E4S: Extreme-scale Scientific Software Stack

Scalable Tools Workshop

10:30am – 11:00am PDT,
Granlibakken Resort, Lake Tahoe, CA

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https://e4s.io/talks/E4S_Scalable_Tools23.pdf

UNIVERSITY
OF OREGON

E4S

EXASCALE
COMPUTING
PROJECT

Challenges

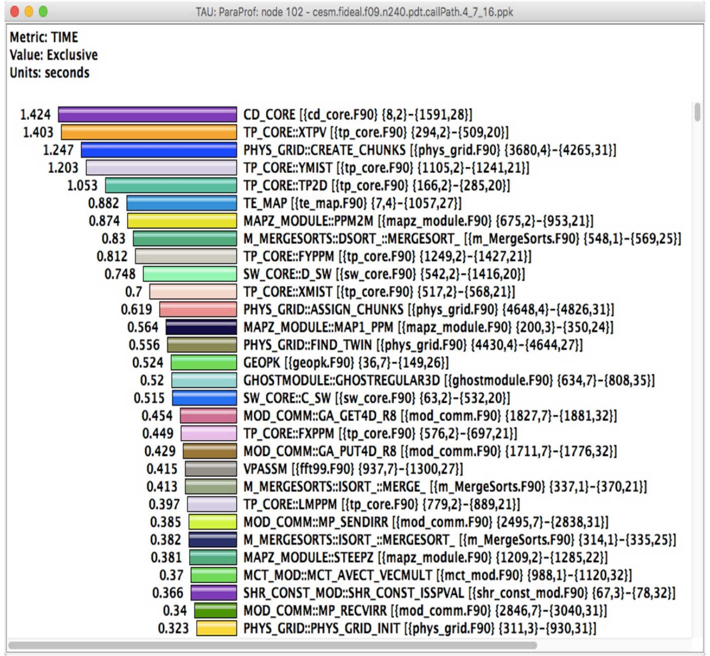
- As our software gets more complex, it is getting harder to measure the performance of, and install tools and libraries correctly in an integrated and interoperable software stack!
- Can E4S provide a stable platform for tool development?
- What are we missing?

TAU Performance System®

Portable profiling and tracing toolkit for performance analysis of HPC parallel programs

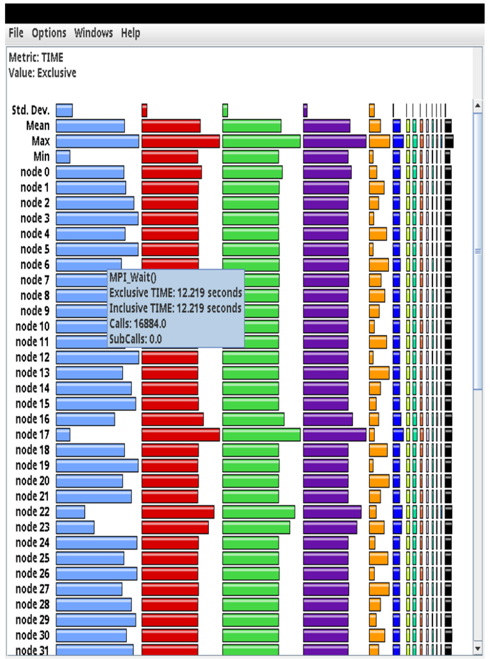
- Supports most parallel execution models
- Provides instrumentation and measurement
- Parallel profiling analysis and data mining
- Open source: http://tau.uoregon.edu

TAU runs on most HPC platforms


TAU: ParaProf: node 102 - cesm.fideal.f09.n240.pdt.callPath.4_7_16.ppk

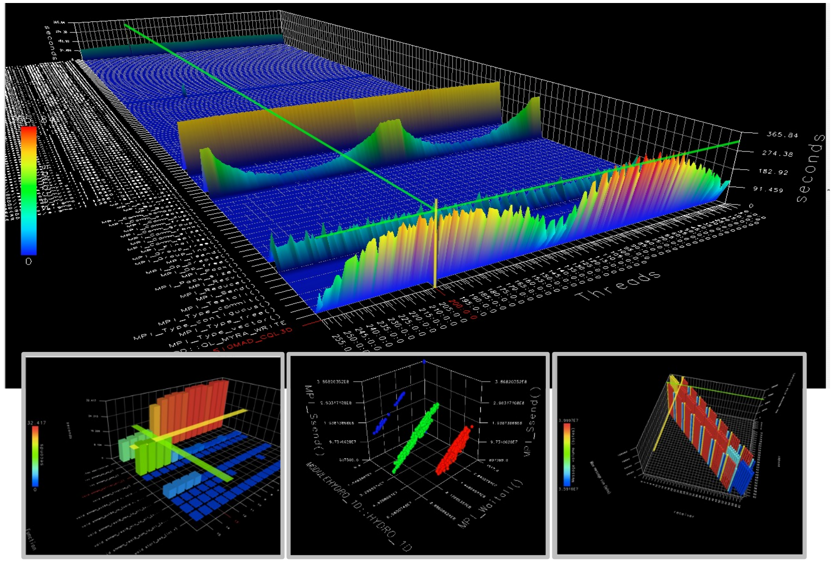
Metric: TIME
Value: Exclusive
Units: seconds

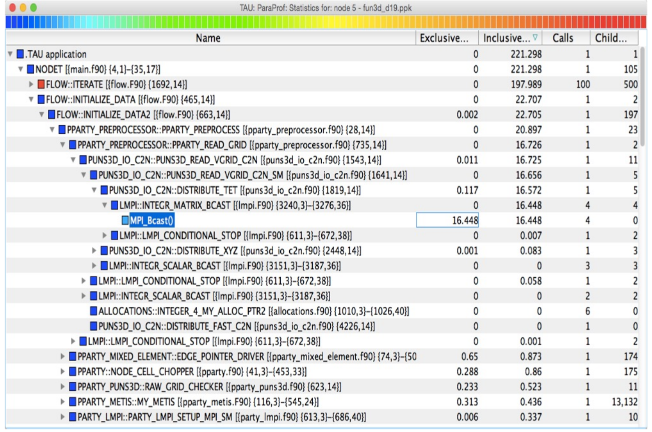
1.424	CD_CORE [{cd_core.F90} {8,2}-{1591,28}]
1.403	TP_CORE::XTPV [{tp_core.F90} {294,2}-{509,20}]
1.247	PHYS_GRID::CREATE_CHUNKS [{phys_grid.F90} {3680,4}-{4265,31}]
1.203	TP_CORE::YMIST [{tp_core.F90} {1105,2}-{1241,21}]
1.053	TP_CORE::TP2D [{tp_core.F90} {166,2}-{285,20}]
0.882	TE_MAP [{te_map.F90} {7,4}-{1057,27}]
0.874	MAPZ_MODULE::PPM2M [{mapz_module.F90} {675,2}-{953,21}]
0.83	M_MERGESORTS::DSORT_::MERGESORT_ [{m_MergeSorts.F90} {548,1}-{569,25}]
0.812	TP_CORE::FYPPM [{tp_core.F90} {1249,2}-{1427,21}]
0.748	SW_CORE::D_SW [{sw_core.F90} {542,2}-{1416,20}]
0.7	TP_CORE::XMIST [{tp_core.F90} {517,2}-{568,21}]
0.619	PHYS_GRID::ASSIGN_CHUNKS [{phys_grid.F90} {4648,4}-{4826,31}]
0.564	MAPZ_MODULE::MAP1_PPM [{mapz_module.F90} {200,3}-{350,24}]
0.556	PHYS_GRID::FIND_TWIN [{phys_grid.F90} {4430,4}-{4644,27}]
0.524	GEOPK [{geopk.F90} {36,7}-{149,26}]
0.52	GHOSTMODULE::GHOSTREGULAR3D [{ghostmodule.F90} {634,7}-{808,35}]
0.515	SW_CORE::C_SW [{sw_core.F90} {63,2}-{532,20}]
0.454	MOD_COMM::GA_GET4D_R8 [{mod_comm.F90} {1827,7}-{1881,32}]
0.449	TP_CORE::FXPPM [{tp_core.F90} {576,2}-{697,21}]
0.429	MOD_COMM::GA_PUT4D_R8 [{mod_comm.F90} {1711,7}-{1776,32}]
0.415	VPASSM [{fft99.F90} {937,7}-{1300,27}]
0.413	M_MERGESORTS::ISORT_::MERGE_ [{m_MergeSorts.F90} {337,1}-{370,21}]
0.397	TP_CORE::LMPPM [{tp_core.F90} {779,2}-{889,21}]
0.385	MOD_COMM::MP_SENDIRR [{mod_comm.F90} {2495,7}-{2838,31}]
0.382	M_MERGESORTS::ISORT_::MERGESORT_ [{m_MergeSorts.F90} {314,1}-{335,25}]
0.381	MAPZ_MODULE::STEEPZ [{mapz_module.F90} {1209,2}-{1285,22}]
0.37	MCT_MOD::MCT_AVECT_VECMULT [{mct_mod.F90} {988,1}-{1120,32}]
0.366	SHR_CONST_MOD::SHR_CONST_ISSPVAL [{shr_const_mod.F90} {67,3}-{78,32}]
0.34	MOD_COMM::MP_RECVIRR [{mod_comm.F90} {2846,7}-{3040,31}]
0.323	PHYS_GRID::PHYS_GRID_INIT [{phys_grid.F90} {311,3}-{930,31}]



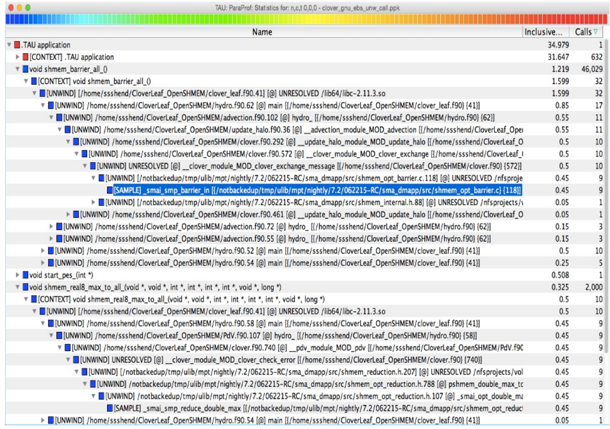
Metric: TIME
Value: Exclusive

MPI_Wait()
Exclusive TIME: 12.219 seconds
Inclusive TIME: 12.219 seconds
Calls: 16884.0
SubCalls: 0.0





Name	Exclusive...	Inclusive... ▽	Calls	Child...
.TAU application	0	221.298	1	1
NODET [{main.f90} {4,1}-{35,17}]	0	221.298	1	105
FLOW::ITERATE [{flow.F90} {1692,14}]	0	197.989	100	500
FLOW::INITIALIZE_DATA [{flow.F90} {465,14}]	0	22.707	1	2
FLOW::INITIALIZE_DATA2 [{flow.F90} {663,14}]	0.002	22.705	1	197
PPARTY_PREPROCESSOR::PPARTY_PREPROCESS [{pparty_preprocessor.f90} {28,14}]	0	20.897	1	23
PPARTY_PREPROCESSOR::PPARTY_READ_GRID [{pparty_preprocessor.f90} {735,14}]	0	16.726	1	2
PUNS3D_IO_C2N::PUNS3D_READ_VGRID_C2N [{puns3d_io_c2n.f90} {1543,14}]	0.011	16.725	1	11
PUNS3D_IO_C2N::PUNS3D_READ_VGRID_C2N_SM [{puns3d_io_c2n.f90} {1641,14}]	0	16.656	1	5
PUNS3D_IO_C2N::DISTRIBUTE_TET [{puns3d_io_c2n.f90} {1819,14}]	0.117	16.572	1	5
LMPI::INTEGR_MATRIX_BCAST [{lmpi.F90} {3240,3}-{3276,36}]	0	16.448	4	4
MPI_Bcast()	16.448	16.448	4	0
LMPI::LMPI_CONDITIONAL_STOP [{lmpi.F90} {611,3}-{672,38}]	0	0.007	1	2
PUNS3D_IO_C2N::DISTRIBUTE_XYZ [{puns3d_io_c2n.f90} {2448,14}]	0.001	0.083	1	3
LMPI::INTEGR_SCALAR_BCAST [{lmpi.F90} {3151,3}-{3187,36}]	0	0	3	3
LMPI::LMPI_CONDITIONAL_STOP [{lmpi.F90} {611,3}-{672,38}]	0	0.058	1	2
LMPI::INTEGR_SCALAR_BCAST [{lmpi.F90} {3151,3}-{3187,36}]	0	0	2	2
ALLOCATIONS::INTEGER_4_MY_ALLOC_PTR2 [{allocations.f90} {1010,3}-{1026,40}]	0	0	6	0
PUNS3D_IO_C2N::DISTRIBUTE_FAST_C2N [{puns3d_io_c2n.f90} {4226,14}]	0	0	1	0
LMPI::LMPI_CONDITIONAL_STOP [{lmpi.F90} {611,3}-{672,38}]	0	0.001	1	2
PPARTY_MIXED_ELEMENT::EDGE_POINTER_DRIVER [{pparty_mixed_element.f90} {74,3}-{50	0.65	0.873	1	174
PPARTY::NODE_CELL_CHOPPER [{pparty.f90} {41,3}-{453,33}]	0.288	0.86	1	175
PPARTY_PUNS3D::RAW_GRID_CHECKER [{pparty_puns3d.f90} {623,14}]	0.233	0.523	1	11
PPARTY_METIS::MY_METIS [{pparty_metis.F90} {116,3}-{545,24}]	0.313	0.436	1	13,132
PARTY_LMPI::PARTY_LMPI_SETUP_MPI_SM [{party_lmpi.f90} {613,3}-{686,40}]	0.006	0.337	1	10

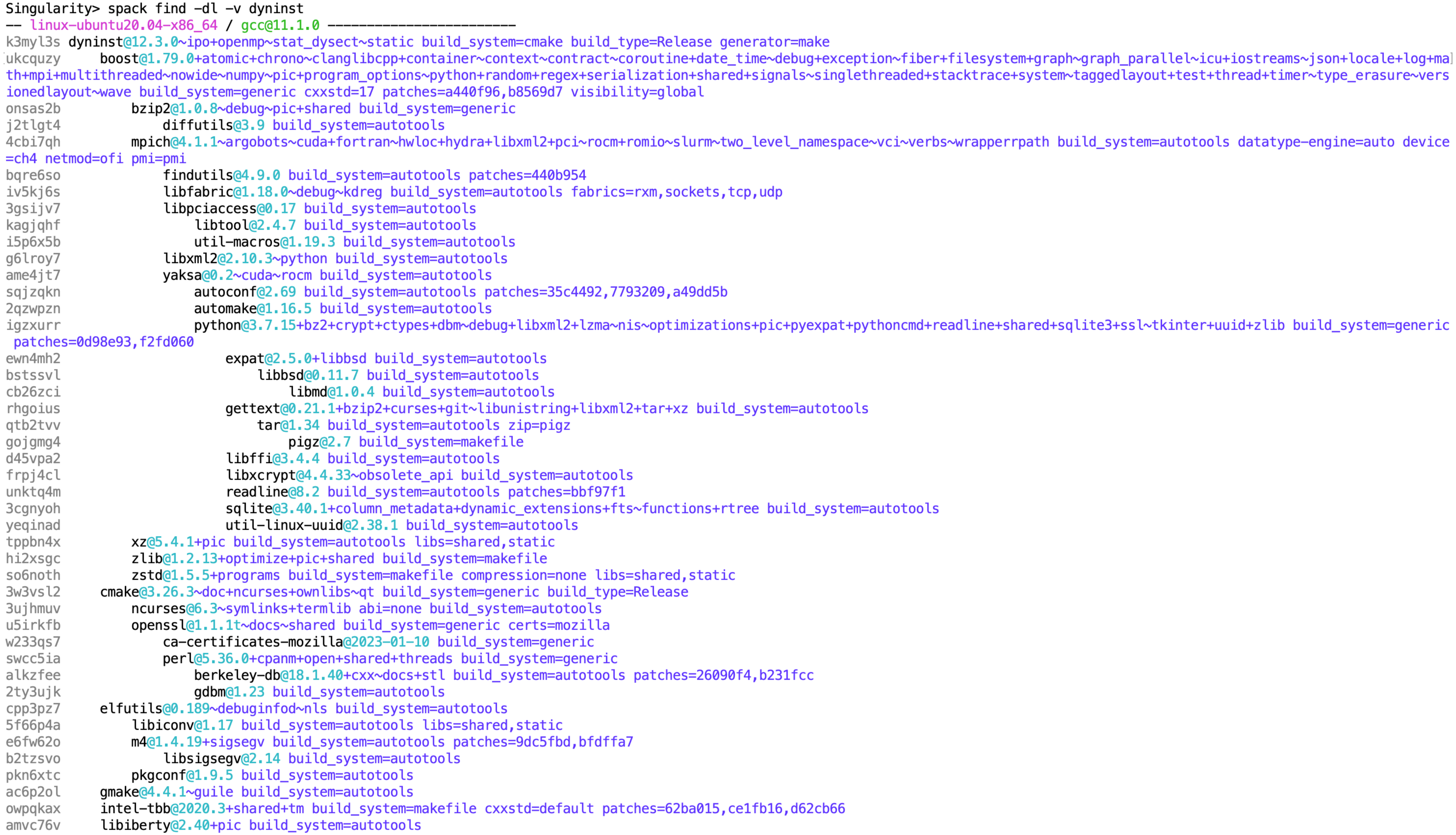

TAU: ParaProf: Statistics for: n,c,t 0,0,0 - clover_gnu_ebs_unw_call.ppk

Name	Inclusive...	Calls ▽
.TAU application	34.979	1
[CONTEXT] .TAU application	31.647	632
void shmem_barrier_all_()	1.219	46,029
[CONTEXT] void shmem_barrier_all_()	1.599	32
[UNWIND] [/home/ssshend/CloverLeaf_OpenSHMEM/clover_leaf.f90.41] [@] UNRESOLVED /lib64/libc-2.11.3.so	1.599	32
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/hydro.f90.62 [@] main [{/home/ssshend/CloverLeaf_OpenSHMEM/clover_leaf.f90} {41}]	0.85	17
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/advection.f90.102 [@] hydro_ [{/home/ssshend/CloverLeaf_OpenSHMEM/hydro.f90} {62}]	0.55	11
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/update_halo.f90.36 [@] __advection_module_MOD_advection [{/home/ssshend/CloverLeaf_Ope	0.55	11
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/clover.f90.292 [@] __update_halo_module_MOD_update_halo [{/home/ssshend/CloverLeaf_O	0.5	10
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/clover.f90.572 [@] __clover_module_MOD_clover_exchange [{/home/ssshend/CloverLeaf_	0.5	10
[UNWIND] UNRESOLVED [@] __clover_module_MOD_clover_exchange_message [{/home/ssshend/CloverLeaf_OpenSHMEM/clover.f90} {572}]	0.5	10
[UNWIND] [/notbackedup/tmp/ulib/mpt/nightly/7.2/062215-RC/sma_dmapp/src/shmem_opt_barrier.c.118] [@] UNRESOLVED /nfsproje	0.45	9
[SAMPLE] _smai_smp_barrier_in [{/notbackedup/tmp/ulib/mpt/nightly/7.2/062215-RC/sma_dmapp/src/shmem_opt_barrier.c} {118}]	0.45	9
[UNWIND] [/notbackedup/tmp/ulib/mpt/nightly/7.2/062215-RC/sma_dmapp/src/shmem_internal.h.88] [@] UNRESOLVED /nfsprojects/	0.05	1
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/clover.f90.461 [@] __update_halo_module_MOD_update_halo [{/home/ssshend/CloverLeaf_O	0.05	1
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/advection.f90.72 [@] hydro_ [{/home/ssshend/CloverLeaf_OpenSHMEM/hydro.f90} {62}]	0.15	3
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/advection.f90.55 [@] hydro_ [{/home/ssshend/CloverLeaf_OpenSHMEM/hydro.f90} {62}]	0.15	3
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/hydro.f90.52 [@] main [{/home/ssshend/CloverLeaf_OpenSHMEM/clover_leaf.f90} {41}]	0.5	10
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/hydro.f90.54 [@] main [{/home/ssshend/CloverLeaf_OpenSHMEM/clover_leaf.f90} {41}]	0.25	5
void start_pes_(int *)	0.508	1
void shmem_real8_max_to_all_(void *, void *, int *, int *, int *, int *, void *, long *)	0.325	2,000
[CONTEXT] void shmem_real8_max_to_all_(void *, void *, int *, int *, int *, int *, void *, long *)	0.5	10
[UNWIND] [/home/ssshend/CloverLeaf_OpenSHMEM/clover_leaf.f90.41] [@] UNRESOLVED /lib64/libc-2.11.3.so	0.5	10
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/hydro.f90.58 [@] main [{/home/ssshend/CloverLeaf_OpenSHMEM/clover_leaf.f90} {41}]	0.45	9
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/PdV.f90.107 [@] hydro_ [{/home/ssshend/CloverLeaf_OpenSHMEM/hydro.f90} {58}]	0.45	9
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/clover.f90.740 [@] __pdv_module_MOD_pdv [{/home/ssshend/CloverLeaf_OpenSHMEM/PdV.f9C	0.45	9
[UNWIND] UNRESOLVED [@] __clover_module_MOD_clover_check_error [{/home/ssshend/CloverLeaf_OpenSHMEM/clover.f90} {740}]	0.45	9
[UNWIND] [/notbackedup/tmp/ulib/mpt/nightly/7.2/062215-RC/sma_dmapp/src/shmem_reduction.h.207] [@] UNRESOLVED /nfsprojects/vol	0.45	9
[UNWIND] /notbackedup/tmp/ulib/mpt/nightly/7.2/062215-RC/sma_dmapp/src/shmem_opt_reduction.h.788 [@] pshmem_double_max_tc	0.45	9
[UNWIND] /notbackedup/tmp/ulib/mpt/nightly/7.2/062215-RC/sma_dmapp/src/shmem_opt_reduction.h.107 [@] _smai_opt_double_ma	0.45	9
[SAMPLE] _smai_smp_reduce_double_max [{/notbackedup/tmp/ulib/mpt/nightly/7.2/062215-RC/sma_dmapp/src/shmem_opt_reduc	0.45	9
[UNWIND] /home/ssshend/CloverLeaf_OpenSHMEM/hydro.f90.54 [@] main [{/home/ssshend/CloverLeaf_OpenSHMEM/clover_leaf.f90} {41}]	0.05	1

Our performance evaluation tools are getting complex to install!

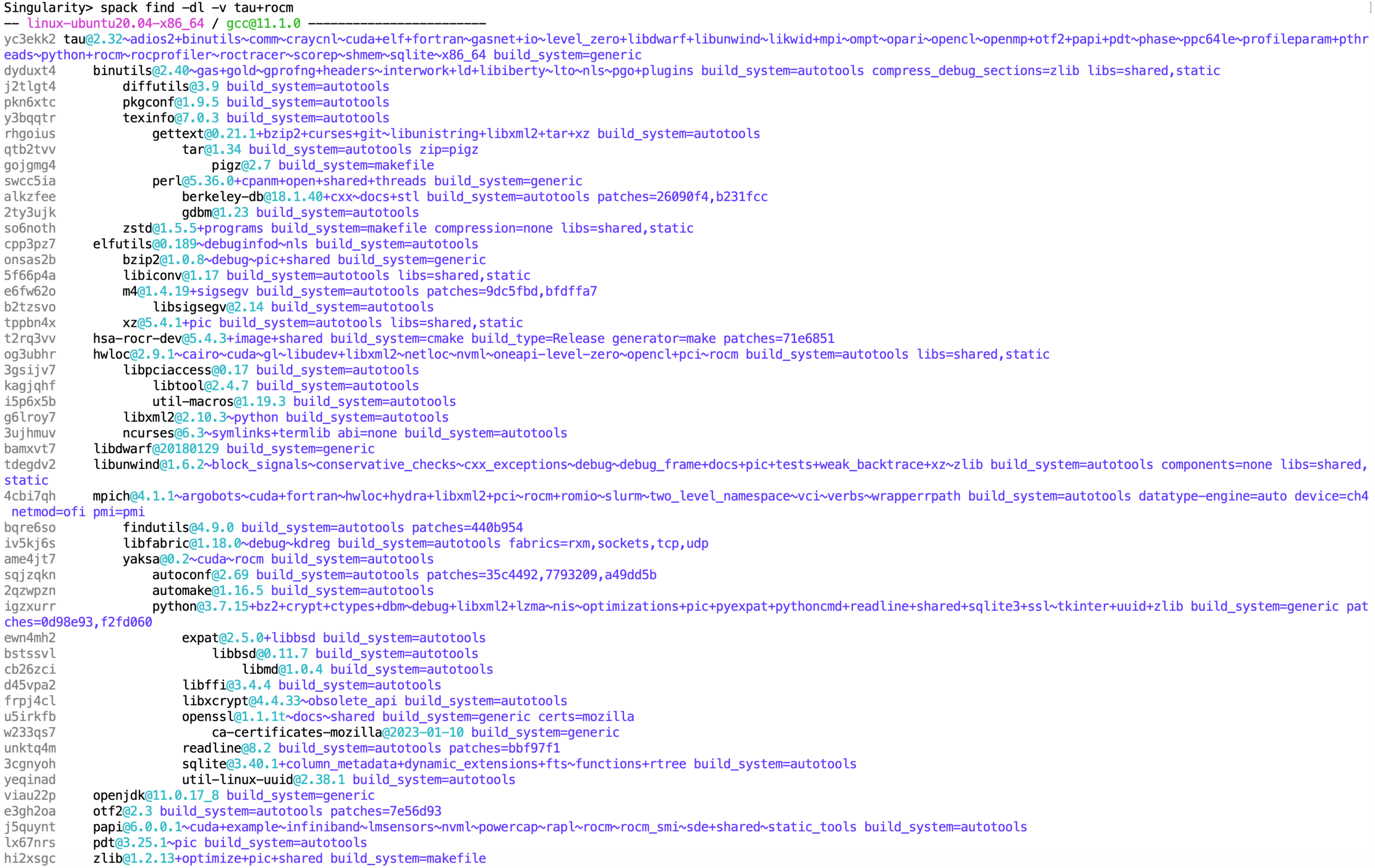
- GPU Runtimes: ROCm, CUDA, oneAPI
- Tool interfaces: ROCprofiler V1/ROCtracer V2/Rocprofiler v2, CUPTI, Level Zero, OpenCL, OMPT, Kokkos, Caliper, CAMTimers, PerfStubs, …
- Tool dependencies:
  - Binutils, libunwind, libdwarf installed just right (-fPIC used to compile .o files that are used in DSOs)
  - GPU runtimes
  - Qt5, Java, Python, perl, bash, sed, awk, cmake…
  - PAPI
  - Compilers: LLVM, GNU, Intel, AMD, NVHPC, PrgEnv-{cray,amd,nvidia,intel,gnu-amd} on HPE CPE
  - MPI
  - Intel TBB
  - Boost
  - Other third-party libraries…
- Installing these tools and their dependencies by hand is hard!

DyninstAPI’s dependency tree



```
Singularity> spack find -dl -v dyninst
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
k3myl3s dyninst@12.3.0~ipo+openmp~stat_dysect~static build_system=cmake build_type=Release generator=make
ukcquzy     boost@1.79.0+atomic+chrono~clanglibcpp+container~context~contract~coroutine+date_time~debug+exception~fiber+filesystem+graph~graph_parallel~icu+iostreams~json+locale+log+ma
th+mpi+multithreaded~nowide~numpy~pic+program_options~python+random+regex+serialization+shared+signals~singlethreaded+stacktrace+system~taggedlayout+test+thread+timer~type_erasure~vers
ionedlayout~wave build_system=generic cxxstd=17 patches=a440f96,b8569d7 visibility=global
onsas2b         bzip2@1.0.8~debug~pic+shared build_system=generic
j2tlgt4             diffutils@3.9 build_system=autotools
4cbi7qh         mpich@4.1.1~argobots~cuda+fortran~hwloc+hydra+libxml2+pci~rocm+romio~slurm~two_level_namespace~vci~verbs~wrapperrpath build_system=autotools datatype-engine=auto device
=ch4 netmod=ofi pmi=pmi
bqre6so             findutils@4.9.0 build_system=autotools patches=440b954
iv5kj6s             libfabric@1.18.0~debug~kdreg build_system=autotools fabrics=rxm,sockets,tcp,udp
3gsijv7             libpciaccess@0.17 build_system=autotools
kagjqhf                 libtool@2.4.7 build_system=autotools
i5p6x5b                 util-macros@1.19.3 build_system=autotools
g6lroy7             libxml2@2.10.3~python build_system=autotools
ame4jt7             yaksa@0.2~cuda~rocm build_system=autotools
sqjzqkn                 autoconf@2.69 build_system=autotools patches=35c4492,7793209,a49dd5b
2qzwpzn                 automake@1.16.5 build_system=autotools
igzxurr                 python@3.7.15+bz2+crypt+ctypes+dbm~debug+libxml2+lzma~nis~optimizations+pic+pyexpat+pythoncmd+readline+shared+sqlite3+ssl~tkinter+uuid+zlib build_system=generic
 patches=0d98e93,f2fd060
ewn4mh2                     expat@2.5.0+libbsd build_system=autotools
bstssvl                         libbsd@0.11.7 build_system=autotools
cb26zci                             libmd@1.0.4 build_system=autotools
rhgoius                     gettext@0.21.1+bzip2+curses+git~libunistring+libxml2+tar+xz build_system=autotools
qtb2tvv                         tar@1.34 build_system=autotools zip=pigz
gojgmg4                             pigz@2.7 build_system=makefile
d45vpa2                     libffi@3.4.4 build_system=autotools
frpj4cl                     libxcrypt@4.4.33~obsolete_api build_system=autotools
unktq4m                     readline@8.2 build_system=autotools patches=bbf97f1
3cgnyoh                     sqlite@3.40.1+column_metadata+dynamic_extensions+fts~functions+rtree build_system=autotools
yeqinad                     util-linux-uuid@2.38.1 build_system=autotools
tppbn4x         xz@5.4.1+pic build_system=autotools libs=shared,static
hi2xsgc         zlib@1.2.13+optimize+pic+shared build_system=makefile
so6noth         zstd@1.5.5+programs build_system=makefile compression=none libs=shared,static
3w3vsl2     cmake@3.26.3~doc+ncurses+ownlibs~qt build_system=generic build_type=Release
3ujhmuv         ncurses@6.3~symlinks+termlib abi=none build_system=autotools
u5irkfb         openssl@1.1.1t~docs~shared build_system=generic certs=mozilla
w233qs7             ca-certificates-mozilla@2023-01-10 build_system=generic
swcc5ia             perl@5.36.0+cpanm+open+shared+threads build_system=generic
alkzfee                 berkeley-db@18.1.40+cxx~docs+stl build_system=autotools patches=26090f4,b231fcc
2ty3ujk                 gdbm@1.23 build_system=autotools
cpp3pz7     elfutils@0.189~debuginfod~nls build_system=autotools
5f66p4a         libiconv@1.17 build_system=autotools libs=shared,static
e6fw62o         m4@1.4.19+sigsegv build_system=autotools patches=9dc5fbd,bfdffa7
b2tzsvo             libsigsegv@2.14 build_system=autotools
pkn6xtc         pkgconf@1.9.5 build_system=autotools
ac6p2ol     gmake@4.4.1~guile build_system=autotools
owpqkax     intel-tbb@2020.3+shared+tm build_system=makefile cxxstd=default patches=62ba015,ce1fb16,d62cb66
amvc76v     libiberty@2.40+pic build_system=autotools
```

TAU’s dependency tree

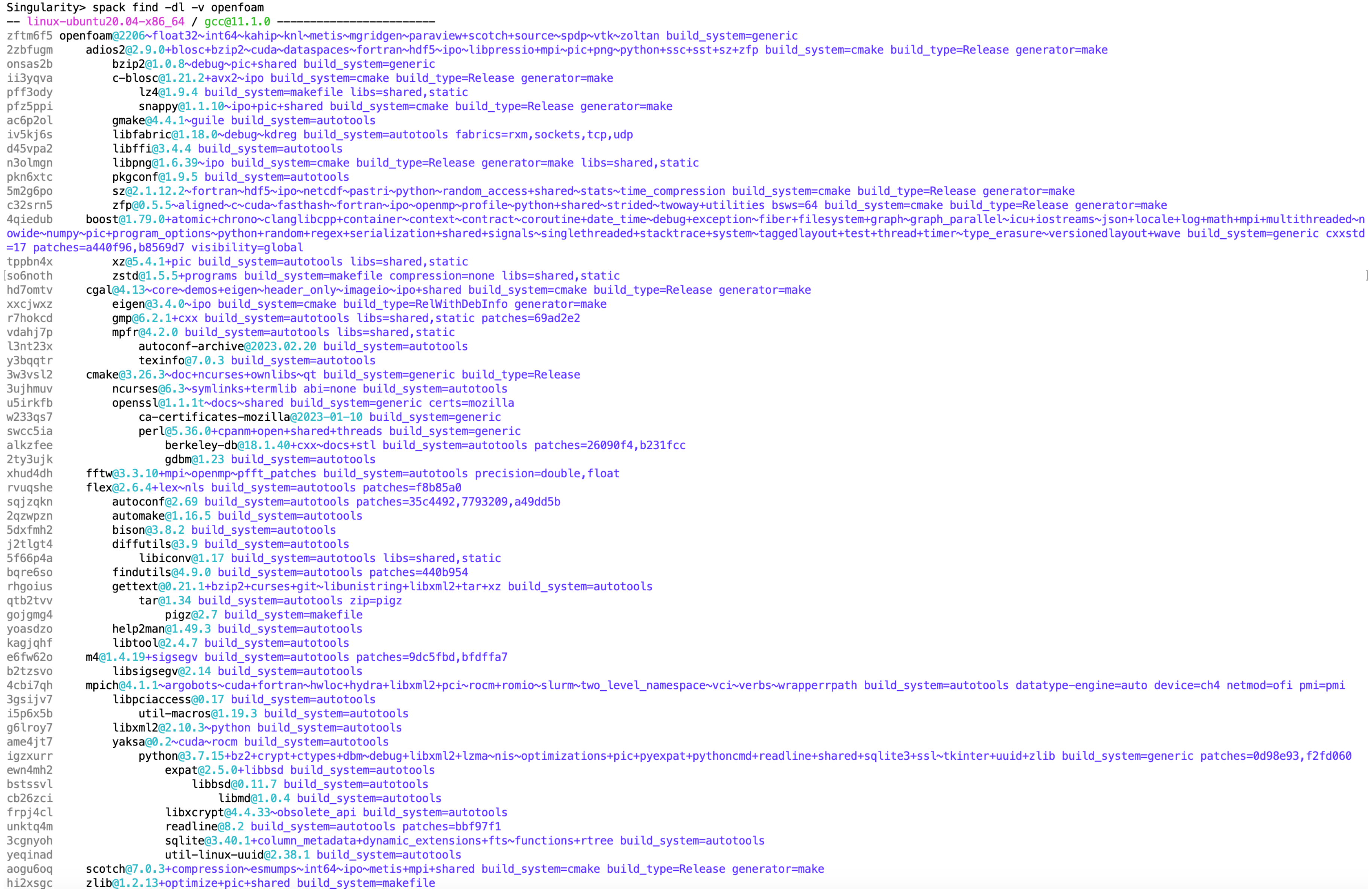


```
Singularity> spack find -dl -v tau+rocm
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
yc3ekk2 tau@2.32~adios2+binutils~comm~craycnl~cuda+elf+fortran~gasnet+io~level_zero+libdwarf+libunwind~likwid+mpi~ompt~opari~opencl~openmp+otf2+papi+pdt~phase~ppc64le~profileparam+pthr
eads~python+rocm~rocprofiler~roctracer~scorep~shmem~sqlite~x86_64 build_system=generic
dyduxt4     binutils@2.40~gas+gold~gprofng+headers~interwork+ld+libiberty~lto~nls~pgo+plugins build_system=autotools compress_debug_sections=zlib libs=shared,static
j2tlgt4         diffutils@3.9 build_system=autotools
pkn6xtc         pkgconf@1.9.5 build_system=autotools
y3bqqtr         texinfo@7.0.3 build_system=autotools
rhgoius             gettext@0.21.1+bzip2+curses+git~libunistring+libxml2+tar+xz build_system=autotools
qtb2tvv                 tar@1.34 build_system=autotools zip=pigz
gojgmg4                     pigz@2.7 build_system=makefile
swcc5ia             perl@5.36.0+cpanm+open+shared+threads build_system=generic
alkzfee                 berkeley-db@18.1.40+cxx~docs+stl build_system=autotools patches=26090f4,b231fcc
2ty3ujk                 gdbm@1.23 build_system=autotools
so6noth         zstd@1.5.5+programs build_system=makefile compression=none libs=shared,static
cpp3pz7     elfutils@0.189~debuginfod~nls build_system=autotools
onsas2b         bzip2@1.0.8~debug~pic+shared build_system=generic
5f66p4a         libiconv@1.17 build_system=autotools libs=shared,static
e6fw62o         m4@1.4.19+sigsegv build_system=autotools patches=9dc5fbd,bfdffa7
b2tzsvo             libsigsegv@2.14 build_system=autotools
tppbn4x         xz@5.4.1+pic build_system=autotools libs=shared,static
t2rq3vv     hsa-rocr-dev@5.4.3+image+shared build_system=cmake build_type=Release generator=make patches=71e6851
og3ubhr     hwloc@2.9.1~cairo~cuda~gl~libudev+libxml2~netloc~nvml~oneapi-level-zero~opencl+pci~rocm build_system=autotools libs=shared,static
3gsijv7         libpciaccess@0.17 build_system=autotools
kagjqhf             libtool@2.4.7 build_system=autotools
i5p6x5b             util-macros@1.19.3 build_system=autotools
g6lroy7         libxml2@2.10.3~python build_system=autotools
3ujhmuv         ncurses@6.3~symlinks+termlib abi=none build_system=autotools
bamxvt7     libdwarf@20180129 build_system=generic
tdegdv2     libunwind@1.6.2~block_signals~conservative_checks~cxx_exceptions~debug~debug_frame+docs+pic+tests+weak_backtrace+xz~zlib build_system=autotools components=none libs=shared,
static
4cbi7qh     mpich@4.1.1~argobots~cuda+fortran~hwloc+hydra+libxml2+pci~rocm+romio~slurm~two_level_namespace~vci~verbs~wrapperrpath build_system=autotools datatype-engine=auto device=ch4
 netmod=ofi pmi=pmi
bqre6so         findutils@4.9.0 build_system=autotools patches=440b954
iv5kj6s         libfabric@1.18.0~debug~kdreg build_system=autotools fabrics=rxm,sockets,tcp,udp
ame4jt7         yaksa@0.2~cuda~rocm build_system=autotools
sqjzqkn             autoconf@2.69 build_system=autotools patches=35c4492,7793209,a49dd5b
2qzwpzn             automake@1.16.5 build_system=autotools
igzxurr             python@3.7.15+bz2+crypt+ctypes+dbm~debug+libxml2+lzma~nis~optimizations+pic+pyexpat+pythoncmd+readline+shared+sqlite3+ssl~tkinter+uuid+zlib build_system=generic pat
ches=0d98e93,f2fd060
ewn4mh2                 expat@2.5.0+libbsd build_system=autotools
bstssvl                     libbsd@0.11.7 build_system=autotools
cb26zci                         libmd@1.0.4 build_system=autotools
d45vpa2                 libffi@3.4.4 build_system=autotools
frpj4cl                 libxcrypt@4.4.33~obsolete_api build_system=autotools
u5irkfb                 openssl@1.1.1t~docs~shared build_system=generic certs=mozilla
w233qs7                     ca-certificates-mozilla@2023-01-10 build_system=generic
unktq4m                 readline@8.2 build_system=autotools patches=bbf97f1
3cgnyoh                 sqlite@3.40.1+column_metadata+dynamic_extensions+fts~functions+rtree build_system=autotools
yeqinad                 util-linux-uuid@2.38.1 build_system=autotools
viau22p     openjdk@11.0.17_8 build_system=generic
e3gh2oa     otf2@2.3 build_system=autotools patches=7e56d93
j5quynt     papi@6.0.0.1~cuda+example~infiniband~lmsensors~nvml~powercap~rapl~rocm~rocm_smi~sde+shared~static_tools build_system=autotools
lx67nrs     pdt@3.25.1~pic build_system=autotools
hi2xsgc     zlib@1.2.13+optimize+pic+shared build_system=makefile
```

HPCToolkit’s dependency tree

```
Singularity> spack find -dl -v hpctoolkit+rocm
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
pqqcf4f hpctoolkit@2023.03.01~cray~cuda~debug~level_zero+mpi~opencl+papi~python+rocm+viewer build_system=autotools
ukcquzy     boost@1.79.0+atomic+chrono~clanglibcpp+container~context~contract~coroutine+date_time~debug+exception~fiber+filesystem+graph~graph_parallel~icu+iostreams~json+locale+log+math+mpi+multithreaded~nowide~numpy
~pic+program_options~python+random+regex+serialization+shared+signals~singlethreaded+stacktrace+system~taggedlayout+test+thread+timer~type_erasure~versionedlayout~wave build_system=generic cxxstd=17 patches=a440f96,b8
569d7 visibility=global
so6noth         zstd@1.5.5+programs build_system=makefile compression=none libs=shared,static
onsas2b     bzip2@1.0.8~debug~pic+shared build_system=generic
j2tlgt4         diffutils@3.9 build_system=autotools
k3myl3s     dyninst@12.3.0~ipo+openmp~stat_dysect~static build_system=cmake build_type=Release generator=make
3w3vsl2         cmake@3.26.3~doc+ncurses+ownlibs~qt build_system=generic build_type=Release
3ujhmuv             ncurses@6.3~symlinks+termlib abi=none build_system=autotools
u5irkfb             openssl@1.1.1t~docs~shared build_system=generic certs=mozilla
w233qs7                 ca-certificates-mozilla@2023-01-10 build_system=generic
ac6p2ol         gmake@4.4.1~guile build_system=autotools
cpp3pz7     elfutils@0.189~debuginfod~nls build_system=autotools
5f66p4a         libiconv@1.17 build_system=autotools libs=shared,static
e6fw62o         m4@1.4.19+sigsegv build_system=autotools patches=9dc5fbd,bfdffa7
b2tzsvo             libsigsegv@2.14 build_system=autotools
pkn6xtc         pkgconf@1.9.5 build_system=autotools
s3u7fv6     hip@5.4.3~cuda~ipo+rocm build_system=cmake build_type=Release generator=make patches=5068750,ca523f1
2diathq     hpcviewer@2023.04 build_system=generic
viau22p         openjdk@11.0.17_8 build_system=generic
ikj6txu     hsa-rocr-dev@5.4.3+image~ipo+shared build_system=cmake build_type=Release generator=make patches=71e6851
owpqkax     intel-tbb@2020.3+shared+tm build_system=makefile cxxstd=default patches=62ba015,ce1fb16,d62cb66
5xnbu3x     intel-xed@2022.10.11~debug+pic build_system=generic
igzxurr         python@3.7.15+bz2+crypt+ctypes+dbm~debug+libxml2+lzma~nis~optimizations+pic+pyexpat+pythoncmd+readline+shared+sqlite3+ssl~tkinter+uuid+zlib build_system=generic patches=0d98e93,f2fd060
ewn4mh2             expat@2.5.0+libbsd build_system=autotools
bstssvl                 libbsd@0.11.7 build_system=autotools
cb26zci                     libmd@1.0.4 build_system=autotools
2ty3ujk             gdbm@1.23 build_system=autotools
rhgoius             gettext@0.21.1+bzip2+curses+git~libunistring+libxml2+tar+xz build_system=autotools
qtb2tvv                 tar@1.34 build_system=autotools zip=pigz
gojgmg4                     pigz@2.7 build_system=makefile
d45vpa2             libffi@3.4.4 build_system=autotools
frpj4cl             libxcrypt@4.4.33~obsolete_api build_system=autotools
unktq4m             readline@8.2 build_system=autotools patches=bbf97f1
3cgnyoh             sqlite@3.40.1+column_metadata+dynamic_extensions+fts~functions+rtree build_system=autotools
yeqinad             util-linux-uuid@2.38.1 build_system=autotools
amvc76v     libiberty@2.40+pic build_system=autotools
3btazyw     libmonitor@2023.03.15~commrank~dlopen+hpctoolkit build_system=autotools
tdegdv2     libunwind@1.6.2~block_signals~conservative_checks~cxx_exceptions~debug~debug_frame+docs+pic+tests+weak_backtrace+xz~zlib build_system=autotools components=none libs=shared,static
2cgjsln     memkind@1.13.0 build_system=autotools
sqjzqkn         autoconf@2.69 build_system=autotools patches=35c4492,7793209,a49dd5b
swcc5ia             perl@5.36.0+cpanm+open+shared+threads build_system=generic
alkzfee                 berkeley-db@18.1.40+cxx~docs+stl build_system=autotools patches=26090f4,b231fcc
2qzwpzn         automake@1.16.5 build_system=autotools
kagjqhf         libtool@2.4.7 build_system=autotools
geg3gor         numactl@2.0.14 build_system=autotools patches=4e1d78c,62fc8a8,ff37630
4cbi7qh     mpich@4.1.1~argobots~cuda+fortran~hwloc+hydra+libxml2+pci~rocm+romio~slurm~two_level_namespace~vci~verbs~wrapperrpath build_system=autotools datatype-engine=auto device=ch4 netmod=ofi pmi=pmi
bqre6so         findutils@4.9.0 build_system=autotools patches=440b954
iv5kj6s         libfabric@1.18.0~debug~kdreg build_system=autotools fabrics=rxm,sockets,tcp,udp
3gsijv7         libpciaccess@0.17 build_system=autotools
i5p6x5b             util-macros@1.19.3 build_system=autotools
g6lroy7         libxml2@2.10.3~python build_system=autotools
ame4jt7         yaksa@0.2~cuda~rocm build_system=autotools
j5quynt     papi@6.0.0.1~cuda+example~infiniband~lmsensors~nvml~powercap~rapl~rocm~rocm_smi~sde+shared~static_tools build_system=autotools
ftwupzv     rocprofiler-dev@5.4.3~ipo build_system=cmake build_type=Release generator=make patches=16754a1,c482eee
lju4qds     roctracer-dev@4.5.3~ipo~rocm build_system=cmake build_type=Release generator=make
d2sre54     xerces-c@3.2.4 build_system=autotools cxxstd=default netaccessor=curl transcoder=iconv
24lnuny         curl@8.0.1~gssapi~ldap~libidn2~librtmp~libssh~libssh2~nghttp2 build_system=autotools libs=shared,static tls=openssl
tppbn4x     xz@5.4.1+pic build_system=autotools libs=shared,static
mde4ok3     yaml-cpp@0.7.0~ipo+pic+shared~tests build_system=cmake build_type=Release generator=make
hi2xsgc     zlib@1.2.13+optimize+pic+shared build_system=makefile
```

Our HPC applications are equally complex!



```
Singularity> spack find -dl -v openfoam
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 -------------------------
zftm6f5 openfoam@2206~float32~int64~kahip~knl~metis~mgridgen~paraview+scotch+source~spdp~vtk~zoltan build_system=generic
2zbfugm     adios2@2.9.0+blosc+bzip2~cuda~dataspaces~fortran~hdf5~ipo~libpressio+mpi~pic+png~python+ssc+sst+sz+zfp build_system=cmake build_type=Release generator=make
onsas2b         bzip2@1.0.8~debug~pic+shared build_system=generic
ii3yqva         c-blosc@1.21.2+avx2~ipo build_system=cmake build_type=Release generator=make
pff3ody             lz4@1.9.4 build_system=makefile libs=shared,static
pfz5ppi             snappy@1.1.10~ipo+pic+shared build_system=cmake build_type=Release generator=make
ac6p2ol         gmake@4.4.1~guile build_system=autotools
iv5kj6s         libfabric@1.18.0~debug~kdreg build_system=autotools fabrics=rxm,sockets,tcp,udp
d45vpa2         libffi@3.4.4 build_system=autotools
n3olmgn         libpng@1.6.39~ipo build_system=cmake build_type=Release generator=make libs=shared,static
pkn6xtc         pkgconf@1.9.5 build_system=autotools
5m2g6po         sz@2.1.12.2~fortran~hdf5~ipo~netcdf~pastri~python~random_access+shared~stats~time_compression build_system=cmake build_type=Release generator=make
c32srn5         zfp@0.5.5~aligned~c~cuda~fasthash~fortran~ipo~openmp~profile~python+shared~strided~twoway+utilities bsws=64 build_system=cmake build_type=Release generator=make
4qiedub     boost@1.79.0+atomic+chrono~clanglibcpp+container~context~contract~coroutine+date_time~debug+exception~fiber+filesystem+graph~graph_parallel~icu+iostreams~json+locale+log+math+mpi+multithreaded~n
owide~numpy~pic+program_options~python+random+regex+serialization+shared+signals~singlethreaded+stacktrace+system~taggedlayout+test+thread+timer~type_erasure~versionedlayout+wave build_system=generic cxxstd
=17 patches=a440f96,b8569d7 visibility=global
tppbn4x         xz@5.4.1+pic build_system=autotools libs=shared,static
so6noth         zstd@1.5.5+programs build_system=makefile compression=none libs=shared,static
hd7omtv     cgal@4.13~core~demos+eigen~header_only~imageio~ipo+shared build_system=cmake build_type=Release generator=make
xxcjwxz         eigen@3.4.0~ipo build_system=cmake build_type=RelWithDebInfo generator=make
r7hokcd         gmp@6.2.1+cxx build_system=autotools libs=shared,static patches=69ad2e2
vdahj7p         mpfr@4.2.0 build_system=autotools libs=shared,static
l3nt23x             autoconf-archive@2023.02.20 build_system=autotools
y3bqqtr             texinfo@7.0.3 build_system=autotools
3w3vsl2     cmake@3.26.3~doc+ncurses+ownlibs~qt build_system=generic build_type=Release
3ujhmuv         ncurses@6.3~symlinks+termlib abi=none build_system=autotools
u5irkfb         openssl@1.1.1t~docs~shared build_system=generic certs=mozilla
w233qs7             ca-certificates-mozilla@2023-01-10 build_system=generic
swcc5ia             perl@5.36.0+cpanm+open+shared+threads build_system=generic
alkzfee                 berkeley-db@18.1.40+cxx~docs+stl build_system=autotools patches=26090f4,b231fcc
2ty3ujk                 gdbm@1.23 build_system=autotools
xhud4dh     fftw@3.3.10+mpi~openmp~pfft_patches build_system=autotools precision=double,float
rvuqshe     flex@2.6.4+lex~nls build_system=autotools patches=f8b85a0
sqjzqkn         autoconf@2.69 build_system=autotools patches=35c4492,7793209,a49dd5b
2qzwpzn         automake@1.16.5 build_system=autotools
5dxfmh2         bison@3.8.2 build_system=autotools
j2tlgt4         diffutils@3.9 build_system=autotools
5f66p4a             libiconv@1.17 build_system=autotools libs=shared,static
bqre6so         findutils@4.9.0 build_system=autotools patches=440b954
rhgoius         gettext@0.21.1+bzip2+curses+git~libunistring+libxml2+tar+xz build_system=autotools
qtb2tvv             tar@1.34 build_system=autotools zip=pigz
gojgmg4                 pigz@2.7 build_system=makefile
yoasdzo         help2man@1.49.3 build_system=autotools
kagjqhf         libtool@2.4.7 build_system=autotools
e6fw62o     m4@1.4.19+sigsegv build_system=autotools patches=9dc5fbd,bfdffa7
b2tzsvo         libsigsegv@2.14 build_system=autotools
4cbi7qh     mpich@4.1.1~argobots~cuda+fortran~hwloc+hydra+libxml2+pci~rocm+romio~slurm~two_level_namespace~vci~verbs~wrapperrpath build_system=autotools datatype-engine=auto device=ch4 netmod=ofi pmi=pmi
3gsijv7         libpciaccess@0.17 build_system=autotools
i5p6x5b             util-macros@1.19.3 build_system=autotools
g6lroy7         libxml2@2.10.3~python build_system=autotools
ame4jt7         yaksa@0.2~cuda~rocm build_system=autotools
igzxurr             python@3.7.15+bz2+crypt+ctypes+dbm~debug+libxml2+lzma~nis~optimizations+pic+pyexpat+pythoncmd+readline+shared+sqlite3+ssl~tkinter+uuid+zlib build_system=generic patches=0d98e93,f2fd060
ewn4mh2                 expat@2.5.0+libbsd build_system=autotools
bstssvl                     libbsd@0.11.7 build_system=autotools
cb26zci                         libmd@1.0.4 build_system=autotools
frpj4cl                 libxcrypt@4.4.33~obsolete_api build_system=autotools
unktq4m                 readline@8.2 build_system=autotools patches=bbf97f1
3cgnyoh                 sqlite@3.40.1+column_metadata+dynamic_extensions+fts~functions+rtree build_system=autotools
yeqinad                 util-linux-uuid@2.38.1 build_system=autotools
aogu6oq     scotch@7.0.3+compression~esmumps~int64~ipo~metis+mpi+shared build_system=cmake build_type=Release generator=make
hi2xsgc     zlib@1.2.13+optimize+pic+shared build_system=makefile
```

Openfoam

How can we build a software stack to help tool developers?

- Tool dependencies should be pre-installed
- A consistent environment that we can share with other tool developers to report bugs
- Can containers help here?
- Build your tools with the dependencies inside a container
  - Same kernel as the host OS
  - Can support a different OS
  - Docker/podman and Singularity/Apptainer are popular container runtimes
- Need a base container that can provide the dependencies
- E4S provides a rich set of containers with tools and libraries

Extreme-scale Scientific Software Stack (E4S)

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

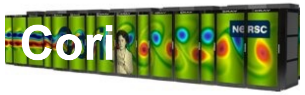
ORNL
Cray/AMD/NVIDIA

ANL
IBM BG/Q

LLNL
IBM BG/Q

Theta
THETA

ANL
Cray/Intel KNL



LBNL
Cray/Intel Xeon/KNL

LANL/SNL
Cray/Intel Xeon/KNL

ORNL
IBM/NVIDIA

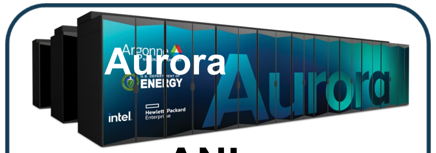
Sierra
NNSA

LLNL
IBM/NVIDIA

NERSC
Perlmutter

LBNL
HPE/AMD/NVIDIA

ORNL
HPE/AMD


Aurora
ENERGY
intel
Aurora

ANL
Intel/HPE

Exascale Systems

CROSSROADS

LANL/SNL
HPE/Intel

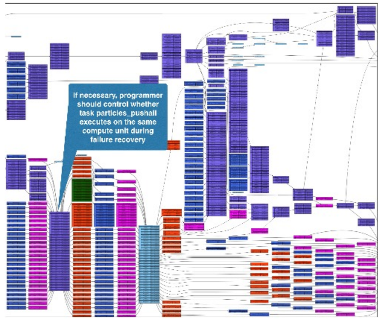
LLNL
HPE/AMD

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


If necessary, programmer should control whether task particles_pushall executes on the same compute unit during failure recovery

Extreme-scale Scientific Software Stack (E4S)

Spack

- 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 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

E4S

https://e4s.io

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

ECP EXASCALE COMPUTING PROJECT

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, 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_May23.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

https://e4s.io

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

- E4S containers support replacement of MPI libraries using MPICH ABI compatibility layer 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:

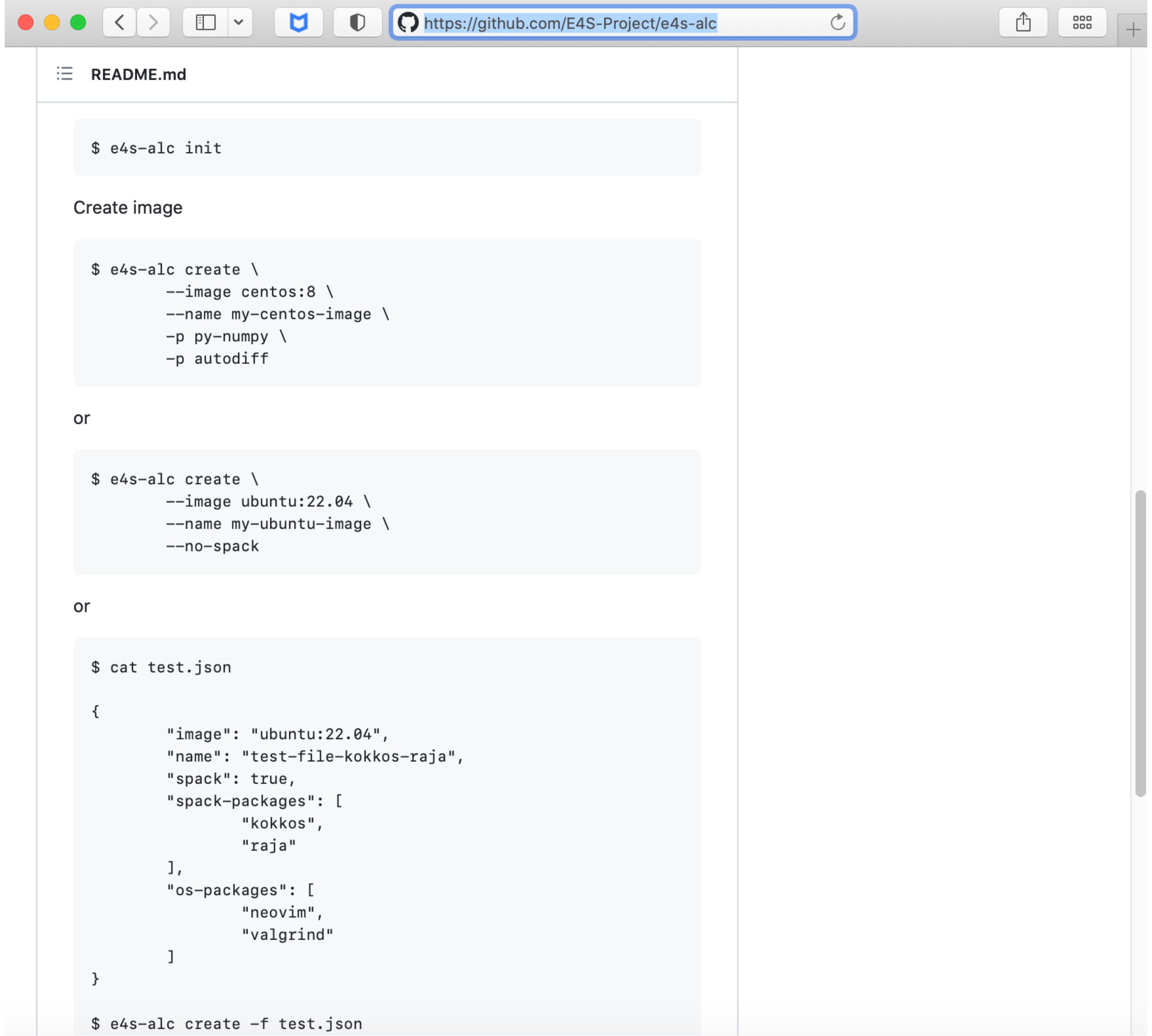
```
e4s-cl init --backend singularity --image ~/images/e4s-gpu-x86.sif --source ~/source.sh

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-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 with Docker/podman & Singularity/Apptainer!

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

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

EXASCALE
COMPUTING
PROJECT

The Spack community is growing rapidly

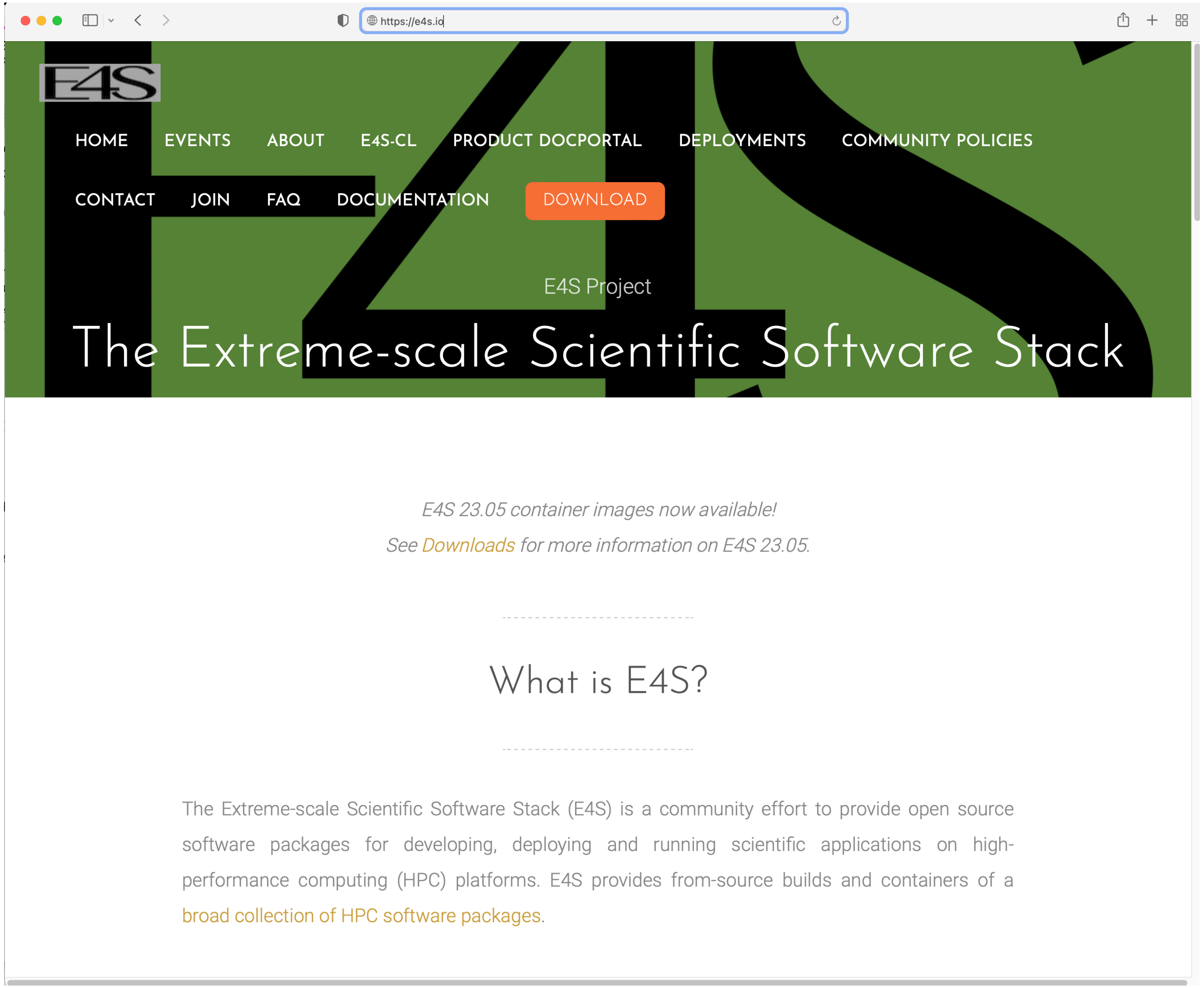
- **Spack simplifies HPC software for:**
  - Users
  - Developers
  - Cluster installations
  - The largest HPC facilities
- **Spack is central to ECP's software strategy**
  - Enable software reuse for developers and users
  - Allow the facilities to consume the entire ECP stack
- **The roadmap is packed 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



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E4S Project

The Extreme-scale Scientific Software Stack

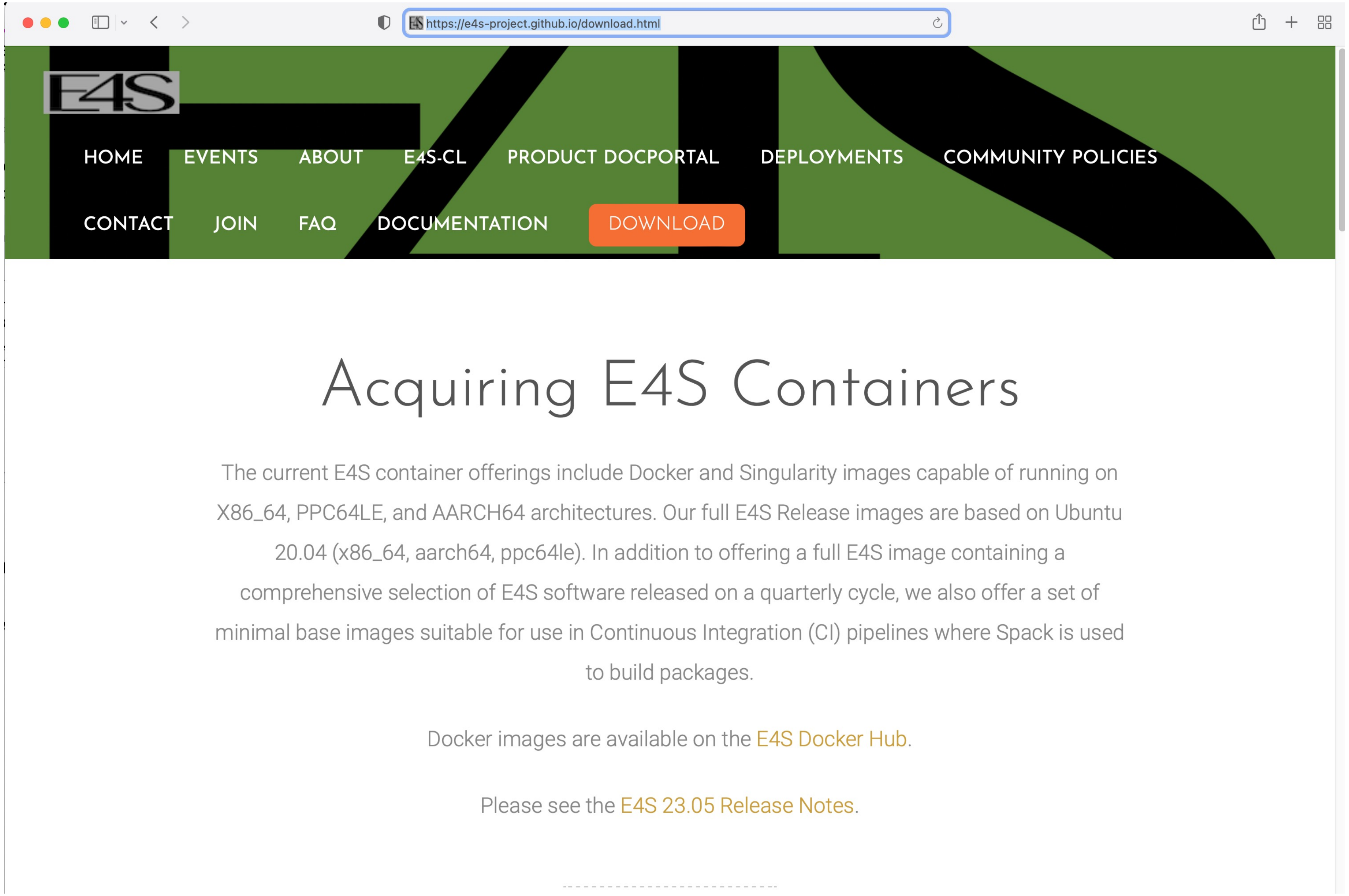
E4S 23.05 container images now available!

See Downloads for more information on E4S 23.05.

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 Container Download from https://e4s.io



https://e4s-project.github.io/download.html
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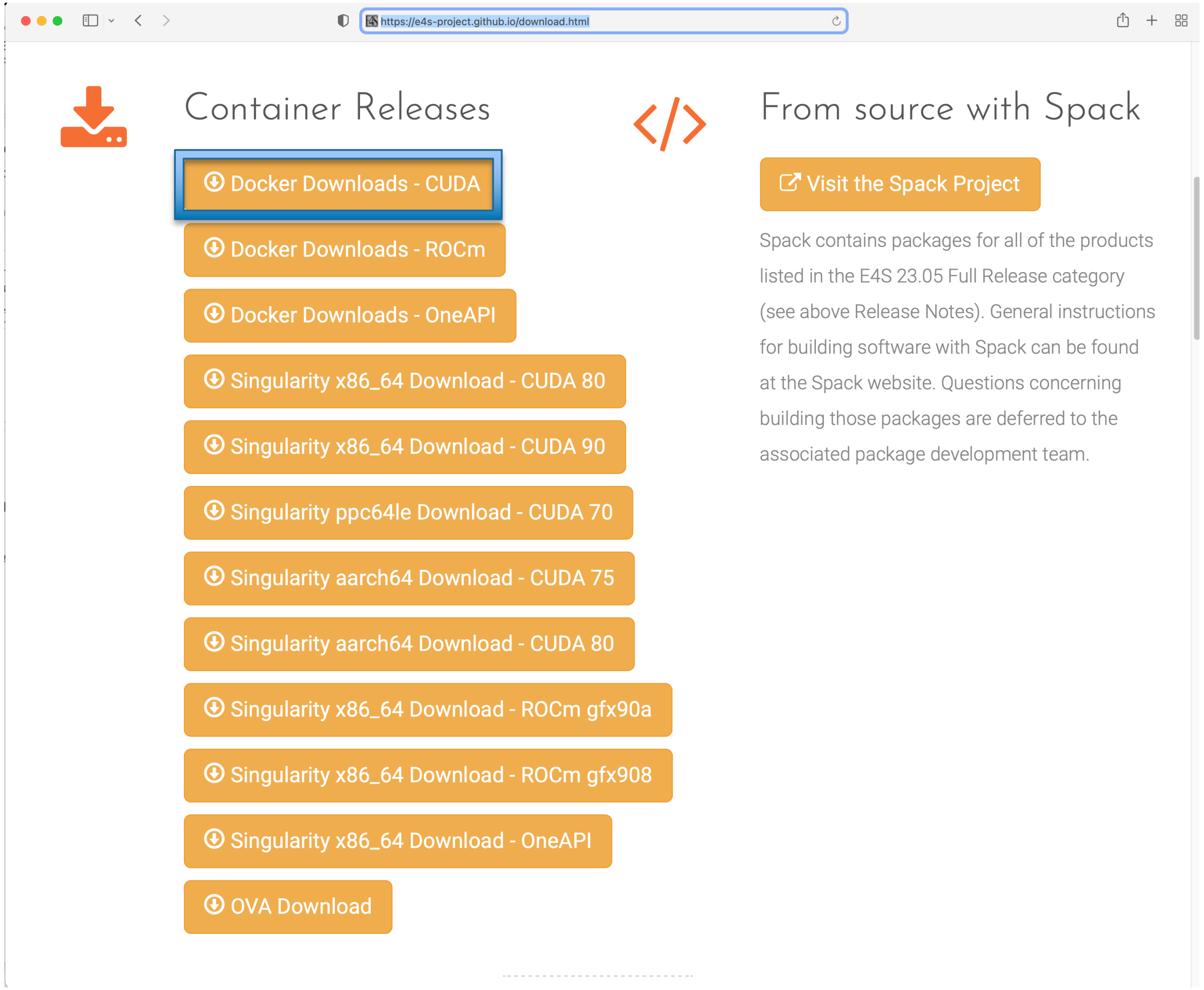
Acquiring E4S Containers

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


https://e4s-project.github.io/download.html
Docker Downloads - CUDA
Docker Downloads - ROCm
Docker Downloads - OneAPI
Singularity x86_64 Download - CUDA 80
Singularity x86_64 Download - CUDA 90
Singularity ppc64le Download - CUDA 70
Singularity aarch64 Download - CUDA 75
Singularity aarch64 Download - CUDA 80
Singularity x86_64 Download - ROCm gfx90a
Singularity x86_64 Download - ROCm gfx908
Singularity x86_64 Download - OneAPI
OVA Download
Visit the Spack Project

Container Releases

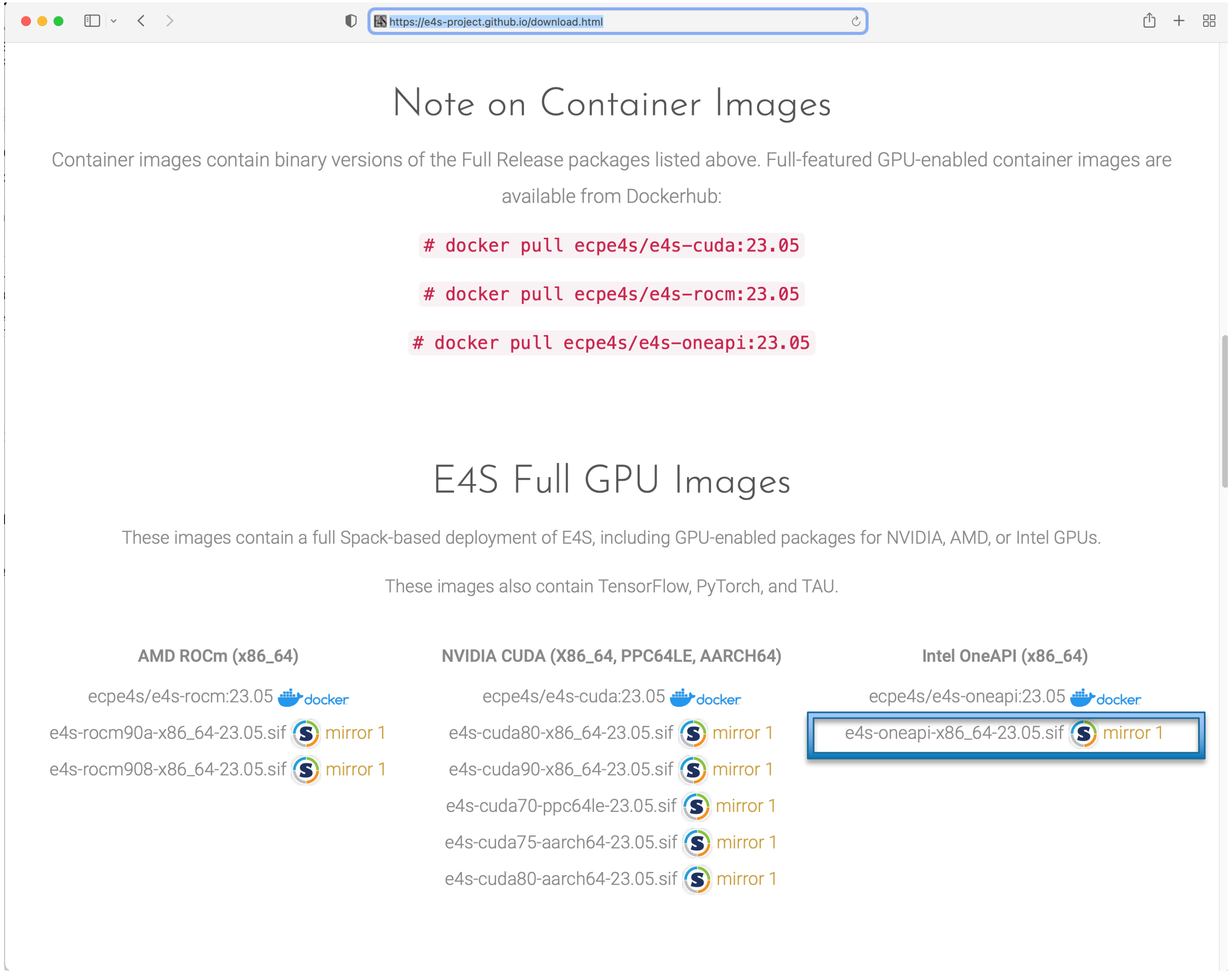
From source with Spack

Spack contains packages for all of the products listed in the E4S 23.05 Full Release category (see above Release Notes). General instructions for building software with Spack can be found at the Spack website. Questions concerning building those packages are deferred to the associated package development team.

- 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



Note on Container Images

Container images contain binary versions of the Full Release packages listed above. Full-featured GPU-enabled container images are available from Dockerhub:

```
# docker pull ecpe4s/e4s-cuda:23.05
# docker pull ecpe4s/e4s-rocm:23.05
# docker pull ecpe4s/e4s-oneapi:23.05
```

E4S Full GPU Images

These images contain a full Spack-based deployment of E4S, including GPU-enabled packages for NVIDIA, AMD, or Intel GPUs.

These images also contain TensorFlow, PyTorch, and TAU.

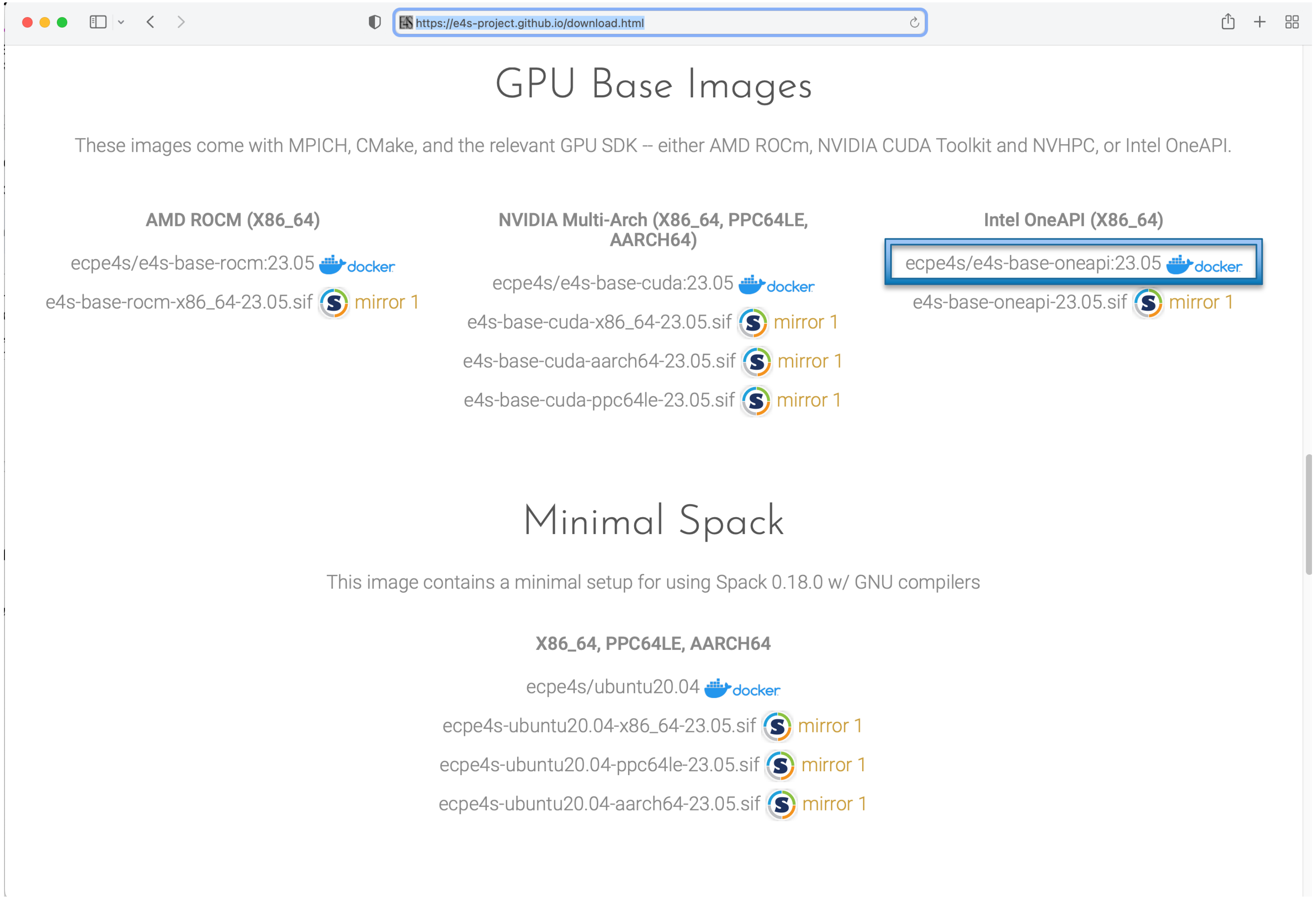
AMD ROCm (x86_64)	NVIDIA CUDA (X86_64, PPC64LE, AARCH64)	Intel OneAPI (x86_64)
ecpe4s/e4s-rocm:23.05 docker	ecpe4s/e4s-cuda:23.05 docker	ecpe4s/e4s-oneapi:23.05 docker
e4s-rocm90a-x86_64-23.05.sif mirror 1	e4s-cuda80-x86_64-23.05.sif mirror 1	e4s-oneapi-x86_64-23.05.sif mirror 1
e4s-rocm908-x86_64-23.05.sif mirror 1	e4s-cuda90-x86_64-23.05.sif mirror 1	
	e4s-cuda70-ppc64le-23.05.sif mirror 1	
	e4s-cuda75-aarch64-23.05.sif mirror 1	
	e4s-cuda80-aarch64-23.05.sif mirror 1	

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



GPU Base Images

These images come with MPICH, CMake, and the relevant GPU SDK -- either AMD ROCm, NVIDIA CUDA Toolkit and NVHPC, or Intel OneAPI.

AMD ROCM (X86_64)

ecpe4s/e4s-base-rocm:23.05 docker

e4s-base-rocm-x86_64-23.05.sif mirror 1

NVIDIA Multi-Arch (X86_64, PPC64LE, AARCH64)

ecpe4s/e4s-base-cuda:23.05 docker

e4s-base-cuda-x86_64-23.05.sif mirror 1

e4s-base-cuda-aarch64-23.05.sif mirror 1

e4s-base-cuda-ppc64le-23.05.sif mirror 1

Intel OneAPI (X86_64)

ecpe4s/e4s-base-oneapi:23.05 docker

e4s-base-oneapi-23.05.sif mirror 1

Minimal Spack

This image contains a minimal setup for using Spack 0.18.0 w/ GNU compilers

X86_64, PPC64LE, AARCH64

ecpe4s/ubuntu20.04 docker

ecpe4s-ubuntu20.04-x86_64-23.05.sif mirror 1

ecpe4s-ubuntu20.04-ppc64le-23.05.sif mirror 1

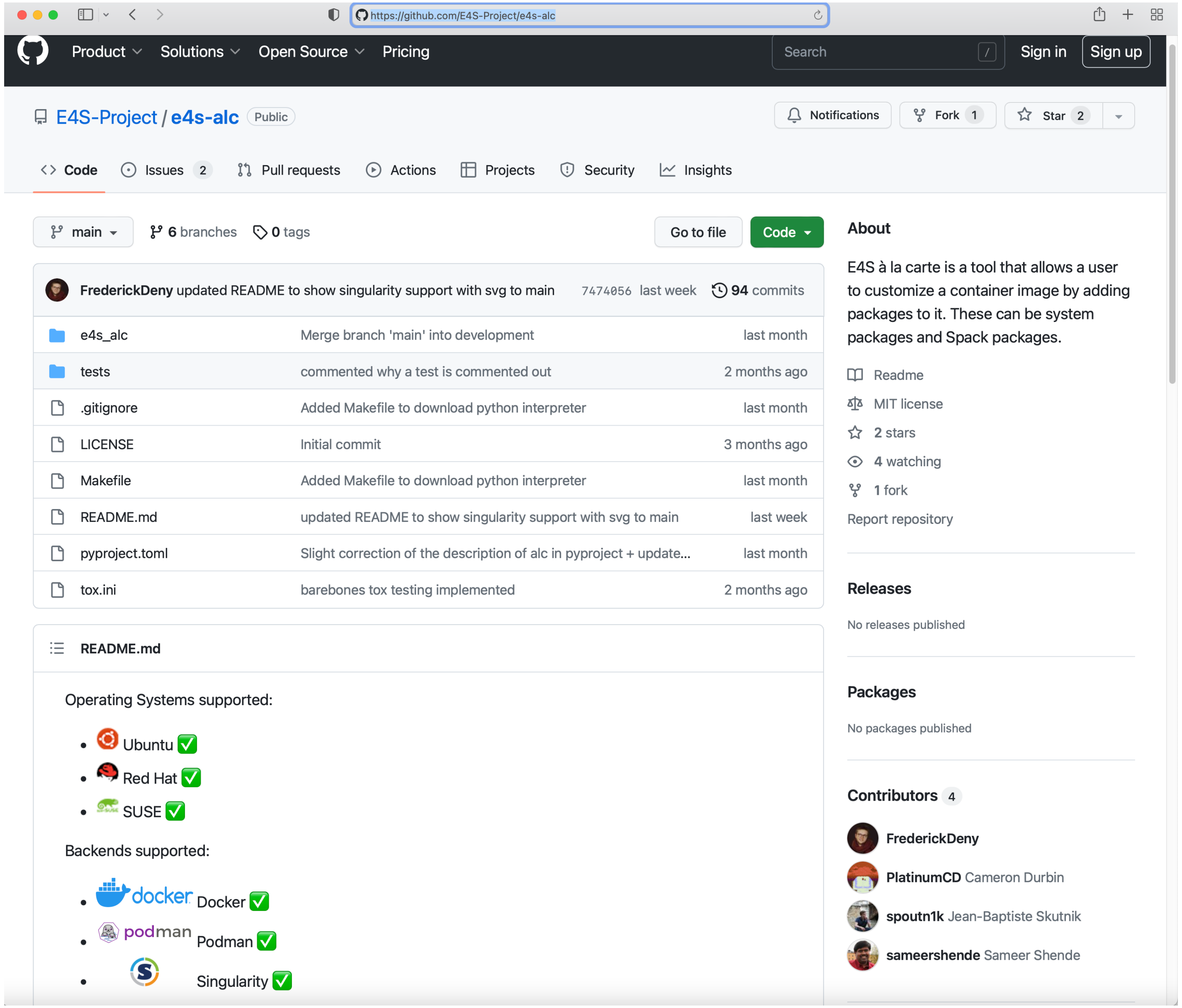
ecpe4s-ubuntu20.04-aarch64-23.05.sif mirror 1

- Intel oneAPI
- AMD ROCm
- NVIDIA NVHPC

  and CUDA

https://e4s.io

e4s-alc: a new tool to customize container images


https://github.com/E4S-Project/e4s-alc
Product
Solutions
Open Source
Pricing
Search
Sign in
Sign up
Notifications
Fork 1
Star 2
Code
Issues 2
Pull requests
Actions
Projects
Security
Insights
main
6 branches
0 tags
Go to file
Code

E4S-Project / e4s-alc Public

FrederickDeny updated README to show singularity support with svg to main 7474056 last week 94 commits

e4s_alc	Merge branch 'main' into development	last month
tests	commented why a test is commented out	2 months ago
.gitignore	Added Makefile to download python interpreter	last month
LICENSE	Initial commit	3 months ago
Makefile	Added Makefile to download python interpreter	last month
README.md	updated README to show singularity support with svg to main	last week
pyproject.toml	Slight correction of the description of alc in pyproject + update...	last month
tox.ini	barebones tox testing implemented	2 months ago

README.md

Operating Systems supported:

- Ubuntu ✅
- Red Hat ✅
- SUSE ✅

Backends supported:

- docker Docker ✅
- podman Podman ✅
- Singularity ✅

About

E4S à la carte is a tool that allows a user to customize a container image by adding packages to it. These can be system packages and Spack packages.

Readme
MIT license
2 stars
4 watching
1 fork
Report repository

Releases

No releases published

Packages

No packages published

Contributors 4

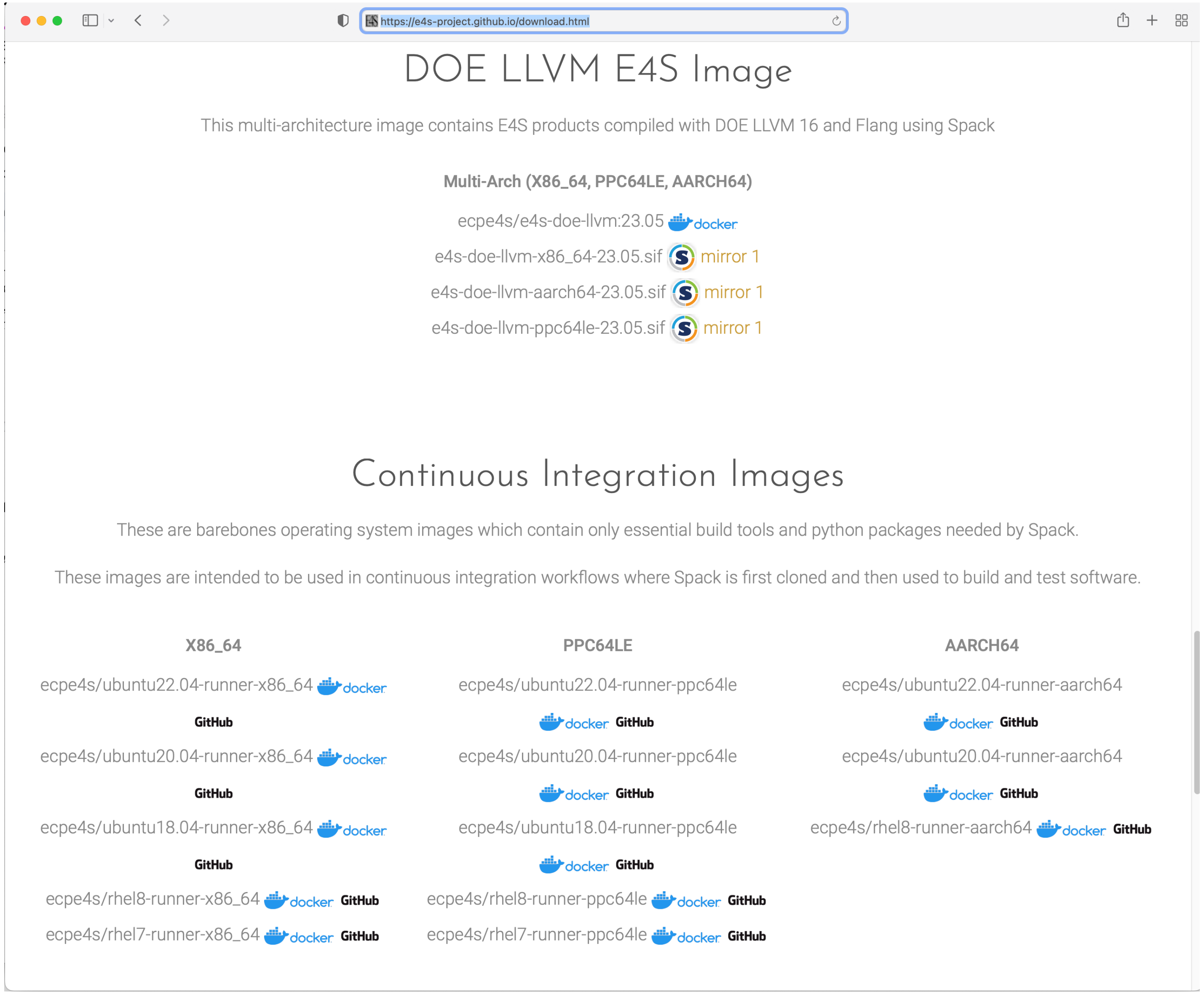
FrederickDeny
PlatinumCD Cameron Durbin
spoutn1k Jean-Baptiste Skutnik
sameershende Sameer Shende

Add to a base image:

- Spack packages
- OS packages
- Tarballs

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

E4S 23.05 DOE LLVM and CI images



DOE LLVM E4S Image

This multi-architecture image contains E4S products compiled with DOE LLVM 16 and Flang using Spack

Multi-Arch (X86_64, PPC64LE, AARCH64)

ecpe4s/e4s-doe-llvm:23.05 docker
e4s-doe-llvm-x86_64-23.05.sif mirror 1
e4s-doe-llvm-aarch64-23.05.sif mirror 1
e4s-doe-llvm-ppc64le-23.05.sif mirror 1

Continuous Integration Images

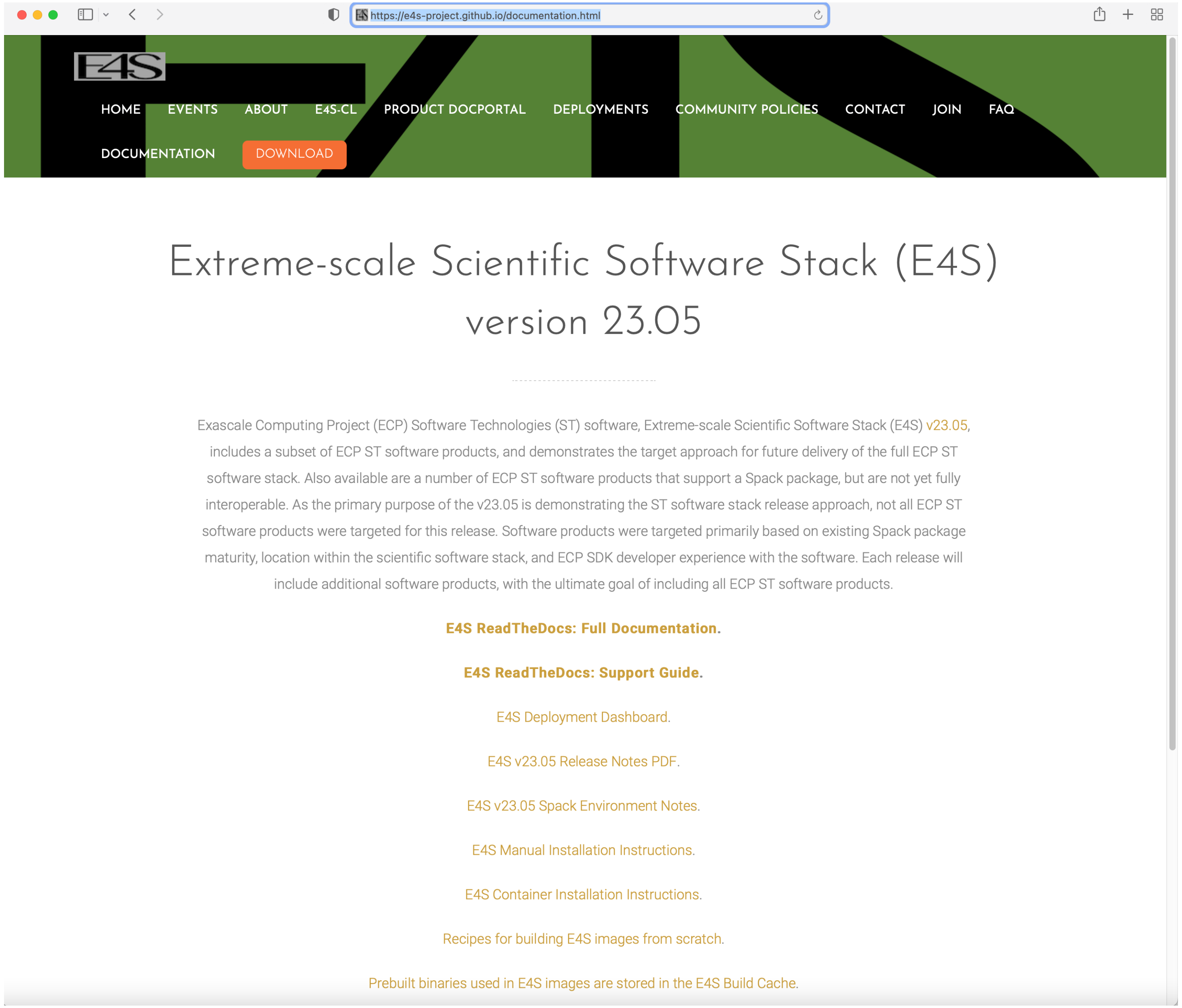
These are barebones operating system images which contain only essential build tools and python packages needed by Spack.

These images are intended to be used in continuous integration workflows where Spack is first cloned and then used to build and test software.

X86_64	PPC64LE	AARCH64
ecpe4s/ubuntu22.04-runner-x86_64 docker GitHub	ecpe4s/ubuntu22.04-runner-ppc64le docker GitHub	ecpe4s/ubuntu22.04-runner-aarch64 docker GitHub
ecpe4s/ubuntu20.04-runner-x86_64 docker GitHub	ecpe4s/ubuntu20.04-runner-ppc64le docker GitHub	ecpe4s/ubuntu20.04-runner-aarch64 docker GitHub
ecpe4s/ubuntu18.04-runner-x86_64 docker GitHub	ecpe4s/ubuntu18.04-runner-ppc64le docker GitHub	ecpe4s/rhel8-runner-aarch64 docker GitHub
ecpe4s/rhel8-runner-x86_64 docker GitHub	ecpe4s/rhel8-runner-ppc64le docker GitHub	
ecpe4s/rhel7-runner-x86_64 docker GitHub	ecpe4s/rhel7-runner-ppc64le docker GitHub	

https://e4s.io

E4S 23.05 Detailed Documentation for Bare-metal Installation


https://e4s-project.github.io/documentation.html
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E4S-CL
PRODUCT DOCPORTAL
DEPLOYMENTS
COMMUNITY POLICIES
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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.

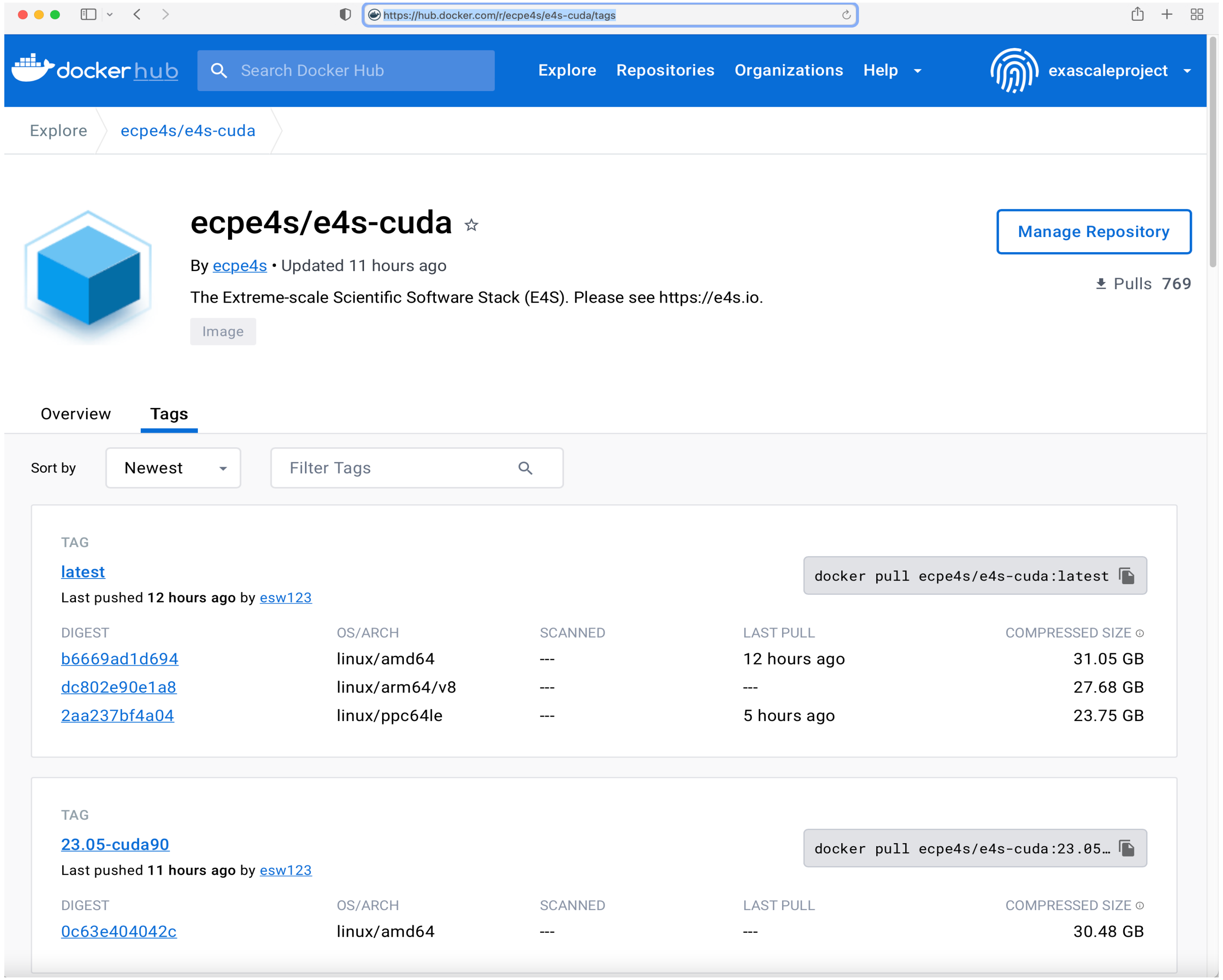
E4S Manual Installation Instructions.

E4S Container Installation Instructions.

Recipes for building E4S images from scratch.

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

E4S 23.05 full featured container release on Dockerhub


https://hub.docker.com/r/ecpe4s/e4s-cuda/tags
docker hub
Search Docker Hub
Explore
Repositories
Organizations
Help
exascaleproject
Explore
ecpe4s/e4s-cuda
Manage Repository
Image
Overview
Tags
Sort by
Newest
Filter Tags

ecpe4s/e4s-cuda ☆

By ecpe4s • Updated 11 hours ago

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

Pulls 769

TAG

latest

Last pushed **12 hours ago** by esw123

`docker pull ecpe4s/e4s-cuda:latest`

DIGEST	OS/ARCH	SCANNED	LAST PULL	COMPRESSED SIZE
b6669ad1d694	linux/amd64	---	12 hours ago	31.05 GB
dc802e90e1a8	linux/arm64/v8	---	---	27.68 GB
2aa237bf4a04	linux/ppc64le	---	5 hours ago	23.75 GB

TAG

23.05-cuda90

Last pushed **11 hours ago** by esw123

`docker pull ecpe4s/e4s-cuda:23.05…`

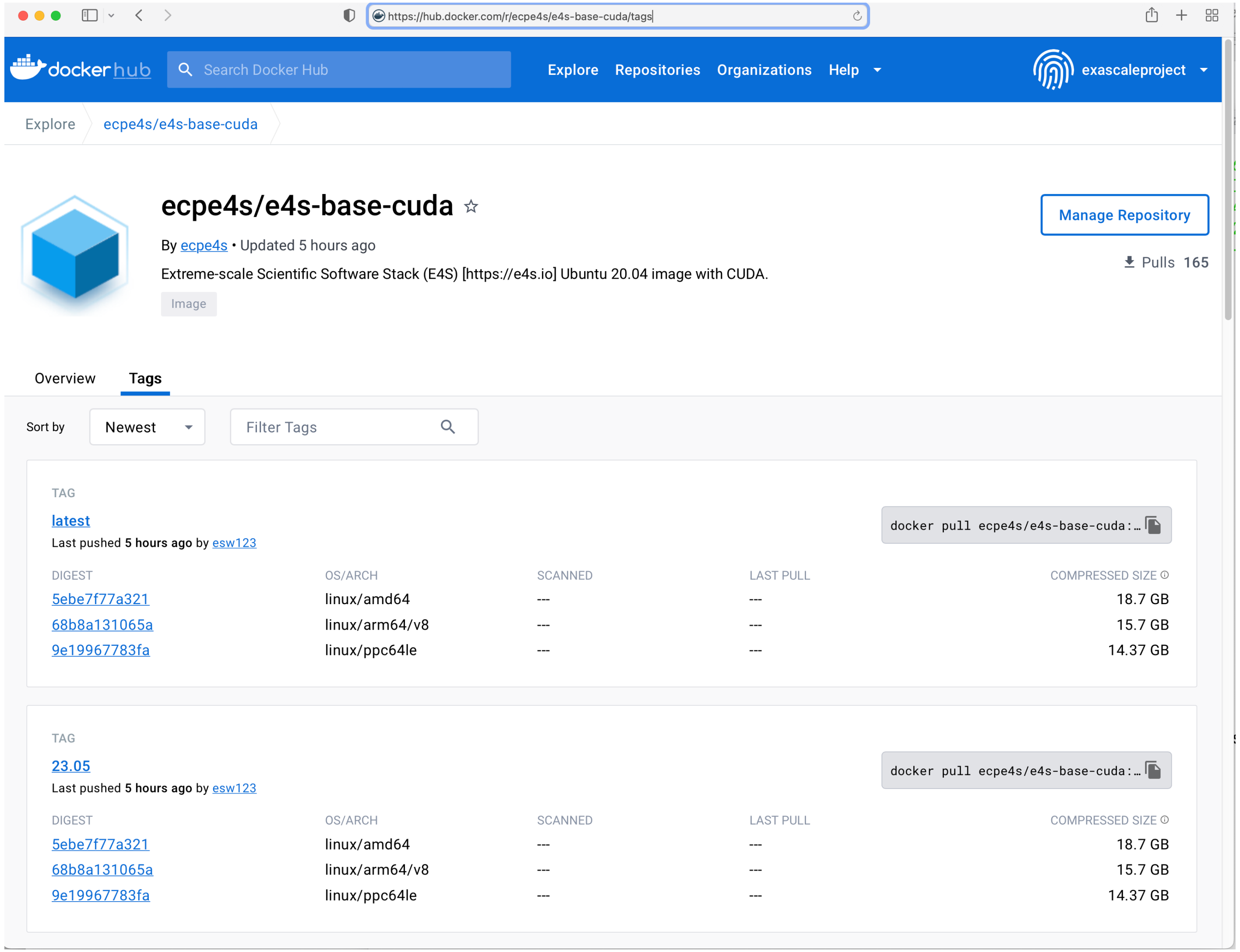
DIGEST	OS/ARCH	SCANNED	LAST PULL	COMPRESSED SIZE
0c63e404042c	linux/amd64	---	---	30.48 GB

```
docker pull ecpe4s/e4s-cuda:23.05
```

Architectures:
- x86_64
- aarch64
- ppc64le

Software:
- CUDA 12.0
- NVHPC 23.3
- oneAPI 2023.1

E4S 23.05 base container release on DockerHub


https://hub.docker.com/r/ecpe4s/e4s-base-cuda/tags
docker hub
Search Docker Hub
Explore
Repositories
Organizations
Help
exascaleproject
Explore
ecpe4s/e4s-base-cuda
Manage Repository
Pulls 165
Image
Overview
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Sort by
Newest
Filter Tags

ecpe4s/e4s-base-cuda ☆

By ecpe4s • Updated 5 hours ago

Extreme-scale Scientific Software Stack (E4S) [https://e4s.io] Ubuntu 20.04 image with CUDA.

TAG

latest

Last pushed **5 hours ago** by esw123

`docker pull ecpe4s/e4s-base-cuda:…`

DIGEST	OS/ARCH	SCANNED	LAST PULL	COMPRESSED SIZE
5ebe7f77a321	linux/amd64	---	---	18.7 GB
68b8a131065a	linux/arm64/v8	---	---	15.7 GB
9e19967783fa	linux/ppc64le	---	---	14.37 GB

TAG

23.05

Last pushed **5 hours ago** by esw123

`docker pull ecpe4s/e4s-base-cuda:…`

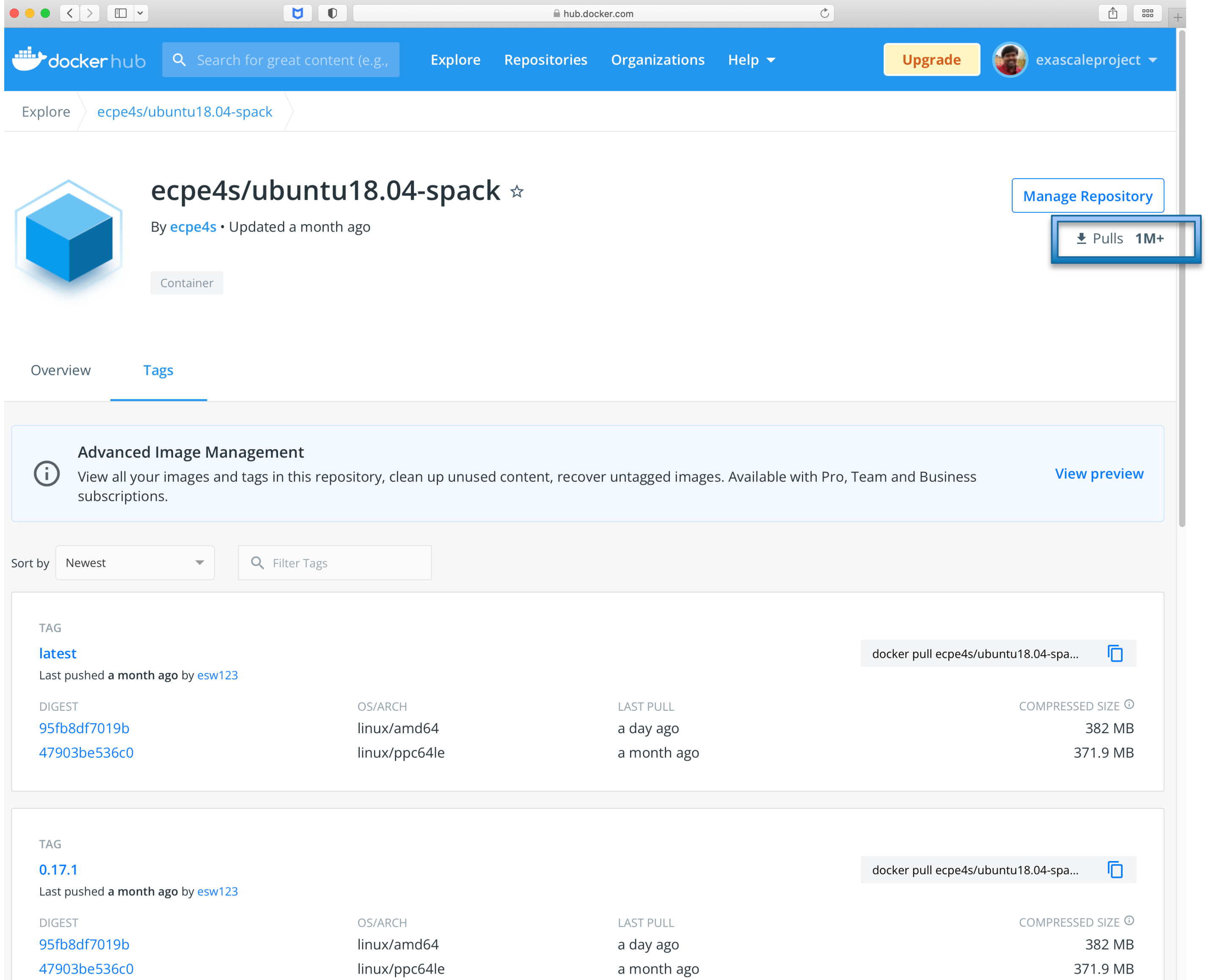
DIGEST	OS/ARCH	SCANNED	LAST PULL	COMPRESSED SIZE
5ebe7f77a321	linux/amd64	---	---	18.7 GB
68b8a131065a	linux/arm64/v8	---	---	15.7 GB
9e19967783fa	linux/ppc64le	---	---	14.37 GB

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


hub.docker.com
docker hub
Search for great content (e.g.,
Explore
Repositories
Organizations
Help
Upgrade
exascaleproject
Explore
ecpe4s/ubuntu18.04-spack
Manage Repository
Pulls 1M+
Container
Overview
Tags
View preview
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ecpe4s/ubuntu18.04-spack ☆

By ecpe4s • Updated a month ago

Advanced Image Management

View all your images and tags in this repository, clean up unused content, recover untagged images. Available with Pro, Team and Business subscriptions.

TAG

latest

Last pushed **a month ago** by esw123

`docker pull ecpe4s/ubuntu18.04-spa...`

DIGEST	OS/ARCH	LAST PULL	COMPRESSED SIZE
95fb8df7019b	linux/amd64	a day ago	382 MB
47903be536c0	linux/ppc64le	a month ago	371.9 MB

TAG

0.17.1

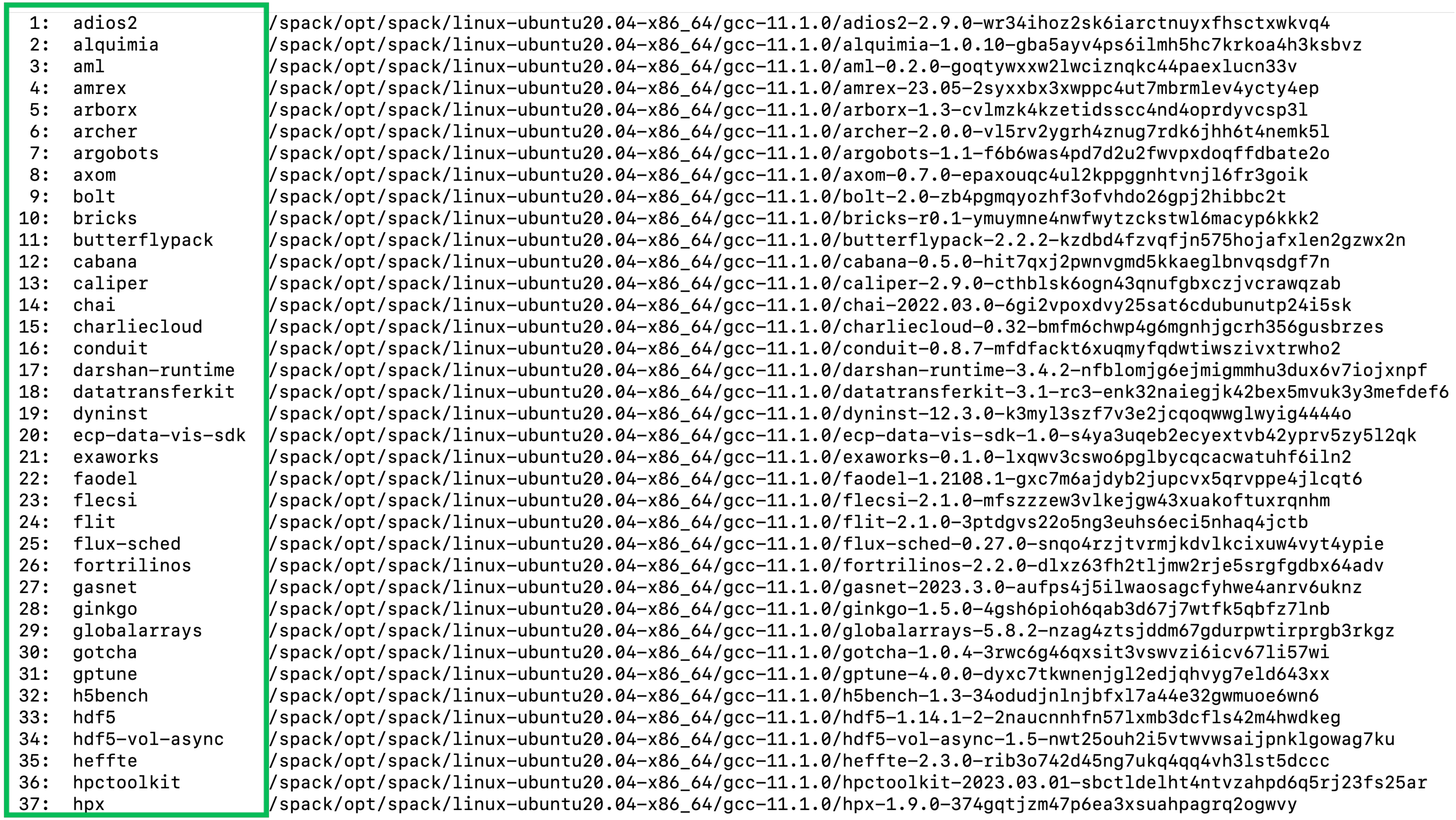
Last pushed **a month ago** by esw123

`docker pull ecpe4s/ubuntu18.04-spa...`

DIGEST	OS/ARCH	LAST PULL	COMPRESSED SIZE
95fb8df7019b	linux/amd64	a day ago	382 MB
47903be536c0	linux/ppc64le	a month ago	371.9 MB

- Create custom container images
- 1M+ downloads!

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



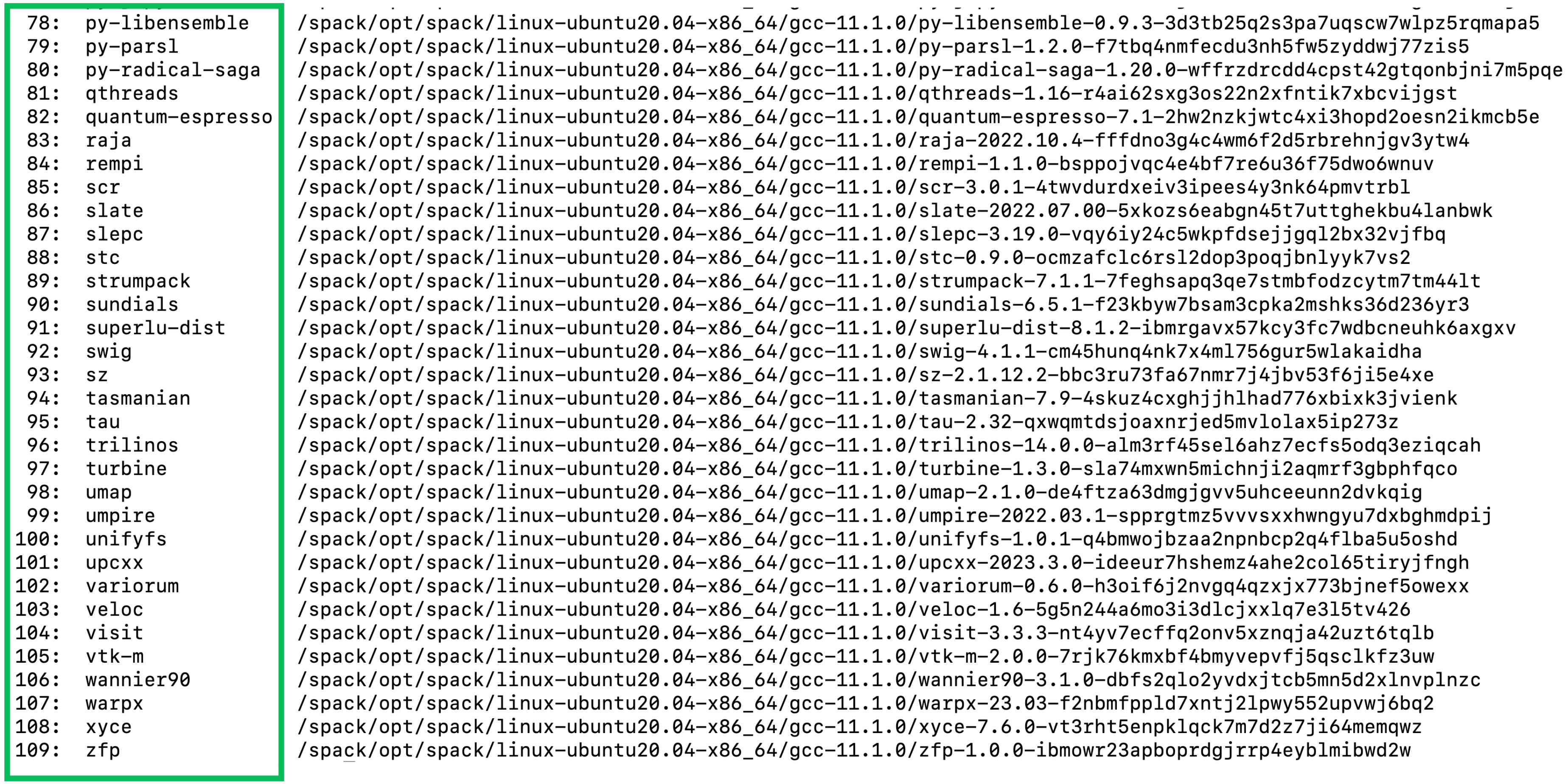
```
 1:  adios2            /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/adios2-2.9.0-wr34ihoz2sk6iarctnuyxfhsctxwkvq4
 2:  alquimia          /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/alquimia-1.0.10-gba5ayv4ps6ilmh5hc7krkoa4h3ksbvz
 3:  aml               /spack/opt/spack/linux-ubuntu20.04-x86_64/gcc-11.1.0/aml-0.2.0-goqtywxxw2lwciznqkc44paexlucn33v
 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-dapbrjq25hsqg2czteuusqkismcpnbu
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
```

23.02 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

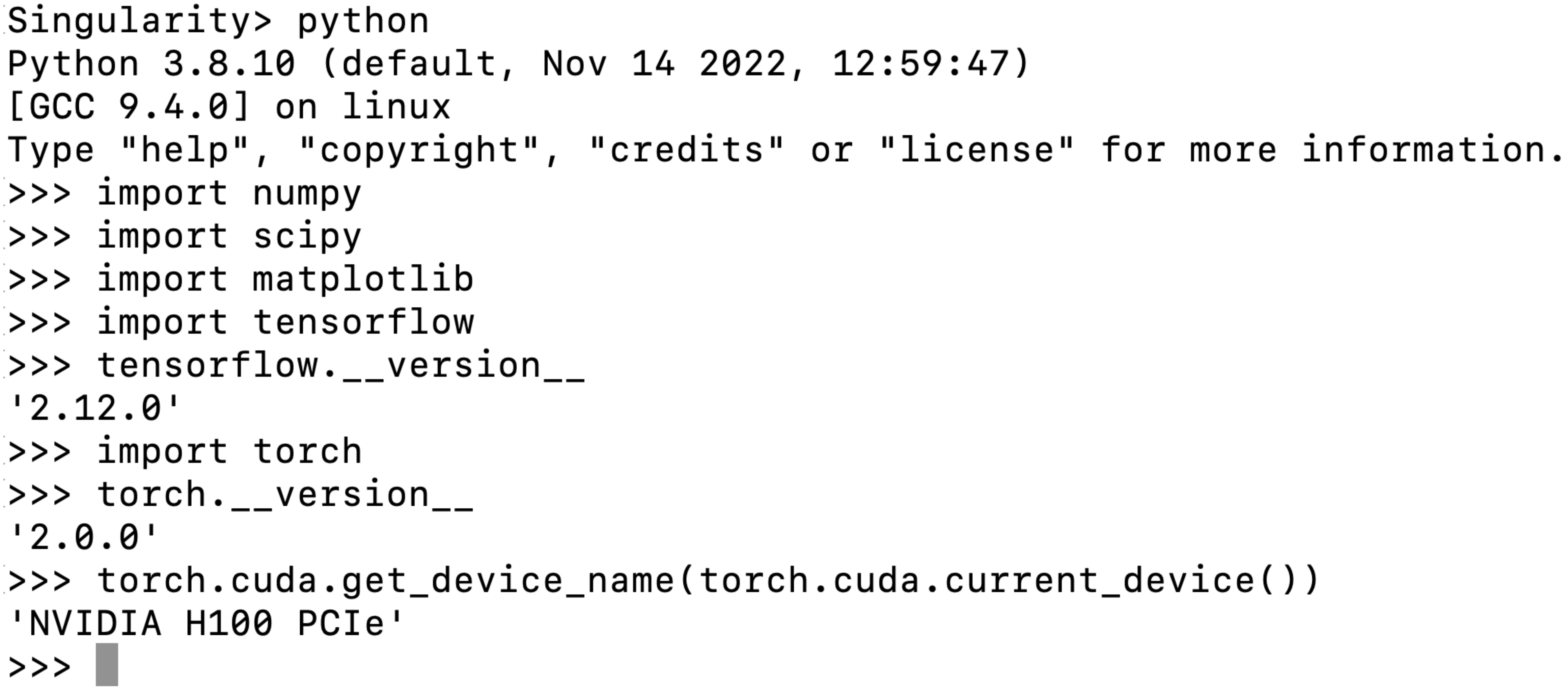
AI products with GPU support
- Tensorflow
- Pytorch

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

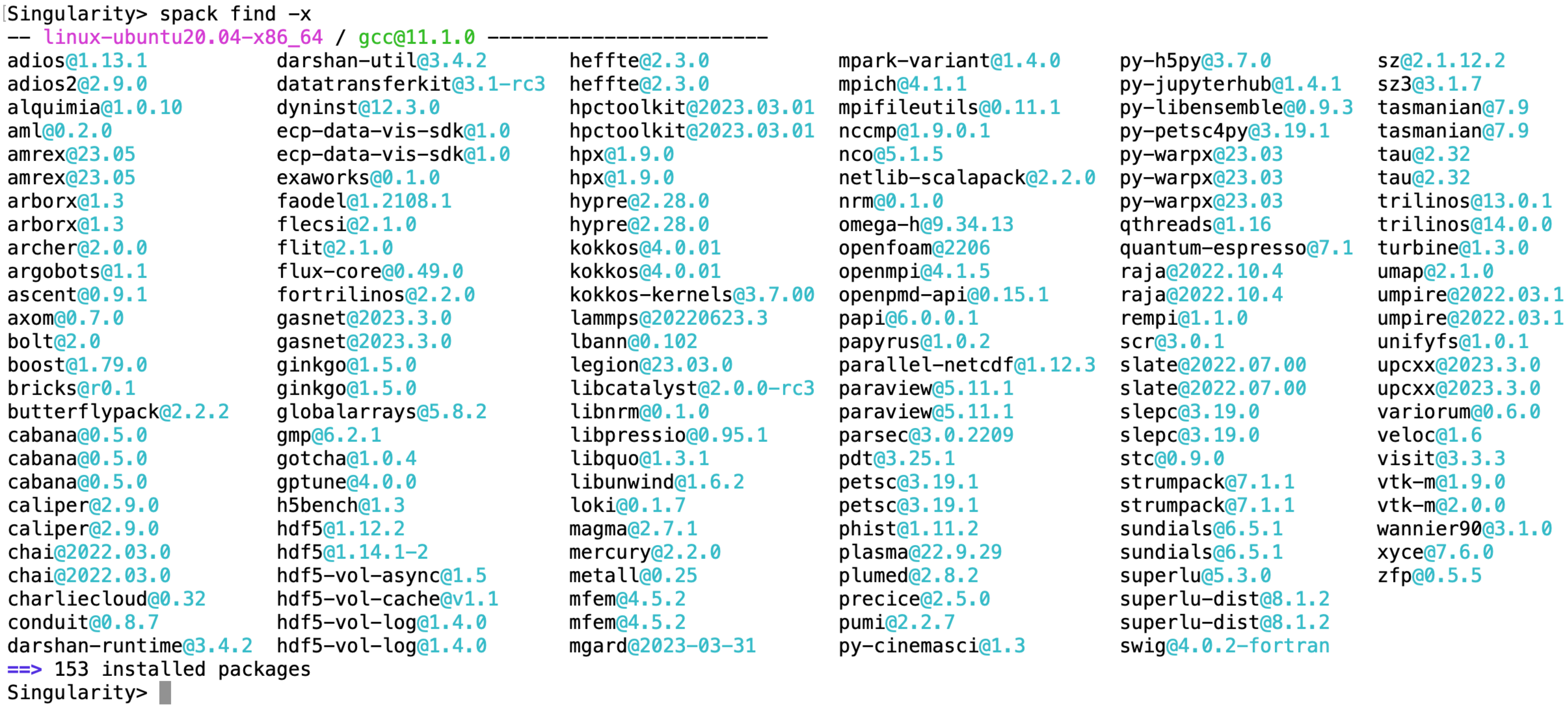
E4S Support for AI/ML frameworks with V100, A100, and H100 GPUs



```
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'
>>> 
```

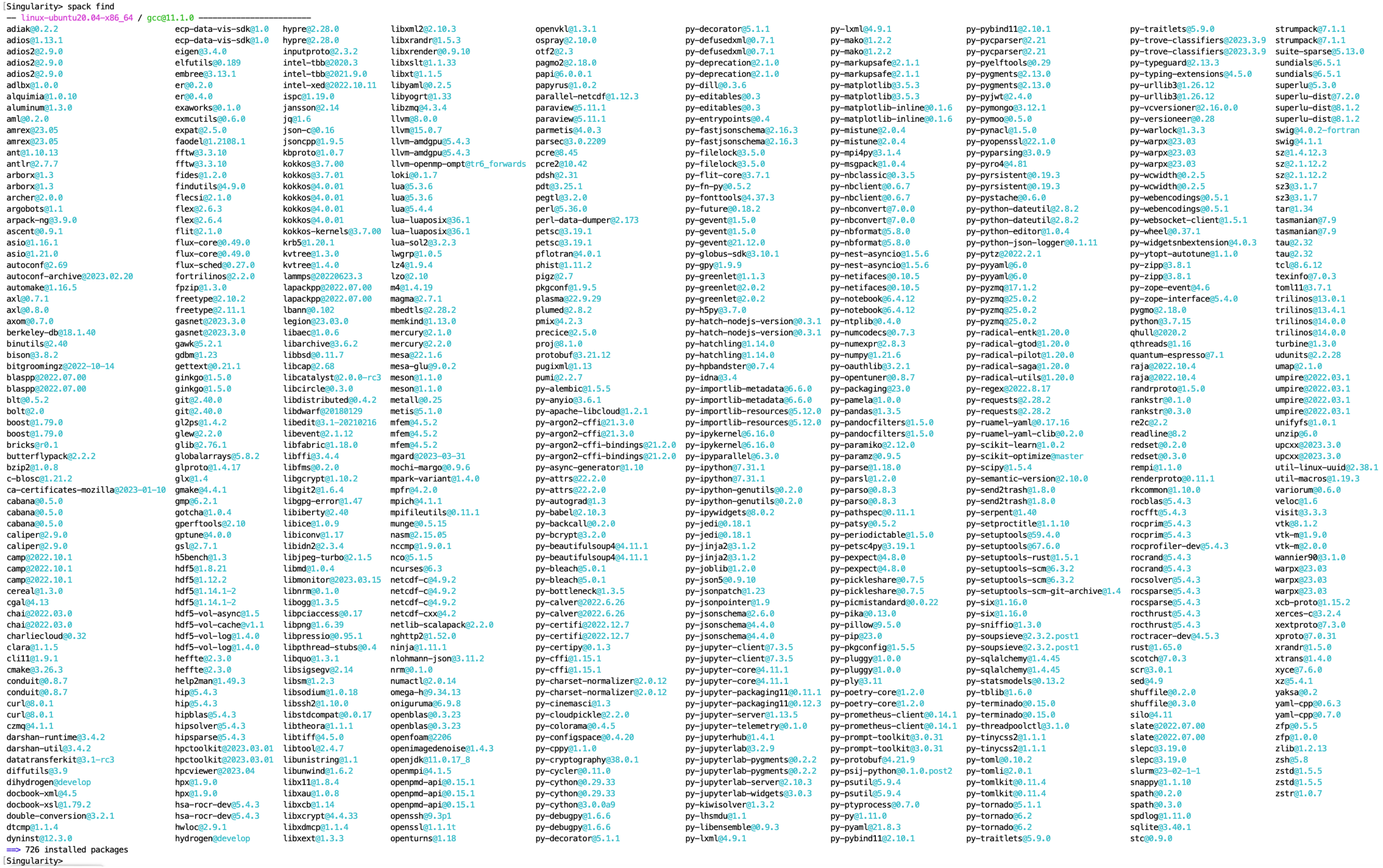
E4S 23.05 supports NVIDIA H100 GPUs with TensorFlow 2.12.0 and PyTorch 2.0.0

E4S 23.05 container with ROCm: Top level specs



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

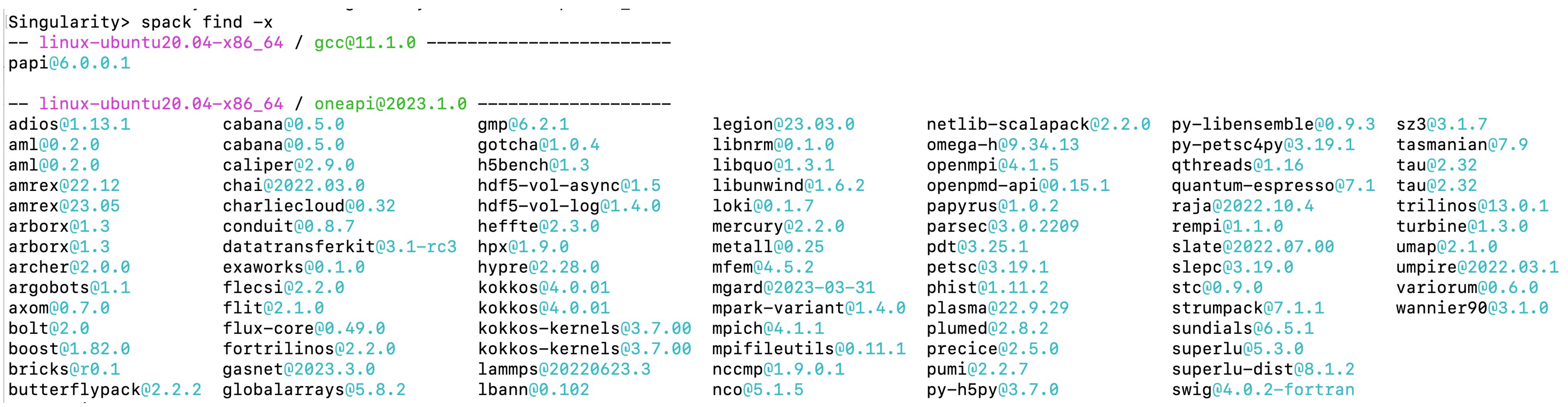
E4S 23.05 : All Spack packages including dependencies!



```
[Singularity> spack find
-- linux-ubuntu20.04-x86_64 / gcc@11.1.0 ------------------------
adiak@0.2.2                        ecp-data-vis-sdk@1.0  hypre@2.28.0          libxml2@2.10.3                openvkl@1.3.1                  py-decorator@5.1.1            py-lxml@4.9.1               py-pybind11@2.10.1                py-traitlets@5.9.0            strumpack@7.1.1
adios@1.13.1                       ecp-data-vis-sdk@1.0  hypre@2.28.0          libxrandr@1.5.3               ospray@2.10.0                  py-defusedxml@0.7.1           py-mako@1.2.2               py-pycparser@2.21                 py-trove-classifiers@2023.3.9 strumpack@7.1.1
adios2@2.9.0                       eigen@3.4.0           inputproto@2.3.2      libxrender@0.9.10             otf2@2.3                       py-defusedxml@0.7.1           py-mako@1.2.2               py-pycparser@2.21                 py-trove-classifiers@2023.3.9 suite-sparse@5.13.0
adios2@2.9.0                       elfutils@0.189        intel-tbb@2020.3      libxslt@1.1.33                pagmo2@2.18.0                  py-deprecation@2.1.0          py-markupsafe@2.1.1         py-pyelftools@0.29                py-typeguard@2.13.3           sundials@6.5.1
adios2@2.9.0                       embree@3.13.1         intel-tbb@2021.9.0    libxt@1.1.5                   papi@6.0.0.1                   py-deprecation@2.1.0          py-markupsafe@2.1.1         py-pygments@2.13.0                py-typing-extensions@4.5.0    sundials@6.5.1
adlbx@1.0.0                        er@0.2.0              intel-xed@2022.10.11  libyaml@0.2.5                 papyrus@1.0.2                  py-dill@0.3.6                 py-matplotlib@3.5.3         py-pygments@2.13.0                py-urllib3@1.26.12            superlu@5.3.0
alquimia@1.0.10                    er@0.4.0              ispc@1.19.0           libyogrt@1.33                 parallel-netcdf@1.12.3         py-editables@0.3              py-matplotlib@3.5.3         py-pyjwt@2.4.0                    py-urllib3@1.26.12            superlu-dist@7.2.0
aluminum@1.3.0                     exaworks@0.1.0        jansson@2.14          libzmq@4.3.4                  paraview@5.11.1                py-editables@0.3              py-matplotlib-inline@0.1.6  py-pymongo@3.12.1                 py-vcversioner@2.16.0.0       superlu-dist@8.1.2
aml@0.2.0                          exmcutils@0.6.0       jq@1.6                llvm@8.0.0                    paraview@5.11.1                py-entrypoints@0.4            py-matplotlib-inline@0.1.6  py-pymoo@0.5.0                    py-versioneer@0.28            superlu-dist@8.1.2
amrex@23.05                        expat@2.5.0           json-c@0.16           llvm@15.0.7                   parmetis@4.0.3                 py-fastjsonschema@2.16.3      py-mistune@2.0.4            py-pynacl@1.5.0                   py-warlock@1.3.3              swig@4.0.2-fortran
amrex@23.05                        faodel@1.2108.1       jsoncpp@1.9.5         llvm-amdgpu@5.4.3             parsec@3.0.2209                py-fastjsonschema@2.16.3      py-mistune@2.0.4            py-pyopenssl@22.1.0               py-warpx@23.03                swig@4.1.1
ant@1.10.13                        fftw@3.3.10           kbproto@1.0.7         llvm-amdgpu@5.4.3             pcre@8.45                      py-filelock@3.5.0             py-mpi4py@3.1.4             py-pyparsing@3.0.9                py-warpx@23.03                sz@1.4.12.3
antlr@2.7.7                        fftw@3.3.10           kokkos@3.7.00         llvm-openmp-ompt@tr6_forwards pcre2@10.42                    py-filelock@3.5.0             py-msgpack@1.0.4            py-pyro4@4.81                     py-warpx@23.03                sz@2.1.12.2
arborx@1.3                         fides@1.2.0           kokkos@3.7.01         loki@0.1.7                    pdsh@2.31                      py-flit-core@3.7.1            py-nbclassic@0.3.5          py-pyrsistent@0.19.3              py-wcwidth@0.2.5              sz@2.1.12.2
arborx@1.3                         findutils@4.9.0       kokkos@4.0.01         lua@5.3.6                     pdt@3.25.1                     py-fn-py@0.5.2                py-nbclient@0.6.7           py-pyrsistent@0.19.3              py-wcwidth@0.2.5              sz3@3.1.7
archer@2.0.0                       flecsi@2.1.0          kokkos@4.0.01         lua@5.3.6                     pegtl@3.2.0                    py-fonttools@4.37.3           py-nbclient@0.6.7           py-pystache@0.6.0                 py-webencodings@0.5.1         sz3@3.1.7
argobots@1.1                       flex@2.6.3            kokkos@4.0.01         lua@5.4.4                     perl@5.36.0                    py-future@0.18.2              py-nbconvert@7.0.0          py-python-dateutil@2.8.2          py-webencodings@0.5.1         tar@1.34
arpack-ng@3.9.0                    flex@2.6.4            kokkos@4.0.01         lua-luaposix@36.1             perl-data-dumper@2.173         py-gevent@1.5.0               py-nbconvert@7.0.0          py-python-dateutil@2.8.2          py-websocket-client@1.5.1     tasmanian@7.9
ascent@0.9.1                       flit@2.1.0            kokkos-kernels@3.7.00 lua-luaposix@36.1             petsc@3.19.1                   py-gevent@1.5.0               py-nbformat@5.8.0           py-python-editor@1.0.4            py-wheel@0.37.1               tasmanian@7.9
asio@1.16.1                        flux-core@0.49.0      krb5@1.20.1           lua-sol2@3.2.3                petsc@3.19.1                   py-gevent@21.12.0             py-nbformat@5.8.0           py-python-json-logger@0.1.11      py-widgetsnbextension@4.0.3   tau@2.32
asio@1.21.0                        flux-core@0.49.0      kvtree@1.3.0          lwgrp@1.0.5                   pflotran@4.0.1                 py-globus-sdk@3.10.1          py-nest-asyncio@1.5.6       py-pytz@2022.2.1                  py-ytopt-autotune@1.1.0       tau@2.32
autoconf@2.69                      flux-sched@0.27.0     kvtree@1.4.0          lz4@1.9.4                     phist@1.11.2                   py-gpy@1.9.9                  py-nest-asyncio@1.5.6       py-pyyaml@6.0                     py-zipp@3.8.1                 tcl@8.6.12
autoconf-archive@2023.02.20        fortrilinos@2.2.0     lammps@20220623.3     lzo@2.10                      pigz@2.7                       py-greenlet@1.1.3             py-netifaces@0.10.5         py-pyyaml@6.0                     py-zipp@3.8.1                 texinfo@7.0.3
automake@1.16.5                    fpzip@1.3.0           lapackpp@2022.07.00   m4@1.4.19                     pkgconf@1.9.5                  py-greenlet@2.0.2             py-netifaces@0.10.5         py-pyzmq@17.1.2                   py-zope-event@4.6             toml11@3.7.1
axl@0.7.1                          freetype@2.10.2       lapackpp@2022.07.00   magma@2.7.1                   plasma@22.9.29                 py-greenlet@2.0.2             py-notebook@6.4.12          py-pyzmq@25.0.2                   py-zope-interface@5.4.0       trilinos@13.0.1
axl@0.8.0                          freetype@2.11.1       lbann@0.102           mbedtls@2.28.2                plumed@2.8.2                   py-h5py@3.7.0                 py-notebook@6.4.12          py-pyzmq@25.0.2                   pygmo@2.18.0                  trilinos@13.4.1
axom@0.7.0                         gasnet@2023.3.0       legion@23.03.0        memkind@1.13.0                pmix@4.2.3                     py-hatch-nodejs-version@0.3.1 py-ntplib@0.4.0             py-pyzmq@25.0.2                   python@3.7.15                 trilinos@14.0.0
berkeley-db@18.1.40                gasnet@2023.3.0       libaec@1.0.6          mercury@2.1.0                 precice@2.5.0                  py-hatch-nodejs-version@0.3.1 py-numcodecs@0.7.3          py-radical-entk@1.20.0            qhull@2020.2                  trilinos@14.0.0
binutils@2.40                      gawk@5.2.1            libarchive@3.6.2      mercury@2.2.0                 proj@8.1.0                     py-hatchling@1.14.0           py-numexpr@2.8.3            py-radical-gtod@1.20.0            qthreads@1.16                 turbine@1.3.0
bison@3.8.2                        gdbm@1.23             libbsd@0.11.7         mesa@22.1.6                   protobuf@3.21.12               py-hatchling@1.14.0           py-numpy@1.21.6             py-radical-pilot@1.20.0           quantum-espresso@7.1          udunits@2.2.28
bitgroomingz@2022-10-14            gettext@0.21.1        libcap@2.68           mesa-glu@9.0.2                pugixml@1.13                   py-hpbandster@0.7.4           py-oauthlib@3.2.1           py-radical-saga@1.20.0            raja@2022.10.4                umap@2.1.0
blaspp@2022.07.00                  ginkgo@1.5.0          libcatalyst@2.0.0-rc3 meson@1.1.0                   pumi@2.2.7                     py-idna@3.4                   py-opentuner@0.8.7          py-radical-utils@1.20.0           raja@2022.10.4                umpire@2022.03.1
blaspp@2022.07.00                  ginkgo@1.5.0          libcircle@0.3.0       meson@1.1.0                   py-alembic@1.5.5               py-importlib-metadata@6.6.0   py-packaging@23.0           py-regex@2022.8.17                randrproto@1.5.0              umpire@2022.03.1
blt@0.5.2                          git@2.40.0            libdistributed@0.4.2  metall@0.25                   py-anyio@3.6.1                 py-importlib-metadata@6.6.0   py-pamela@1.0.0             py-requests@2.28.2                rankstr@0.1.0                 umpire@2022.03.1
bolt@2.0                           git@2.40.0            libdwarf@20180129     metis@5.1.0                   py-apache-libcloud@1.2.1       py-importlib-resources@5.12.0 py-pandas@1.3.5             py-requests@2.28.2                rankstr@0.3.0                 umpire@2022.03.1
boost@1.79.0                       gl2ps@1.4.2           libedit@3.1-20210216  mfem@4.5.2                    py-argon2-cffi@21.3.0          py-importlib-resources@5.12.0 py-pandocfilters@1.5.0      py-ruamel-yaml@0.17.16            re2c@2.2                      unifyfs@1.0.1
boost@1.79.0                       glew@2.2.0            libevent@2.1.12       mfem@4.5.2                    py-argon2-cffi@21.3.0          py-ipykernel@6.16.0           py-pandocfilters@1.5.0      py-ruamel-yaml-clib@0.2.0         readline@8.2                  unzip@6.0
bricks@r0.1                        glib@2.76.1           libfabric@1.18.0      mfem@4.5.2                    py-argon2-cffi-bindings@21.2.0 py-ipykernel@6.16.0           py-paramiko@2.12.0          py-scikit-learn@1.0.2             redset@0.2.0                  upcxx@2023.3.0
butterflypack@2.2.2                globalarrays@5.8.2    libffi@3.4.4          mgard@2023-03-31              py-argon2-cffi-bindings@21.2.0 py-ipyparallel@6.3.0          py-paramz@0.9.5             py-scikit-optimize@master         redset@0.3.0                  upcxx@2023.3.0
bzip2@1.0.8                        glproto@1.4.17        libfms@0.2.0          mochi-margo@0.9.6             py-async-generator@1.10        py-ipython@7.31.1             py-parse@1.18.0             py-scipy@1.5.4                    rempi@1.1.0                   util-linux-uuid@2.38.1
c-blosc@1.21.2                     glx@1.4               libgcrypt@1.10.2      mpark-variant@1.4.0           py-attrs@22.2.0                py-ipython@7.31.1             py-parsl@1.2.0              py-semantic-version@2.10.0        renderproto@0.11.1            util-macros@1.19.3
ca-certificates-mozilla@2023-01-10 gmake@4.4.1           libgit2@1.6.4         mpfr@4.2.0                    py-attrs@22.2.0                py-ipython-genutils@0.2.0     py-parso@0.8.3              py-send2trash@1.8.0               rkcommon@1.10.0               variorum@0.6.0
cabana@0.5.0                       gmp@6.2.1             libgpg-error@1.47     mpich@4.1.1                   py-autograd@1.3                py-ipython-genutils@0.2.0     py-parso@0.8.3              py-send2trash@1.8.0               rocblas@5.4.3                 veloc@1.6
cabana@0.5.0                       gotcha@1.0.4          libiberty@2.40        mpifileutils@0.11.1           py-babel@2.10.3                py-ipywidgets@8.0.2           py-pathspec@0.11.1          py-serpent@1.40                   rocfft@5.4.3                  visit@3.3.3
cabana@0.5.0                       gperftools@2.10       libice@1.0.9          munge@0.5.15                  py-backcall@0.2.0              py-jedi@0.18.1                py-patsy@0.5.2              py-setproctitle@1.1.10            rocprim@5.4.3                 vtk@8.1.2
caliper@2.9.0                      gptune@4.0.0          libiconv@1.17         nasm@2.15.05                  py-bcrypt@3.2.0                py-jedi@0.18.1                py-periodictable@1.5.0      py-setuptools@59.4.0              rocprim@5.4.3                 vtk-m@1.9.0
caliper@2.9.0                      gsl@2.7.1             libidn2@2.3.4         nccmp@1.9.0.1                 py-beautifulsoup4@4.11.1       py-jinja2@3.1.2               py-petsc4py@3.19.1          py-setuptools@67.6.0              rocprofiler-dev@5.4.3         vtk-m@2.0.0
camp@2022.10.1                     h5bench@1.3           libjpeg-turbo@2.1.5   nco@5.1.5                     py-beautifulsoup4@4.11.1       py-jinja2@3.1.2               py-pexpect@4.8.0            py-setuptools-rust@1.5.1          rocrand@5.4.3                 wannier90@3.1.0
camp@2022.10.1                     hdf5@1.8.21           libmd@1.0.4           ncurses@6.3                   py-bleach@5.0.1                py-joblib@1.2.0               py-pexpect@4.8.0            py-setuptools-scm@6.3.2           rocrand@5.4.3                 warpx@23.03
camp@2022.10.1                     hdf5@1.12.2           libmonitor@2023.03.15 netcdf-c@4.9.2                py-bleach@5.0.1                py-json5@0.9.10               py-pickleshare@0.7.5        py-setuptools-scm@6.3.2           rocsolver@5.4.3               warpx@23.03
cereal@1.3.0                       hdf5@1.14.1-2         libnrm@0.1.0          netcdf-c@4.9.2                py-bottleneck@1.3.5            py-jsonpatch@1.23             py-pickleshare@0.7.5        py-setuptools-scm-git-archive@1.4 rocsparse@5.4.3               warpx@23.03
cgal@4.13                          hdf5@1.14.1-2         libogg@1.3.5          netcdf-c@4.9.2                py-calver@2022.6.26            py-jsonpointer@1.9            py-picmistandard@0.0.22     py-six@1.16.0                     rocsparse@5.4.3               xcb-proto@1.15.2
chai@2022.03.0                     hdf5-vol-async@1.5    libpciaccess@0.17     netcdf-cxx@4.2                py-calver@2022.6.26            py-jsonschema@2.6.0           py-pika@0.13.0              py-six@1.16.0                     rocthrust@5.4.3               xerces-c@3.2.4
chai@2022.03.0                     hdf5-vol-cache@v1.1   libpng@1.6.39         netlib-scalapack@2.2.0        py-certifi@2022.12.7           py-jsonschema@4.4.0           py-pillow@9.5.0             py-sniffio@1.3.0                  rocthrust@5.4.3               xextproto@7.3.0
charliecloud@0.32                  hdf5-vol-log@1.4.0    libpressio@0.95.1     nghttp2@1.52.0                py-certifi@2022.12.7           py-jsonschema@4.4.0           py-pip@23.0                 py-soupsieve@2.3.2.post1          roctracer-dev@4.5.3           xproto@7.0.31
clara@1.1.5                        hdf5-vol-log@1.4.0    libpthread-stubs@0.4  ninja@1.11.1                  py-certipy@0.1.3               py-jupyter-client@7.3.5       py-pkgconfig@1.5.5          py-soupsieve@2.3.2.post1          rust@1.65.0                   xrandr@1.5.0
cli11@1.9.1                        heffte@2.3.0          libquo@1.3.1          nlohmann-json@3.11.2          py-cffi@1.15.1                 py-jupyter-client@7.3.5       py-pluggy@1.0.0             py-sqlalchemy@1.4.45              scotch@7.0.3                  xtrans@1.4.0
cmake@3.26.3                       heffte@2.3.0          libsigsegv@2.14       nrm@0.1.0                     py-cffi@1.15.1                 py-jupyter-core@4.11.1        py-pluggy@1.0.0             py-sqlalchemy@1.4.45              scr@3.0.1                     xyce@7.6.0
conduit@0.8.7                      help2man@1.49.3       libsm@1.2.3           numactl@2.0.14                py-charset-normalizer@2.0.12   py-jupyter-core@4.11.1        py-ply@3.11                 py-statsmodels@0.13.2             sed@4.9                       xz@5.4.1
conduit@0.8.7                      hip@5.4.3             libsodium@1.0.18      omega-h@9.34.13               py-charset-normalizer@2.0.12   py-jupyter-packaging11@0.11.1 py-poetry-core@1.2.0        py-tblib@1.6.0                    shuffile@0.2.0                yaksa@0.2
curl@8.0.1                         hip@5.4.3             libssh2@1.10.0        oniguruma@6.9.8               py-cinemasci@1.3               py-jupyter-packaging11@0.12.3 py-poetry-core@1.2.0        py-terminado@0.15.0               shuffile@0.3.0                yaml-cpp@0.6.3
curl@8.0.1                         hipblas@5.4.3         libstdcompat@0.0.17   openblas@0.3.23               py-cloudpickle@2.2.0           py-jupyter-server@1.13.5      py-prometheus-client@0.14.1 py-terminado@0.15.0               silo@4.11                     yaml-cpp@0.7.0
czmq@4.1.1                         hipsolver@5.4.3       libtheora@1.1.1       openblas@0.3.23               py-colorama@0.4.5              py-jupyter-telemetry@0.1.0    py-prometheus-client@0.14.1 py-threadpoolctl@3.1.0            slate@2022.07.00              zfp@0.5.5
darshan-runtime@3.4.2              hipsparse@5.4.3       libtiff@4.5.0         openfoam@2206                 py-configspace@0.4.20          py-jupyterhub@1.4.1           py-prompt-toolkit@3.0.31    py-tinycss2@1.1.1                 slate@2022.07.00              zfp@1.0.0
darshan-util@3.4.2                 hpctoolkit@2023.03.01 libtool@2.4.7         openimagedenoise@1.4.3        py-cppy@1.1.0                  py-jupyterlab@3.2.9           py-prompt-toolkit@3.0.31    py-tinycss2@1.1.1                 slepc@3.19.0                  zlib@1.2.13
datatransferkit@3.1-rc3            hpctoolkit@2023.03.01 libunistring@1.1      openjdk@11.0.17_8             py-cryptography@38.0.1         py-jupyterlab-pygments@0.2.2  py-protobuf@4.21.9          py-toml@0.10.2                    slepc@3.19.0                  zsh@5.8
diffutils@3.9                      hpcviewer@2023.04     libunwind@1.6.2       openmpi@4.1.5                 py-cycler@0.11.0               py-jupyterlab-pygments@0.2.2  py-psij-python@0.1.0.post2  py-tomli@2.0.1                    slurm@23-02-1-1               zstd@1.5.5
dihydrogen@develop                 hpx@1.9.0             libx11@1.8.4          openpmd-api@0.15.1            py-cython@0.29.33              py-jupyterlab-server@2.10.3   py-psutil@5.9.4             py-tomlkit@0.11.4                 snappy@1.1.10                 zstd@1.5.5
docbook-xml@4.5                    hpx@1.9.0             libxau@1.0.8          openpmd-api@0.15.1            py-cython@0.29.33              py-jupyterlab-widgets@3.0.3   py-psutil@5.9.4             py-tomlkit@0.11.4                 spath@0.2.0                   zstr@1.0.7
docbook-xsl@1.79.2                 hsa-rocr-dev@5.4.3    libxcb@1.14           openpmd-api@0.15.1            py-cython@3.0.0a9              py-kiwisolver@1.3.2           py-ptyprocess@0.7.0         py-tornado@5.1.1                  spath@0.3.0
double-conversion@3.2.1            hsa-rocr-dev@5.4.3    libxcrypt@4.4.33      openssh@9.3p1                 py-debugpy@1.6.6               py-lhsmdu@1.1                 py-py@1.11.0                py-tornado@6.2                    spdlog@1.11.0
dtcmp@1.1.4                        hwloc@2.9.1           libxdmcp@1.1.4        openssl@1.1.1t                py-debugpy@1.6.6               py-libensemble@0.9.3          py-pyaml@21.8.3             py-tornado@6.2                    sqlite@3.40.1
dyninst@12.3.0                     hydrogen@develop      libxext@1.3.3         openturns@1.18                py-decorator@5.1.1             py-lxml@4.9.1                 py-pybind11@2.10.1          py-traitlets@5.9.0                stc@0.9.0
==> 726 installed packages
[Singularity>
```

726 packages!

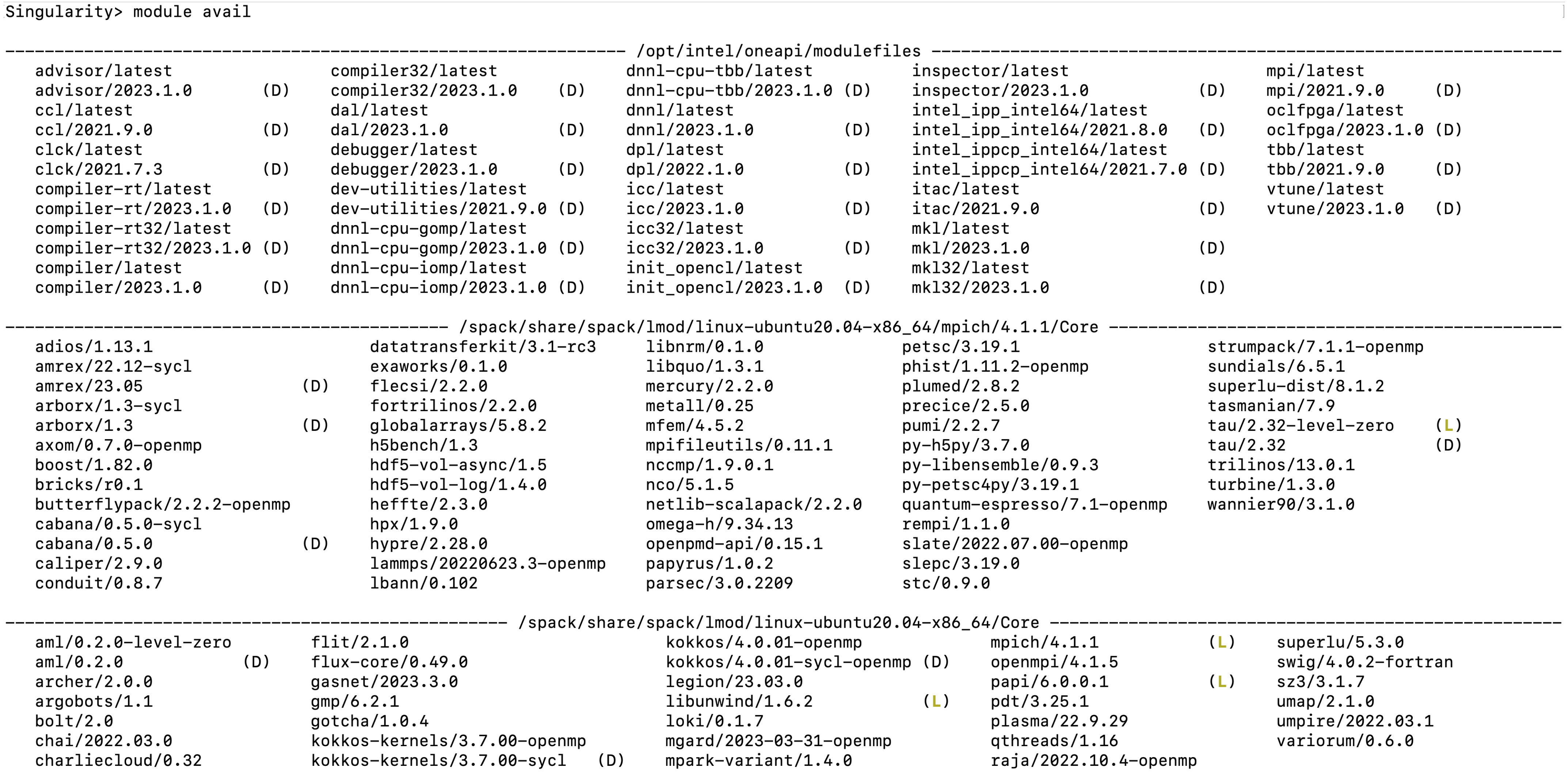
E4S 23.05 Intel oneAPI 2023.1: Packages built with Intel compilers



```
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

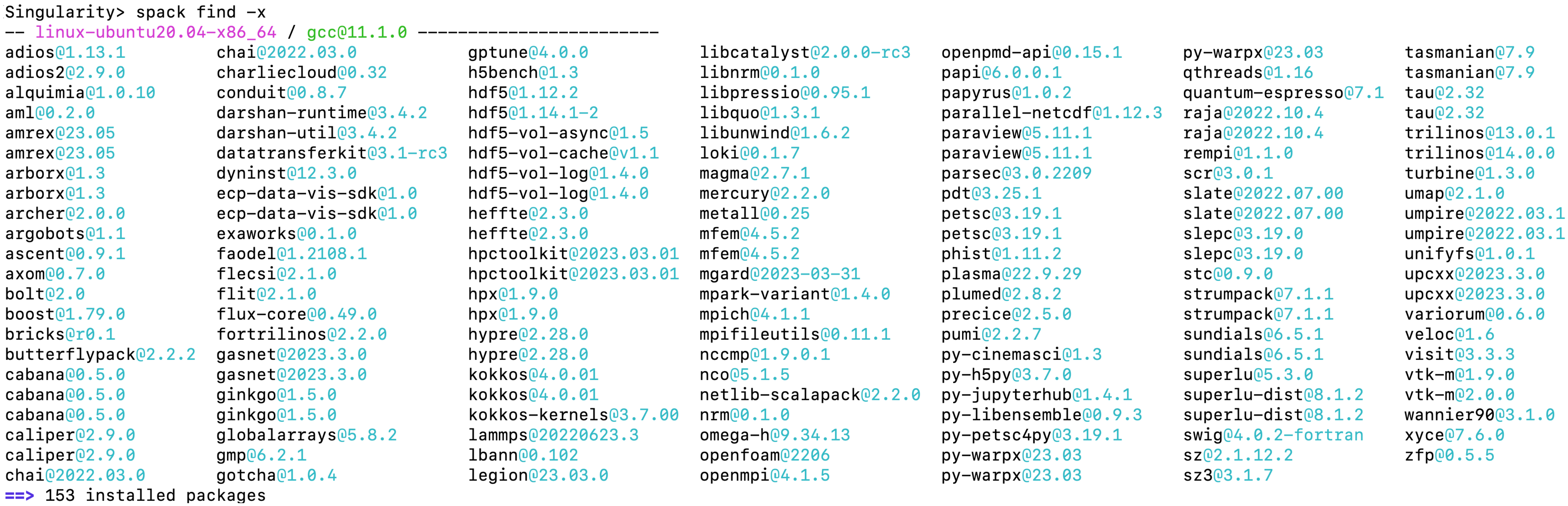
E4S 23.05 Intel oneAPI 2023.1: Packages built with Intel compilers



```
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        heffte/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

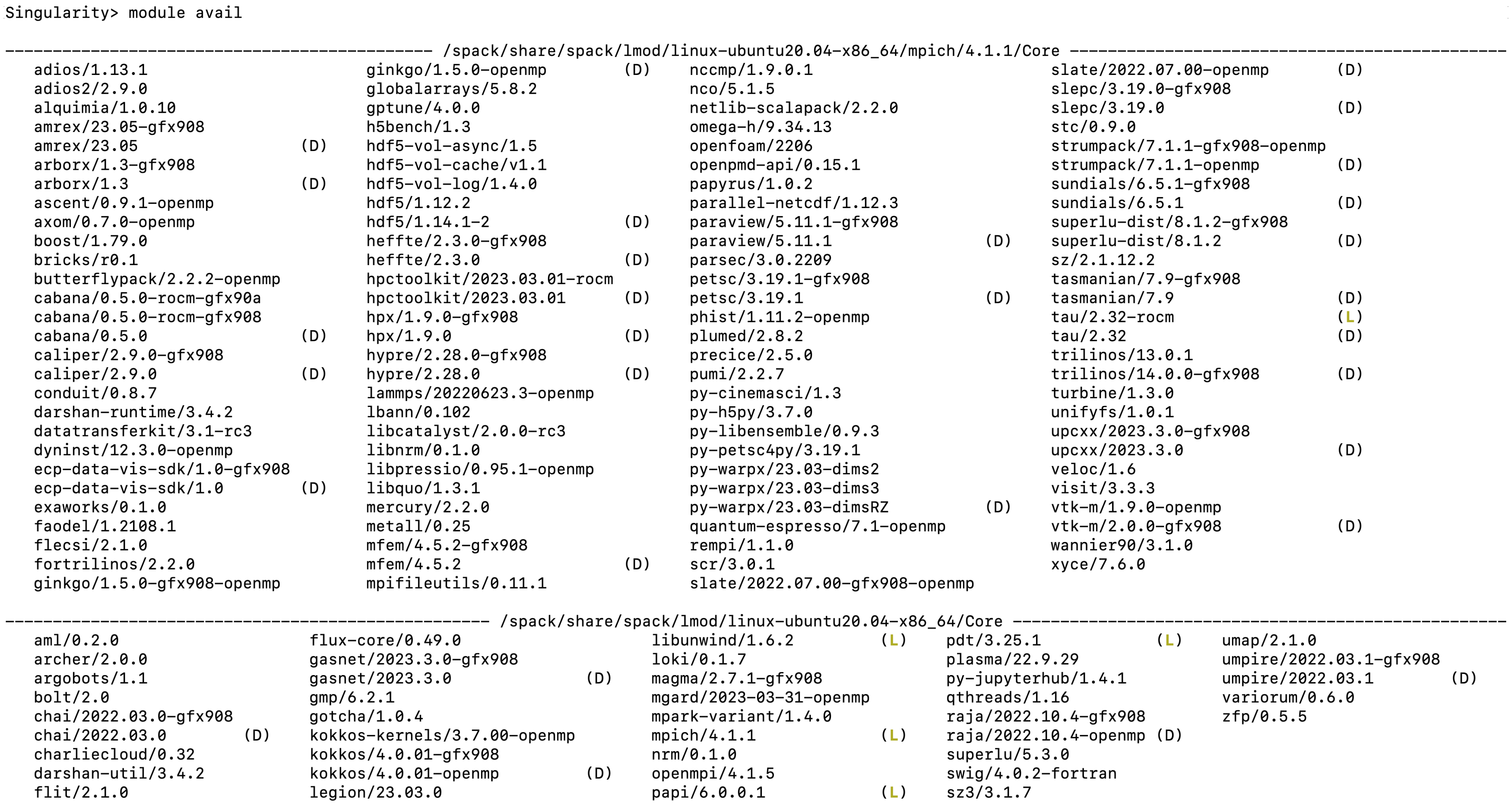
E4S Support for ROCm variants for MI250X (gfx90a) on x86_64



```
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

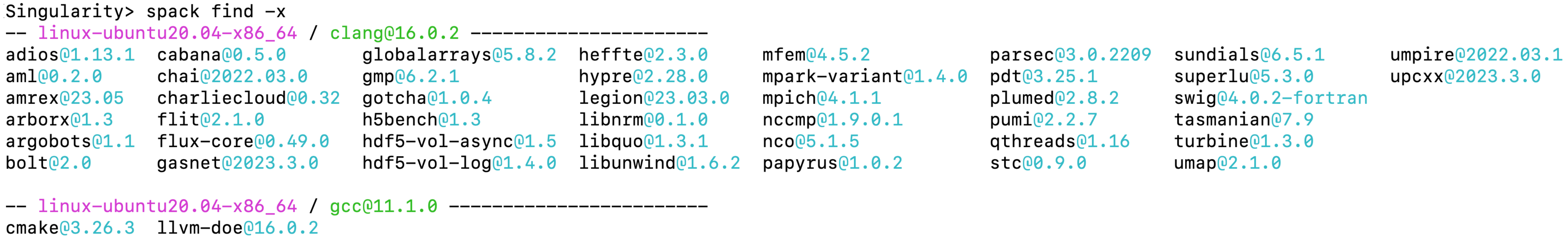
E4S Support for ROCm variants for MI250X (gfx90a) on x86_64



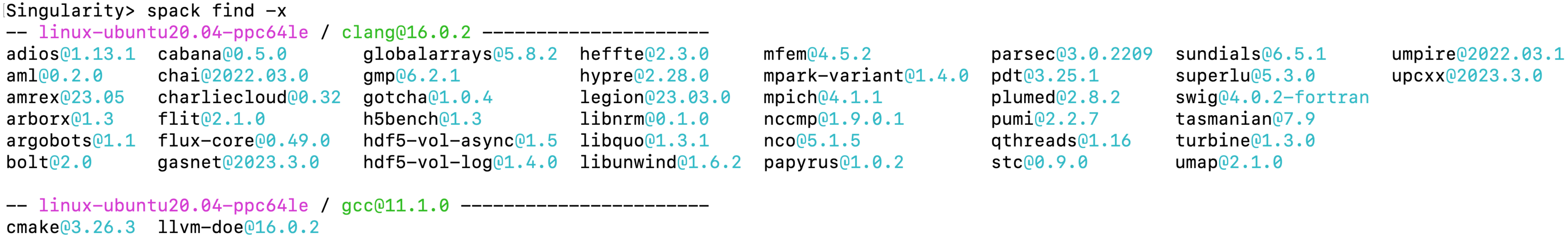
```
Singularity> module avail

--------------------------------------------- /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

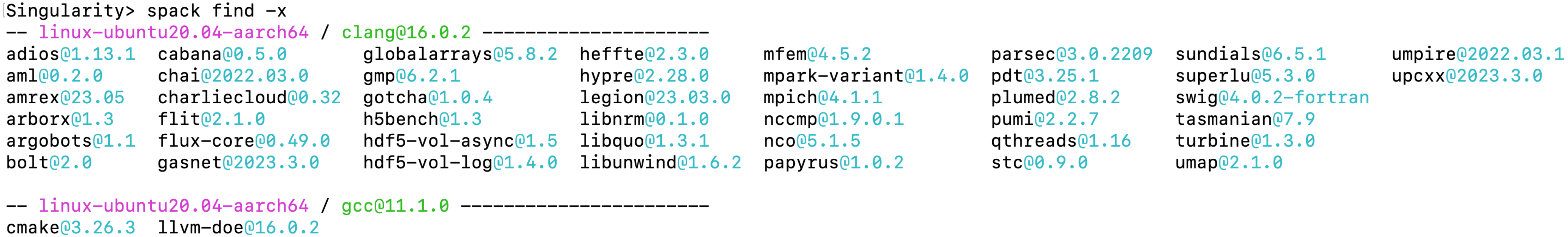
E4S 23.05 DOE LLVM Release: x86_64, ppc64le, and aarch64



```
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
```

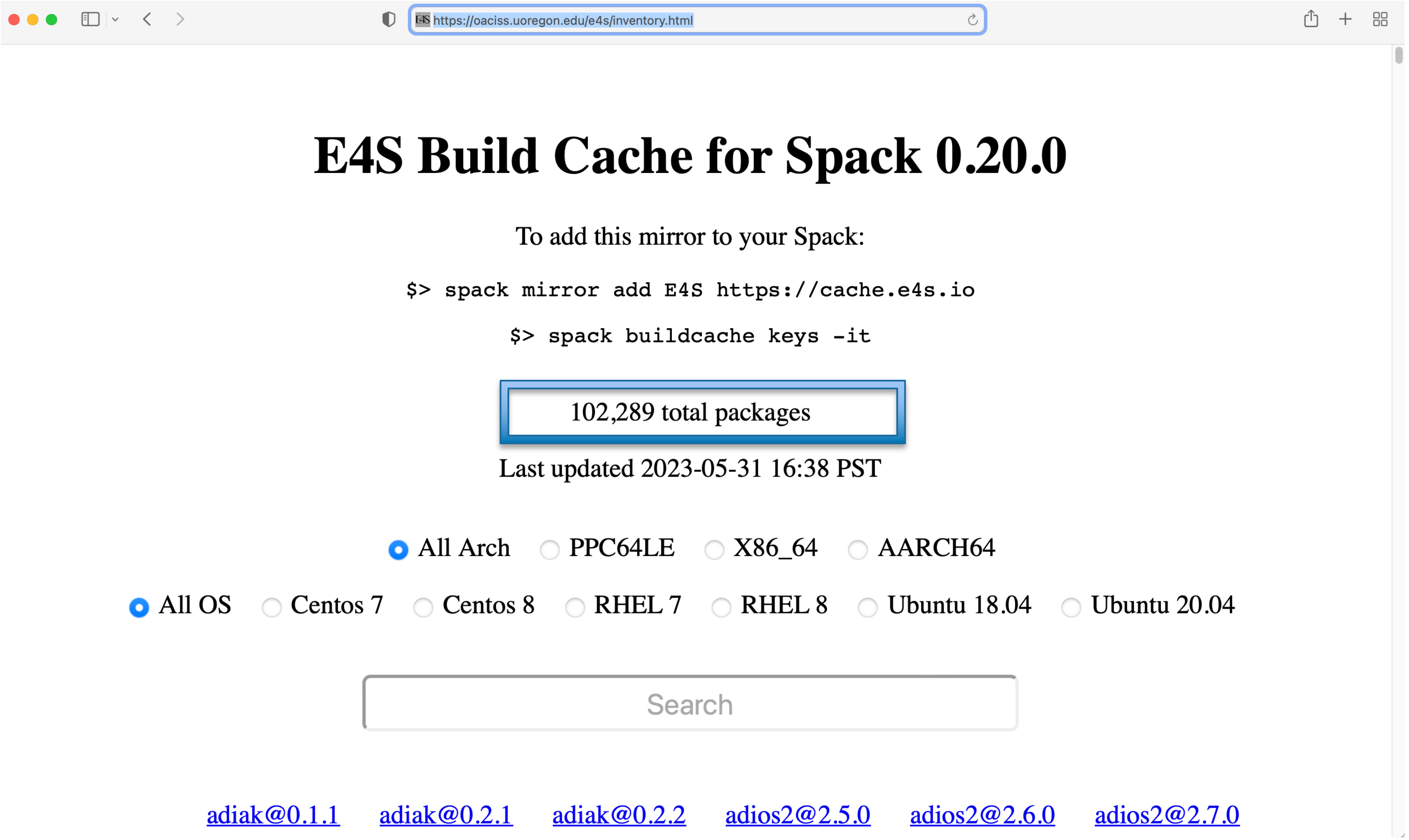


```
Singularity> spack find -x
-- linux-ubuntu20.04-ppc64le / clang@16.0.2 ---------------------
adios@1.13.1  cabana@0.5.0       globalarrays@5.8.2  heffte@2.3.0     mfem@4.5.2           parsec@3.0.2209  sundials@6.5.1      umpire@2022.03.1
aml@0.2.0     chai@2022.03.0     gmp@6.2.1           hypre@2.28.0     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



E4S Build Cache for Spack 0.20.0

To add this mirror to your Spack:

```
$> spack mirror add E4S https://cache.e4s.io
$> spack buildcache keys -it
```

102,289 total packages

Last updated 2023-05-31 16:38 PST

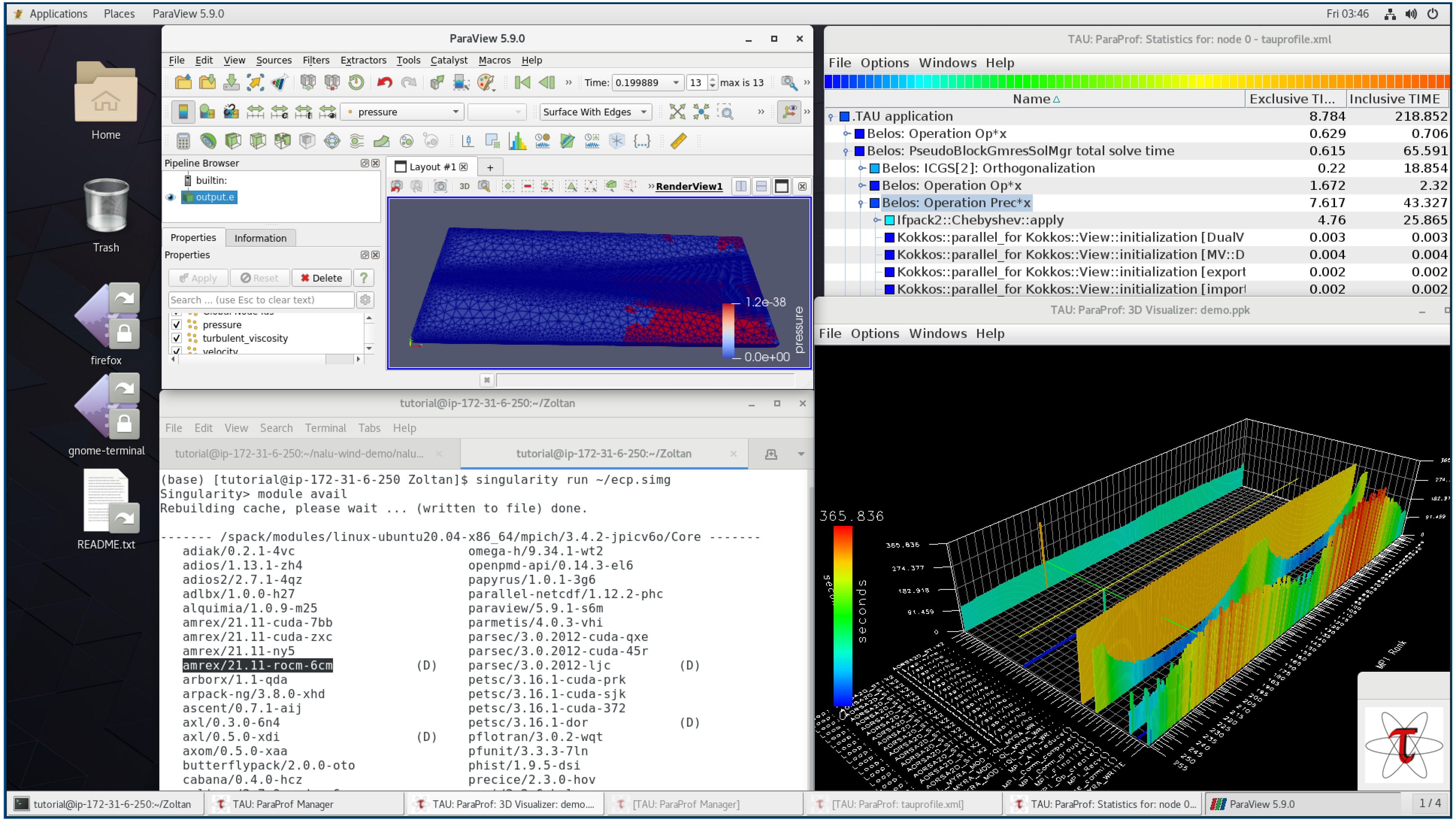
● All Arch ○ PPC64LE ○ X86_64 ○ AARCH64

● All OS ○ Centos 7 ○ Centos 8 ○ RHEL 7 ○ RHEL 8 ○ Ubuntu 18.04 ○ Ubuntu 20.04

adiak@0.1.1 adiak@0.2.1 adiak@0.2.2 adios2@2.5.0 adios2@2.6.0 adios2@2.7.0

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

E4S 23.02 AWS image: US-West2 (OR)


Applications
Places
ParaView 5.9.0
Fri 03:46
Home
Trash
firefox
gnome-terminal
README.txt
ParaView 5.9.0
File Edit View Sources Filters Extractors Tools Catalyst Macros Help
Time: 0.199889
13
max is 13
pressure
Surface With Edges
Pipeline Browser
builtin:
output.e
Properties
Information
Apply
Reset
Delete
Search ... (use Esc to clear text)
pressure
turbulent_viscosity
velocity
Layout #1
RenderView1
1.2e-38
0.0e+00
pressure
tutorial@ip-172-31-6-250:~/Zoltan
File Edit View Search Terminal Tabs Help
tutorial@ip-172-31-6-250:~/nalu-wind-demo/nalu...
tutorial@ip-172-31-6-250:~/Zoltan
TAU: ParaProf: Statistics for: node 0 - tauprofile.xml
File Options Windows Help
TAU: ParaProf: 3D Visualizer: demo.ppk
File Options Windows Help
365.836
seconds
365.836
274.377
182.918
91.459
0
MPI Rank
tutorial@ip-172-31-6-250:~/Zoltan
TAU: ParaProf Manager
TAU: ParaProf: 3D Visualizer: demo....
[TAU: ParaProf Manager]
[TAU: ParaProf: tauprofile.xml]
TAU: ParaProf: Statistics for: node 0...
ParaView 5.9.0
1 / 4

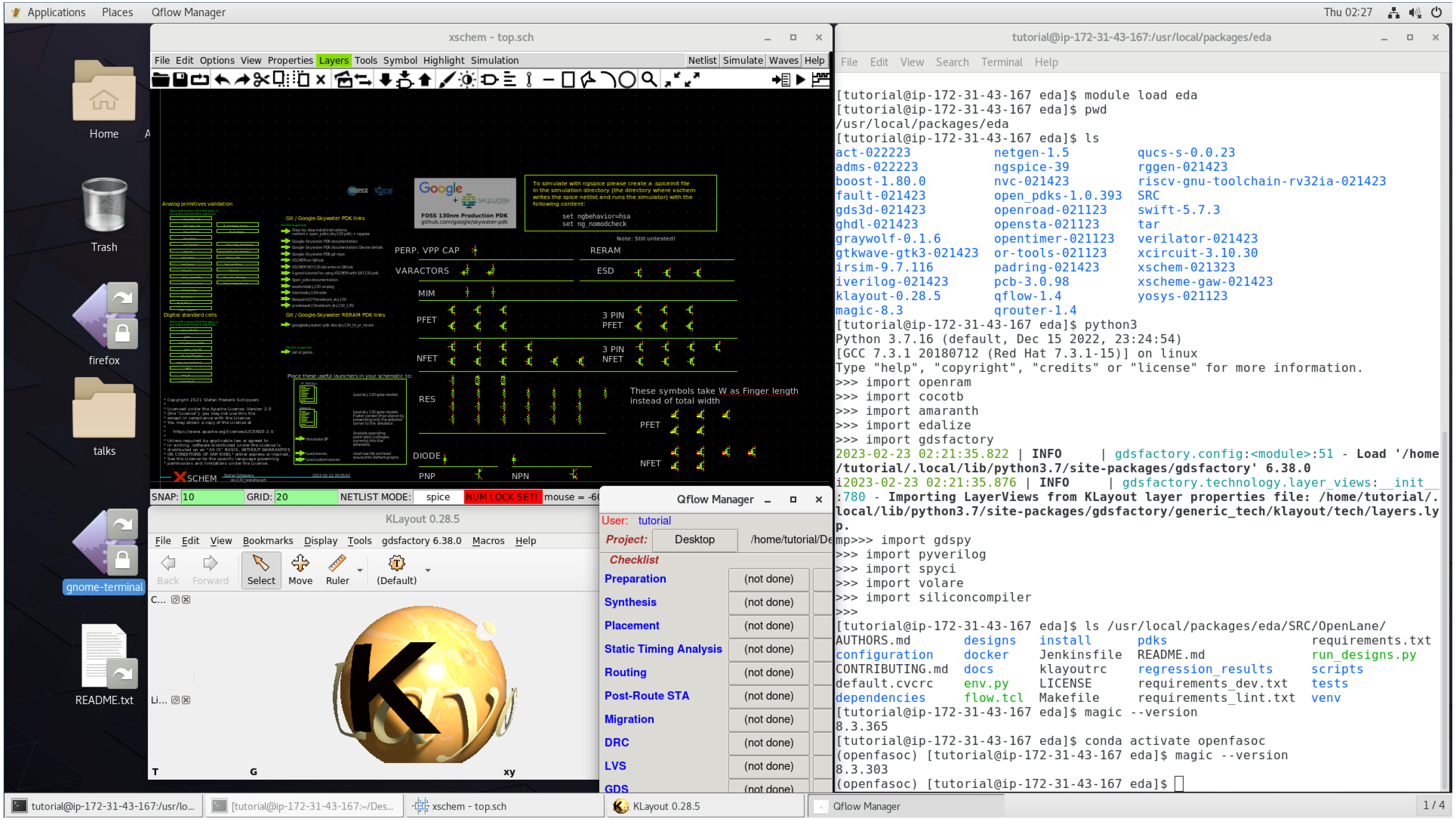
```
(base) [tutorial@ip-172-31-6-250 Zoltan]$ singularity run ~/ecp.simg
Singularity> module avail
Rebuilding cache, please wait ... (written to file) done.

------- /spack/modules/linux-ubuntu20.04-x86_64/mpich/3.4.2-jpicv6o/Core -------
   adiak/0.2.1-4vc                         omega-h/9.34.1-wt2
   adios/1.13.1-zh4                        openpmd-api/0.14.3-el6
   adios2/2.7.1-4qz                        papyrus/1.0.1-3g6
   adlbx/1.0.0-h27                         parallel-netcdf/1.12.2-phc
   alquimia/1.0.9-m25                      paraview/5.9.1-s6m
   amrex/21.11-cuda-7bb                    parmetis/4.0.3-vhi
   amrex/21.11-cuda-zxc                    parsec/3.0.2012-cuda-qxe
   amrex/21.11-ny5                         parsec/3.0.2012-cuda-45r
   amrex/21.11-rocm-6cm             (D)    parsec/3.0.2012-ljc              (D)
   arborx/1.1-qda                          petsc/3.16.1-cuda-prk
   arpack-ng/3.8.0-xhd                     petsc/3.16.1-cuda-sjk
   ascent/0.7.1-aij                        petsc/3.16.1-cuda-372
   axl/0.3.0-6n4                           petsc/3.16.1-dor                 (D)
   axl/0.5.0-xdi                    (D)    pflotran/3.0.2-wqt
   axom/0.5.0-xaa                          pfunit/3.3.3-7ln
   butterflypack/2.0.0-oto                 phist/1.9.5-dsi
   cabana/0.4.0-hcz                        precice/2.3.0-hov
```

Name	Exclusive TI...	Inclusive TIME
.TAU application	8.784	218.852
Belos: Operation Op*x	0.629	0.706
Belos: PseudoBlockGmresSolMgr total solve time	0.615	65.591
Belos: ICGS[2]: Orthogonalization	0.22	18.854
Belos: Operation Op*x	1.672	2.32
Belos: Operation Prec*x	7.617	43.327
Ifpack2::Chebyshev::apply	4.76	25.865
Kokkos::parallel_for Kokkos::View::initialization [DualV	0.003	0.003
Kokkos::parallel_for Kokkos::View::initialization [MV::D	0.004	0.004
Kokkos::parallel_for Kokkos::View::initialization [export	0.002	0.002
Kokkos::parallel_for Kokkos::View::initialization [import	0.002	0.002

E4S 23.02 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…

E4S for Commercial Cloud Platforms for EDA on AWS

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



```
[tutorial@ip-172-31-43-167 eda]$ module load eda
[tutorial@ip-172-31-43-167 eda]$ pwd
/usr/local/packages/eda
[tutorial@ip-172-31-43-167 eda]$ ls
act-022223          netgen-1.5          qucs-s-0.0.23
adms-022223         ngspice-39          rggen-021423
boost-1.80.0        nvc-021423          riscv-gnu-toolchain-rv32ia-021423
fault-021423        open_pdks-1.0.393   SRC
gds3d-021423        openroad-021123     swift-5.7.3
ghdl-021423         opensta-021123      tar
graywolf-0.1.6      opentimer-021123    verilator-021423
gtkwave-gtk3-021423 or-tools-021123     xcircuit-3.10.30
irsim-9.7.116       padring-021423      xschem-021323
iverilog-021423     pcb-3.0.98          xscheme-gaw-021423
klayout-0.28.5      qflow-1.4           yosys-021123
magic-8.3           qrouter-1.4
[tutorial@ip-172-31-43-167 eda]$ python3
Python 3.7.16 (default, Dec 15 2022, 23:24:54)
[GCC 7.3.1 20180712 (Red Hat 7.3.1-15)] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> import openram
>>> import cocotb
>>> import amaranth
>>> import edalize
>>> import gdsfactory
2023-02-23 02:21:35.822 | INFO     | gdsfactory.config:<module>:51 - Load '/home
/tutorial/.local/lib/python3.7/site-packages/gdsfactory' 6.38.0
i2023-02-23 02:21:35.876 | INFO     | gdsfactory.technology.layer_views:__init__
:780 - Importing LayerViews from KLayout layer properties file: /home/tutorial/.
local/lib/python3.7/site-packages/gdsfactory/generic_tech/klayout/tech/layers.ly
p.
mp>>> import gdspy
>>> import pyverilog
>>> import spyci
>>> import volare
>>> import siliconcompiler
>>>
[tutorial@ip-172-31-43-167 eda]$ ls /usr/local/packages/eda/SRC/OpenLane/
AUTHORS.md       designs    install      pdks                    requirements.txt
configuration    docker     Jenkinsfile  README.md               run_designs.py
CONTRIBUTING.md  docs       klayoutrc    regression_results      scripts
default.cvcrc    env.py     LICENSE      requirements_dev.txt    tests
dependencies     flow.tcl   Makefile     requirements_lint.txt   venv
[tutorial@ip-172-31-43-167 eda]$ magic --version
8.3.365
[tutorial@ip-172-31-43-167 eda]$ conda activate openfasoc
(openfasoc) [tutorial@ip-172-31-43-167 eda]$ magic --version
8.3.303
(openfasoc) [tutorial@ip-172-31-43-167 eda]$
```

User: tutorial
Project: Desktop /home/tutorial/De
Checklist
Preparation (not done)
Synthesis (not done)
Placement (not done)
Static Timing Analysis (not done)
Routing (not done)
Post-Route STA (not done)
Migration (not done)
DRC (not done)
LVS (not done)
GDS (not done)

SNAP: 10 GRID: 20 NETLIST MODE: spice NUM LOCK SET! mouse = -6

Applications
Places
Qflow Manager
Thu 02:27
Home
Trash
firefox
talks
gnome-terminal
README.txt
xschem - top.sch
File Edit Options View Properties Layers Tools Symbol Highlight Simulation
Netlist Simulate Waves Help
tutorial@ip-172-31-43-167:/usr/local/packages/eda
File Edit View Search Terminal Help
Analog primitives validation
Digital standard cells
Google + SkyWater
FOSS 130nm Production PDK
github.com/google/skywater-pdk
Git / Google-Skywater PDK links
Git / Google-Skywater RERAM PDK links
To simulate with ngspice please create a .spiceinit file in the simulation directory (the directory where xschem writes the spice netlist and runs the simulator) with the following content:
set ngbehavior=hsa
set ng_nomodcheck
Note: Still untested!
PERP. VPP CAP
RERAM
VARACTORS
ESD
MIM
PFET
3 PIN PFET
NFET
3 PIN NFET
RES
These symbols take W as Finger length instead of total width
PFET
NFET
DIODE
PNP
NPN
XSCHEM
Place these useful launchers in your schematic to:
KLayout 0.28.5
File Edit View Bookmarks Display Tools gdsfactory 6.38.0 Macros Help
Back
Forward
Select
Move
Ruler
(Default)
T
G
xy
Qflow Manager
tutorial@ip-172-31-43-167:/usr/lo...
[tutorial@ip-172-31-43-167:~/Des...
xschem - top.sch
KLayout 0.28.5
Qflow Manager
1 / 4

E4S EDA on AWS

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

EXASCALE COMPUTING PROJECT

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

#	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

- E4S: 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

Can E4S help provide a stable platform for tool development?

- Bare-metal installation as well as containers built with Spack
- Base containers that can be customized with e4s-alc
- Replace MPI in containerized E4S application with system MPI using e4s-cl
- What are we missing?

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.

EXASCALE COMPUTING PROJECT

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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001100
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