xqwprzdg
69:  pdt              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/pdt-3.25.1-lx67nrs24pkbnmnj7am3t75swtowtfc5
70:  petsc            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/petsc-3.19.1-bonrfxf3arijwtulzcck4xqyd3ceik63
71:  phist            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/phist-1.11.2-qz36u6cuvuupj3gj5v7hmm4sdbrzdljv
72:  plasma           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/plasma-22.9.29-2qwdll5vjs74mymdiugdhd32iiibm2v3
73:  plumed           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/plumed-2.8.2-oq5243vtzgcl6ex6zookbxqgaeofkzxh
74:  precice          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/precice-2.5.0-b7eniikqkee5veujb5xnuukfnz7wiwm2
75:  pumi             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/pumi-2.2.7-57q5bidz4mzlldkfpwaovebwqhvxgps3
76:  py-cinemasci     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-cinemasci-1.3-5tnt5kqnzrin5j5dmse6gdq77mteiiyz
77:  py-jupyterhub    /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-jupyterhub-1.4.1-awj3cwfv2d3irsm24dmr37gbhd5xniju
```

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

```
 78:  py-libensemble   /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-libensemble-0.9.3-3d3tb25q2s3pa7uqscw7wlpz5rqmapa5
 79:  py-parsl         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-parsl-1.2.0-f7tbq4nmfecdu3nh5fw5zyddwj77zis5
 80:  py-radical-saga  /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/py-radical-saga-1.20.0-wffrzdrcdd4cpst42gtqonbjni7m5pqe
 81:  qthreads         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/qthreads-1.16-r4ai62sxg3os22n2xfntik7xbcvijgst
 82:  quantum-espresso /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/quantum-espresso-7.1-2hw2nzkjwtc4xi3hopd2oesn2ikmcb5e
 83:  raja             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/raja-2022.10.4-fffdno3g4c4wm6f2d5rbrehnjgv3ytw4
 84:  rempi            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/rempi-1.1.0-bsppojvqc4e4bf7re6u36f75dwo6wnuv
 85:  scr              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/scr-3.0.1-4twvdurdxeiv3ipees4y3nk64pmvtrbl
 86:  slate            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/slate-2022.07.00-5xkozs6eabgn45t7uttghekbu4lanbwk
 87:  slepc            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/slepc-3.19.0-vqy6iy24c5wkpfdsejjgql2bx32vjfbq
 88:  stc              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/stc-0.9.0-ocmzafclc6rsl2dop3poqjbnlyyk7vs2
 89:  strumpack        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/strumpack-7.1.1-7feghsapq3qe7stmbfodzcytm7tm44lt
 90:  sundials         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/sundials-6.5.1-f23kbyw7bsam3cpka2mshks36d236yr3
 91:  superlu-dist     /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/superlu-dist-8.1.2-ibmrgavx57kcy3fc7wdbcneuhk6axgxv
 92:  swig             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/swig-4.1.1-cm45hunq4nk7x4ml756gur5wlakaidha
 93:  sz               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/sz-2.1.12.2-bbc3ru73fa67nmr7j4jbv53f6ji5e4xe
 94:  tasmanian        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/tasmanian-7.9-4skuz4cxghjjhlhad776xbixk3jvienk
 95:  tau              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/tau-2.32-qxwqmtdsjoaxnrjed5mvlolax5ip273z
 96:  trilinos         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/trilinos-14.0.0-alm3rf45sel6ahz7ecfs5odq3eziqcah
 97:  turbine          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/turbine-1.3.0-sla74mxwn5michnji2aqmrf3gbphfqco
 98:  umap             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/umap-2.1.0-de4ftza63dmgjgvv5uhceeunn2dvkqig
 99:  umpire           /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/umpire-2022.03.1-spprgtmz5vvvsxxhwngyu7dxbghmdpij
100:  unifyfs          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/unifyfs-1.0.1-q4bmwojbzaa2npnbcp2q4flba5u5oshd
101:  upcxx            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/upcxx-2023.3.0-ideeur7hshemz4ahe2col65tiryjfngh
102:  variorum         /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/variorum-0.6.0-h3oif6j2nvgq4qzxjx773bjnef5owexx
103:  veloc            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/veloc-1.6-5g5n244a6mo3i3dlcjxxlq7e3l5tv426
104:  visit            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/visit-3.3.3-nt4yv7ecffq2onv5xznqja42uzt6tqlb
105:  vtk-m            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/vtk-m-2.0.0-7rjk76kmxbf4bmyvepvfj5qsclkfz3uw
106:  wannier90        /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/wannier90-3.1.0-dbfs2qlo2yvdxjtcb5mn5d2xlnvplnzc
107:  warpx            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/warpx-23.03-f2nbmfppld7xntj2lpwy552upvwj6bq2
108:  xyce             /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/xyce-7.6.0-vt3rht5enpklqck7m7d2z7ji64memqwz
109:  zfp              /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/zfp-1.0.0-ibmowr23apboprdgjrrp4eyblmibwd2w
```

Languages:
- Julia with support for MPI, and CUDA
- Python

AI products with GPU support
- Tensorflow
- Pytorch

EDA Tools:
- Xyce

3D Visualization
- Paraview
- VisIt
- TAU's paraprof …

E4S 23.05 adds support for NVIDIA A100 (sm80), V100 (sm70), and H100 (sm90) GPUs

# E4S 23.05 Intel oneAPI 2023.1: Packages built with Intel compilers

```
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 -----------------------
papi@6.0.0.1

-- linux-ubuntu20.04-x86_64 / oneapi@2023.1.0 ------------------
adios@1.13.1         cabana@0.5.0         gmp@6.2.1            legion@23.03.0       netlib-scalapack@2.2.0  py-libensemble@0.9.3  sz3@3.1.7
aml@0.2.0            cabana@0.5.0         gotcha@1.0.4         libnrm@0.1.0         omega-h@9.34.13         py-petsc4py@3.19.1    tasmanian@7.9
aml@0.2.0            caliper@2.9.0        h5bench@1.3          libquo@1.3.1         openmpi@4.1.5           qthreads@1.16         tau@2.32
amrex@22.12          chai@2022.03.0       hdf5-vol-async@1.5   libunwind@1.6.2      openpmd-api@0.15.1      quantum-espresso@7.1  tau@2.32
amrex@23.05          charliecloud@0.32    hdf5-vol-log@1.4.0   loki@0.1.7           papyrus@1.0.2           raja@2022.10.4        trilinos@13.0.1
arborx@1.3           conduit@0.8.7        heffte@2.3.0         mercury@2.2.0        parsec@3.0.2209         rempi@1.1.0           turbine@1.3.0
arborx@1.3           datatransferkit@3.1-rc3  hpx@1.9.0        metall@0.25          pdt@3.25.1              slate@2022.07.00      umap@2.1.0
archer@2.0.0         exaworks@0.1.0       hypre@2.28.0         mfem@4.5.2           petsc@3.19.1            slepc@3.19.0          umpire@2022.03.1
argobots@1.1         flecsi@2.2.0         kokkos@4.0.01        mgard@2023-03-31     phist@1.11.2            stc@0.9.0             variorum@0.6.0
axom@0.7.0           flit@2.1.0           kokkos@4.0.01        mpark-variant@1.4.0  plasma@22.9.29          strumpack@7.1.1       wannier90@3.1.0
bolt@2.0             flux-core@0.49.0     kokkos-kernels@3.7.00  mpich@4.1.1        plumed@2.8.2            sundials@6.5.1
boost@1.82.0         fortrilinos@2.2.0    kokkos-kernels@3.7.00  mpifileutils@0.11.1  precice@2.5.0         superlu@5.3.0
bricks@r0.1          gasnet@2023.3.0      lammps@20220623.3    nccmp@1.9.0.1        pumi@2.2.7              superlu-dist@8.1.2
butterflypack@2.2.2  globalarrays@5.8.2   lbann@0.102          nco@5.1.5            py-h5py@3.7.0           swig@4.0.2-fortran
```

Use of Intel oneAPI BaseKit and HPCToolkit is subject to acceptance of Intel EULA by the user

# E4S 23.05 Intel oneAPI 2023.1: Packages built with Intel compilers

```
Singularity> module avail

---------------------------------------- /opt/intel/oneapi/modulefiles ----------------------------------------
   advisor/latest                  compiler32/latest             dnnl-cpu-tbb/latest          inspector/latest                           mpi/latest
   advisor/2023.1.0      (D)       compiler32/2023.1.0   (D)     dnnl-cpu-tbb/2023.1.0 (D)    inspector/2023.1.0            (D)           mpi/2021.9.0     (D)
   ccl/latest                      dal/latest                    dnnl/latest                  intel_ipp_intel64/latest                   oclfpga/latest
   ccl/2021.9.0          (D)       dal/2023.1.0          (D)     dnnl/2023.1.0         (D)     intel_ipp_intel64/2021.8.0   (D)           oclfpga/2023.1.0 (D)
   clck/latest                     debugger/latest               dpl/latest                   intel_ippcp_intel64/latest                 tbb/latest
   clck/2021.7.3         (D)       debugger/2023.1.0     (D)     dpl/2022.1.0          (D)     intel_ippcp_intel64/2021.7.0 (D)           tbb/2021.9.0     (D)
   compiler-rt/latest              dev-utilities/latest          icc/latest                   itac/latest                                vtune/latest
   compiler-rt/2023.1.0  (D)       dev-utilities/2021.9.0 (D)    icc/2023.1.0          (D)     itac/2021.9.0                (D)           vtune/2023.1.0   (D)
   compiler-rt32/latest            dnnl-cpu-gomp/latest          icc32/latest                 mkl/latest
   compiler-rt32/2023.1.0 (D)      dnnl-cpu-gomp/2023.1.0 (D)    icc32/2023.1.0        (D)     mkl/2023.1.0                 (D)
   compiler/latest                 dnnl-cpu-iomp/latest          init_opencl/latest           mkl32/latest
   compiler/2023.1.0     (D)       dnnl-cpu-iomp/2023.1.0 (D)    init_opencl/2023.1.0  (D)     mkl32/2023.1.0               (D)

---------------------------------------- /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/mpich/4.1.1/Core ----------------------------------------
   adios/1.13.1                    datatransferkit/3.1-rc3       libnrm/0.1.0                 petsc/3.19.1                   strumpack/7.1.1-openmp
   amrex/22.12-sycl                exaworks/0.1.0                libquo/1.3.1                 phist/1.11.2-openmp            sundials/6.5.1
   amrex/23.05            (D)      flecsi/2.2.0                  mercury/2.2.0                plumed/2.8.2                   superlu-dist/8.1.2
   arborx/1.3-sycl                 fortrilinos/2.2.0             metall/0.25                  precice/2.5.0                  tasmanian/7.9
   arborx/1.3             (D)      globalarrays/5.8.2            mfem/4.5.2                   pumi/2.2.7                     tau/2.32-level-zero    (L)
   axom/0.7.0-openmp               h5bench/1.3                   mpifileutils/0.11.1          py-h5py/3.7.0                  tau/2.32               (D)
   boost/1.82.0                    hdf5-vol-async/1.5            nccmp/1.9.0.1                py-libensemble/0.9.3           trilinos/13.0.1
   bricks/r0.1                     hdf5-vol-log/1.4.0            nco/5.1.5                    py-petsc4py/3.19.1             turbine/1.3.0
   butterflypack/2.2.2-openmp      hefkte/2.3.0                  netlib-scalapack/2.2.0       quantum-espresso/7.1-openmp    wannier90/3.1.0
   cabana/0.5.0-sycl               hpx/1.9.0                     omega-h/9.34.13              rempi/1.1.0
   cabana/0.5.0          (D)       hypre/2.28.0                  openpmd-api/0.15.1           slate/2022.07.00-openmp
   caliper/2.9.0                   lammps/20220623.3-openmp      papyrus/1.0.2                slepc/3.19.0
   conduit/0.8.7                   lbann/0.102                   parsec/3.0.2209              stc/0.9.0

---------------------------------------- /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/Core ----------------------------------------
   aml/0.2.0-level-zero            flit/2.1.0                    kokkos/4.0.01-openmp          mpich/4.1.1              (L)   superlu/5.3.0
   aml/0.2.0             (D)       flux-core/0.49.0              kokkos/4.0.01-sycl-openmp (D) openmpi/4.1.5                  swig/4.0.2-fortran
   archer/2.0.0                    gasnet/2023.3.0               legion/23.03.0                papi/6.0.0.1             (L)   sz3/3.1.7
   argobots/1.1                    gmp/6.2.1                     libunwind/1.6.2          (L)  pdt/3.25.1                     umap/2.1.0
   bolt/2.0                        gotcha/1.0.4                  loki/0.1.7                    plasma/22.9.29                 umpire/2022.03.1
   chai/2022.03.0                  kokkos-kernels/3.7.00-openmp  mgard/2023-03-31-openmp       qthreads/1.16                  variorum/0.6.0
   charliecloud/0.32               kokkos-kernels/3.7.00-sycl (D) mpark-variant/1.4.0          raja/2022.10.4-openmp
```

Use of Intel oneAPI BaseKit and HPCToolkit is subject to acceptance of Intel EULA by the user

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

```
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 -----------------------
adios@1.13.1          chai@2022.03.0        gptune@4.0.0          libcatalyst@2.0.0-rc3  openpmd-api@0.15.1    py-warpx@23.03        tasmanian@7.9
adios2@2.9.0          charliecloud@0.32     h5bench@1.3           libnrm@0.1.0           papi@6.0.0.1          qthreads@1.16         tasmanian@7.9
alquimia@1.0.10       conduit@0.8.7         hdf5@1.12.2           libpressio@0.95.1      papyrus@1.0.2         quantum-espresso@7.1  tau@2.32
aml@0.2.0             darshan-runtime@3.4.2 hdf5@1.14.1-2         libquo@1.3.1           parallel-netcdf@1.12.3 raja@2022.10.4       tau@2.32
amrex@23.05           darshan-util@3.4.2    hdf5-vol-async@1.5    libunwind@1.6.2        paraview@5.11.1       raja@2022.10.4        trilinos@13.0.1
amrex@23.05           datatransferkit@3.1-rc3 hdf5-vol-cache@v1.1 loki@0.1.7            paraview@5.11.1       rempi@1.1.0           trilinos@14.0.0
arborx@1.3            dyninst@12.3.0        hdf5-vol-log@1.4.0     magma@2.7.1            parsec@3.0.2209       scr@3.0.1             turbine@1.3.0
arborx@1.3            ecp-data-vis-sdk@1.0  hdf5-vol-log@1.4.0     mercury@2.2.0          pdt@3.25.1            slate@2022.07.00      umap@2.1.0
archer@2.0.0          ecp-data-vis-sdk@1.0  heffte@2.3.0          metall@0.25            petsc@3.19.1          slate@2022.07.00      umpire@2022.03.1
argobots@1.1          exaworks@0.1.0        heffte@2.3.0          mfem@4.5.2             petsc@3.19.1          slepc@3.19.0          umpire@2022.03.1
ascent@0.9.1          faodel@1.2108.1       hpctoolkit@2023.03.01 mfem@4.5.2             phist@1.11.2          slepc@3.19.0          unifyfs@1.0.1
axom@0.7.0            flecsi@2.1.0          hpctoolkit@2023.03.01 mgard@2023-03-31       plasma@22.9.29        stc@0.9.0             upcxx@2023.3.0
bolt@2.0              flit@2.1.0            hpx@1.9.0             mpark-variant@1.4.0    plumed@2.8.2          strumpack@7.1.1       upcxx@2023.3.0
boost@1.79.0          flux-core@0.49.0      hpx@1.9.0             mpich@4.1.1            precice@2.5.0         strumpack@7.1.1       variorum@0.6.0
bricks@r0.1           fortrilinos@2.2.0     hypre@2.28.0          mpifileutils@0.11.1    pumi@2.2.7            sundials@6.5.1        veloc@1.6
butterflypack@2.2.2   gasnet@2023.3.0       hypre@2.28.0          nccmp@1.9.0.1          py-cinemasci@1.3      sundials@6.5.1        visit@3.3.3
cabana@0.5.0          gasnet@2023.3.0       kokkos@4.0.01         nco@5.1.5              py-h5py@3.7.0         superlu@5.3.0         vtk-m@1.9.0
cabana@0.5.0          ginkgo@1.5.0          kokkos@4.0.01         netlib-scalapack@2.2.0 py-jupyterhub@1.4.1   superlu-dist@8.1.2    vtk-m@2.0.0
cabana@0.5.0          ginkgo@1.5.0          kokkos-kernels@3.7.00 nrm@0.1.0             py-libensemble@0.9.3  superlu-dist@8.1.2    wannier90@3.1.0
caliper@2.9.0         globalarrays@5.8.2    lammps@20220623.3     omega-h@9.34.13        py-petsc4py@3.19.1    swig@4.0.2-fortran    xyce@7.6.0
caliper@2.9.0         gmp@6.2.1             lbann@0.102           openfoam@2206          py-warpx@23.03        sz@2.1.12.2           zfp@0.5.5
chai@2022.03.0        gotcha@1.0.4          legion@23.03.0        openmpi@4.1.5          py-warpx@23.03        sz3@3.1.7
==> 153 installed packages
```

E4S 23.05 supports AMD MI100 (gfx908) as well as MI250X (gfx90a) GPUs

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

```
Singularity> module avail

-------------------------------------- /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/mpich/4.1.1/Core --------------------------------------
    adios/1.13.1                         ginkgo/1.5.0-openmp          (D)   nccmp/1.9.0.1                      slate/2022.07.00-openmp          (D)
    adios2/2.9.0                         globalarrays/5.8.2                 nco/5.1.5                          slepc/3.19.0-gfx908
    alquimia/1.0.10                      gptune/4.0.0                       netlib-scalapack/2.2.0            slepc/3.19.0                     (D)
    amrex/23.05-gfx908                   h5bench/1.3                        omega-h/9.34.13                   stc/0.9.0
    amrex/23.05                    (D)   hdf5-vol-async/1.5                 openfoam/2206                      strumpack/7.1.1-gfx908-openmp
    arborx/1.3-gfx908                    hdf5-vol-cache/v1.1                openpmd-api/0.15.1                strumpack/7.1.1-openmp          (D)
    arborx/1.3                     (D)   hdf5-vol-log/1.4.0                 papyrus/1.0.2                      sundials/6.5.1-gfx908
    ascent/0.9.1-openmp                  hdf5/1.12.2                        parallel-netcdf/1.12.3           sundials/6.5.1                   (D)
    axom/0.7.0-openmp                    hdf5/1.14.1-2                (D)   paraview/5.11.1-gfx908           superlu-dist/8.1.2-gfx908
    boost/1.79.0                         heffte/2.3.0-gfx908                paraview/5.11.1             (D)   superlu-dist/8.1.2               (D)
    bricks/r0.1                          heffte/2.3.0                (D)   parsec/3.0.2209                   sz/2.1.12.2
    butterflypack/2.2.2-openmp           hpctoolkit/2023.03.01-rocm         petsc/3.19.1-gfx908               tasmanian/7.9-gfx908
    cabana/0.5.0-rocm-gfx90a             hpctoolkit/2023.03.01       (D)   petsc/3.19.1                (D)   tasmanian/7.9                    (D)
    cabana/0.5.0-rocm-gfx908             hpx/1.9.0-gfx908                   phist/1.11.2-openmp               tau/2.32-rocm                    (L)
    cabana/0.5.0                   (D)   hpx/1.9.0                    (D)   plumed/2.8.2                      tau/2.32                         (D)
    caliper/2.9.0-gfx908                 hypre/2.28.0-gfx908                precice/2.5.0                     trilinos/13.0.1
    caliper/2.9.0                  (D)   hypre/2.28.0                (D)   pumi/2.2.7                        trilinos/14.0.0-gfx908           (D)
    conduit/0.8.7                        lammps/20220623.3-openmp           py-cinemasci/1.3                  turbine/1.3.0
    darshan-runtime/3.4.2                lbann/0.102                        py-h5py/3.7.0                     unifyfs/1.0.1
    datatransferkit/3.1-rc3              libcatalyst/2.0.0-rc3              py-libensemble/0.9.3              upcxx/2023.3.0-gfx908
    dyninst/12.3.0-openmp                libnrm/0.1.0                       py-petsc4py/3.19.1               upcxx/2023.3.0                   (D)
    ecp-data-vis-sdk/1.0-gfx908          libpressio/0.95.1-openmp           py-warpx/23.03-dims2             veloc/1.6
    ecp-data-vis-sdk/1.0           (D)   libquo/1.3.1                       py-warpx/23.03-dims3             visit/3.3.3
    exaworks/0.1.0                       mercury/2.2.0                      py-warpx/23.03-dimsRZ       (D)   vtk-m/1.9.0-openmp
    faodel/1.2108.1                      metall/0.25                        quantum-espresso/7.1-openmp       vtk-m/2.0.0-gfx908               (D)
    flecsi/2.1.0                         mfem/4.5.2-gfx908                  rempi/1.1.0                       wannier90/3.1.0
    fortrilinos/2.2.0                    mfem/4.5.2                   (D)   scr/3.0.1                         xyce/7.6.0
    ginkgo/1.5.0-gfx908-openmp           mpifileutils/0.11.1                slate/2022.07.00-gfx908-openmp

-------------------------------------- /spack/share/spack/lmod/linux-ubuntu20.04-x86_64/Core --------------------------------------
    aml/0.2.0                    flux-core/0.49.0             libunwind/1.6.2        (L)   pdt/3.25.1             (L)   umap/2.1.0
    archer/2.0.0                 gasnet/2023.3.0-gfx908       loki/0.1.7                   plasma/22.9.29               umpire/2022.03.1-gfx908
    argobots/1.1                 gasnet/2023.3.0        (D)   magma/2.7.1-gfx908           py-jupyterhub/1.4.1          umpire/2022.03.1          (D)
    bolt/2.0                     gmp/6.2.1                    mgard/2023-03-31-openmp      qthreads/1.16                variorum/0.6.0
    chai/2022.03.0-gfx908        gotcha/1.0.4                 mpark-variant/1.4.0          raja/2022.10.4-gfx908        zfp/0.5.5
    chai/2022.03.0         (D)   kokkos-kernels/3.7.00-openmp mpich/4.1.1            (L)   raja/2022.10.4-openmp (D)
    charliecloud/0.32            kokkos/4.0.01-gfx908         nrm/0.1.0                    superlu/5.3.0
    darshan-util/3.4.2           kokkos/4.0.01-openmp   (D)   openmpi/4.1.5                swig/4.0.2-fortran
    flit/2.1.0                   legion/23.03.0               papi/6.0.0.1           (L)   sz3/3.1.7
```

E4S 23.05 supports AMD MI100 (gfx908) as well as MI250X (gfx90a) GPUs

# E4S 23.05 DOE LLVM Release: x86_64, ppc64le, and aarch64

```
Singularity> spack find -x
-- linux-ubuntu20.04-x86_64 / clang@16.0.2 ----------------------
adios@1.13.1   cabana@0.5.0        globalarrays@5.8.2  heffte@2.3.0    mfem@4.5.2           parsec@3.0.2209  sundials@6.5.1    umpire@2022.03.1
aml@0.2.0      chai@2022.03.0      gmp@6.2.1           hypre@2.28.0    mpark-variant@1.4.0  pdt@3.25.1       superlu@5.3.0     upcxx@2023.3.0
amrex@23.05    charliecloud@0.32   gotcha@1.0.4        legion@23.03.0  mpich@4.1.1          plumed@2.8.2     swig@4.0.2-fortran
arborx@1.3     flit@2.1.0          h5bench@1.3         libnrm@0.1.0    nccmp@1.9.0.1        pumi@2.2.7       tasmanian@7.9
argobots@1.1   flux-core@0.49.0    hdf5-vol-async@1.5  libquo@1.3.1    nco@5.1.5            qthreads@1.16    turbine@1.3.0
bolt@2.0       gasnet@2023.3.0     hdf5-vol-log@1.4.0  libunwind@1.6.2 papyrus@1.0.2        stc@0.9.0        umap@2.1.0

-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ----------------------
cmake@3.26.3   llvm-doe@16.0.2

Singularity> spack find -x
-- linux-ubuntu20.04-ppc64le / clang@16.0.2 ----------------------
adios@1.13.1   cabana@0.5.0        globalarrays@5.8.2  heffte@2.3.0    mfem@4.5.2           parsec@3.0.2209  sundials@6.5.1    umpire@2022.03.1
aml@0.2.0      chai@2022.03.0      gmp@6.2.1           hypre@2.28.0    mpark-variant@1.4.0  pdt@3.25.1       superlu@5.3.0     upcxx@2023.3.0
amrex@23.05    charliecloud@0.32   gotcha@1.0.4        legion@23.03.0  mpich@4.1.1          plumed@2.8.2     swig@4.0.2-fortran
arborx@1.3     flit@2.1.0          h5bench@1.3         libnrm@0.1.0    nccmp@1.9.0.1        pumi@2.2.7       tasmanian@7.9
argobots@1.1   flux-core@0.49.0    hdf5-vol-async@1.5  libquo@1.3.1    nco@5.1.5            qthreads@1.16    turbine@1.3.0
bolt@2.0       gasnet@2023.3.0     hdf5-vol-log@1.4.0  libunwind@1.6.2 papyrus@1.0.2        stc@0.9.0        umap@2.1.0

-- linux-ubuntu20.04-ppc64le / gcc@11.1.0 ----------------------
cmake@3.26.3   llvm-doe@16.0.2

Singularity> spack find -x
-- linux-ubuntu20.04-aarch64 / clang@16.0.2 ----------------------
adios@1.13.1   cabana@0.5.0        globalarrays@5.8.2  heffte@2.3.0    mfem@4.5.2           parsec@3.0.2209  sundials@6.5.1    umpire@2022.03.1
aml@0.2.0      chai@2022.03.0      gmp@6.2.1           hypre@2.28.0    mpark-variant@1.4.0  pdt@3.25.1       superlu@5.3.0     upcxx@2023.3.0
amrex@23.05    charliecloud@0.32   gotcha@1.0.4        legion@23.03.0  mpich@4.1.1          plumed@2.8.2     swig@4.0.2-fortran
arborx@1.3     flit@2.1.0          h5bench@1.3         libnrm@0.1.0    nccmp@1.9.0.1        pumi@2.2.7       tasmanian@7.9
argobots@1.1   flux-core@0.49.0    hdf5-vol-async@1.5  libquo@1.3.1    nco@5.1.5            qthreads@1.16    turbine@1.3.0
bolt@2.0       gasnet@2023.3.0     hdf5-vol-log@1.4.0  libunwind@1.6.2 papyrus@1.0.2        stc@0.9.0        umap@2.1.0

-- linux-ubuntu20.04-aarch64 / gcc@11.1.0 ----------------------
cmake@3.26.3   llvm-doe@16.0.2
```
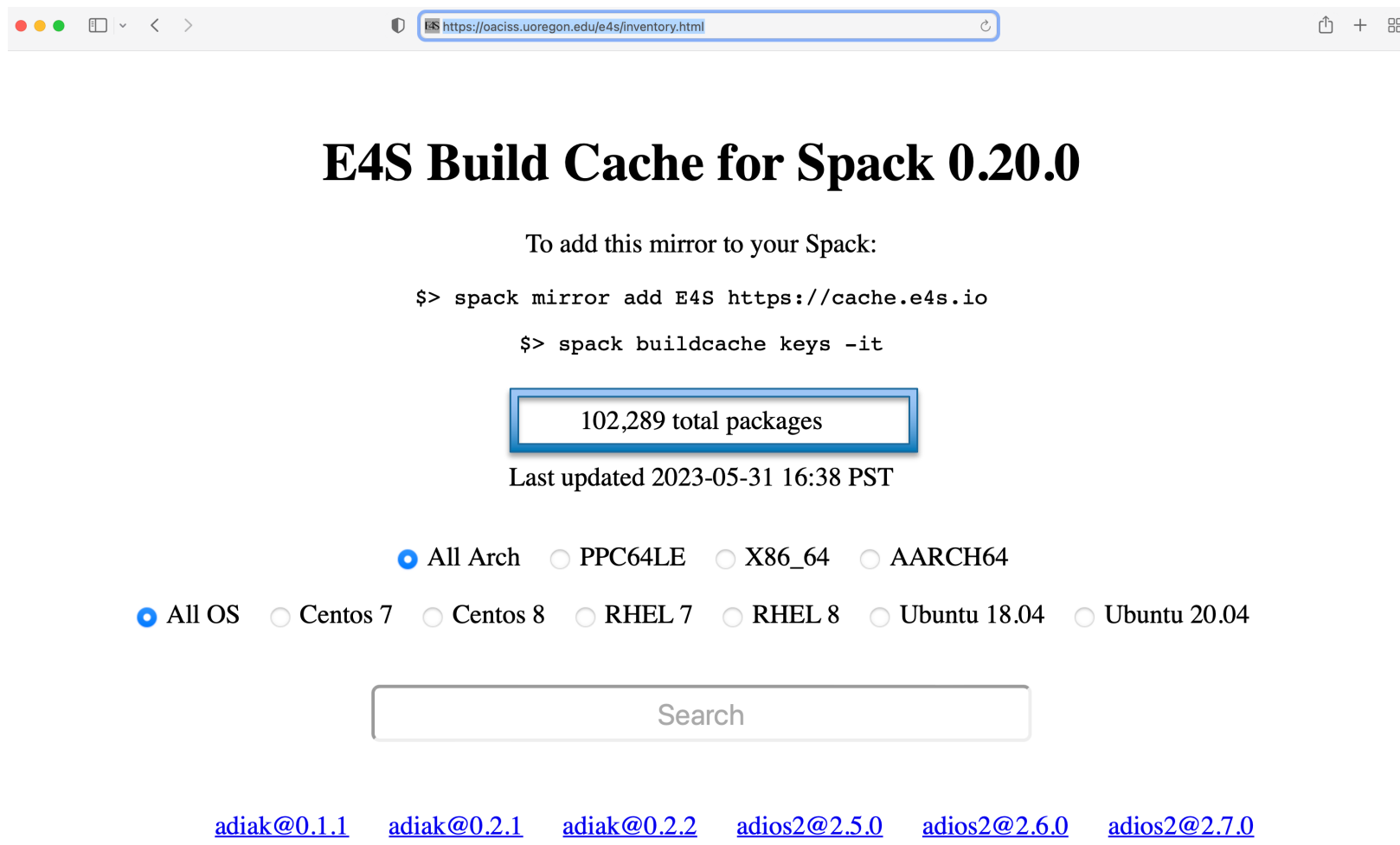
# E4S Build Cache for Spack 0.19.1 hosted at U. Oregon



- Over 100K binaries!
- No need to recompile from source code.

# 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:

```
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

# E4S: A Container Platform for High Throughput Computing

- E4S singularity containers supporting NVIDIA GPUs and Intel runtimes are now available on OSG-HTC [https://osg-htc.org]:
  - `/cvmfs/singularity.opensciencegrid.org/ecpe4s/e4s-cuda:23.05`
  - `/cvmfs/singularity.opensciencegrid.org/ecpe4s/e4s-oneapi:23.05`

- E4S containers include vendor runtimes (NVIDIA CUDA/NVHPC and Intel oneAPI)

- E4S containers include full-featured Python with support for AI/ML tools with support for GPUs
  - PyTorch 2.0.0, TensorFlow 2.12.0
  - Numpy, scipy, keras, matplotlib,…
  - pip3 install --user other packages in your workflow

- E4S containers include 100+ HPC tools installed using the Spack package manager

- E4S features base containers as well as full-featured containers and tools to customize containers

- E4S containers will continue to be supported in future releases on OSG-HTC and provides a viable platform for tool integration for high throughput computing

# Thank you

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**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.