DOE Exascale Computing Project

Update for the June ASCAC Meeting

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ECP Director

Crystal City, Arlington, VA
June 12-13, 2023

This document includes NDA
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The ECP team has been very busy since our last update

- Large focus on meeting ECP KPPs for applications and software technology
- Independent project review in early May
- Leadership transition in early June
- Preparing for project close out
- Preparing for the post-ECP era; Interactions with stakeholders

- Complementing this talk
  - Sameer Shende will discuss E4S and extending it’s reach beyond ECP
  - Ryan Prout will discuss software deployment activities
  - Bronson Messer is discussing early science on Frontier
  - Susan Coghlan is giving an update on Aurora

Progress toward completion of ECP's Key Performance Parameters

Frontier

Compute Node
1 64-core AMD "Optimized 3rd Gen EPYC" CPU
4 AMD Instinct MI250X GPUs
CPU & GPUs fully connected AMD Infinity Fabric

Node Memory
512 GiB HBM2e memory
512 GiB DDR4 memory
Cache Coherent Memory across entire node

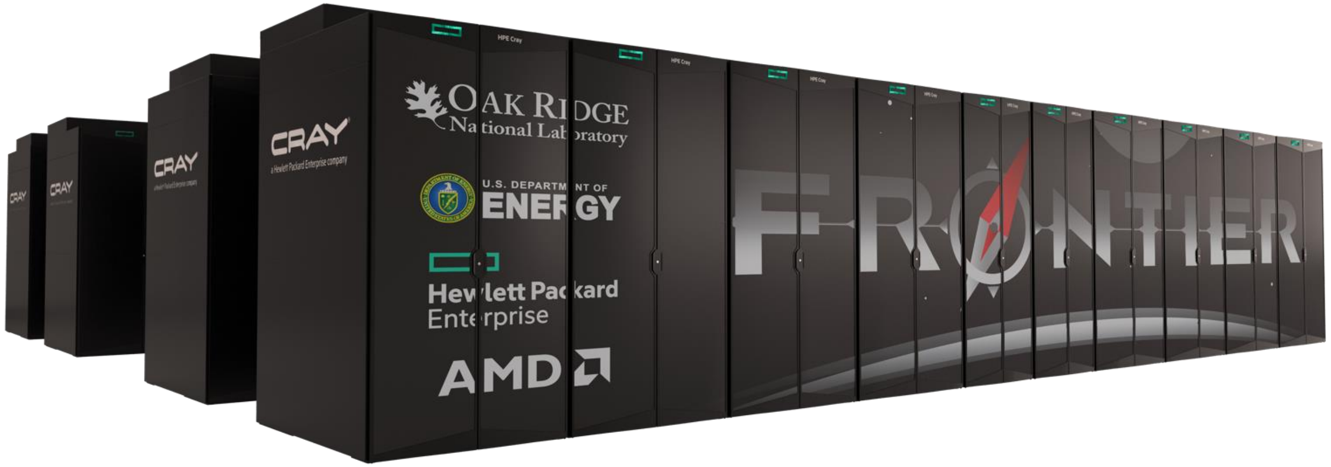
System Interconnect
HPE Slingshot. Four 200 Gbps (25 GB/s) NICs per node provides a node-injection bandwidth of 800 Gbps (100 GB/s)

High-Performance Storage
716 PB at 9.4 TB/s plus 11 Billion IOPS from
36 PB node local storage at 65 TB/s

Programming Models
MPI, OpenMP, OpenACC, HIP, C/C++, Fortran, DPC++, RAJA, Kokkos, and others

Node Performance
214 TF double precision

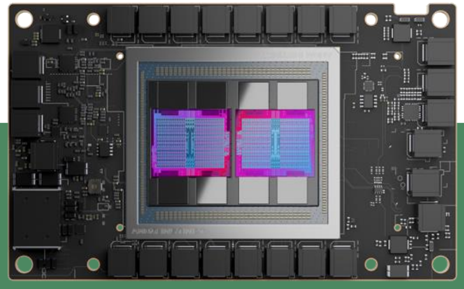
System Size
9,472 nodes


CRAY
Oak Ridge National Laboratory
U.S. Department of Energy
Hewlett Packard Enterprise
AMD
FRONTIER

FRONTIER
HPE Cray EX

PEAK PERFORMANCE
≥2.0 Exaflop DP

FRONTIER COMPUTE NODE
1 64-core AMD CPU
4 AMD MI250X GPUs
4 TB NVM local storage



- ECP gained access on April 5, 2023; initial feedback has been very positive
- ECP teams transition to early science once they've hit their KPP
- 6 ECP teams were awarded INCITE allocations on Frontier for science campaigns
- Overall usage by ECP teams is just over 2.1M node hours to date

Frontier supports, at a minimum, all non-ADTM threshold metrics for KPP-1, KPP-2, and KPP-3
Secure early access systems at LLNL support ATDM metrics for KPP-2 and KPP-3

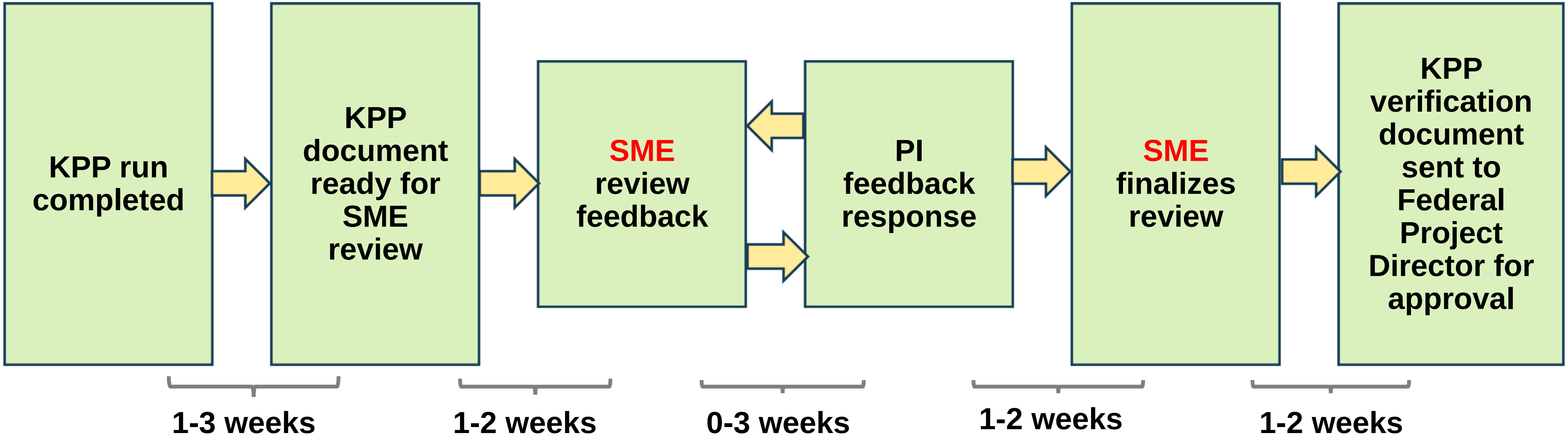
ECP’s KPPs: Quantified with Explicit Targets

KPP ID	Description of Scope	Threshold KPP	Objective KPP	Verification Action/Evidence
KPP-1	11 selected applications demonstrate performance improvement for mission-critical problems	✓ 6 of 11 applications demonstrate Figure of Merit improvement ≥50 on their base challenge problem	All 11 selected applications demonstrate their stretch challenge problem	Independent assessment of measured FOM results and base challenge problem demonstration evidence
KPP-2	14 selected applications broaden the reach of exascale science and mission capability	5 of 10 DOE Science and Applied Energy applications *and* 2 of 4 NNSA applications demonstrate their base challenge problem	All 14 selected applications demonstrate their stretch challenge problem	Independent assessment of base challenge problem demonstration evidence
KPP-3	76 software products selected to meet an aggregate capability integration score	Software products achieve an aggregate capability integration score of at least 34 out of a possible score of 68 points	Software products achieve the maximum aggregate capability integration score of 68 points	Independent assessment of each software product’s capability integration score
KPP-4	Delivery of 267 vendor baselined milestones in the PathForward element	✓ Vendors meet 214 out of the total possible 267 PathForward milestones	✓ Vendors meet all 267 possible PathForward milestones	Independent review of the PathForward milestones to assure they meet the contract requirements; evidence is the final milestone deliverable

ECP’s KPPs: Quantified with Explicit Targets

KPP ID	Description of Scope	Threshold KPP	Objective KPP	Threshold Completion Status (2/27/22)
KPP-1	11 selected applications demonstrate performance improvement for mission-critical problems	✓ 6 of 11 applications demonstrate Figure of Merit improvement ≥50 on their base challenge problem	All 11 selected applications demonstrate their stretch challenge problem	✓ **7 SC apps (1 complete, 4 under review, 2 preparing)** • **3 more very close**
KPP-2	14 selected applications broaden the reach of exascale science and mission capability	✓ 5 of 10 DOE Science and Applied Energy applications *and* 2 of 4 NNSA applications demonstrate their base challenge problem	All 14 selected applications demonstrate their stretch challenge problem	✓ **5 SC apps (2 under review, 3 preparing)** ✓ **3 ATDM apps under review** • **1 more very close**
KPP-3	76 software products selected to meet an aggregate capability integration score	Software products achieve an aggregate capability integration score of at least 34 out of a possible score of 68 points	Software products achieve the maximum aggregate capability integration score of 68 points	• **27.5 integration points (5 complete, 17 in closeout with FPD, 5.5 more under review)**
KPP-4	Delivery of 267 vendor baselined milestones in the PathForward element	✓ Vendors meet 214 out of the total possible 267 PathForward milestones	✓ Vendors meet all 267 possible PathForward milestones	✓ **267 PathForward milestones**

The full KPP verification process is rigorous and time consuming



KPP run completed

KPP document ready for SME review

SME review feedback

PI feedback response

SME finalizes review

KPP verification document sent to Federal Project Director for approval

1-3 weeks

1-2 weeks

0-3 weeks

1-2 weeks

1-2 weeks

KPP Completion Tracking Status

Frontier KPP Status	Details
Verified KPP Completion	KPP completion has been confirmed by the lead SME and federal project director
KPP Under Review	The KPP verification document has been assembled and submitted to the L3 with all artifacts needed by SMEs to confirm KPP completion
Successful KPP Run	The team has successfully executed the simulations that they believe demonstrate their KPP
Ready to Run KPP	The team is ready to attempt their KPP run, just waiting for time
Preparing for KPP	The team is not blocked but work remains before the team can attempt a KPP run
Minor Issues	There are minor issues that need to be addressed before the team can run their challenge problem or (for co-design) satisfy their KPP-3
Major Issues	The team is blocked by issues outside of their control. Support ticket(s) should be filed with OLCF and/or vendors.
Active Code Development	Code development and/or debugging needs to be completed before the team is ready to attempt KPP runs.
Not on	The team has not yet begun testing on Frontier.

Status of KPP-1 Completion on Frontier

7 out of 11 KPP-1 applications tentative complete: achieves threshold!

KPP-1 Project	Frontier Status	Comment or Results/Status or Current State or Status Details
LatticeQCD	Preparing for KPP	Close: 5/6 calculations complete
NWChemEx	Preparing for KPP	300-node Frontier runs have shown good results. Scaling work remains
EXAALT ✓	Successful KPP Run	FOM speedup: ~400
QMCPACK	Major Issues	OpenMP/library bugs
ExaSMR ✓	KPP Under Review	FOM Speedup: ~70
WDMApp ✓	KPP Under Review	FOM Speedup: ~150
WarpX ✓	KPP Under Review	FOM Speedup: ~500
ExaSky ✓	Verified KPP Completion	FOM Speedup: ~270
EQSIM ✓	KPP Under Review	FOM Speedup: ~3500
E3SM-MMF✓	Successful KPP Run	Achieved KPP on 5K nodes with FOM speedup: ~490
CANDLE	Preparing for KPP	Verifying if recent run met KPP

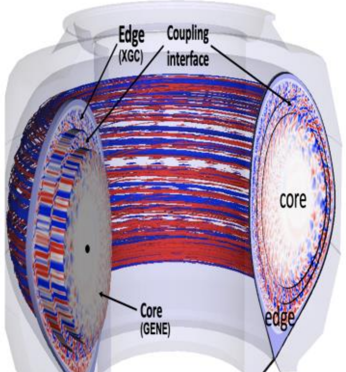
Status of KPP-2 Completion on Frontier

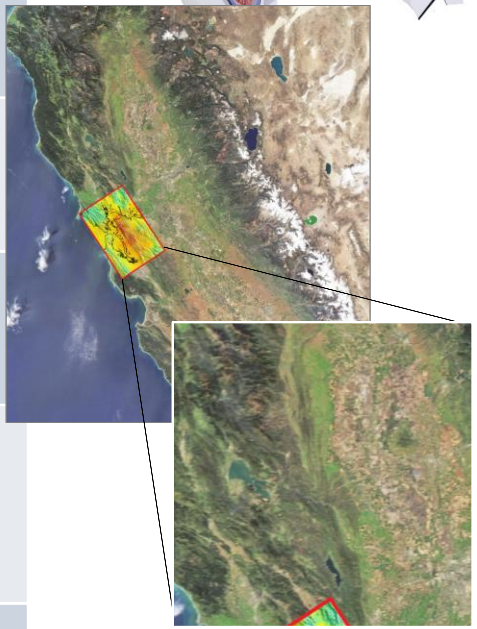
5 of 10 SC applications and 3 of 4 NNSA applications have tentatively achieved their KPP goals

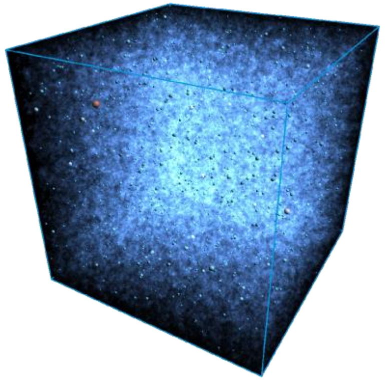
KPP-2 Project	Frontier Status	Status
GAMESS	Minor Issues	OpenMP Bugs
ExaAM ✓	Successful KPP run	Scaling up Coupled Workflow
ExaWind	Active code development	Sparse solver Performance
Combustion-PELE ✓	KPP Under Review	KPP Demo used 7K Nodes
MFIX-Exa ✓	KPP Under Review	Sparse solver Performance
ExaStar	Minor issues	Compiler bug
Subsurface	Minor Issues	Hypre (solver) bug
ExaSGD ✓	Successful KPP run	Close: minor system issues
ExaBiome ✓	Successful KPP run	Successful 9K node run with 50TB dataset
ExaFEL	Active code development	Scalability
Ristra (LANL)	Using EAS-3 / El Capitan	SME review not successful
MAPP (LLNL)✓	Using EAS-3 / El Capitan	SME review successful
SPARC (SNL)✓	Using EAS-3 / El Capitan	SME review successful
EMPIRE (SNL)✓	Using EAS-3 / El Capitan	SME review successful

Example KPP-1 Application Runs

Project	Challenge Problem	FOM Speedup	Nodes Used	ST/CD Tools
WDMApp: Fusion Tokamaks	Gyrokinetic simulation of the full ITER plasma to predict the height and width of the edge pedestal	150	6156	CODAR, CoPA, PETSc, ADIOS, VTK-m
ExaSMR: Small Modular Reactors	NuScale-style Small Module Reactor (SMR) with depleted fuel and natural circulation	70	6400	CEED, Trilinos
EXAALT: Molecular Dynamics	Damaged surface of Tungsten in conditions relevant to plasma facing materials in fusion reactors	398.5	7000	Kokkos, CoPa
EQSIM: Earthquake Modeling and Risk	Impacts of Mag 7 rupture on the Hayward Fault on the bay area.	3467	5088	RAJA, HDF5
WarpX: Plasma Wakefield Accelerators	Wakefield plasma accelerator with a 1PW laser drive	500	8576	AMReX, libEnsemble, ADIOS, HDF5, VTK-m, ALPINE
ExaSky: Cosmology	Two large cosmology simulations • gravity-only • hydrodynamics	271.6	8192	CoPa, VTK-m, CINEMA, HDF5





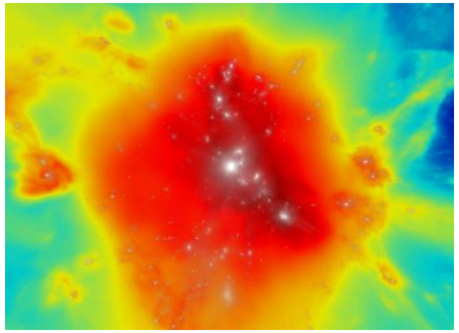


ExaSky: Computing the Sky at Extreme Scales

ECP *Challenge Problem*

The challenge problem consists of two HACC simulations, 1) a gravity-only run which will be the basis for the most detailed large-area synthetic sky maps ever made, 2) a large-volume, survey-scale, gravity + hydro simulation for multiple cosmology probe predictions, including cross-correlations.

Key Simulation Milestone



High dynamic range, survey-scale cosmic simulations, including gas dynamics and detailed models of subgrid physics for multi-wavelength in-survey and cross-survey studies

Hours of run-time on Frontier

Software Products Delivered

Core Modeling Capabilities	• Extreme-scale gravity + hydro cosmological simulations • Subgrid models for star and black hole formation, astrophysical feedback mechanisms • Detailed modeling of observations for high-fidelity synthetic sky catalogs
Codes	• HACC/CosmoTools, Nyx, SWFFT
Target Domains	• Multi-wavelength sky surveys • Plasma physics, particle transport
Key Software Dependencies	• ArborX, SZ, VeloC (HACC) • AMReX, SUNDIALS (Nyx)

FOM on 8192 Frontier nodes is ~230X baseline run on ANL Theta system

ECP Team

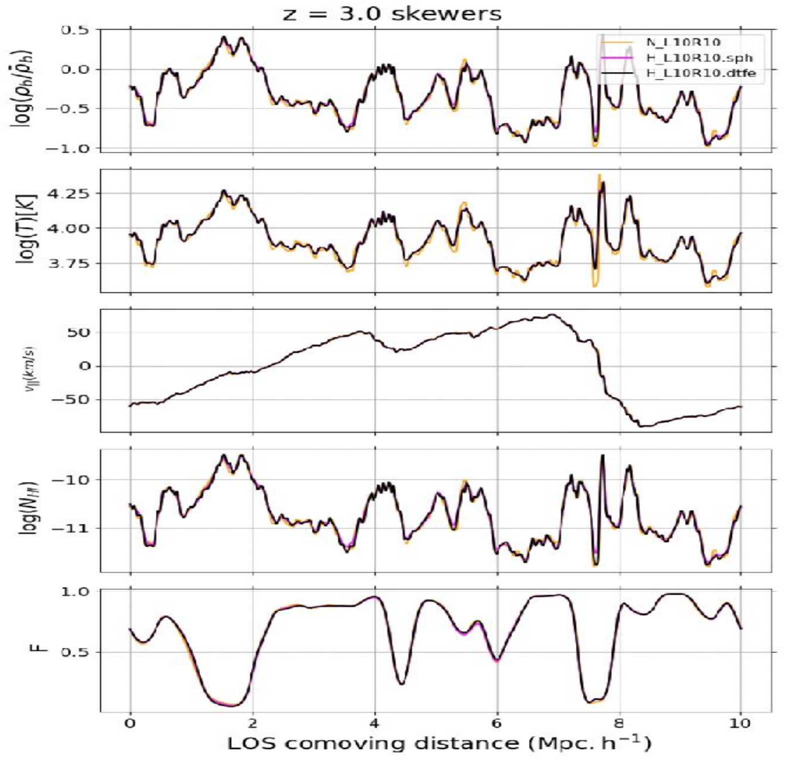
Argonne	JD Emberson, Nicholas Frontiere, Salman Habib, Katrin Heitmann, Adrian Pope, Esteban Rangel
LANL	Pascal Grosset
LBNL	Jean Sexton, Zarija Lukic

Exascale and Beyond

- New generation of astrophysical subgrid models, hydro solvers, radiation transport/hydrodynamics
- Sustained code/algorithm evolution for future (specialized) hardware; support of community science effort
- AI/ML methods for increased dynamic range, new physics, and subgrid model speed-up
- New science applications within and outside current domains (e.g., multi-messenger astrophysics, plasma physics)

ExaSky: Progress on Multiple GPU Platforms

- **HACC:**
  - Design focuses performance on a small number (~10) of compact kernels that are separately optimized for each system
  - Increased accuracy through more resolution (particles) and higher order SPH algorithms
  - Performance validated on AMD, Intel, NVIDIA GPUs
  - Early science runs on Crusher, Perlmutter, Polaris (ongoing), test runs on Frontier
- **Nyx:**
  - Ready for Frontier testing (running on Crusher), running on Perlmutter, tests on Intel devices ongoing
  - Successful transition from CPU to CPU-GPU systems based on AMReX framework advances under ECP; good performance enhancements achieved
- **Use of ECP Software Technology:**
  - HACC uses ArborX (fast analysis), VeloC (checkpointing), SZ (data compression); Nyx (based on AMReX), uses HDF5, SUNDIALS (ODE solvers), SZ

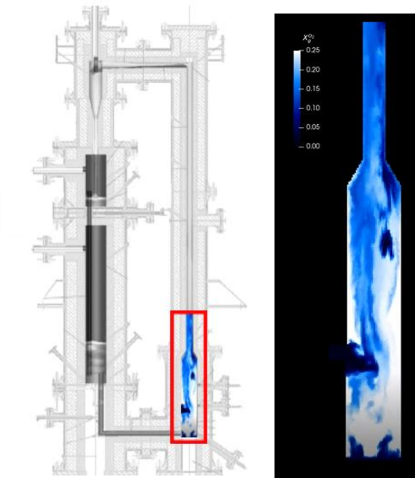


HACC and Nyx comparison (Chabanier et al. arXiv:2207.05023) for Ly-alpha simulations; agreement is at the 1% level, the best between Lagrangian and Eulerian codes ever achieved.

MFIX-Exa: Exascale modeling of carbon capture reactors

Goal: Demonstrate commercial-scale transformational energy technologies that **curb fossil fuel plant CO2 emission** by 2030.

Key Simulation Milestone



1486 Summit Nodes

Simulation of CLR air reactor at full scale resolution with interphase heat mass, momentum coupling. Oxygen reduction in gas (white) illustrates uptake by solids carrier.

ECP Challenge Problem

CFD-DEM (discrete element method) simulation of NETL's 50 kW chemical looping reactor (CLR), containing 5 billion particles and including the full-loop CLR geometry covering all five flow regimes including interphase momentum, mass, and energy transfer.

Software Products Delivered

Core Modeling Capabilities	• Low-Mach, fully coupled reactive gas-particle flows • CFD and DEM on block-AMR structured grids with embedded boundaries
Codes	• MFIX-Exa • CSG-EB lib
Target Domains	• Decarbonization technologies • Bioreactors • Pharmaceuticals • Geological Sciences
Key Software Dependencies	• AMReX • hypre • ALPINE

ECP Team

NETL	Jordan Musser, William Fullmer, Roberto Porcu, Deepak Rangarajan
LBL	Ann Almgren, Hengjie Wang

Exascale and Beyond

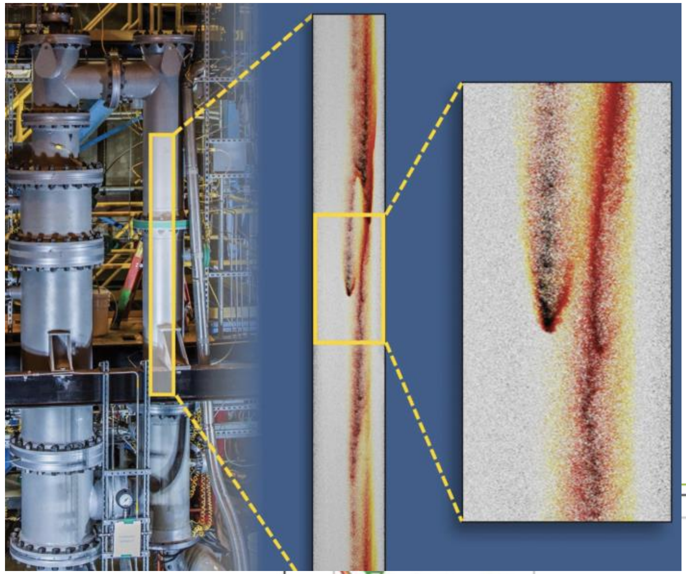
- Gas-solids reactor design, diagnostics and optimization:
  - Decarbonization technologies
  - U.S. manufacturing (e.g., iron reduction furnaces)
- Base funding needed to sustain growing ecosystem & user-base
- Key research areas
  - Fluidization, particle transport, granular materials
  - Low-Mach CFD on block-AMR grids with embedded boundaries
  - Interphase transfer

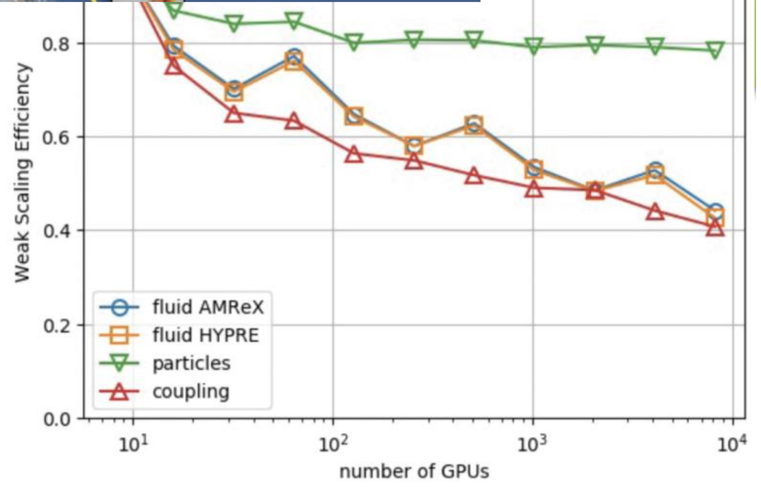
The MFIX-Exa project is targeting a 1000X increase in capabilities through new algorithms and exascale computing

PI: Madhava Syamlal, NETL

ECP accomplishments:

- Added CFD discrete element method to AMReX adaptive mesh refinement framework
- Extended physical modeling capabilities to include heat and mass transfer, species composition and chemical reactions
- Added a lower-fidelity particle-in-cell (PIC) to enable initial condition bootstrapping and save computational resources for evolving the (guessed) initial condition to a fully-developed state.
- Fully ported the code from CPUs to GPUs
- Performed weak scaling studies up to 8,192 GPUs on OLCF’s Summit supercomputer, nearly 30% of the machine
- Modeled a lab-scale demonstration of one of NETL’s cylindrical spouted beds containing 2.2 million HDPE particles fluidized by a central high-speed gas jet.





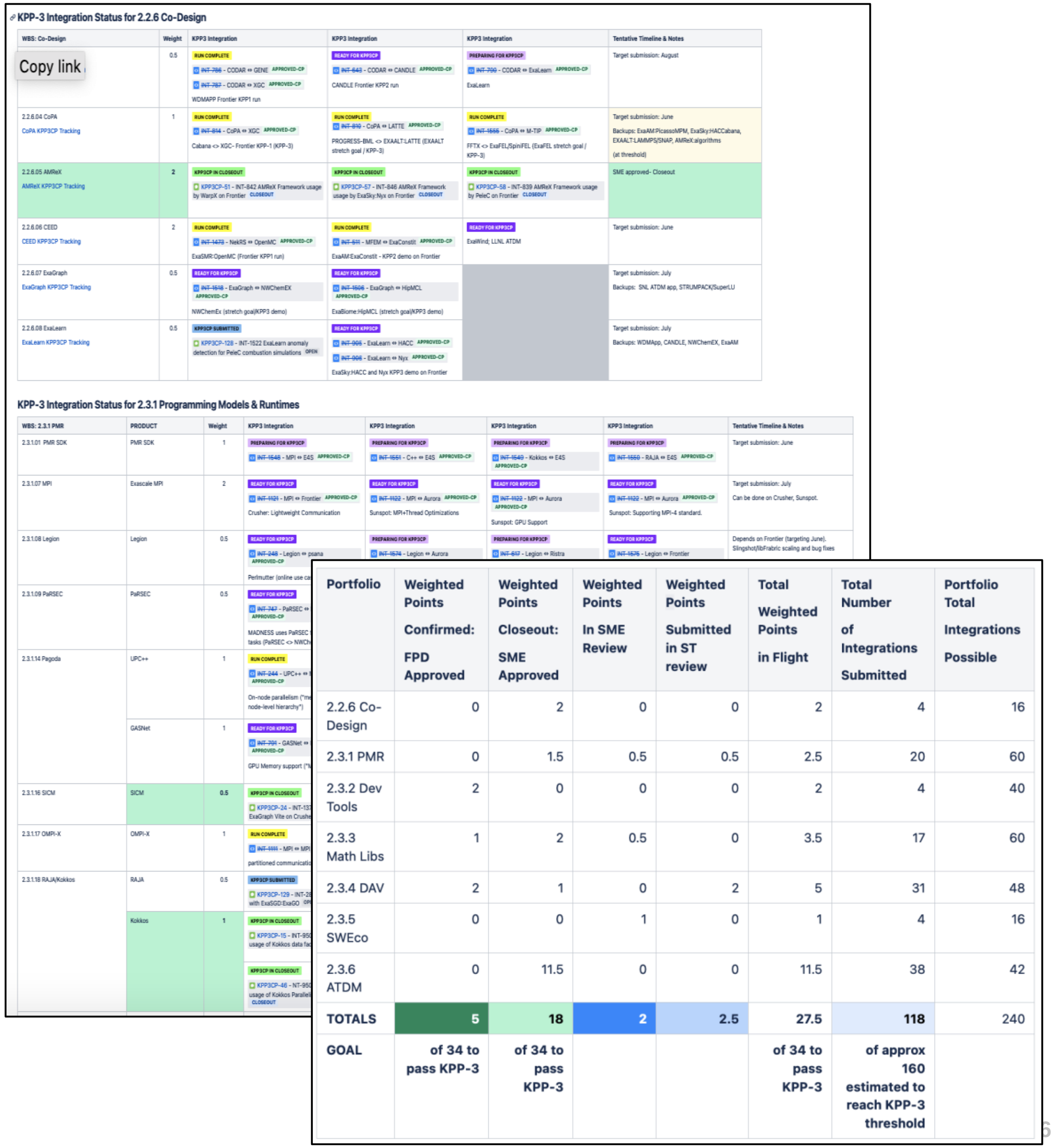
New capabilities give orders of magnitude improvements in size and complexity of systems that can be studied; earlier models only allowed for smaller, simplified geometries

BERKELEY LAB

NATIONAL ENERGY TECHNOLOGY LABORATORY

Managing the KPP-3 integration process is complex

- The first time our community has explicitly tried to put this kind of metric of success in place
- Definition: A KPP-3 integration is the use of a significant capability by a client (application, other library, facility, etc.) in a sustained way in the exascale ecosystem
- Definition: A KPP-3 weighted point is obtained when a team shows evidence of 4 (typically) integrations
- KPP-3 has 68 total possible weighted points; 34 needed for threshold
- 290 possible integrations; 160 needed to pass KPP-3
- Terry Turton and Joshua Sartin (LANL) have developed numerous dashboards and processes to make this tractable
- Planning a KPP-3 reviewer ‘jamboree’ in late June



KPP-3 Integration Status for 2.2.6 Co-Design

WBS: Co-Design	Weight	KPP3 Integration	KPP3 Integration	KPP3 Integration	Tentative Timeline & Notes
Copy link	0.5	RUN COMPLETE ~~INT-786~~ - CODAR ⇔ GENE APPROVED-CP ~~INT-787~~ - CODAR ⇔ XGC APPROVED-CP WDMAPP Frontier KPP1 run	READY FOR KPP3CP ~~INT-643~~ - CODAR ⇔ CANDLE APPROVED-CP CANDLE Frontier KPP2 run	PREPARING FOR KPP3CP ~~INT-790~~ - CODAR ⇔ ExaLearn APPROVED-CP ExaLearn	Target submission: August
2.2.6.04 CoPA CoPA KPP3CP Tracking	1	RUN COMPLETE ~~INT-814~~ - CoPA ⇔ XGC APPROVED-CP Cabana <> XGC- Frontier KPP-1 (KPP-3)	RUN COMPLETE ~~INT-810~~ - CoPA ⇔ LATTE APPROVED-CP PROGRESS-BML <> EXAALT:LATTE (EXAALT stretch goal / KPP-3)	RUN COMPLETE ~~INT-1555~~ - CoPA ⇔ M-TIP APPROVED-CP FFTX <> ExaFEL/SpiniFEL (ExaFEL stretch goal / KPP-3)	Target submission: June Backups: ExaAM:PicassoMPM, ExaSky:HACCabana, EXAALT:LAMMPS/SNAP, AMReX:algorithms (at threshold)
2.2.6.05 AMReX AMReX KPP3CP Tracking	**2**	KPP3CP IN CLOSEOUT KPP3CP-51 - INT-842 AMReX Framework usage by WarpX on Frontier CLOSEOUT	KPP3CP IN CLOSEOUT KPP3CP-57 - INT-846 AMReX Framework usage by ExaSky:Nyx on Frontier CLOSEOUT	KPP3CP IN CLOSEOUT KPP3CP-58 - INT-839 AMReX Framework usage by PeleC on Frontier CLOSEOUT	SME approved- Closeout
2.2.6.06 CEED CEED KPP3CP Tracking	2	RUN COMPLETE ~~INT-1473~~ - NekRS ⇔ OpenMC APPROVED-CP ExaSMR:OpenMC (Frontier KPP1 run)	RUN COMPLETE ~~INT-511~~ - MFEM ⇔ ExaConstit APPROVED-CP ExaAM:ExaConstit - KPP2 demo on Frontier	READY FOR KPP3CP ExaWind; LLNL ATDM	Target submission: June
2.2.6.07 ExaGraph ExaGraph KPP3CP Tracking	0.5	READY FOR KPP3CP ~~INT-1518~~ - ExaGraph ⇔ NWChemEX APPROVED-CP NWChemEx (stretch goal/KPP3 demo)	READY FOR KPP3CP ~~INT-1506~~ - ExaGraph ⇔ HipMCL APPROVED-CP ExaBiome:HipMCL (stretch goal/KPP3 demo)		Target submission: July Backups: SNL ATDM app, STRUMPACK/SuperLU
2.2.6.08 ExaLearn ExaLearn KPP3CP Tracking	0.5	KPP3CP SUBMITTED KPP3CP-128 - INT-1522 ExaLearn anomaly detection for PeleC combustion simulations OPEN	READY FOR KPP3CP ~~INT-905~~ - ExaLearn ⇔ HACC APPROVED-CP ~~INT-906~~ - ExaLearn ⇔ Nyx APPROVED-CP ExaSky:HACC and Nyx KPP3 demo on Frontier		Target submission: July Backups: WDMApp, CANDLE, NWChemEX, ExaAM

KPP-3 Integration Status for 2.3.1 Programming Models & Runtimes

WBS: 2.3.1 PMR	PRODUCT	Weight	KPP3 Integration	KPP3 Integration	KPP3 Integration	KPP3 Integration	Tentative Timeline & Notes
2.3.1.01 PMR SDK	PMR SDK	1	PREPARING FOR KPP3CP ~~INT-1548~~ - MPI ⇔ E4S APPROVED-CP	PREPARING FOR KPP3CP ~~INT-1551~~ - C++ ⇔ E4S APPROVED-CP	PREPARING FOR KPP3CP ~~INT-1549~~ - Kokkos ⇔ E4S APPROVED-CP	PREPARING FOR KPP3CP ~~INT-1550~~ - RAJA ⇔ E4S APPROVED-CP	Target submission: June
2.3.1.07 MPI	Exascale MPI	2	READY FOR KPP3CP ~~INT-1121~~ - MPI ⇔ Frontier APPROVED-CP Crusher: Lightweight Communication	READY FOR KPP3CP ~~INT-1122~~ - MPI ⇔ Aurora APPROVED-CP Sunspot: MPI+Thread Optimizations	READY FOR KPP3CP ~~INT-1122~~ - MPI ⇔ Aurora APPROVED-CP Sunspot: GPU Support	READY FOR KPP3CP ~~INT-1122~~ - MPI ⇔ Aurora APPROVED-CP Sunspot: Supporting MPI-4 standard.	Target submission: July Can be done on Crusher, Sunspot.
2.3.1.08 Legion	Legion	0.5	READY FOR KPP3CP ~~INT-248~~ - Legion ⇔ psana APPROVED-CP Perlmutter (online use ca	PREPARING FOR KPP3CP ~~INT-1574~~ - Legion ⇔ Aurora	PREPARING FOR KPP3CP ~~INT-617~~ - Legion ⇔ Ristra	READY FOR KPP3CP ~~INT-1575~~ - Legion ⇔ Frontier	Depends on Frontier (targeting June). Slingshot/libFrabric scaling and bug fixes
2.3.1.09 PaRSEC	PaRSEC	0.5	READY FOR KPP3CP ~~INT-747~~ - PaRSEC ⇔ APPROVED-CP MADNESS uses PaRSEC t tasks (PaRSEC <> NWCh				
2.3.1.14 Pagoda	UPC++	1	RUN COMPLETE ~~INT-244~~ - UPC++ ⇔ APPROVED-CP On-node parallelism ("me node-level hierarchy")				
	GASNet	1	READY FOR KPP3CP ~~INT-791~~ - GASNet ⇔ APPROVED-CP GPU Memory support ("M				
2.3.1.16 SICM	SICM	**0.5**	KPP3CP IN CLOSEOUT KPP3CP-24 - INT-137 ExaGraph Vite on Crushe				
2.3.1.17 OMPI-X	OMPI-X	1	RUN COMPLETE ~~INT-1111~~ - MPI ⇔ MPI partitioned communicatio				
2.3.1.18 RAJA/Kokkos	RAJA	0.5	KPP3CP SUBMITTED KPP3CP-129 - INT-28 with ExaSGD:ExaGO OP				
	Kokkos	**1**	KPP3CP IN CLOSEOUT KPP3CP-15 - INT-950 usage of Kokkos data fac				
			KPP3CP IN CLOSEOUT KPP3CP-46 - NT-950 usage of Kokkos Paralleli CLOSEOUT				

Portfolio	Weighted Points Confirmed: FPD Approved	Weighted Points Closeout: SME Approved	Weighted Points In SME Review	Weighted Points Submitted in ST review	Total Weighted Points in Flight	Total Number of Integrations Submitted	Portfolio Total Integrations Possible
2.2.6 Co-Design	0	2	0	0	2	4	16
2.3.1 PMR	0	1.5	0.5	0.5	2.5	20	60
2.3.2 Dev Tools	2	0	0	0	2	4	40
2.3.3 Math Libs	1	2	0.5	0	3.5	17	60
2.3.4 DAV	2	1	0	2	5	31	48
2.3.5 SWEco	0	0	1	0	1	4	16
2.3.6 ATDM	0	11.5	0	0	11.5	38	42
TOTALS	**5**	**18**	**2**	**2.5**	**27.5**	**118**	240
GOAL	**of 34 to pass KPP-3**	**of 34 to pass KPP-3**			**of 34 to pass KPP-3**	**of approx 160 estimated to reach KPP-3 threshold**	

Inevitably, challenges remain on Frontier

- Software stack
  - Various MPI issues caused in part by the software layer’s interaction with Slingshot interconnect (e.g., GPU-aware MPI)
  - Immaturity with OpenMP target offload, particularly with Fortran
- User errors / knowledge
  - Using a different scheduler (SLURM) relative to other systems (e.g., LSF on Summit),
  - Building source code correctly,
  - Settling on the myriad of environment variables (particularly for MPI)
- Node hardware failures (GPUs, SIVOCS, memory), typical on the front end of the “bathtub curve”, principal cause for MTBF numbers that are lower than that envisioned for steady state operations
- Performance variability at scale remains, e.g., due to global reductions, all-to-all, hanging switches
  - SlingShot network is hanging together better now, e.g., no major “meltdowns”
  - Jobs near full system size (8-9K nodes) having better success than just a few weeks ago

Aurora will provide an important test of exascale portability

- Approximately seven AD teams currently using Sunspot (Aurora TDS system)
  - Several utilizing >= 50% of system
  - Some early excellent results: e.g. OpenMC
- Many teams are eager to exercise their codes at scale on Aurora as soon as it is available.
- ECP is expected to give AD teams a major head start in being able to efficiently take advantage of DOE leadership class compute resources.

- Several teams are on Sunspot (Aurora TDS); about 3000 node hours used to date
- Limited Auroral access expected in July 2023; full access in October 2023

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Hewlett Packard Enterprise
intel
Aurora

Compute Node
2 Intel® Xeon® CPU Max Series processors; 6 Intel® Data Center GPU Max Series GPUs; Unified Memory Architecture; 8 fabric endpoints; RAMBO

GPU Architecture
Intel® Data Center GPU Max Series; Tile-based chiplets, HBM stack, Foveros 3D integration, 7nm

System Interconnect
HPE Slingshot; Dragonfly topology with adaptive routing

Network Switch
25.6 Tb/s per switch, from 64–200 Gbs ports (25 GB/s per direction)

High-Performance Storage
≥230 PB, ≥25 TB/s (DAOS)

Node Performance
>130 TF

System Size
>10,000 nodes

Independent Project Review held May 2-4, 2023 at ORNL

IPR Charge Questions

1 Is the project making adequate progress to address the recommendations and comments from the March 2022 Independent Project Review? YES

2 Is the project on track to meet its threshold KPPs? YES

3 Is the ECP adequately prepared for project close out? YES

4 Are risks adequately identified and managed with appropriate responses? Is there adequate contingency to successfully complete the project? YES

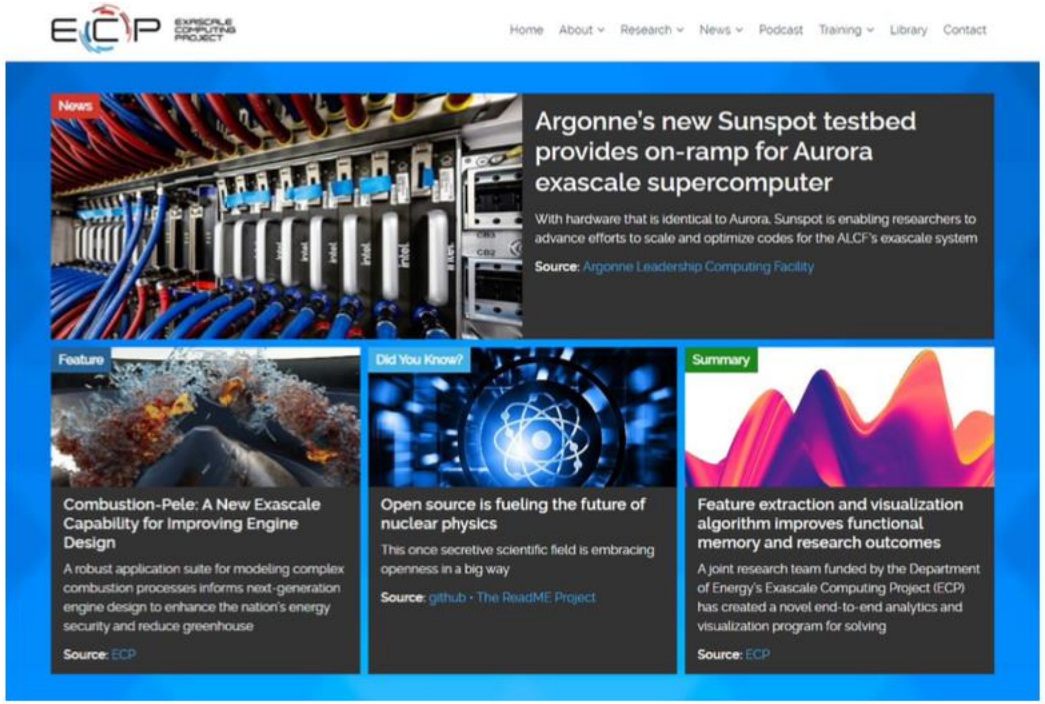
5 Is the overall project being properly managed? YES

Summary of Actionable Comments

- Communicate, Communicate, Communicate
  - Develop articles/podcasts that showcase relevance for a non-technical audience
  - Continue Capabilities Assessment Report for software technologies
  - Follow through on the communications strategy and plan
  - Develop a plan to transition the ECP website and embedded communications
- Update staffing and succession planning for ECP leadership and key technical personnel
- Elucidate the KPP verification process with specific examples and improve progress tracking via dashboards
- Work to ensure codes are robust and reliable once KPPs are met
- Encourage stretch science problems and success on both exascale platforms

ECP Communication Strategy

- ECP has increased staff resources to ‘spread the word’
- Recap: Calendar Year 2022
  - 17 Podcasts Published *(Total now 101 episodes)*
  - > 950 Million Media Impressions Worldwide
  - 3,178 followers on Twitter
  - 3,800 followers on LinkedIn *Exascale Computing*
  - 916 subscribers YouTube channel
  - Exascale Day 2022 *Collaboration with Labs, Vendors and Industry/Agency Council Members)*
    - 45 articles posted
    - 33 video clips and researcher quotes
- Planned
  - Then and Now article series
  - ECP Book
  - Significant presence at SC23
  - Stakeholder meetings



Argonne's new Sunspot testbed provides on-ramp for Aurora exascale supercomputer

With hardware that is identical to Aurora, Sunspot is enabling researchers to advance efforts to scale and optimize codes for the ALCF's exascale system

Source: Argonne Leadership Computing Facility

Combustion-Pele: A New Exascale Capability for Improving Engine Design

A robust application suite for modeling complex combustion processes informs next-generation engine design to enhance the nation's energy security and reduce greenhouse

Source: ECP

Open source is fueling the future of nuclear physics

This once secretive scientific field is embracing openness in a big way

Source: github · The ReadME Project

Feature extraction and visualization algorithm improves functional memory and research outcomes

A joint research team funded by the Department of Energy's Exascale Computing Project (ECP) has created a novel end-to-end analytics and visualization program for solving

Source: ECP

Leadership Transitions

Recent Leadership Changes

Doug Kothe (ORNL) departed ORNL for SNL June 2

Lori Diachin (LLNL) assumed ECP Director role June 1

Ashley Barker (ORNL) named ECP Deputy Director June 1

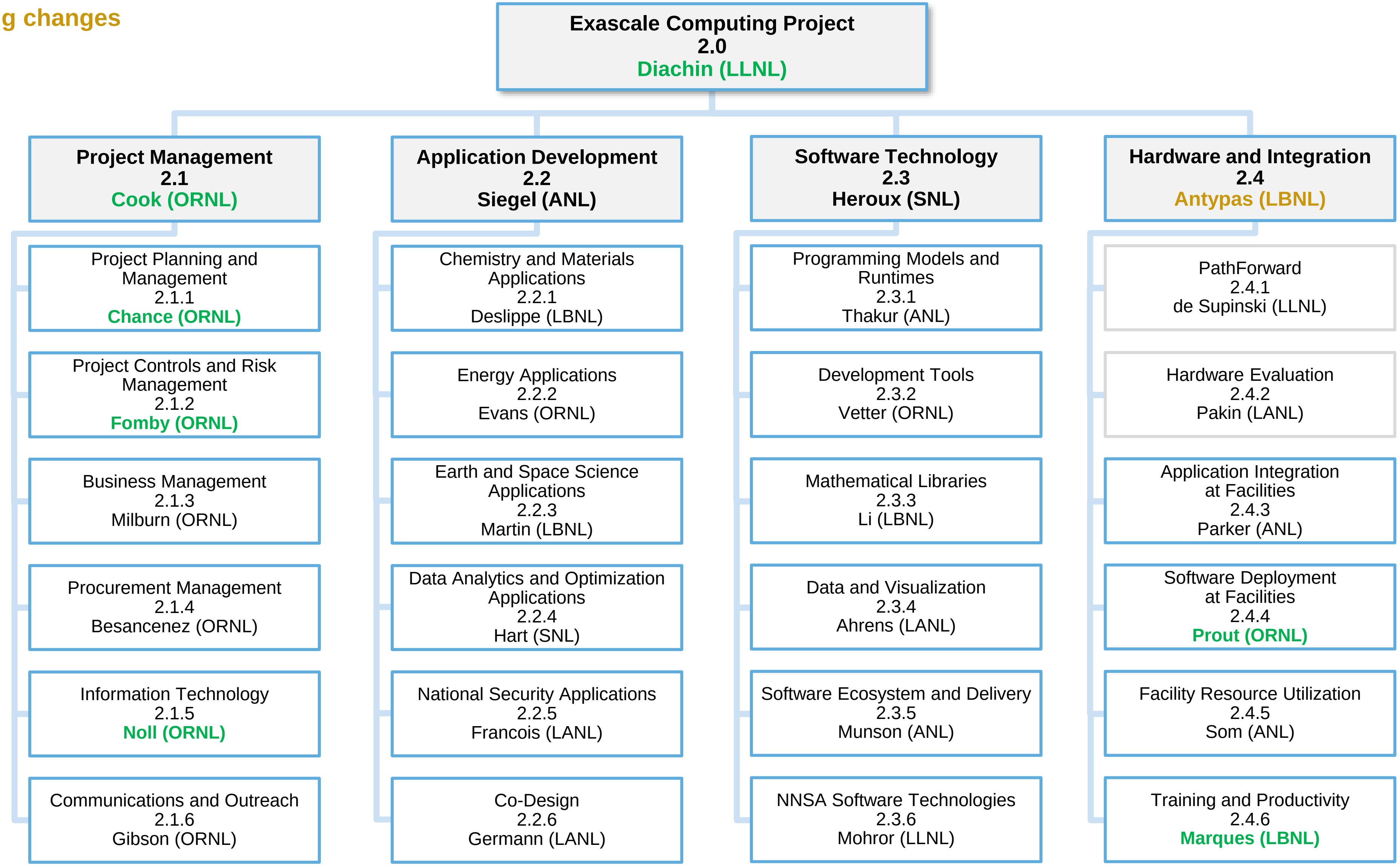
Katie Antypas (LBNL) departing for NSF in early July

Richard Gerber (LBNL) will assume HI Lead Role

ECP continues to enjoy a lot of stability at the L2 and L3 levels

Green: Changes since March 2022

Yellow: Upcoming changes



Exascale Computing Project
2.0
Diachin (LLNL)

Project Management
2.1
Cook (ORNL)

Project Planning and Management
2.1.1
Chance (ORNL)

Project Controls and Risk Management
2.1.2
Fomby (ORNL)

Business Management
2.1.3
Milburn (ORNL)

Procurement Management
2.1.4
Besancenez (ORNL)

Information Technology
2.1.5
Noll (ORNL)

Communications and Outreach
2.1.6
Gibson (ORNL)

Application Development
2.2
Siegel (ANL)

Chemistry and Materials Applications
2.2.1
Deslippe (LBNL)

Energy Applications
2.2.2
Evans (ORNL)

Earth and Space Science Applications
2.2.3
Martin (LBNL)

Data Analytics and Optimization Applications
2.2.4
Hart (SNL)

National Security Applications
2.2.5
Francois (LANL)

Co-Design
2.2.6
Germann (LANL)

Software Technology
2.3
Heroux (SNL)

Programming Models and Runtimes
2.3.1
Thakur (ANL)

Development Tools
2.3.2
Vetter (ORNL)

Mathematical Libraries
2.3.3
Li (LBNL)

Data and Visualization
2.3.4
Ahrens (LANL)

Software Ecosystem and Delivery
2.3.5
Munson (ANL)

NNSA Software Technologies
2.3.6
Mohror (LLNL)

Hardware and Integration
2.4
Antypas (LBNL)

PathForward
2.4.1
de Supinski (LLNL)

Hardware Evaluation
2.4.2
Pakin (LANL)

Application Integration at Facilities
2.4.3
Parker (ANL)

Software Deployment at Facilities
2.4.4
Prout (ORNL)

Facility Resource Utilization
2.4.5
Som (ANL)

Training and Productivity
2.4.6
Marques (LBNL)

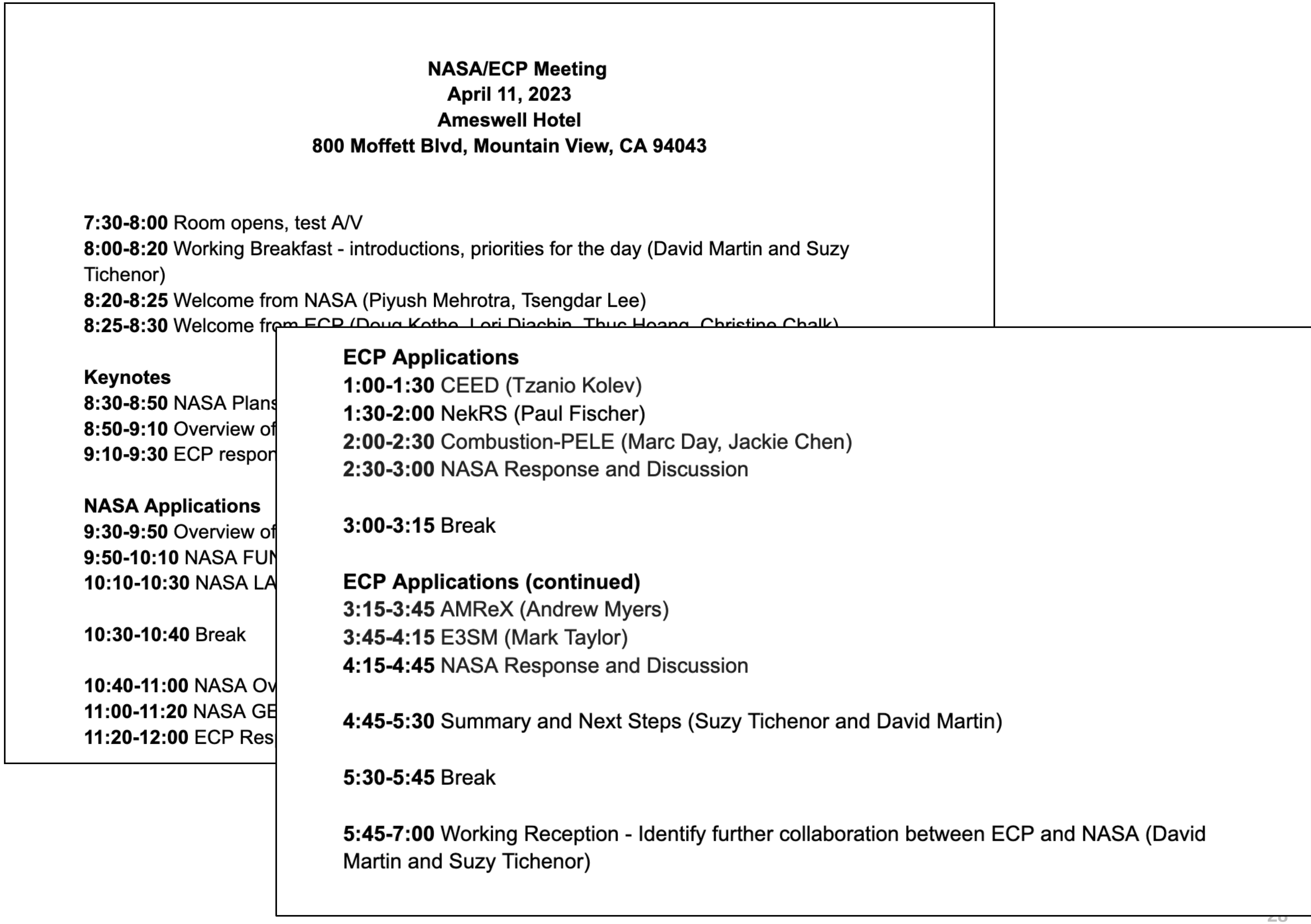
Outreach and Broader Engagement Activities

ECP has been very active with our Industry and Agency Council

Date	ECP Events
October 26-27, 2022	IAC Meeting at ORNL
October 31, 2022	Cloud Computing Workshop (IAC) (virtual)
November 2022	Fortran Workshop (IAC) (virtual)
January 27, 2023	Winter Quarterly IAC (virtual)
February 2023	ECP community BOF days and tutorials
April 11, 2023	NASA Technical Deep dive (AD)
June 1-2, 2023	IAC Spring/Summer meeting
June 2023	NOAA collaboration meeting ORNL
July 2023	NASA Technical Deep dive (ST)

NASA/ECP Technical Deep Dive – April 11, 2023

- Focus on CFD applications and supporting co-design technologies from AMReX and CEED
- ~60 participants
  - 30 from NASA Ames, Langley, Glenn, Goddard, HQ
  - 30 from ECP
- Next steps include identifying targeted collaborations via embedded teaming and longer term (FY25) joint DOE/NASA funding opportunities
- ST deep dive planned for July



NASA/ECP Meeting
April 11, 2023
Ameswell Hotel
800 Moffett Blvd, Mountain View, CA 94043

7:30-8:00 Room opens, test A/V
8:00-8:20 Working Breakfast - introductions, priorities for the day (David Martin and Suzy Tichenor)
8:20-8:25 Welcome from NASA (Piyush Mehrotra, Tsengdar Lee)
8:25-8:30 Welcome from ECP (Doug Kothe, Lori Diachin, Thuc Hoang, Christine Chalk)

Keynotes
8:30-8:50 NASA Plans
8:50-9:10 Overview of
9:10-9:30 ECP respon

NASA Applications
9:30-9:50 Overview of
9:50-10:10 NASA FUN
10:10-10:30 NASA LA

10:30-10:40 Break

10:40-11:00 NASA Ov
11:00-11:20 NASA GE
11:20-12:00 ECP Res

ECP Applications
1:00-1:30 CEED (Tzanio Kolev)
1:30-2:00 NekRS (Paul Fischer)
2:00-2:30 Combustion-PELE (Marc Day, Jackie Chen)
2:30-3:00 NASA Response and Discussion

3:00-3:15 Break

ECP Applications (continued)
3:15-3:45 AMReX (Andrew Myers)
3:45-4:15 E3SM (Mark Taylor)
4:15-4:45 NASA Response and Discussion

4:45-5:30 Summary and Next Steps (Suzy Tichenor and David Martin)

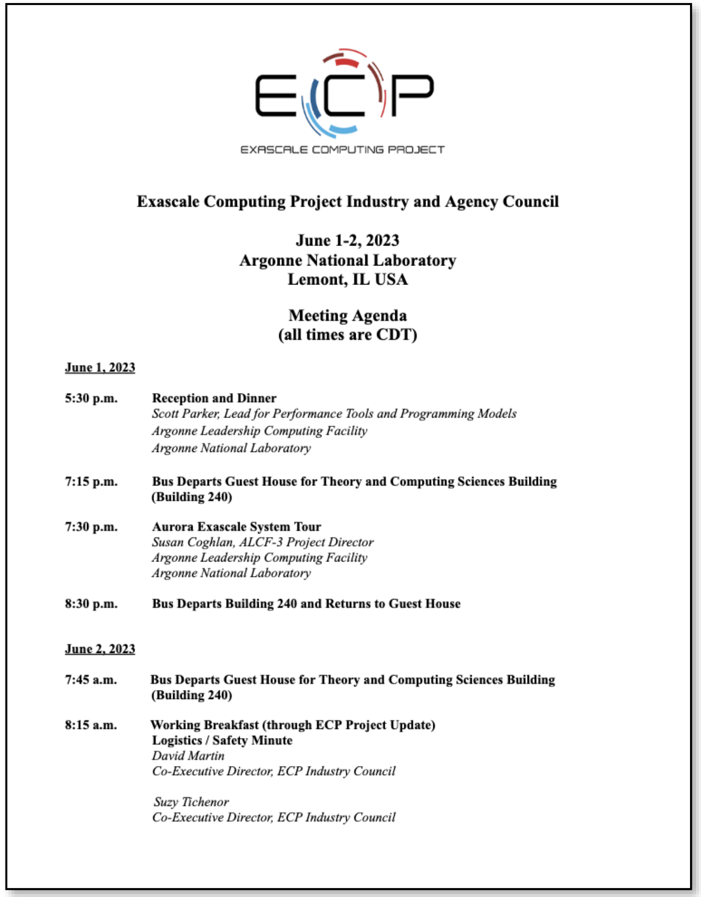
5:30-5:45 Break

5:45-7:00 Working Reception - Identify further collaboration between ECP and NASA (David Martin and Suzy Tichenor)

The most recent Industry and Agency Council Meeting focused on learnings from ECP involvement

- ~20 participants (10 from the IAC; 10 from ECP)
- Special topics:
  - DoD experiences with E4S
  - GE knowledge management system
- Survey results and lightening talks
  - What IAC members have learned from ECP about HPC or other topics
  - Recommendations from the IAC to ECP
- Key take aways
  - Significance of the move to GPUs; in some cases resulting in a change in internal computing strategies
  - The need for software to leverage advanced architectures
  - ECP has de-risked a move to GPUs for many
  - The value of lessons learned and networking with others in the community was highly cited
  - Continue to momentum for ECP applications and software
  - Communicate!

June 1-2, 2023
Argonne National Laboratory



EXASCALE COMPUTING PROJECT

Exascale Computing Project Industry and Agency Council

June 1-2, 2023
Argonne National Laboratory
Lemont, IL USA

Meeting Agenda
(all times are CDT)

June 1, 2023

5:30 p.m. **Reception and Dinner**
Scott Parker, Lead for Performance Tools and Programming Models
Argonne Leadership Computing Facility
Argonne National Laboratory

7:15 p.m. **Bus Departs Guest House for Theory and Computing Sciences Building (Building 240)**

7:30 p.m. **Aurora Exascale System Tour**
Susan Coghlan, ALCF-3 Project Director
Argonne Leadership Computing Facility
Argonne National Laboratory

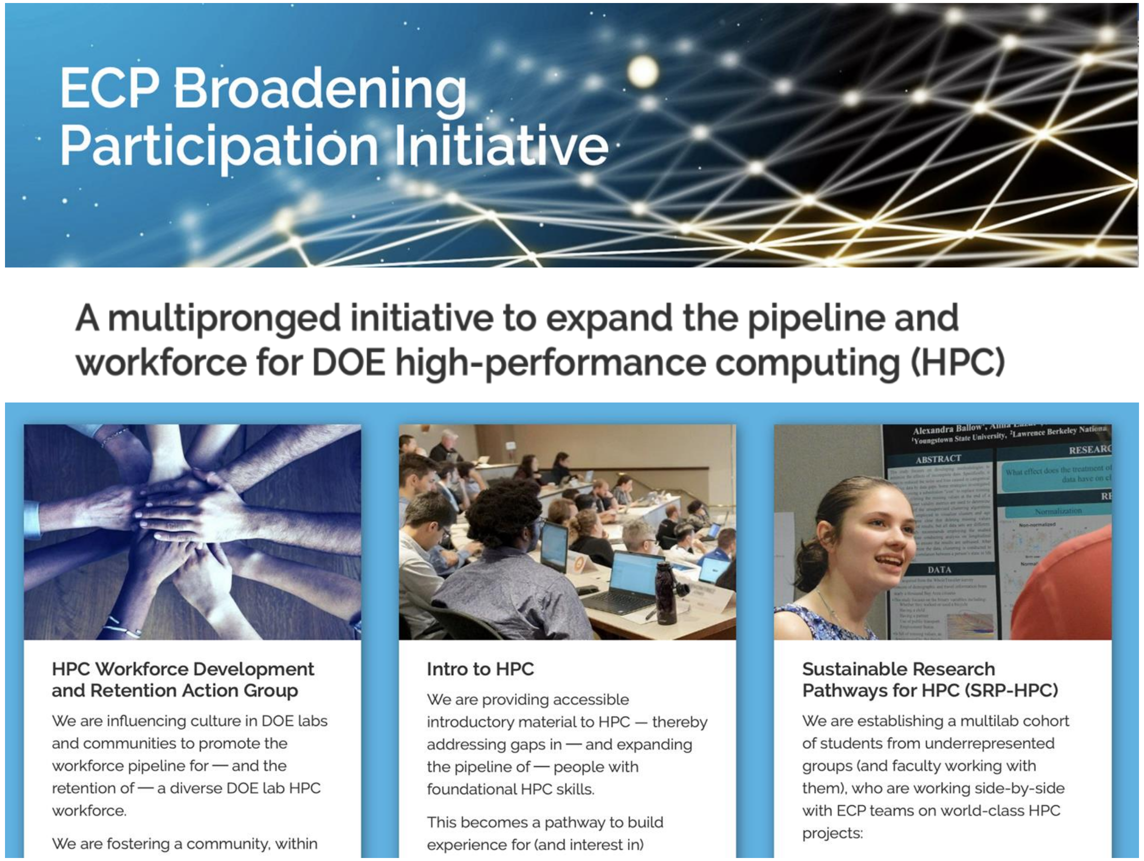
8:30 p.m. **Bus Departs Building 240 and Returns to Guest House**

June 2, 2023

7:45 a.m. **Bus Departs Guest House for Theory and Computing Sciences Building (Building 240)**

8:15 a.m. **Working Breakfast (through ECP Project Update)**
Logistics / Safety Minute
David Martin
Co-Executive Director, ECP Industry Council

Suzy Tichenor
Co-Executive Director, ECP Industry Council



ECP Broadening Participation Initiative

A multipronged initiative to expand the pipeline and workforce for DOE high-performance computing (HPC)

HPC Workforce Development and Retention Action Group

We are influencing culture in DOE labs and communities to promote the workforce pipeline for — and the retention of — a diverse DOE lab HPC workforce.

We are fostering a community, within

Intro to HPC

We are providing accessible introductory material to HPC — thereby addressing gaps in — and expanding the pipeline of — people with foundational HPC skills.

This becomes a pathway to build experience for (and interest in)

Sustainable Research Pathways for HPC (SRP-HPC)

We are establishing a multilab cohort of students from underrepresented groups (and faculty working with them), who are working side-by-side with ECP teams on world-class HPC projects:

Sustainable Research Pathways

SUSTAINABLE HORIZONS INSTITUTE

SRP-HPC students and faculty, summer 2022

Summer 2022:

- 61 participants: 13 student track, 16 faculty track (+29 students), 3 self-funded students
- 82% of overall participants represent at least 1 element of diversity
- Mentors/hosts through ECP and Facilities community
- Matches at all 9 participating labs

Summer 2023:

- Multi-lab CRLC program spanning ECP and other computational and data science projects 60+ faculty and students participating

Trevor Taylor Florida A&M University @ORNL

- Mentor: Veronica G. Melesse Vergara/ORNL
- Privacy Preserving Models Leveraging Mobility Data via HPC
- Smoky Mountain Conference 2022 Data Challenge Best Paper Award in "student/novice"

Aman Rani Texas Tech University @LBNL

- Mentor: Xiaoye Sherry Li/LBNL
- A Bayesian Optimization-Assisted, High-Performance Simulator for Modeling RF Accelerator Cavities
- SC22 Research Poster

Congratulations
to SRP-HPC awardee
Dr. Tanzima Islam
Winner of the
DOE Early Career
Award!

SRP @ LBNL and SRP-HPC @ BNL

SRP-HPC mentors/co-mentors

Dan Martin, LBL
SRP thrust lead
for ECP

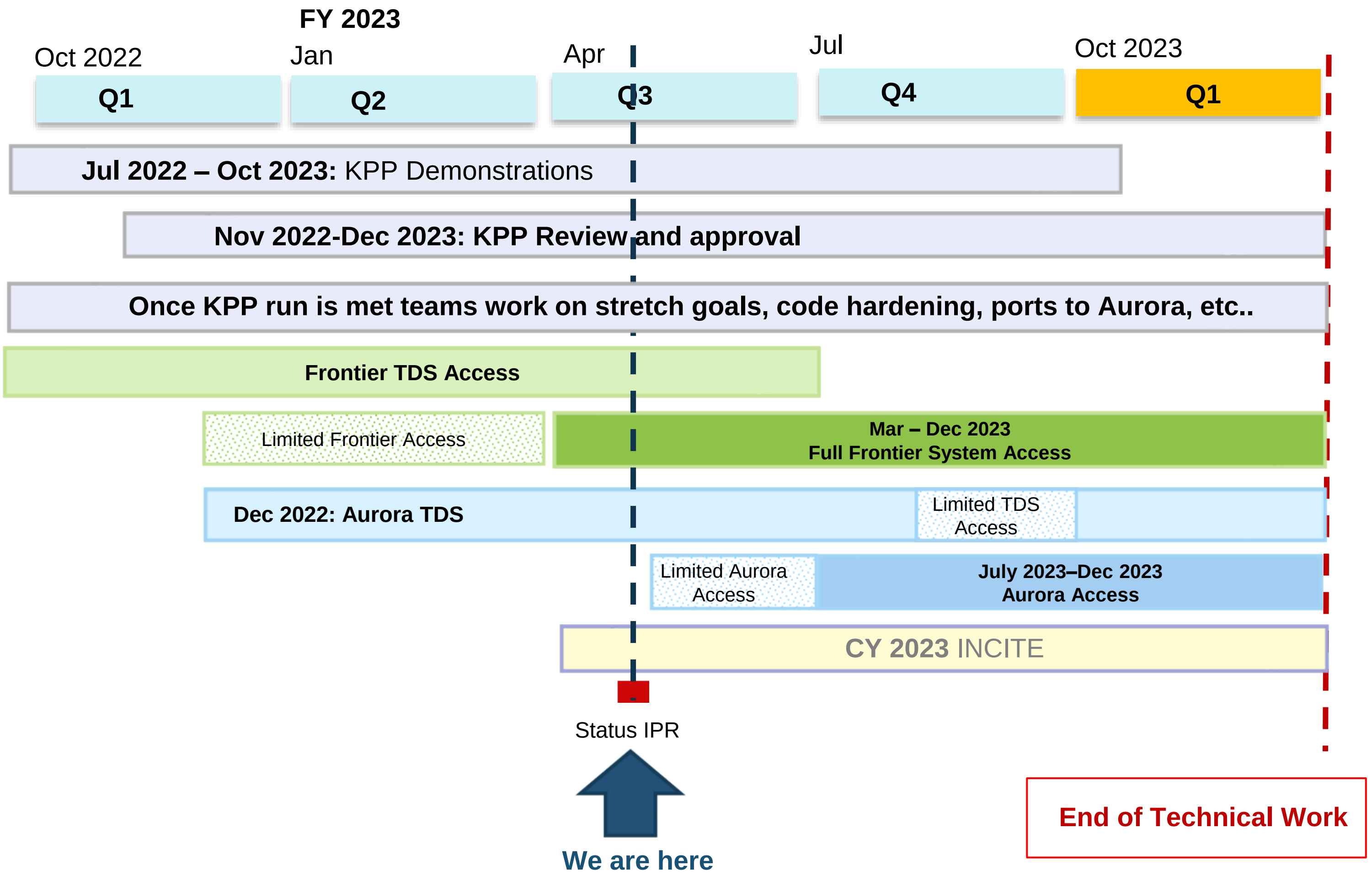
Keisha Moore, SHI
SRP Program
Coordinator

Project Close out

ECP will focus a significant amount of time and energy on project close out over the next 6-12 months

- Complete all technical work including documentation and review of KPPs
- Complete documentation required for a formal 413.3b project
  - Final milestone reports
  - Financial close out plan
  - Transition to operations plan
  - Project Close out report
  - Lessons learned
- Formal review of project completion including estimate of final costs, KPP completion verification, project documentation, etc
- Archive and/or transition project artifacts and project management tools
- Strong focus on outreach and continued stakeholder engagement

ECP will Extend One Quarter to December 31, 2023

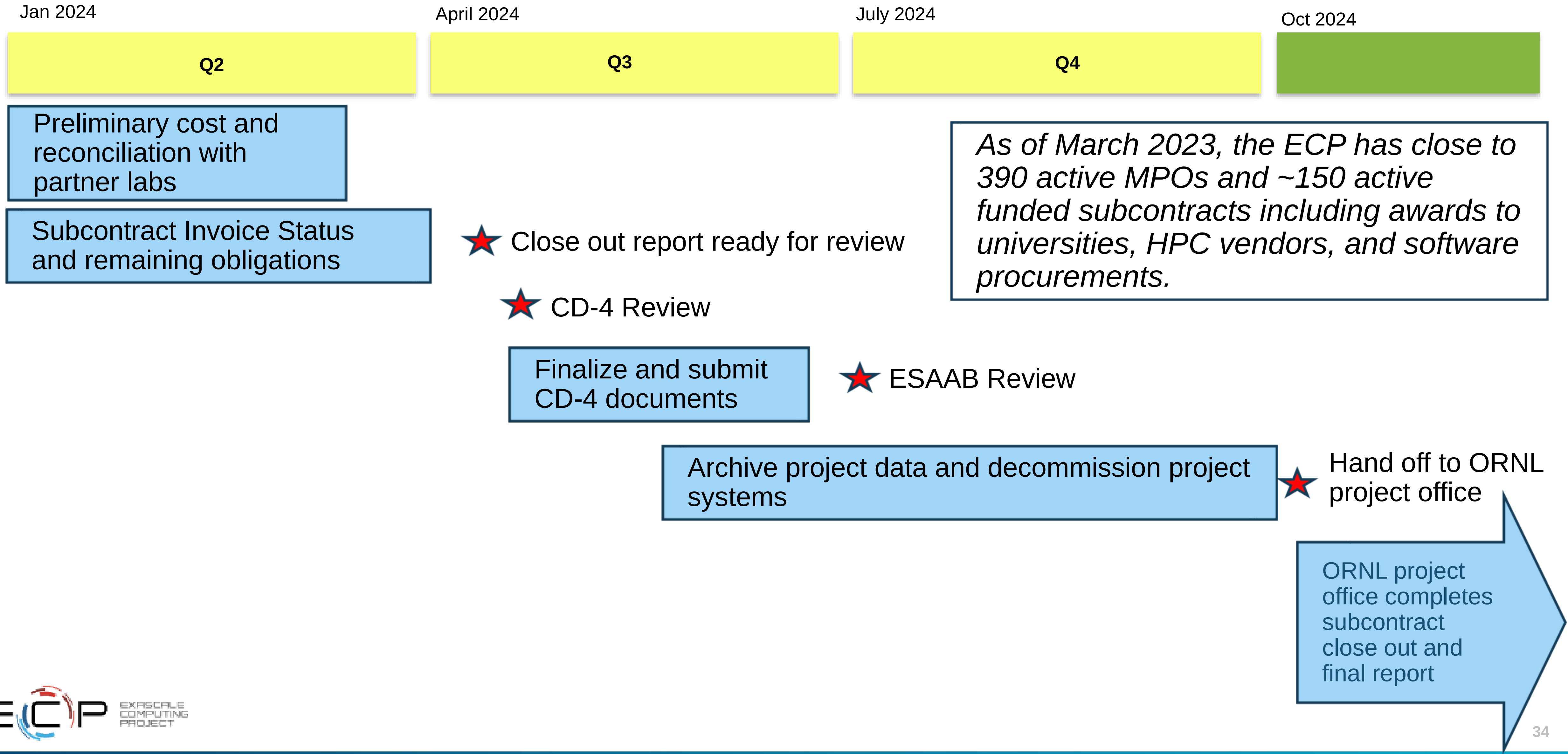


Scope for the final quarter of technical work includes:

- KPP run completions, write up and review for any teams not already done
- KPP stretch goals
- Porting to Aurora
- Final milestone reports
- Outreach activities including conferences, journal articles, etc.
- Code documentation and hardening

Once it is clear ECP will meet KPP thresholds, ECP will return any uncommitted/unneeded contingency to ASCR. Additionally, any unspent funds remaining after Q1 FY24 not needed for project close out will be de-obligated and returned to ASCR.

Timeline of Closeout Activities Once Technical Work is Complete



Jan 2024

April 2024

July 2024

Oct 2024

Q2

Q3

Q4

Preliminary cost and reconciliation with partner labs

Subcontract Invoice Status and remaining obligations

★ Close out report ready for review

★ CD-4 Review

Finalize and submit CD-4 documents

★ ESAAB Review

Archive project data and decommission project systems

★ Hand off to ORNL project office

ORNL project office completes subcontract close out and final report

As of March 2023, the ECP has close to 390 active MPOs and ~150 active funded subcontracts including awards to universities, HPC vendors, and software procurements.

Leadership team will remain engaged through FY24

- Finalizing project documentation
- Preparing for the CD-4 review; following up on any recommendations
- Helping archive project artifacts
- Conducting technical outreach – successes and impact of ECP
  - Stakeholders
  - Broader non-technical audiences
- Continuing to work on post-ECP sustainability (transitioning ECP technologies to ‘operations’)

Post-ECP sustainability

ECP ST team successful in proposing PESO to the ASCR sustainability seedling call

Deploying a hub and spoke model for a wide array of **software product communities**

- Anticipate it will include DOE-sponsored and commercial/community software products
- Shared design space exploration, coordination, etc.
- Already working with three other seed projects for workflows, tools, programming systems

Enabling Cross Cutting Communities of Practice

- Scientific software developers (e.g. IDEAS, HPC best practices)
- Community Outreach (e.g., Center for Scientific collaboration and community engagement)
- Software Foundations (e.g., NumFOCUS, Linsu)
- Workforce development (e.g.,Research software engineers, BSSw Fellows, Sustainabie Resesarch Pathways)

Community Engagements

- Recent workshop at ANL will result in a report
- LSSW meeting – Update on seed projects (June 15) (https://lssw.io/Meeting13)
- PESO meeting – PESO Overview and Panel (June 20) (https://lssw.io/PESOMeeting1)

ECP will continue to engage in significant outreach and stakeholder activities as we bring the project to a close

- Engaging stakeholders on the new capabilities developed
- Engaging industry and other agencies with outreach and lessons learned to broaden the community of exascale-ready applications and technologies
- Gathering feedback on the value and impact of exascale computing in their domains
- We are aware of and targeting possibilities for follow on funding from DOE or other agencies
  - DOE ASCR: SciDAC, EERCs, Research / ACT Division FOAs, Facility Division IRI
  - DOE SC Program (BER, BES, FES, HEP, NP) FOAs
  - DOE Earthshots, microelectronics
  - DOE NNSA (NA-10, NA-20)
- We are committed to being very aggressive in our outreach on all facets of ECP and seek your advice and input in those endeavors

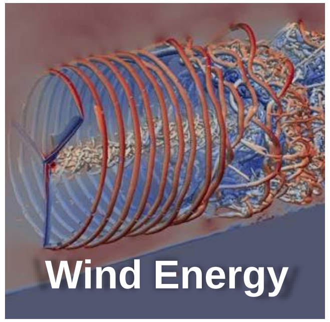
AD stakeholder engagement

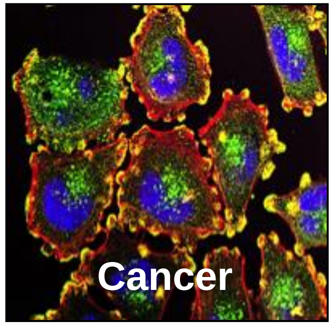
Office	POC	Briefing Date
FECM	Jennifer Wilcox	December 8, 2021
FES	James Van Dam	December 23, 2021 October 13, 2022
HEP	Harriet Kung	June 10, 2022
BES	Linda Horton	June 29, 2022
WETO	Benjamin Hallissy	September 26, 2022
NE	Katie Huff	October 31, 2022
NP	Tim Hallman	May 10, 2023
BER	Gary Geernaert	June 15, 2023
EERE	VTO, GTO, JOET, AMMTO	**TBD**
OE	Gil Bindewald	**TBD**
CESER	Puesh Kumar	**TBD**

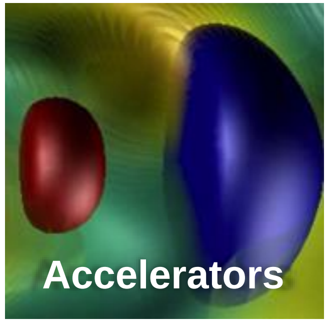
Looking Ahead

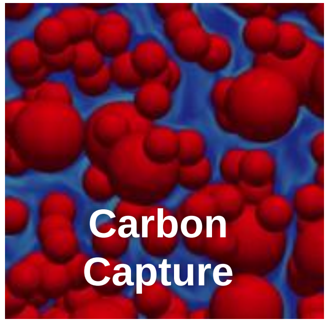
- Frontier
  - Support all 62 ECP teams now on Frontier, with priority for those not yet hitting threshold targets
  - Prioritize KPP-2 application and KPP-3 software product teams (including consumers needed for verification)
  - Strive to knock off KPP-2 and KPP-3 as soon as possible. Optimistic for threshold on both before Q3 FY23
- Aurora
  - Support all 62 ECP teams now on Aurora TDS (Sunspot) with focus on any blocking issues
  - Roll selected AD and ST teams on starting Jul 2023, with priority for teams that may meet their threshold KPP or are otherwise likely to deliver scientific impact (e.g., KPP objective). Full access is expected in Oct 2023
- KPP targets: preference for Frontier due to existing availability
  - KPP-1: Strive for all 11 applications meeting their base challenge problem and performance metrics
  - KPP-2: Expect to meet at least half of 10+4 applications to meet their base challenge problem (6+3)
  - KPP-3: Not unrealistic to see an integration score of 60+ points (out of 68 possible)
- Opportunities
  - Ensure scope post KPP threshold for each AD and ST team targets KPP objective and post ECP uptake
- Closeout: ensure expeditious closeout of all MPOs and subcontracts, success CD-4 review, return of all uncommitted ASCR funds back to ASCR for appropriate rescoping

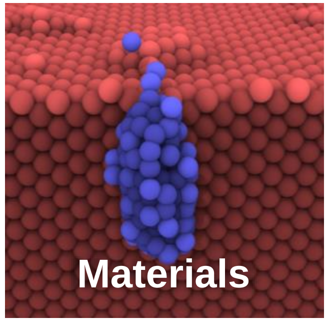
The breadth of ECP applications is remarkable; truly indicative of a change in computing abilities for DOE and the nation

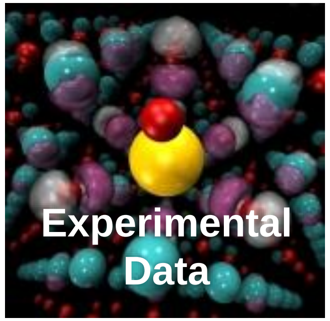

Wind Energy


Cancer

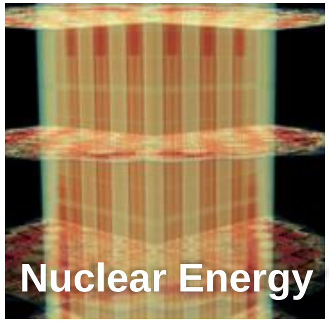

Accelerators

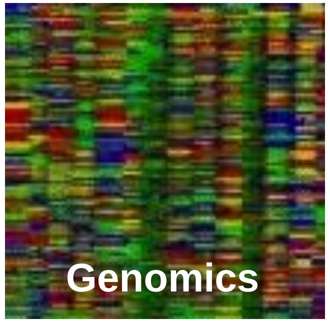

Carbon Capture

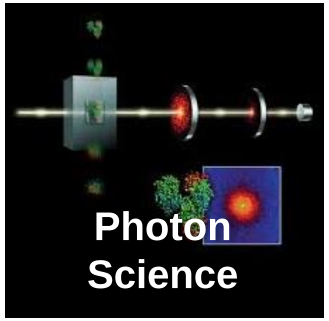

Materials

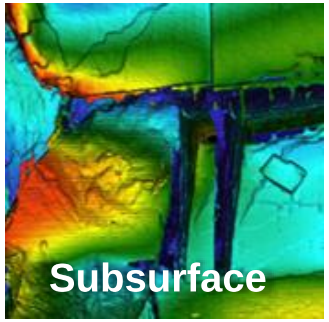

Experimental Data

National Security


Nuclear Energy


Genomics


Photon Science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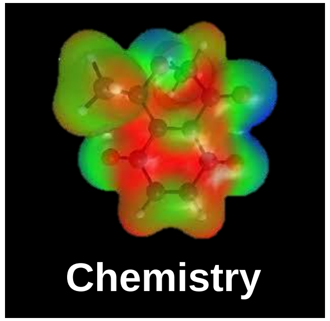
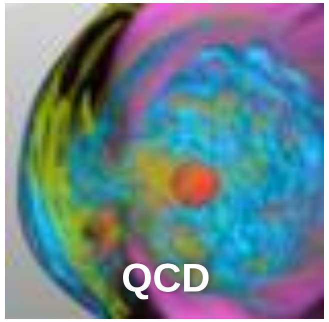
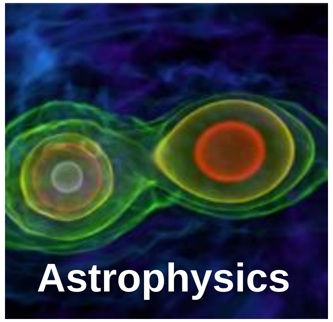

Chemistry

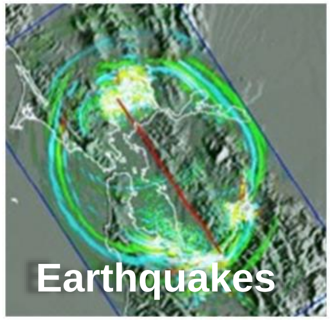

QCD

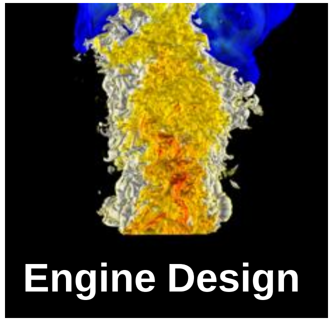

Astrophysics

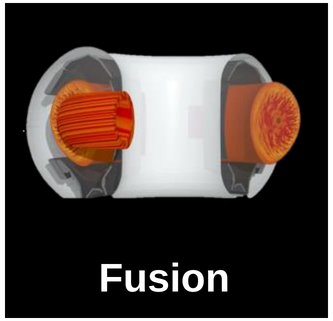
Power Grid

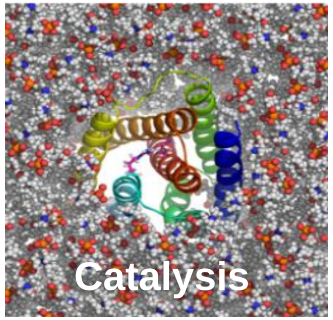
Additive Manufacturing

Climate


Earthquakes


Engine Design


Fusion


Catalysis

Questions?

EXTENDING THE IMPACT OF THE ECP SOFTWARE ECOSYSTEM

ASCAC Meeting

2:30pm – 3:00pm EDT
DoubleTree Hotel, Crystal City, Arlington, VA

Prof. Sameer Shende
Research Professor and Director,
Performance Research Laboratory, OACISS, University of Oregon
President and Director, ParaTools, Inc.

http://e4s.io/talks/Shende_PT_ASCAC23.pptx

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 to deploy our HPC applications to the cloud platforms!

Technology Translation

ParaTools, Inc. was founded in 2004: Prof. Allen D. Malony and Prof. Sameer Shende

- Spinoff from University of Oregon (UO) with equity participation (Office of Technology Transfer)
- Licenses **TAU Performance System®** trademark from UO under a royalty agreement
- Develops HPC business projects by providing consulting services
- Aims to improve the performance and productivity of software on HPC systems

ParaTools business

- Training in HPC performance tools
- HPC performance engineering
- TAU and E4S support
  - Continuous Integration Continuous Deployment (CI/CD)
  - Enhancements, design, installation, maintenance, support, engagement with applications’ teams
- Parallel runtime systems, cloud platforms
- ParaTools provides E4S and TAU support and is optimizing E4S for commercial cloud platforms

ParaTools’ High Performance Software Mission

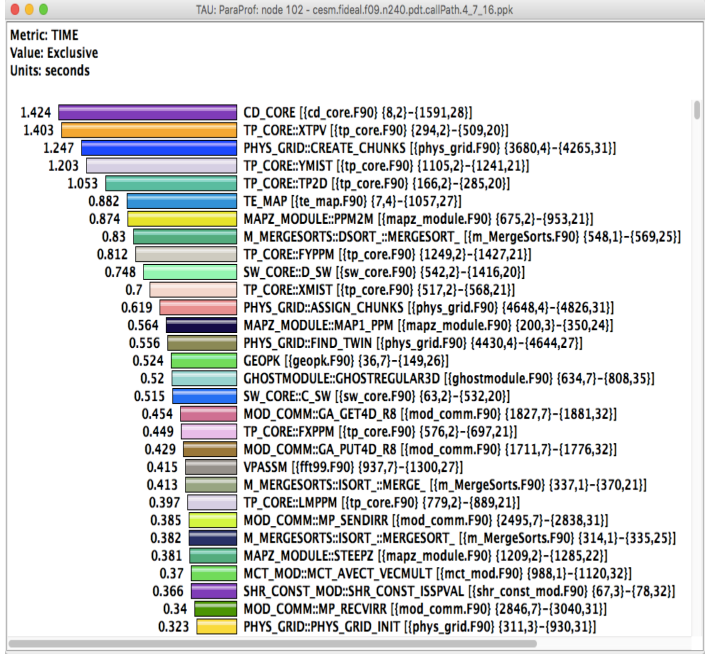
- **Software performance engineering is vital to realizing full capability**
  - Computational performance growth is slowing (*End of Moore’s Law)*
  - Computer systems are more complex and difficult to use than ever
- **Performance engineering tools have not kept pace with industry**
  - Domain experts often lack extensive programming expertise
  - Vendor supplied tools are limited or biased
  - Popular performance engineering software tools are experimental, ad-hoc, unstable, unsupported, or for experts only
- **Customers are developing in-house, ad-hoc tools and workflows**
  - Expensive, time consuming, non-transferable software developed reactively on a case-by-case basis
  - No provenance leaves customer at risk
- **Lack of expertise makes high performance computing (HPC) inaccessible to small- and mid-sized customers**
  - Many manufacturers in the United States experience missed deadlines and restricted product innovation due to computing performance limitations
- **Focus on HPC performance engineering technologies and solutions**
  - Increase performance productivity

TAU Performance System®

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

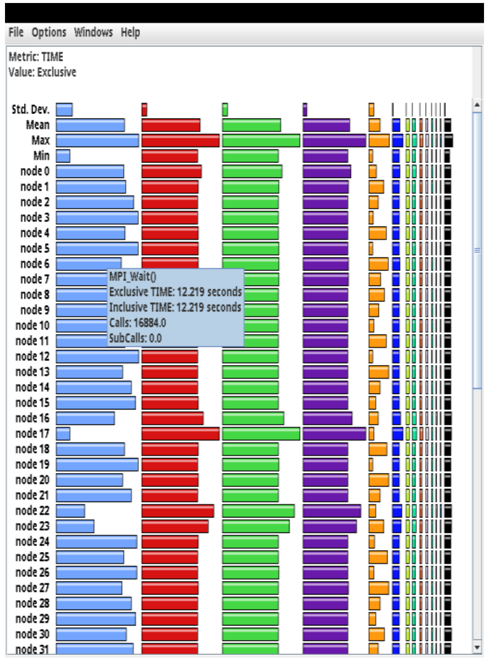
- Supports all parallel execution models
- Provides instrumentation and measurement
- Parallel profiling analysis and data mining
- Open source: https://www.paratools.com/TAU

TAU runs on all HPC platforms


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

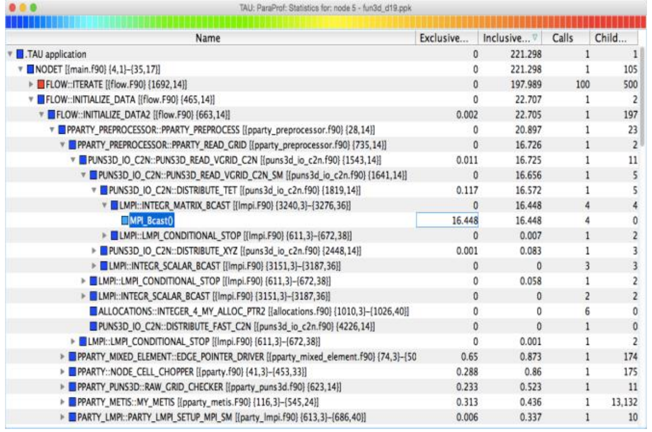
Metric: TIME
Value: Exclusive
Units: seconds

```
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}]
```

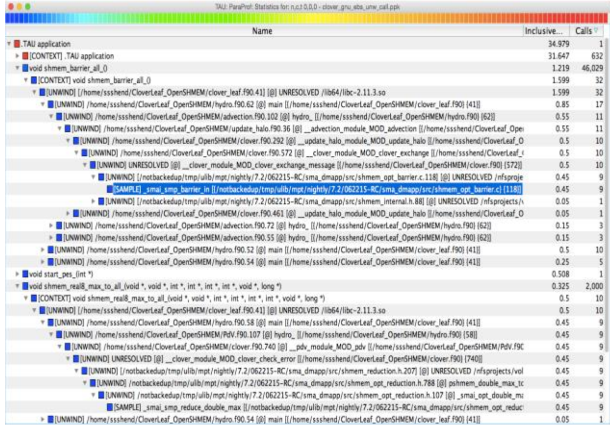


Metric: TIME
Value: Exclusive

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

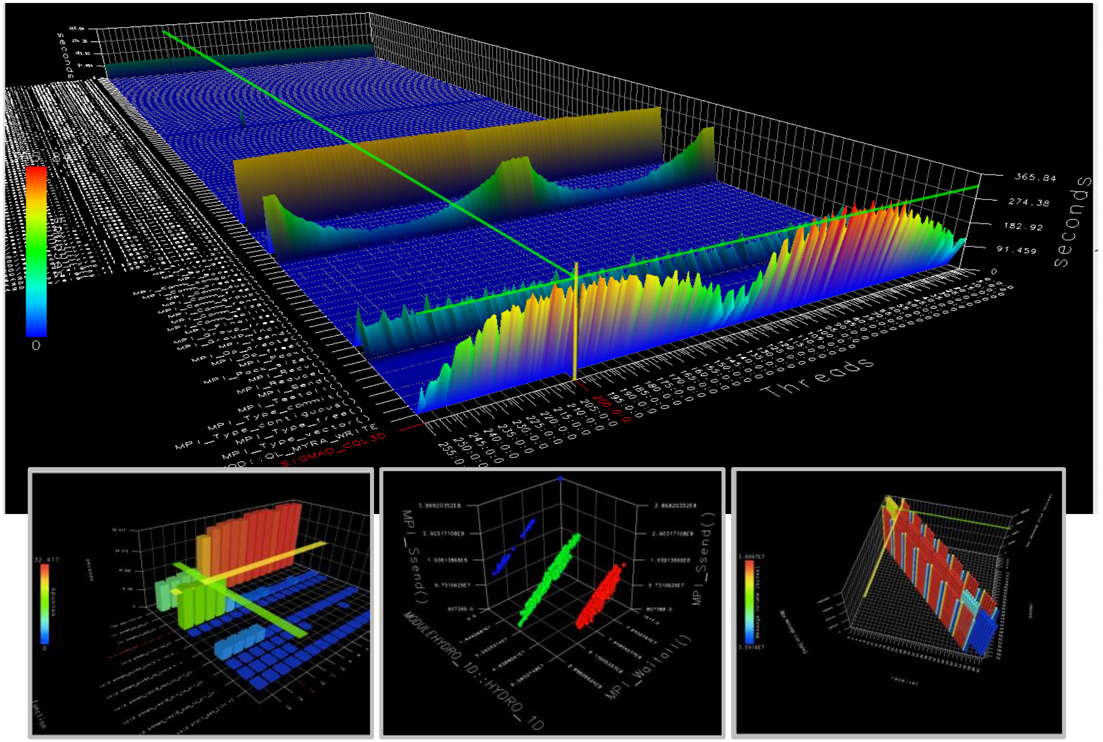

TAU: ParaProf: Statistics for: n,c,t 0,0,0 - clover_gnu_ebs_unw_call.ppk

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_m	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

TAU Commander: Improving the Usability of TAU Performance System®

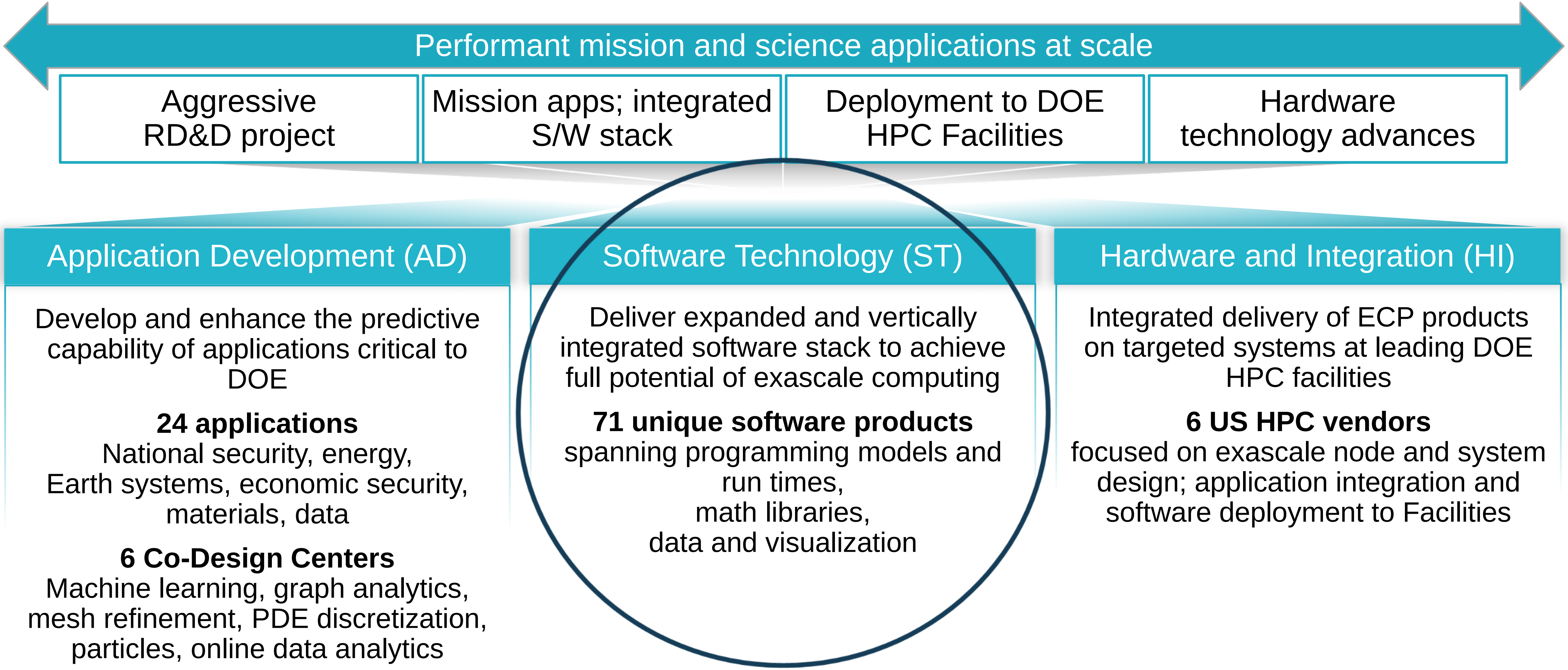
TAU Commander is a powerful environment to assist developers in managing their performance analysis activities and optimizing HPC software It offers capabilities across languages, parallel programming models, and HPC platforms.

Just one command: `tau`



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

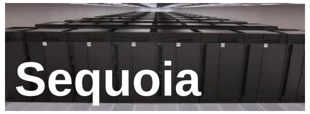
2012-2020

2021-2023

decommissioned

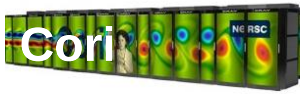
ORNL
Cray/AMD/NVIDIA

ANL
IBM BG/Q



LLNL
IBM BG/Q

ANL
Cray/Intel KNL



LBNL
Cray/Intel Xeon/KNL

LANL/SNL
Cray/Intel Xeon/KNL

ORNL
IBM/NVIDIA

LLNL
IBM/NVIDIA

LBNL
HPE/AMD/NVIDIA

ORNL
HPE/AMD

Exascale Systems

ANL
Intel/HPE

CROSSROADS

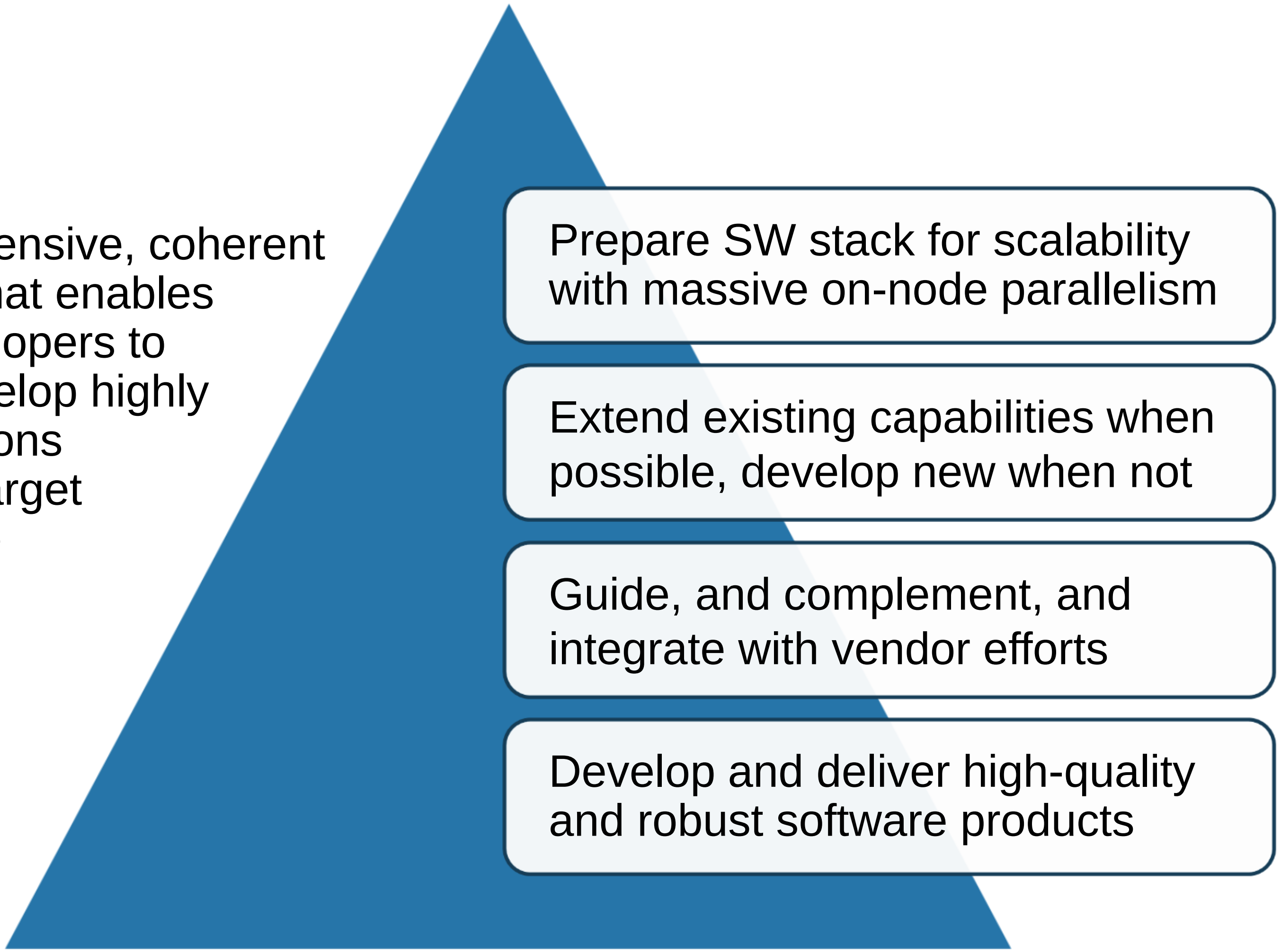
LANL/SNL
HPE/Intel

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

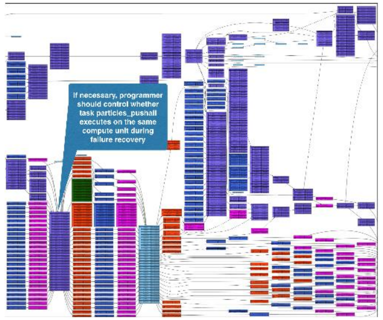


Prepare SW stack for scalability with massive on-node parallelism

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)

- 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

https://e4s.io

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

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

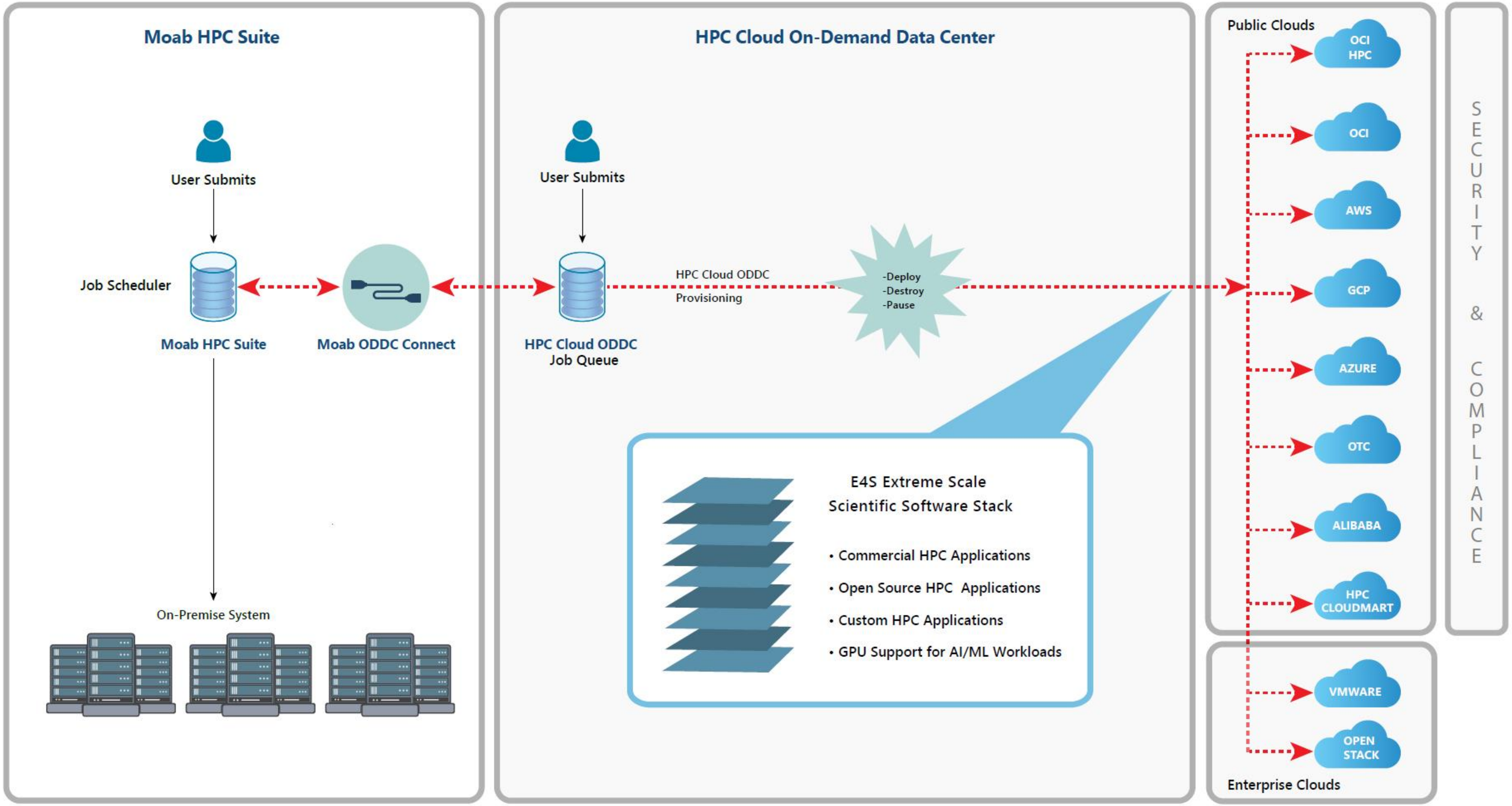
Considerations while deploying HPC/AI workloads to the cloud

- Which cloud provider?
  - AWS, OCI, GCP, Azure, …
  - Why not all?
- HPC and AI/ML workloads need low latency, high bandwidth
  - Which MPI?
- Which image?
  - Base Ubuntu without HPC tools or libraries? Too steep a learning curve
- Provisioning and building the image on different cloud providers
  - Command line interfaces can be cumbersome to use
- Bursting to the cloud from on-prem clusters using batch submission scripts?

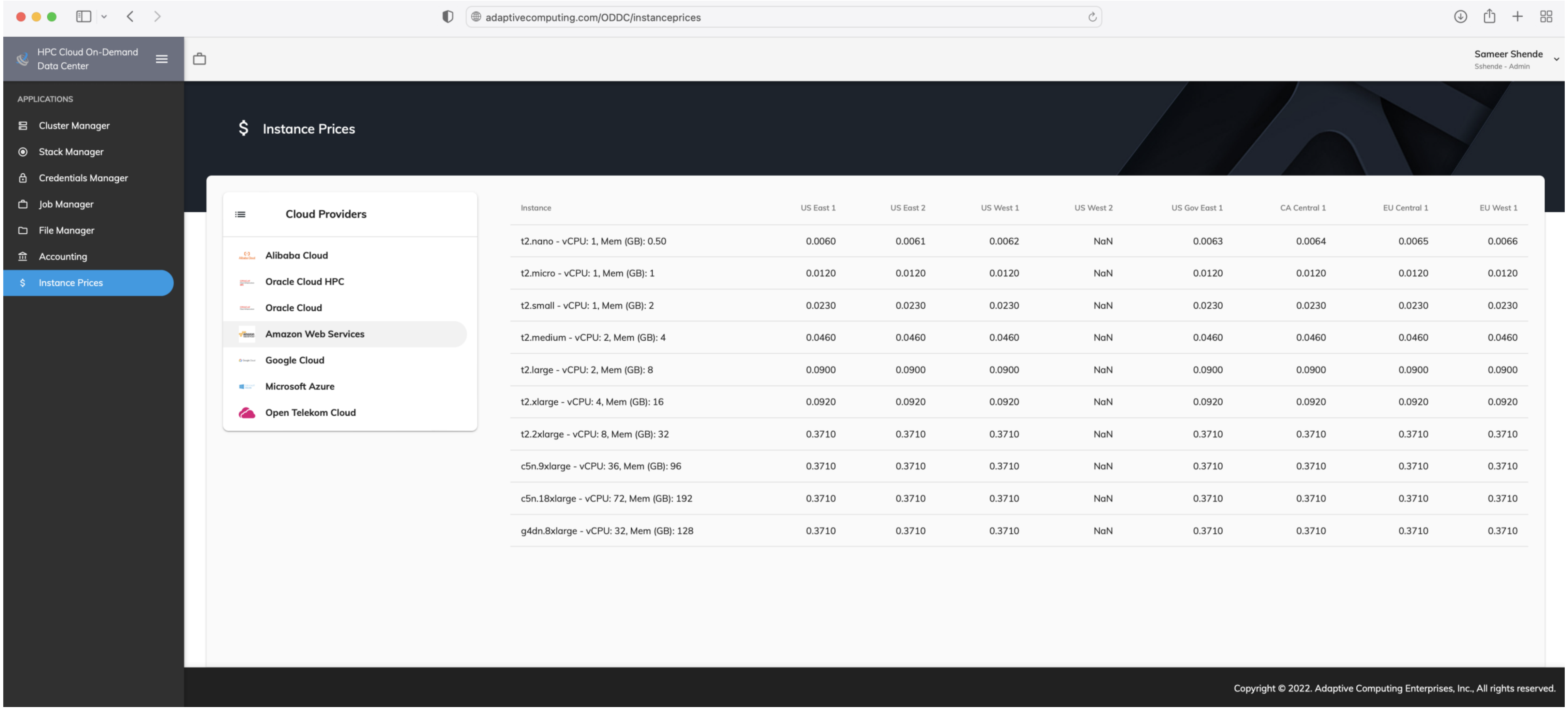
Key considerations for cloud-based deployment for E4S

- MPI - the core inter-node communication library has several implementations
  - Intel MPI, MVAPICH2-X, OpenMPI
  - Interfacing MPI with the job scheduling package (MOAB, Torque, SLURM)
- Cloud providers have different inter-node network adapters:
  - Elastic Fabric Adapter (EFA) on AWS
  - Infiniband on Azure
  - Mellanox Connect-X 5 Ethernet (ROCE) on Oracle Cloud Infrastructure (OCI)
- Intra-node communication with XPMEM (driver and kernel module support is critical)
- GPU Direct Async (GDR) support for communication between GPUs in MVPICH-Plus release
- ParaTools, Inc. building E4S optimized with MVAPICH-Plus for AWS, OCI, GCP, and Azure
- Using Adaptive Computing’s ODDC interface to launch E4S jobs on multiple cloud providers!

Adaptive Computing’s ODDC interface for E4S



Accessing Multiple Commercial Cloud Providers through ODDC



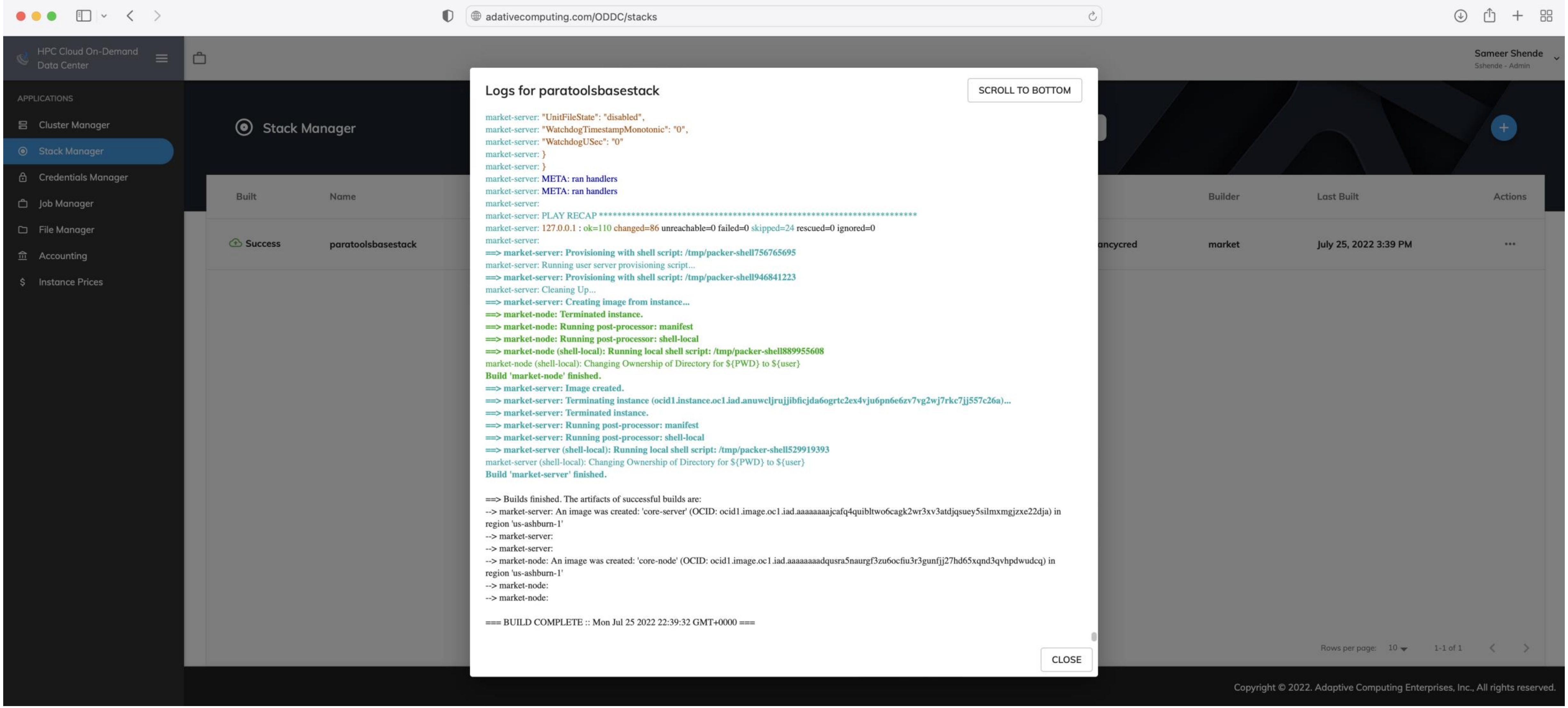
$ Instance Prices

Cloud Providers

- Alibaba Cloud
- Oracle Cloud HPC
- Oracle Cloud
- Amazon Web Services
- Google Cloud
- Microsoft Azure
- Open Telekom Cloud

Instance	US East 1	US East 2	US West 1	US West 2	US Gov East 1	CA Central 1	EU Central 1	EU West 1
t2.nano - vCPU: 1, Mem (GB): 0.50	0.0060	0.0061	0.0062	NaN	0.0063	0.0064	0.0065	0.0066
t2.micro - vCPU: 1, Mem (GB): 1	0.0120	0.0120	0.0120	NaN	0.0120	0.0120	0.0120	0.0120
t2.small - vCPU: 1, Mem (GB): 2	0.0230	0.0230	0.0230	NaN	0.0230	0.0230	0.0230	0.0230
t2.medium - vCPU: 2, Mem (GB): 4	0.0460	0.0460	0.0460	NaN	0.0460	0.0460	0.0460	0.0460
t2.large - vCPU: 2, Mem (GB): 8	0.0900	0.0900	0.0900	NaN	0.0900	0.0900	0.0900	0.0900
t2.xlarge - vCPU: 4, Mem (GB): 16	0.0920	0.0920	0.0920	NaN	0.0920	0.0920	0.0920	0.0920
t2.2xlarge - vCPU: 8, Mem (GB): 32	0.3710	0.3710	0.3710	NaN	0.3710	0.3710	0.3710	0.3710
c5n.9xlarge - vCPU: 36, Mem (GB): 96	0.3710	0.3710	0.3710	NaN	0.3710	0.3710	0.3710	0.3710
c5n.18xlarge - vCPU: 72, Mem (GB): 192	0.3710	0.3710	0.3710	NaN	0.3710	0.3710	0.3710	0.3710
g4dn.8xlarge - vCPU: 32, Mem (GB): 128	0.3710	0.3710	0.3710	NaN	0.3710	0.3710	0.3710	0.3710

Building an image to deploy on cloud platforms



Built	Name		Builder	Last Built	Actions
Success	paratoolsbasestack	ancycred	market	July 25, 2022 3:39 PM	···

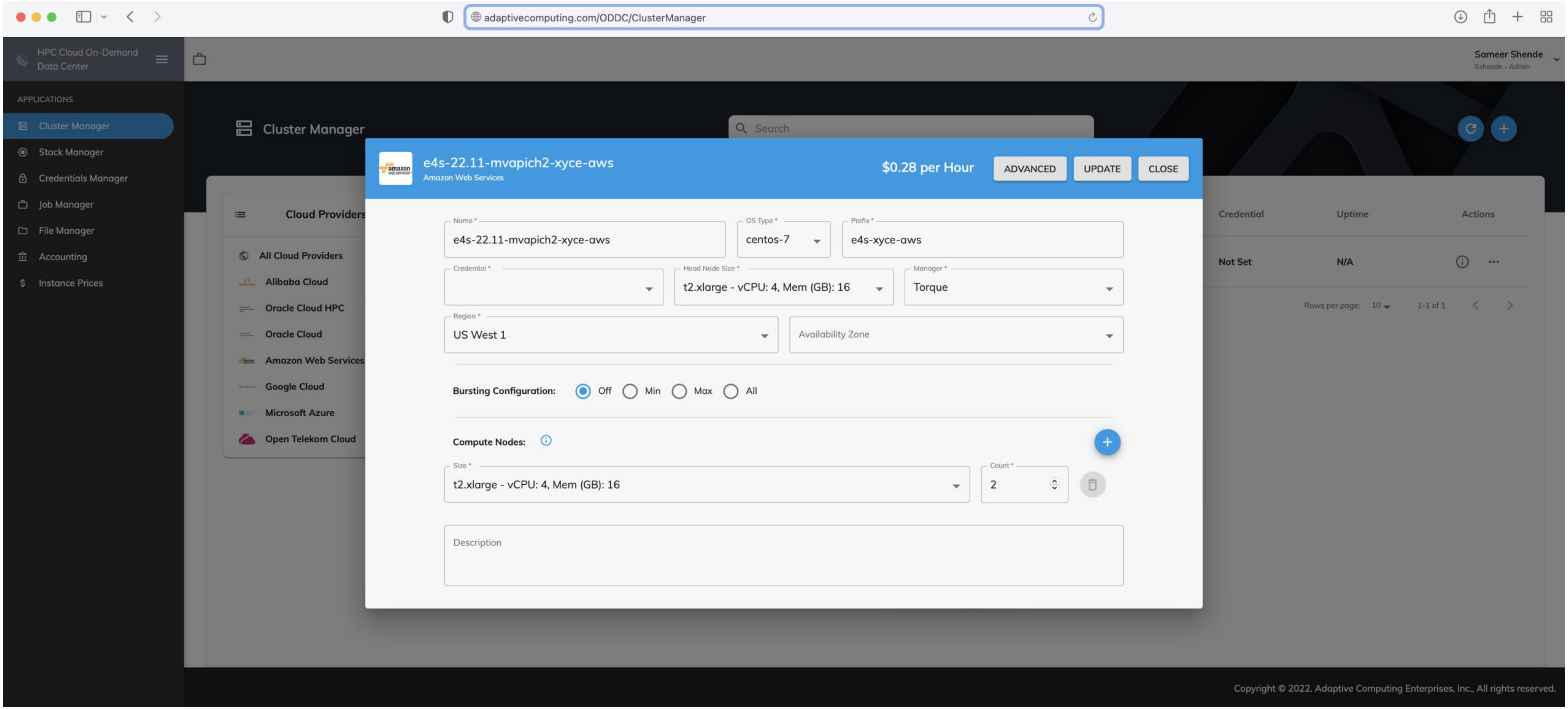
Logs for paratoolsbasestack

```
market-server: "UnitFileState": "disabled",
market-server: "WatchdogTimestampMonotonic": "0",
market-server: "WatchdogUSec": "0"
market-server: }
market-server: }
market-server: META: ran handlers
market-server: META: ran handlers
market-server:
market-server: PLAY RECAP *****************************************************************************
market-server: 127.0.0.1 : ok=110 changed=86 unreachable=0 failed=0 skipped=24 rescued=0 ignored=0
market-server:
==> market-server: Provisioning with shell script: /tmp/packer-shell756765695
market-server: Running user server provisioning script...
==> market-server: Provisioning with shell script: /tmp/packer-shell946841223
market-server: Cleaning Up...
==> market-server: Creating image from instance...
==> market-node: Terminated instance.
==> market-node: Running post-processor: manifest
==> market-node: Running post-processor: shell-local
==> market-node (shell-local): Running local shell script: /tmp/packer-shell889955608
market-node (shell-local): Changing Ownership of Directory for ${PWD} to ${user}
Build 'market-node' finished.
==> market-server: Image created.
==> market-server: Terminating instance (ocid1.instance.oc1.iad.anuwcljrujjibficjda6ogrtc2ex4vju6pn6e6zv7vg2wj7rkc7jj557c26a)...
==> market-server: Terminated instance.
==> market-server: Running post-processor: manifest
==> market-server: Running post-processor: shell-local
==> market-server (shell-local): Running local shell script: /tmp/packer-shell529919393
market-server (shell-local): Changing Ownership of Directory for ${PWD} to ${user}
Build 'market-server' finished.

==> Builds finished. The artifacts of successful builds are:
--> market-server: An image was created: 'core-server' (OCID: ocid1.image.oc1.iad.aaaaaaaajcafq4quibltwo6cagk2wr3xv3atdjqsuey5silmxmgjzxe22dja) in
region 'us-ashburn-1'
--> market-server:
--> market-server:
--> market-node: An image was created: 'core-node' (OCID: ocid1.image.oc1.iad.aaaaaaaadqusra5naurgf3zu6ocfiu3r3gunfjj27hd65xqnd3qvhpdwudcq) in
region 'us-ashburn-1'
--> market-node:
--> market-node:

=== BUILD COMPLETE :: Mon Jul 25 2022 22:39:32 GMT+0000 ===
```

Choosing an instance on AWS to run the image



adaptivecomputing.com/ODDC/ClusterManager

HPC Cloud On-Demand Data Center

Sameer Shende
Sshende - Admin

APPLICATIONS

- Cluster Manager
- Stack Manager
- Credentials Manager
- Job Manager
- File Manager
- Accounting
- Instance Prices

Cluster Manager

Search

Cloud Providers

- All Cloud Providers
- Alibaba Cloud
- Oracle Cloud HPC
- Oracle Cloud
- Amazon Web Services
- Google Cloud
- Microsoft Azure
- Open Telekom Cloud

Credential	Uptime	Actions
Not Set	N/A	

Rows per page: 10 1-1 of 1

e4s-22.11-mvapich2-xyce-aws
Amazon Web Services

$0.28 per Hour

ADVANCED UPDATE CLOSE

Name *: e4s-22.11-mvapich2-xyce-aws
OS Type *: centos-7
Prefix *: e4s-xyce-aws
Credential *:
Head Node Size *: t2.xlarge - vCPU: 4, Mem (GB): 16
Manager *: Torque
Region *: US West 1
Availability Zone

Bursting Configuration: ● Off ○ Min ○ Max ○ All

Compute Nodes:

Size *: t2.xlarge - vCPU: 4, Mem (GB): 16
Count *: 2

Description

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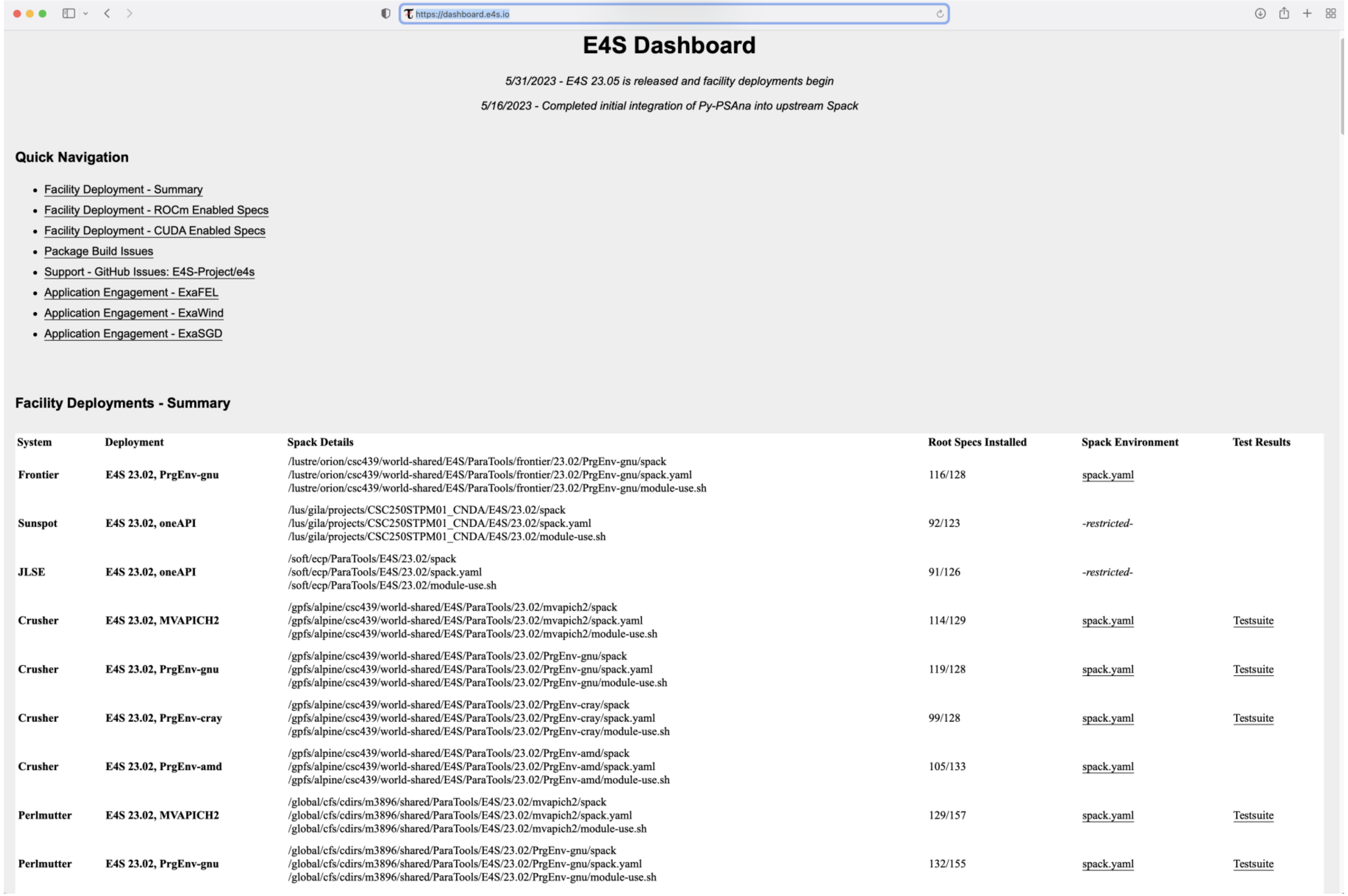
ParaTools, Inc. provides commercial support for E4S

- E4S Support: Maintains an E4S issue tracker
- E4S Installation: Maintains E4S on ALCF, OLCF, and NERSC systems
- E4S AD engagement: ECP applications
  - Nalu-Wind
  - ExaSGD
  - ExaFEL
  - ExaRL
  - WDMApp

  …

E4S Facility Deployment Progress: https://dashboard.e4s.io



E4S Dashboard

5/31/2023 - E4S 23.05 is released and facility deployments begin

5/16/2023 - Completed initial integration of Py-PSAna into upstream Spack

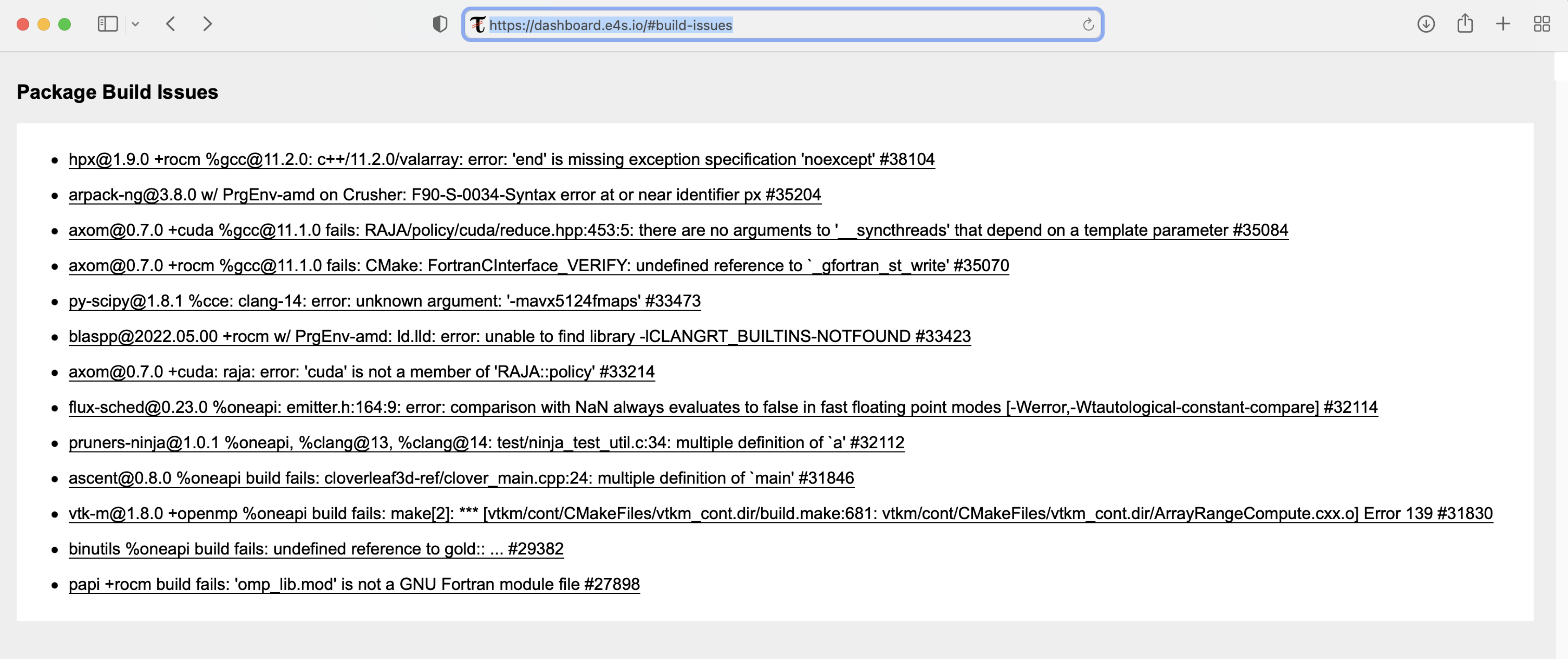
Quick Navigation

- Facility Deployment - Summary
- Facility Deployment - ROCm Enabled Specs
- Facility Deployment - CUDA Enabled Specs
- Package Build Issues
- Support - GitHub Issues: E4S-Project/e4s
- Application Engagement - ExaFEL
- Application Engagement - ExaWind
- Application Engagement - ExaSGD

Facility Deployments - Summary

System	Deployment	Spack Details	Root Specs Installed	Spack Environment	Test Results
Frontier	**E4S 23.02, PrgEnv-gnu**	/lustre/orion/csc439/world-shared/E4S/ParaTools/frontier/23.02/PrgEnv-gnu/spack /lustre/orion/csc439/world-shared/E4S/ParaTools/frontier/23.02/PrgEnv-gnu/spack.yaml /lustre/orion/csc439/world-shared/E4S/ParaTools/frontier/23.02/PrgEnv-gnu/module-use.sh	116/128	spack.yaml	
Sunspot	**E4S 23.02, oneAPI**	/lus/gila/projects/CSC250STPM01_CNDA/E4S/23.02/spack /lus/gila/projects/CSC250STPM01_CNDA/E4S/23.02/spack.yaml /lus/gila/projects/CSC250STPM01_CNDA/E4S/23.02/module-use.sh	92/123	*-restricted-*	
JLSE	**E4S 23.02, oneAPI**	/soft/ecp/ParaTools/E4S/23.02/spack /soft/ecp/ParaTools/E4S/23.02/spack.yaml /soft/ecp/ParaTools/E4S/23.02/module-use.sh	91/126	*-restricted-*	
Crusher	**E4S 23.02, MVAPICH2**	/gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/mvapich2/spack /gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/mvapich2/spack.yaml /gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/mvapich2/module-use.sh	114/129	spack.yaml	Testsuite
Crusher	**E4S 23.02, PrgEnv-gnu**	/gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/PrgEnv-gnu/spack /gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/PrgEnv-gnu/spack.yaml /gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/PrgEnv-gnu/module-use.sh	119/128	spack.yaml	Testsuite
Crusher	**E4S 23.02, PrgEnv-cray**	/gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/PrgEnv-cray/spack /gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/PrgEnv-cray/spack.yaml /gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/PrgEnv-cray/module-use.sh	99/128	spack.yaml	Testsuite
Crusher	**E4S 23.02, PrgEnv-amd**	/gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/PrgEnv-amd/spack /gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/PrgEnv-amd/spack.yaml /gpfs/alpine/csc439/world-shared/E4S/ParaTools/23.02/PrgEnv-amd/module-use.sh	105/133	spack.yaml	
Perlmutter	**E4S 23.02, MVAPICH2**	/global/cfs/cdirs/m3896/shared/ParaTools/E4S/23.02/mvapich2/spack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/23.02/mvapich2/spack.yaml /global/cfs/cdirs/m3896/shared/ParaTools/E4S/23.02/mvapich2/module-use.sh	129/157	spack.yaml	Testsuite
Perlmutter	**E4S 23.02, PrgEnv-gnu**	/global/cfs/cdirs/m3896/shared/ParaTools/E4S/23.02/PrgEnv-gnu/spack /global/cfs/cdirs/m3896/shared/ParaTools/E4S/23.02/PrgEnv-gnu/spack.yaml /global/cfs/cdirs/m3896/shared/ParaTools/E4S/23.02/PrgEnv-gnu/module-use.sh	132/155	spack.yaml	Testsuite

Dashboard for Monitoring Progress: Spack build issues



https://dashboard.e4s.io/#build-issues

Package Build Issues

- hpx@1.9.0 +rocm %gcc@11.2.0: c++/11.2.0/valarray: error: 'end' is missing exception specification 'noexcept' #38104
- arpack-ng@3.8.0 w/ PrgEnv-amd on Crusher: F90-S-0034-Syntax error at or near identifier px #35204
- axom@0.7.0 +cuda %gcc@11.1.0 fails: RAJA/policy/cuda/reduce.hpp:453:5: there are no arguments to '__syncthreads' that depend on a template parameter #35084
- axom@0.7.0 +rocm %gcc@11.1.0 fails: CMake: FortranCInterface_VERIFY: undefined reference to `_gfortran_st_write' #35070
- py-scipy@1.8.1 %cce: clang-14: error: unknown argument: '-mavx5124fmaps' #33473
- blaspp@2022.05.00 +rocm w/ PrgEnv-amd: ld.lld: error: unable to find library -lCLANGRT_BUILTINS-NOTFOUND #33423
- axom@0.7.0 +cuda: raja: error: 'cuda' is not a member of 'RAJA::policy' #33214
- flux-sched@0.23.0 %oneapi: emitter.h:164:9: error: comparison with NaN always evaluates to false in fast floating point modes [-Werror,-Wtautological-constant-compare] #32114
- pruners-ninja@1.0.1 %oneapi, %clang@13, %clang@14: test/ninja_test_util.c:34: multiple definition of `a' #32112
- ascent@0.8.0 %oneapi build fails: cloverleaf3d-ref/clover_main.cpp:24: multiple definition of `main' #31846
- vtk-m@1.8.0 +openmp %oneapi build fails: make[2]: *** [vtkm/cont/CMakeFiles/vtkm_cont.dir/build.make:681: vtkm/cont/CMakeFiles/vtkm_cont.dir/ArrayRangeCompute.cxx.o] Error 139 #31830
- binutils %oneapi build fails: undefined reference to gold:: ... #29382
- papi +rocm build fails: 'omp_lib.mod' is not a GNU Fortran module file #27898

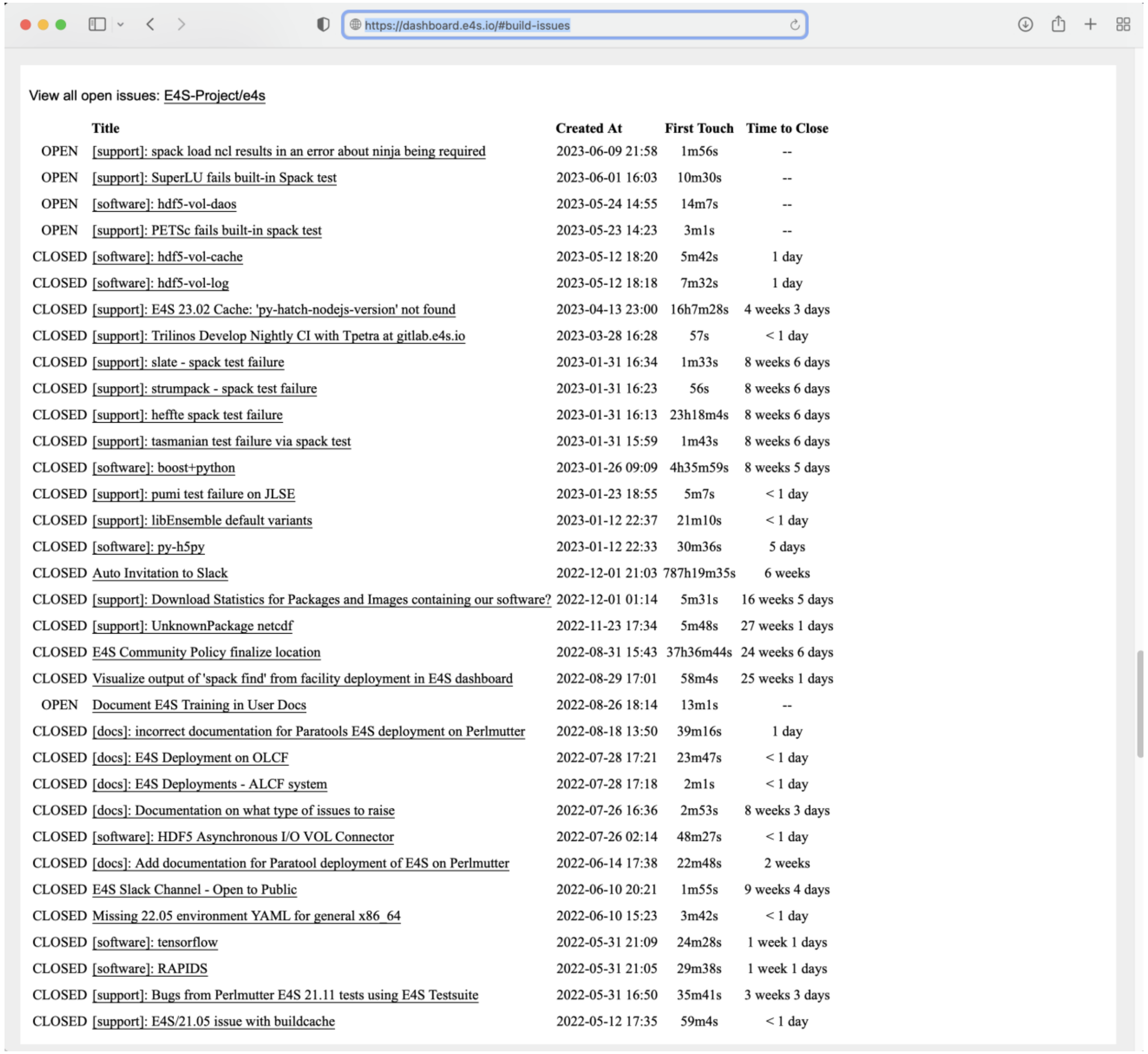
EXASCALE COMPUTING PROJECT

Progress Report of E4S Support by ParaTools, Inc.

E4S Support: Issue Tracker

- Provide a portal for tracking and supporting Tier 2 E4S issues using GitHub issues.
- Curate, resolve, or delegate tickets related to E4S packages with the package developers.
- Maintain the E4S issues portal as a central location for tracking container and bare-metal deployment related issues for E4S installations.
- Assist DOE facilities staff in managing tickets related to E4S.
- https://github.com/E4S-Project/e4s/issues

Dashboard for Monitoring Progress: Support Tickets Open and Resolved



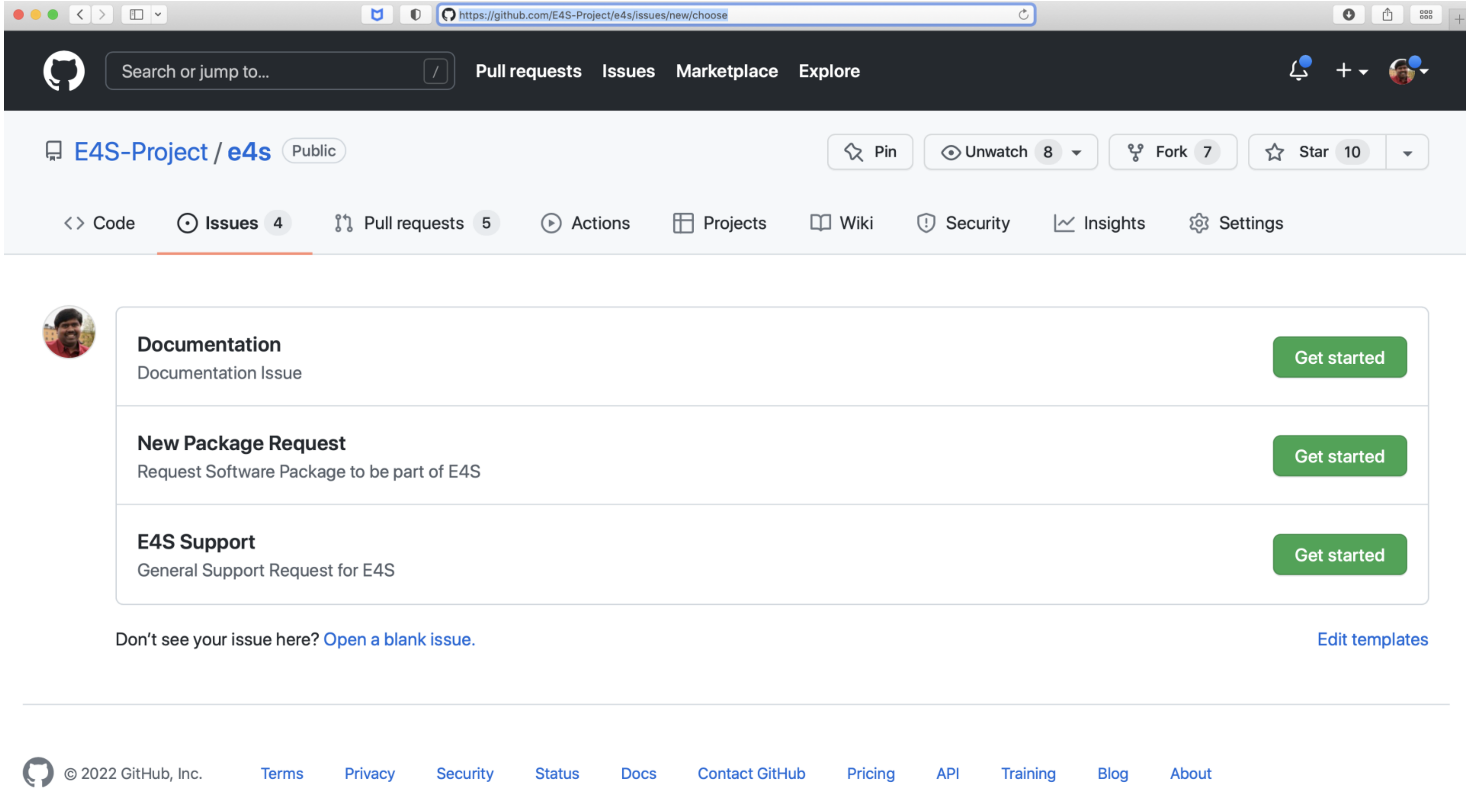
https://dashboard.e4s.io/#build-issues

View all open issues: E4S-Project/e4s

	Title	Created At	First Touch	Time to Close
OPEN	[support]: spack load ncl results in an error about ninja being required	2023-06-09 21:58	1m56s	--
OPEN	[support]: SuperLU fails built-in Spack test	2023-06-01 16:03	10m30s	--
OPEN	[software]: hdf5-vol-daos	2023-05-24 14:55	14m7s	--
OPEN	[support]: PETSc fails built-in spack test	2023-05-23 14:23	3m1s	--
CLOSED	[software]: hdf5-vol-cache	2023-05-12 18:20	5m42s	1 day
CLOSED	[software]: hdf5-vol-log	2023-05-12 18:18	7m32s	1 day
CLOSED	[support]: E4S 23.02 Cache: 'py-hatch-nodejs-version' not found	2023-04-13 23:00	16h7m28s	4 weeks 3 days
CLOSED	[support]: Trilinos Develop Nightly CI with Tpetra at gitlab.e4s.io	2023-03-28 16:28	57s	< 1 day
CLOSED	[support]: slate - spack test failure	2023-01-31 16:34	1m33s	8 weeks 6 days
CLOSED	[support]: strumpack - spack test failure	2023-01-31 16:23	56s	8 weeks 6 days
CLOSED	[support]: heffte spack test failure	2023-01-31 16:13	23h18m4s	8 weeks 6 days
CLOSED	[support]: tasmanian test failure via spack test	2023-01-31 15:59	1m43s	8 weeks 6 days
CLOSED	[software]: boost+python	2023-01-26 09:09	4h35m59s	8 weeks 5 days
CLOSED	[support]: pumi test failure on JLSE	2023-01-23 18:55	5m7s	< 1 day
CLOSED	[support]: libEnsemble default variants	2023-01-12 22:37	21m10s	< 1 day
CLOSED	[software]: py-h5py	2023-01-12 22:33	30m36s	5 days
CLOSED	Auto Invitation to Slack	2022-12-01 21:03	787h19m35s	6 weeks
CLOSED	[support]: Download Statistics for Packages and Images containing our software?	2022-12-01 01:14	5m31s	16 weeks 5 days
CLOSED	[support]: UnknownPackage netcdf	2022-11-23 17:34	5m48s	27 weeks 1 days
CLOSED	E4S Community Policy finalize location	2022-08-31 15:43	37h36m44s	24 weeks 6 days
CLOSED	Visualize output of 'spack find' from facility deployment in E4S dashboard	2022-08-29 17:01	58m4s	25 weeks 1 days
OPEN	Document E4S Training in User Docs	2022-08-26 18:14	13m1s	--
CLOSED	[docs]: incorrect documentation for Paratools E4S deployment on Perlmutter	2022-08-18 13:50	39m16s	1 day
CLOSED	[docs]: E4S Deployment on OLCF	2022-07-28 17:21	23m47s	< 1 day
CLOSED	[docs]: E4S Deployments - ALCF system	2022-07-28 17:18	2m1s	< 1 day
CLOSED	[docs]: Documentation on what type of issues to raise	2022-07-26 16:36	2m53s	8 weeks 3 days
CLOSED	[software]: HDF5 Asynchronous I/O VOL Connector	2022-07-26 02:14	48m27s	< 1 day
CLOSED	[docs]: Add documentation for Paratool deployment of E4S on Perlmutter	2022-06-14 17:38	22m48s	2 weeks
CLOSED	E4S Slack Channel - Open to Public	2022-06-10 20:21	1m55s	9 weeks 4 days
CLOSED	Missing 22.05 environment YAML for general x86_64	2022-06-10 15:23	3m42s	< 1 day
CLOSED	[software]: tensorflow	2022-05-31 21:09	24m28s	1 week 1 days
CLOSED	[software]: RAPIDS	2022-05-31 21:05	29m38s	1 week 1 days
CLOSED	[support]: Bugs from Perlmutter E4S 21.11 tests using E4S Testsuite	2022-05-31 16:50	35m41s	3 weeks 3 days
CLOSED	[support]: E4S/21.05 issue with buildcache	2022-05-12 17:35	59m4s	< 1 day

First touch and time to close statistics.

Reporting New E4S Issues: 3 Choices



Documentation
Documentation Issue
Get started

New Package Request
Request Software Package to be part of E4S
Get started

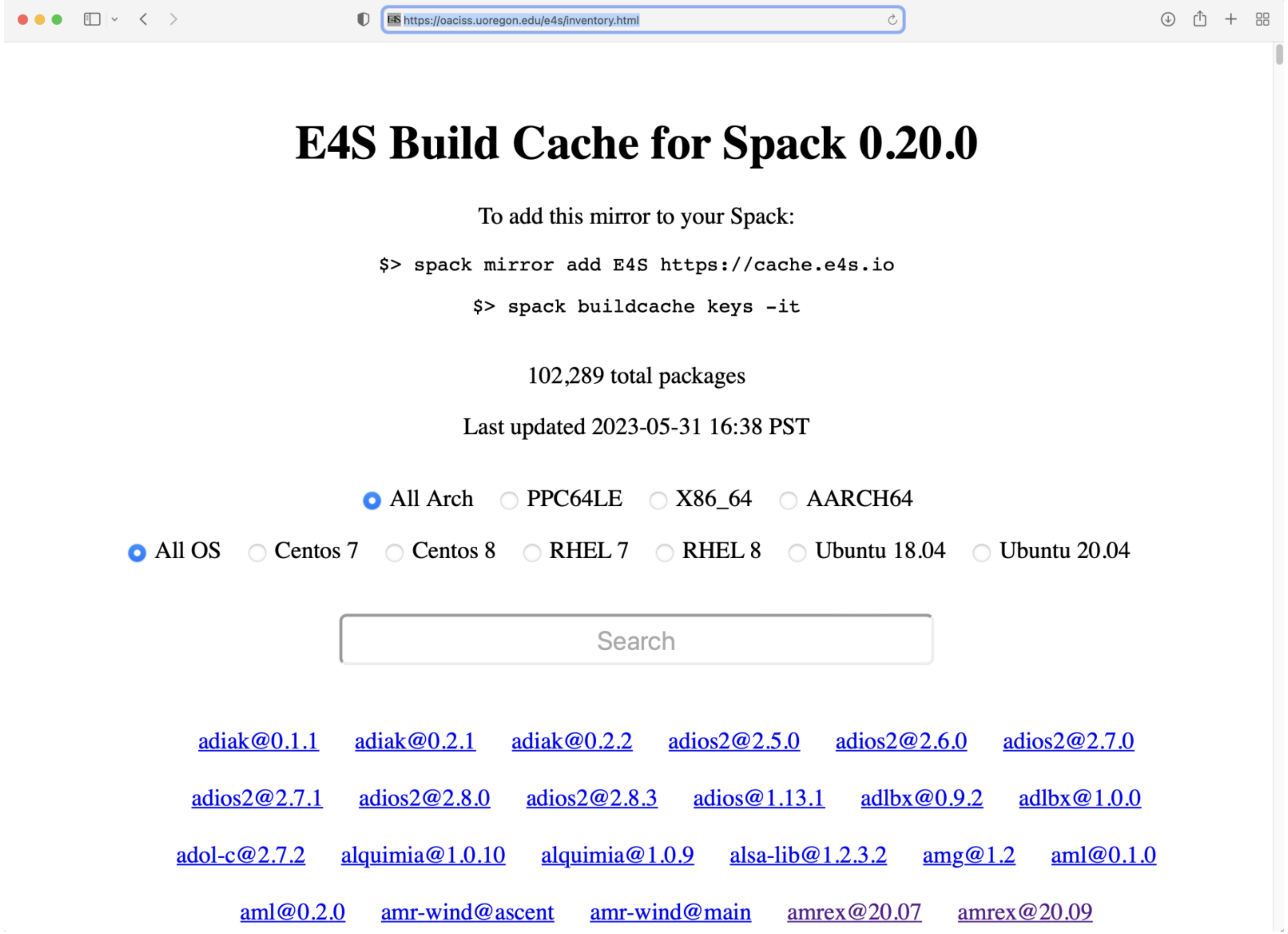
E4S Support
General Support Request for E4S
Get started

Don't see your issue here? Open a blank issue.

Edit templates

https://github.com/E4S-Project/issues/new/choose

E4S Build Cache 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

Search

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

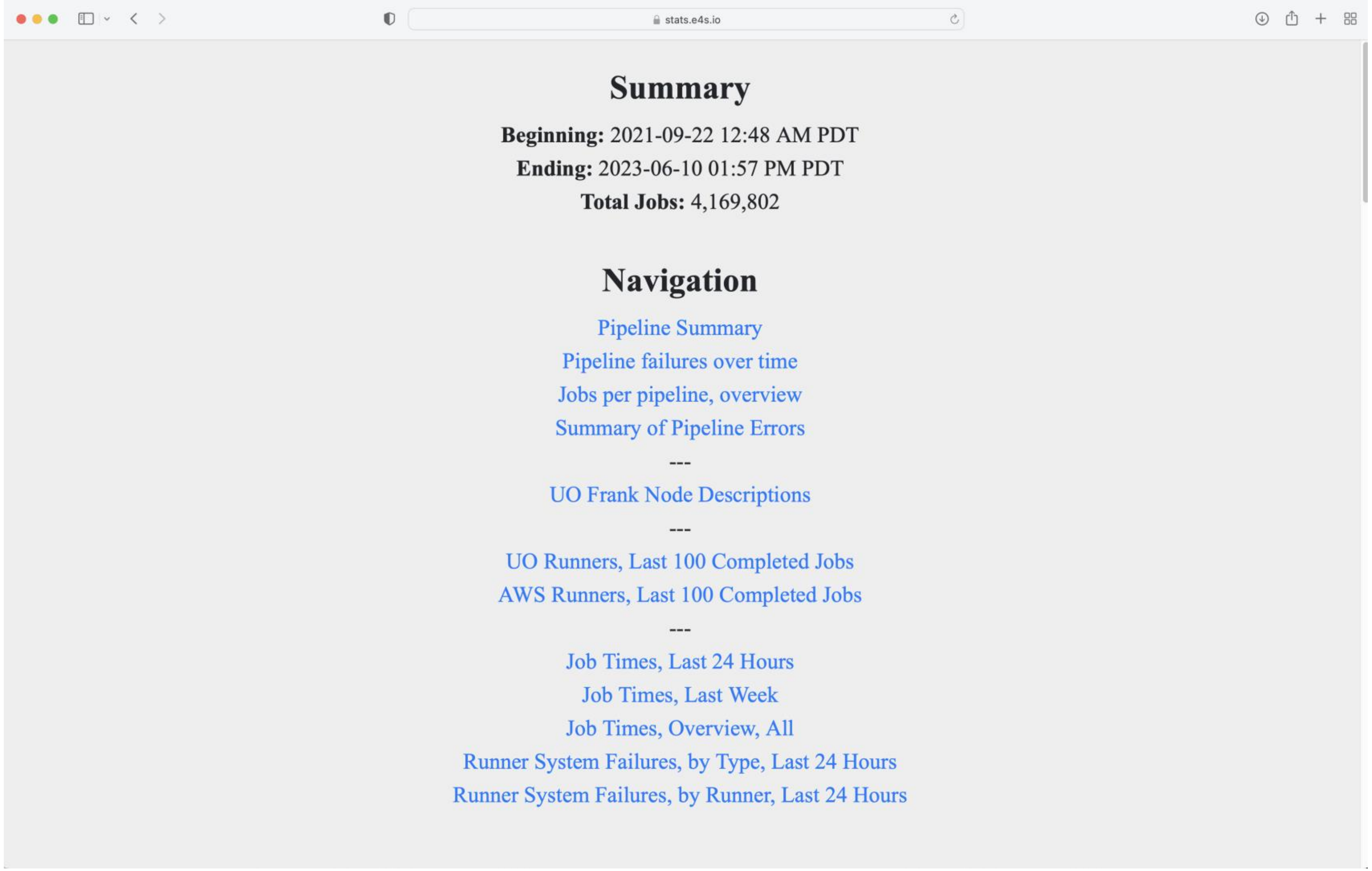
adios2@2.7.1 adios2@2.8.0 adios2@2.8.3 adios@1.13.1 adlbx@0.9.2 adlbx@1.0.0

adol-c@2.7.2 alquimia@1.0.10 alquimia@1.0.9 alsa-lib@1.2.3.2 amg@1.2 aml@0.1.0

aml@0.2.0 amr-wind@ascent amr-wind@main amrex@20.07 amrex@20.09

Over 100K binaries!

Spack Pull Request Merge CI Jobs Running on Frank@UO and AWS



Summary

Beginning: 2021-09-22 12:48 AM PDT
Ending: 2023-06-10 01:57 PM PDT
Total Jobs: 4,169,802

Navigation

Pipeline Summary
Pipeline failures over time
Jobs per pipeline, overview
Summary of Pipeline Errors

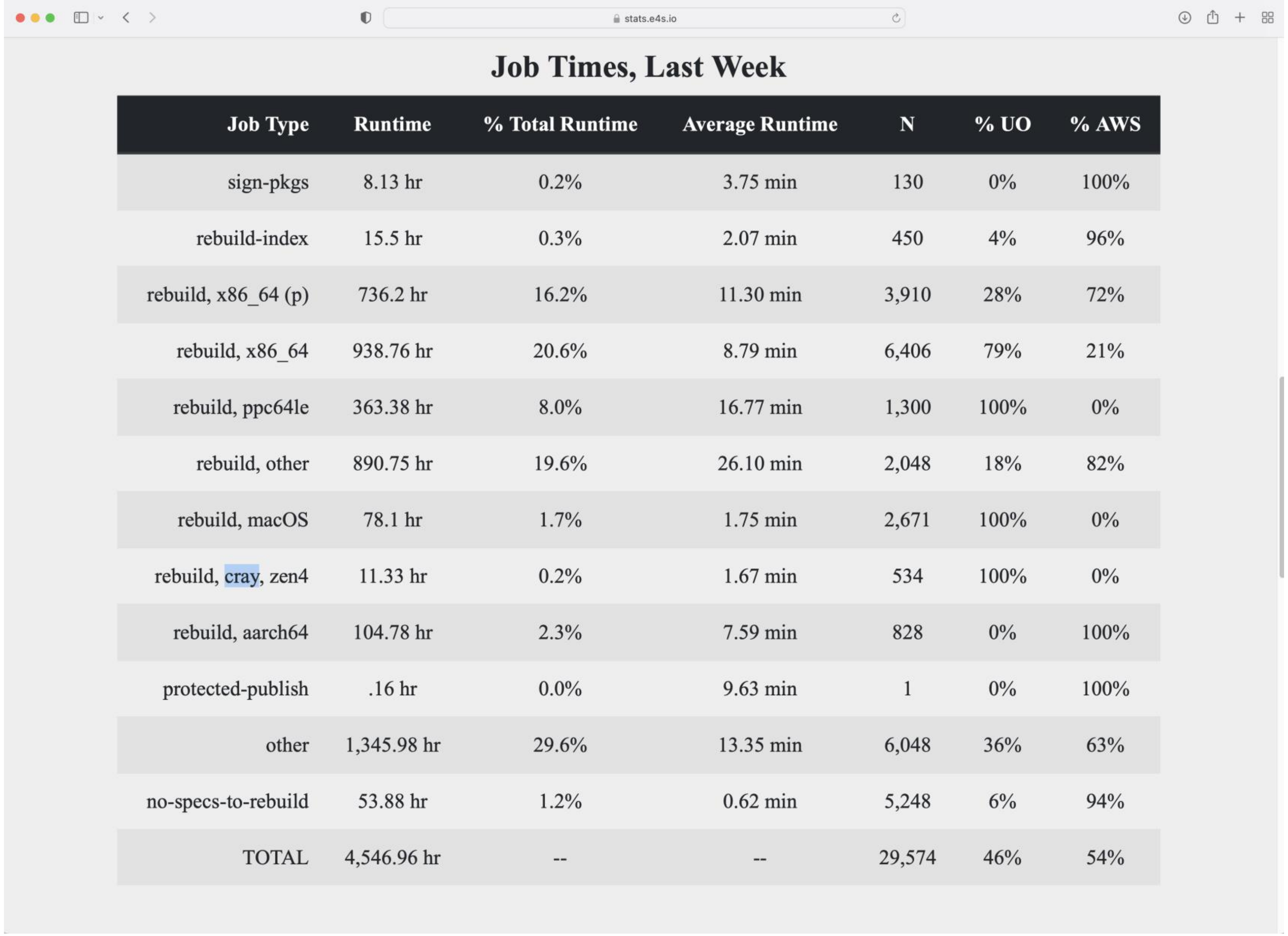
UO Frank Node Descriptions

UO Runners, Last 100 Completed Jobs
AWS Runners, Last 100 Completed Jobs

Job Times, Last 24 Hours
Job Times, Last Week
Job Times, Overview, All
Runner System Failures, by Type, Last 24 Hours
Runner System Failures, by Runner, Last 24 Hours

https://stats.e4s.i

Spack PR Merge Jobs: Frank and AWS statistics

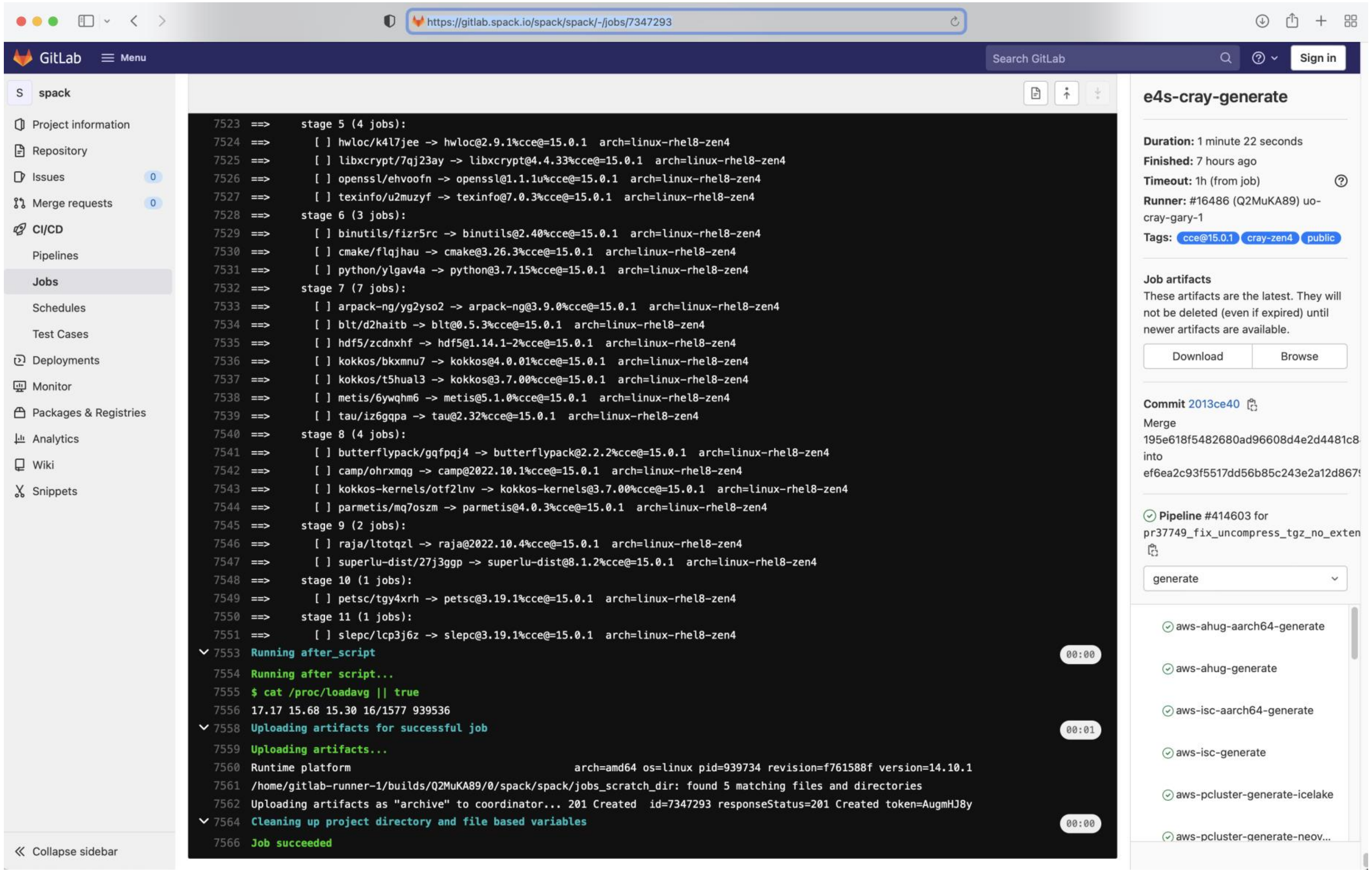


Job Times, Last Week

Job Type	Runtime	% Total Runtime	Average Runtime	N	% UO	% AWS
sign-pkgs	8.13 hr	0.2%	3.75 min	130	0%	100%
rebuild-index	15.5 hr	0.3%	2.07 min	450	4%	96%
rebuild, x86_64 (p)	736.2 hr	16.2%	11.30 min	3,910	28%	72%
rebuild, x86_64	938.76 hr	20.6%	8.79 min	6,406	79%	21%
rebuild, ppc64le	363.38 hr	8.0%	16.77 min	1,300	100%	0%
rebuild, other	890.75 hr	19.6%	26.10 min	2,048	18%	82%
rebuild, macOS	78.1 hr	1.7%	1.75 min	2,671	100%	0%
rebuild, cray, zen4	11.33 hr	0.2%	1.67 min	534	100%	0%
rebuild, aarch64	104.78 hr	2.3%	7.59 min	828	0%	100%
protected-publish	.16 hr	0.0%	9.63 min	1	0%	100%
other	1,345.98 hr	29.6%	13.35 min	6,048	36%	63%
no-specs-to-rebuild	53.88 hr	1.2%	0.62 min	5,248	6%	94%
TOTAL	4,546.96 hr	--	--	29,574	46%	54%

https://stats.e4s.i

Spack PR Merge Jobs on HPE Cray (CPE) on Frank @ U. Oregon



```
==>     stage 5 (4 jobs):
==>       [ ] hwloc/k4l7jee -> hwloc@2.9.1%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] libxcrypt/7qj23ay -> libxcrypt@4.4.33%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] openssl/ehvoofn -> openssl@1.1.1u%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] texinfo/u2muzyf -> texinfo@7.0.3%cce@=15.0.1  arch=linux-rhel8-zen4
==>     stage 6 (3 jobs):
==>       [ ] binutils/fizr5rc -> binutils@2.40%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] cmake/flqjhau -> cmake@3.26.3%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] python/ylgav4a -> python@3.7.15%cce@=15.0.1  arch=linux-rhel8-zen4
==>     stage 7 (7 jobs):
==>       [ ] arpack-ng/yg2yso2 -> arpack-ng@3.9.0%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] blt/d2haitb -> blt@0.5.3%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] hdf5/zcdnxhf -> hdf5@1.14.1-2%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] kokkos/bkxmnu7 -> kokkos@4.0.01%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] kokkos/t5hual3 -> kokkos@3.7.00%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] metis/6ywqhm6 -> metis@5.1.0%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] tau/iz6gqpa -> tau@2.32%cce@=15.0.1  arch=linux-rhel8-zen4
==>     stage 8 (4 jobs):
==>       [ ] butterflypack/gqfpqj4 -> butterflypack@2.2.2%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] camp/ohrxmqg -> camp@2022.10.1%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] kokkos-kernels/otf2lnv -> kokkos-kernels@3.7.00%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] parmetis/mq7oszm -> parmetis@4.0.3%cce@=15.0.1  arch=linux-rhel8-zen4
==>     stage 9 (2 jobs):
==>       [ ] raja/ltotqzl -> raja@2022.10.4%cce@=15.0.1  arch=linux-rhel8-zen4
==>       [ ] superlu-dist/27j3ggp -> superlu-dist@8.1.2%cce@=15.0.1  arch=linux-rhel8-zen4
==>     stage 10 (1 jobs):
==>       [ ] petsc/tgy4xrh -> petsc@3.19.1%cce@=15.0.1  arch=linux-rhel8-zen4
==>     stage 11 (1 jobs):
==>       [ ] slepc/lcp3j6z -> slepc@3.19.1%cce@=15.0.1  arch=linux-rhel8-zen4
Running after_script                                                          00:00
Running after script...
$ cat /proc/loadavg || true
17.17 15.68 15.30 16/1577 939536
Uploading artifacts for successful job                                        00:01
Uploading artifacts...
Runtime platform                                    arch=amd64 os=linux pid=939734 revision=f761588f version=14.10.1
/home/gitlab-runner-1/builds/Q2MuKA89/0/spack/spack/jobs_scratch_dir: found 5 matching files and directories
Uploading artifacts as "archive" to coordinator... 201 Created  id=7347293 responseStatus=201 Created token=AugmHJ8y
Cleaning up project directory and file based variables                        00:00
Job succeeded
```

e4s-cray-generate

Duration: 1 minute 22 seconds

Finished: 7 hours ago

Timeout: 1h (from job)

Runner: #16486 (Q2MuKA89) uo-cray-gary-1

Tags: cce@15.0.1 cray-zen4 public

Job artifacts

These artifacts are the latest. They will not be deleted (even if expired) until newer artifacts are available.

Download | Browse

Commit 2013ce40

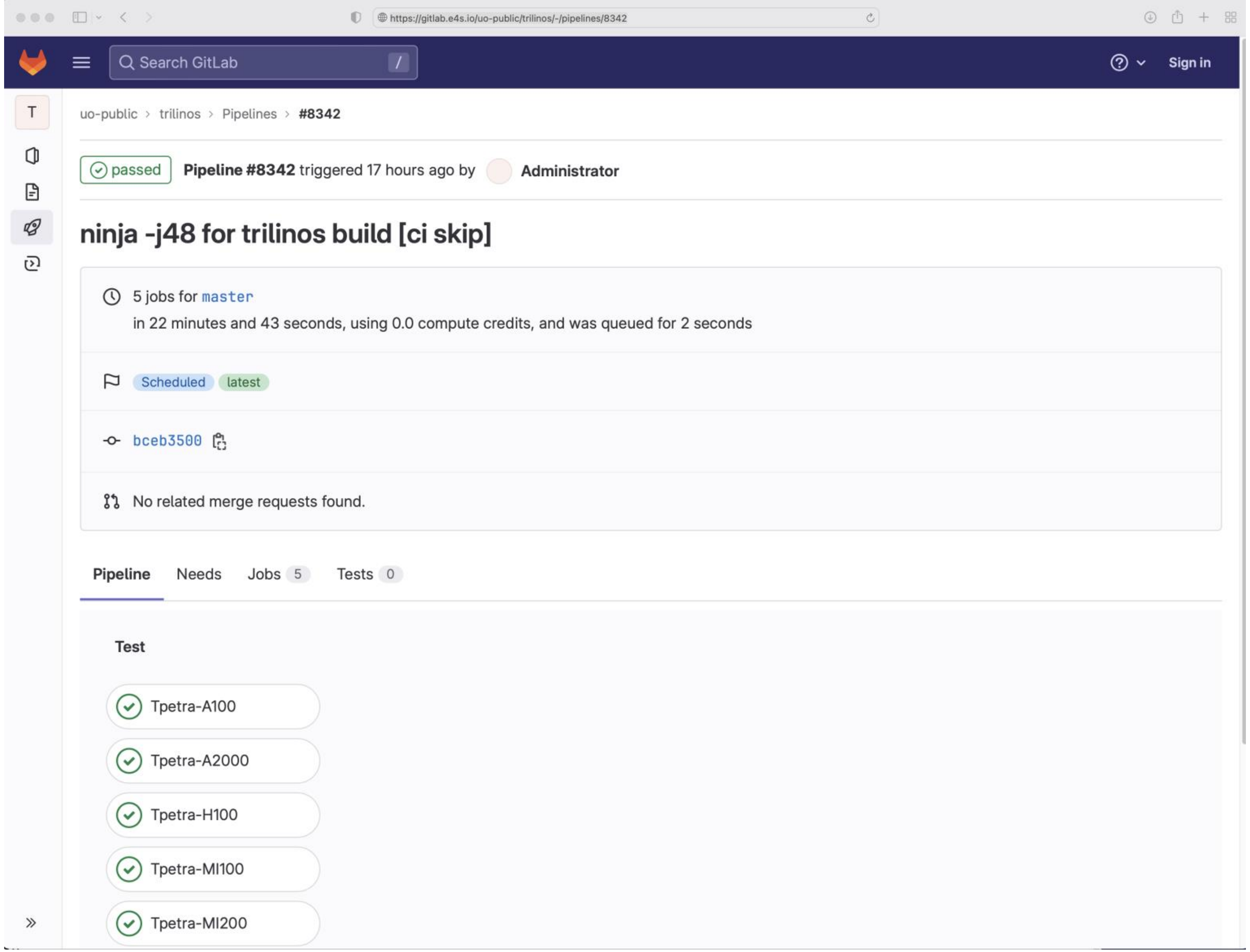
Merge 195e618f5482680ad96608d4e2d4481c8 into ef6ea2c93f5517dd56b85c243e2a12d867

Pipeline #414603 for pr37749_fix_uncompress_tgz_no_exten

generate

- aws-ahug-aarch64-generate
- aws-ahug-generate
- aws-isc-aarch64-generate
- aws-isc-generate
- aws-pcluster-generate-icelake
- aws-pcluster-generate-neov...

Trilinos’ Pipeline on GPUs



https://gitlab.e4s.io/uo-public/trilinos/-/pipelines/8342

uo-public › trilinos › Pipelines › #8342

passed **Pipeline #8342** triggered 17 hours ago by **Administrator**

ninja -j48 for trilinos build [ci skip]

5 jobs for `master`
in 22 minutes and 43 seconds, using 0.0 compute credits, and was queued for 2 seconds

Scheduled latest

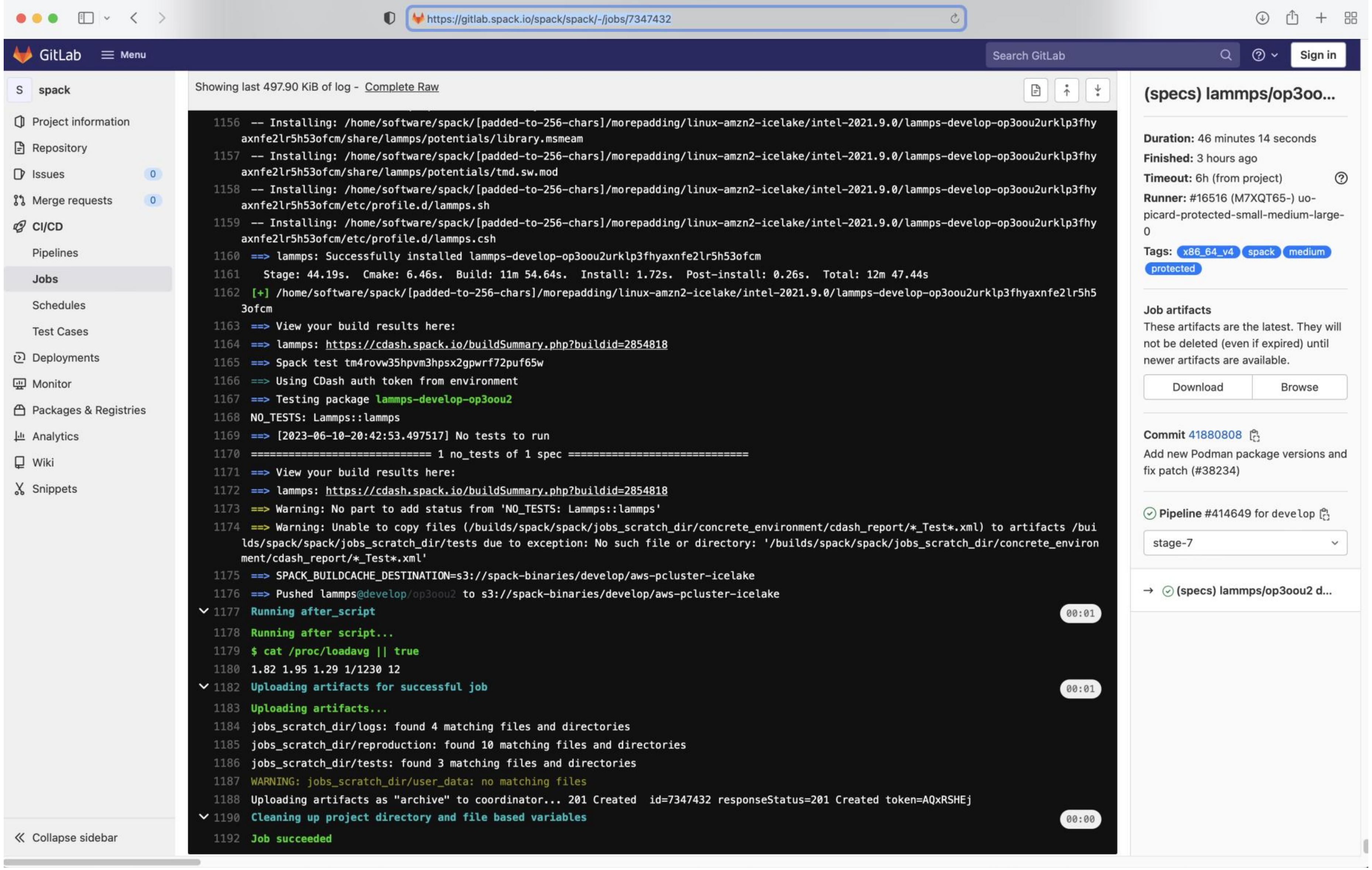
`bceb3500`

No related merge requests found.

Test

- Tpetra-A100
- Tpetra-A2000
- Tpetra-H100
- Tpetra-MI100
- Tpetra-MI200

Trilinos Pipeline on H100 GPUs



Showing last 497.90 KiB of log - Complete Raw

```
-- Installing: /home/software/spack/[padded-to-256-chars]/morepadding/linux-amzn2-icelake/intel-2021.9.0/lammps-develop-op3oou2urklp3fhyaxnfe2lr5h53ofcm/share/lammps/potentials/library.msmeam
-- Installing: /home/software/spack/[padded-to-256-chars]/morepadding/linux-amzn2-icelake/intel-2021.9.0/lammps-develop-op3oou2urklp3fhyaxnfe2lr5h53ofcm/share/lammps/potentials/tmd.sw.mod
-- Installing: /home/software/spack/[padded-to-256-chars]/morepadding/linux-amzn2-icelake/intel-2021.9.0/lammps-develop-op3oou2urklp3fhyaxnfe2lr5h53ofcm/etc/profile.d/lammps.sh
-- Installing: /home/software/spack/[padded-to-256-chars]/morepadding/linux-amzn2-icelake/intel-2021.9.0/lammps-develop-op3oou2urklp3fhyaxnfe2lr5h53ofcm/etc/profile.d/lammps.csh
==> lammps: Successfully installed lammps-develop-op3oou2urklp3fhyaxnfe2lr5h53ofcm
  Stage: 44.19s.  Cmake: 6.46s.  Build: 11m 54.64s.  Install: 1.72s.  Post-install: 0.26s.  Total: 12m 47.44s
[+] /home/software/spack/[padded-to-256-chars]/morepadding/linux-amzn2-icelake/intel-2021.9.0/lammps-develop-op3oou2urklp3fhyaxnfe2lr5h53ofcm
==> View your build results here:
==> lammps: https://cdash.spack.io/buildSummary.php?buildid=2854818
==> Spack test tm4rovw35hpvm3hpsx2gpwrf72puf65w
==> Using CDash auth token from environment
==> Testing package lammps-develop-op3oou2
NO_TESTS: Lammps::lammps
==> [2023-06-10-20:42:53.497517] No tests to run
============================= 1 no_tests of 1 spec =============================
==> View your build results here:
==> lammps: https://cdash.spack.io/buildSummary.php?buildid=2854818
==> Warning: No part to add status from 'NO_TESTS: Lammps::lammps'
==> Warning: Unable to copy files (/builds/spack/spack/jobs_scratch_dir/concrete_environment/cdash_report/*_Test*.xml) to artifacts /builds/spack/spack/jobs_scratch_dir/tests due to exception: No such file or directory: '/builds/spack/spack/jobs_scratch_dir/concrete_environment/cdash_report/*_Test*.xml'
==> SPACK_BUILDCACHE_DESTINATION=s3://spack-binaries/develop/aws-pcluster-icelake
==> Pushed lammps@develop/op3oou2 to s3://spack-binaries/develop/aws-pcluster-icelake
Running after_script                                                        00:01
Running after script...
$ cat /proc/loadavg || true
1.82 1.95 1.29 1/1230 12
Uploading artifacts for successful job                                      00:01
Uploading artifacts...
jobs_scratch_dir/logs: found 4 matching files and directories
jobs_scratch_dir/reproduction: found 10 matching files and directories
jobs_scratch_dir/tests: found 3 matching files and directories
WARNING: jobs_scratch_dir/user_data: no matching files
Uploading artifacts as "archive" to coordinator... 201 Created  id=7347432 responseStatus=201 Created token=AQxRSHEj
Cleaning up project directory and file based variables                      00:00
Job succeeded
```

(specs) lammps/op3oo...

Duration: 46 minutes 14 seconds
Finished: 3 hours ago
Timeout: 6h (from project)
Runner: #16516 (M7XQT65-) uo-picard-protected-small-medium-large-0
Tags: x86_64_v4 spack medium protected

Job artifacts
These artifacts are the latest. They will not be deleted (even if expired) until newer artifacts are available.

Download Browse

Commit 41880808
Add new Podman package versions and fix patch (#38234)

Pipeline #414649 for develop

stage-7

→ (specs) lammps/op3oou2 d...

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

EXASCALE COMPUTING PROJECT

Spack provides the *spec* syntax to describe custom configurations

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

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

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

The Spack community is growing rapidly

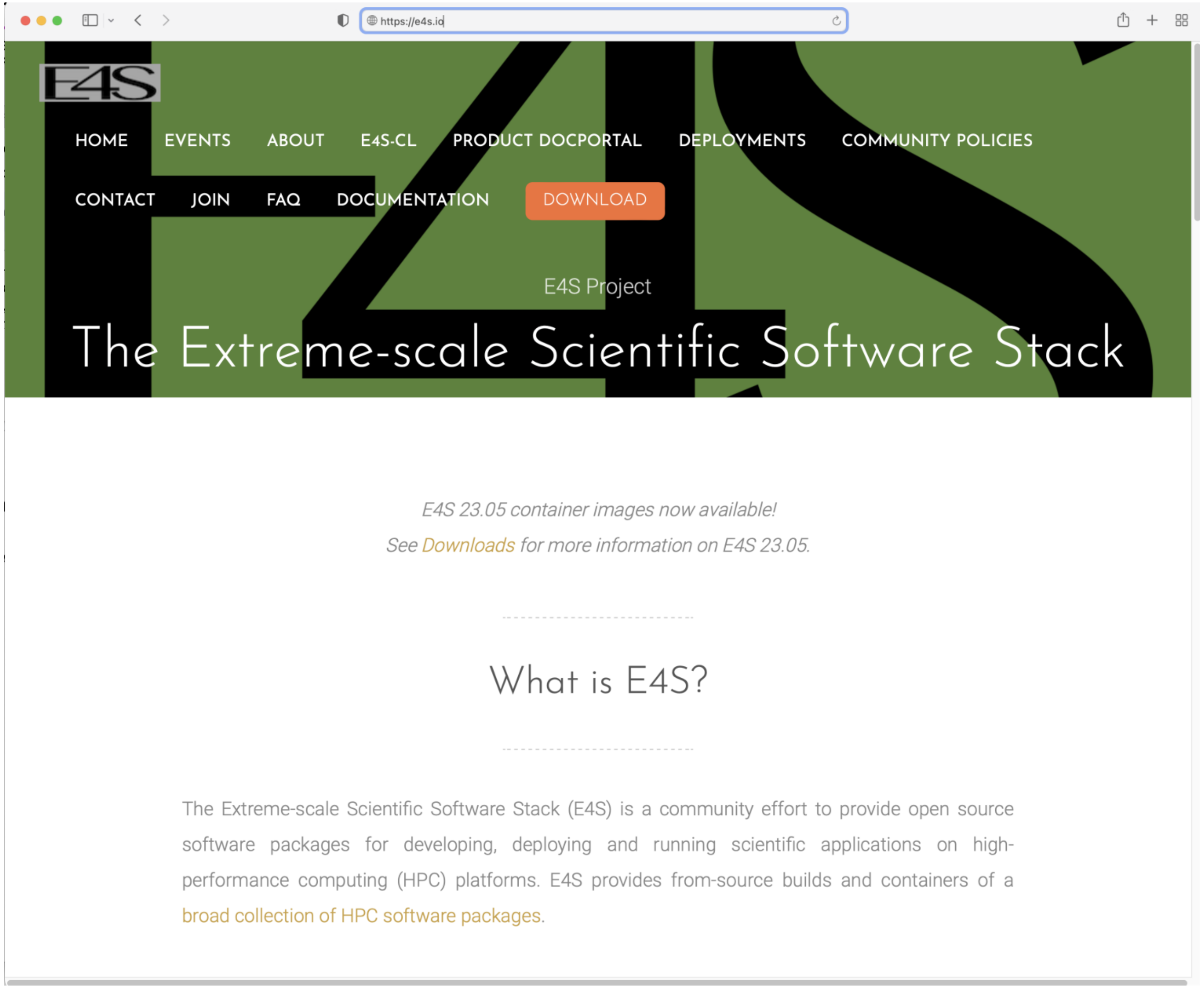
- **Spack simplifies HPC software for:**
  - Users
  - Developers
  - Cluster installations
  - The largest HPC facilities
- **Spack is central to ECP's software strategy**
  - Enable software reuse for developers and users
  - Allow the facilities to consume the entire ECP stack
- **The roadmap is packed with new features:**
  - Building the ECP software distribution
  - Better workflows for building containers
  - Stacks for facilities
  - Chains for rapid dev workflow
  - Optimized binaries
  - Better dependency resolution

Visit spack.io

github.com/spack/spack

@spackpm

E4S Download from https://e4s.io



E4S Project

The Extreme-scale Scientific Software Stack

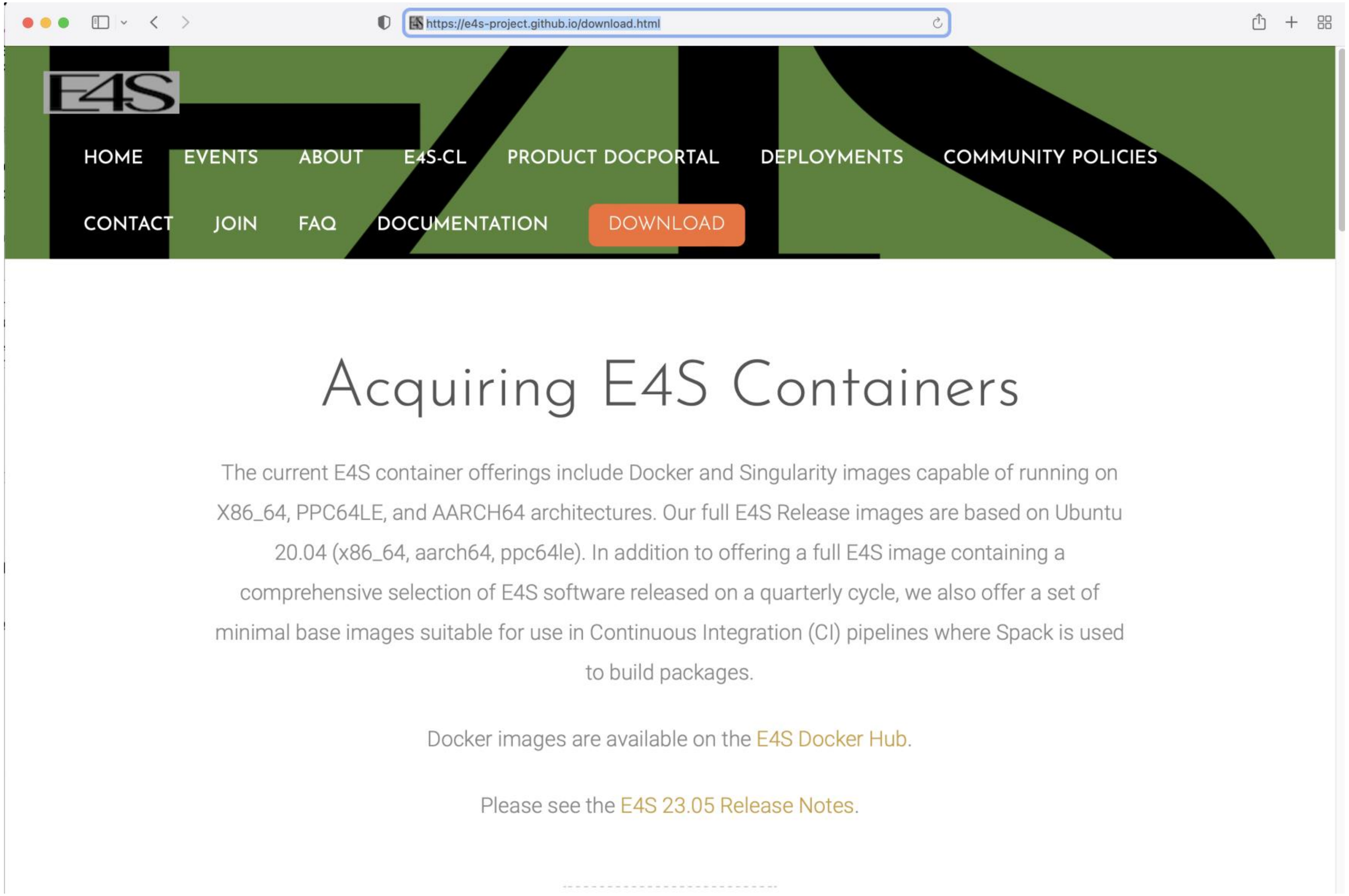
E4S 23.05 container images now available!

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



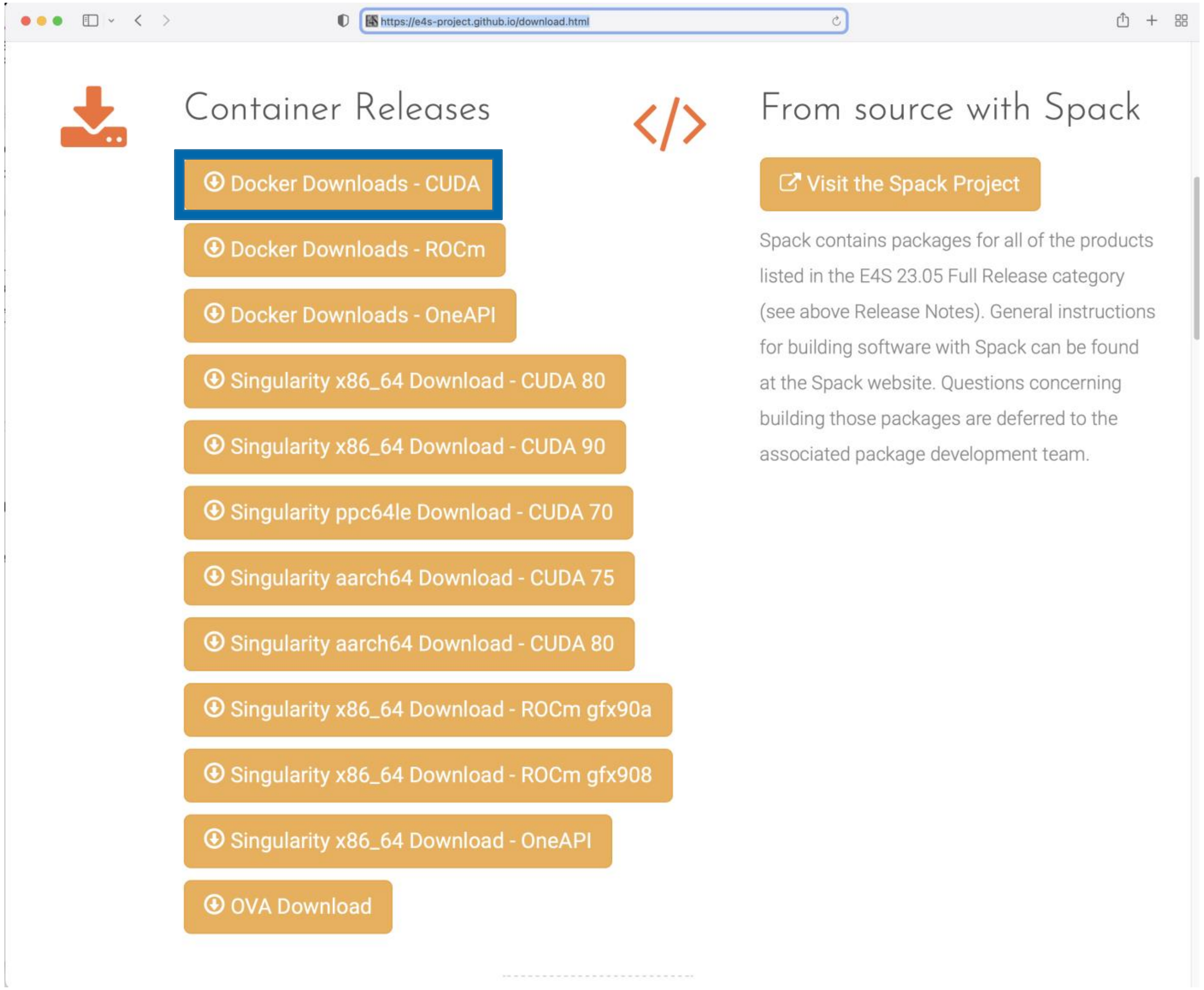
Acquiring E4S Containers

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

Container Releases

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

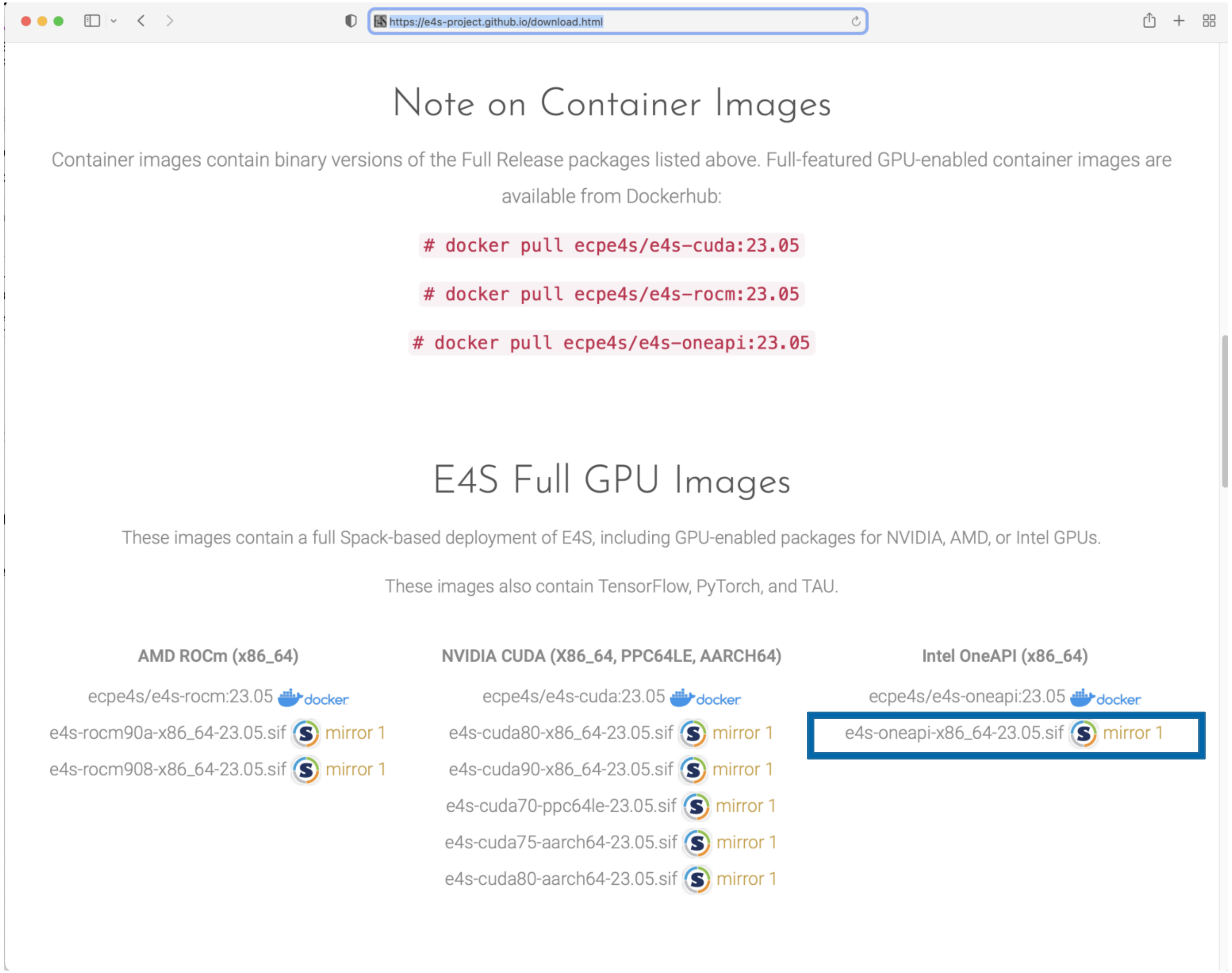
From source with Spack

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



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

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.

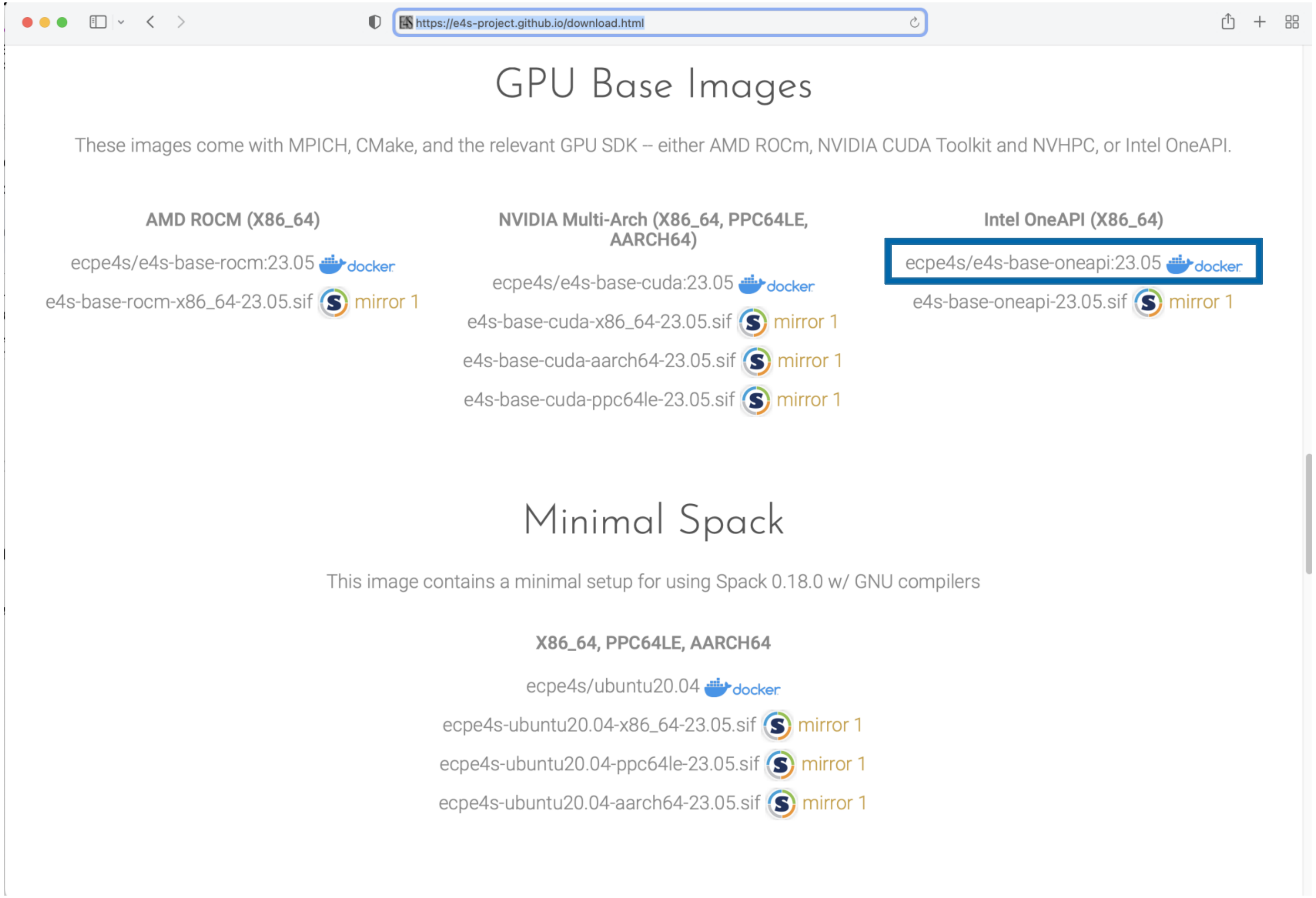
AMD ROCm (x86_64)	NVIDIA CUDA (X86_64, PPC64LE, AARCH64)	Intel OneAPI (x86_64)
ecpe4s/e4s-rocm:23.05 docker	ecpe4s/e4s-cuda:23.05 docker	ecpe4s/e4s-oneapi:23.05 docker
e4s-rocm90a-x86_64-23.05.sif mirror 1	e4s-cuda80-x86_64-23.05.sif mirror 1	e4s-oneapi-x86_64-23.05.sif mirror 1
e4s-rocm908-x86_64-23.05.sif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



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

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

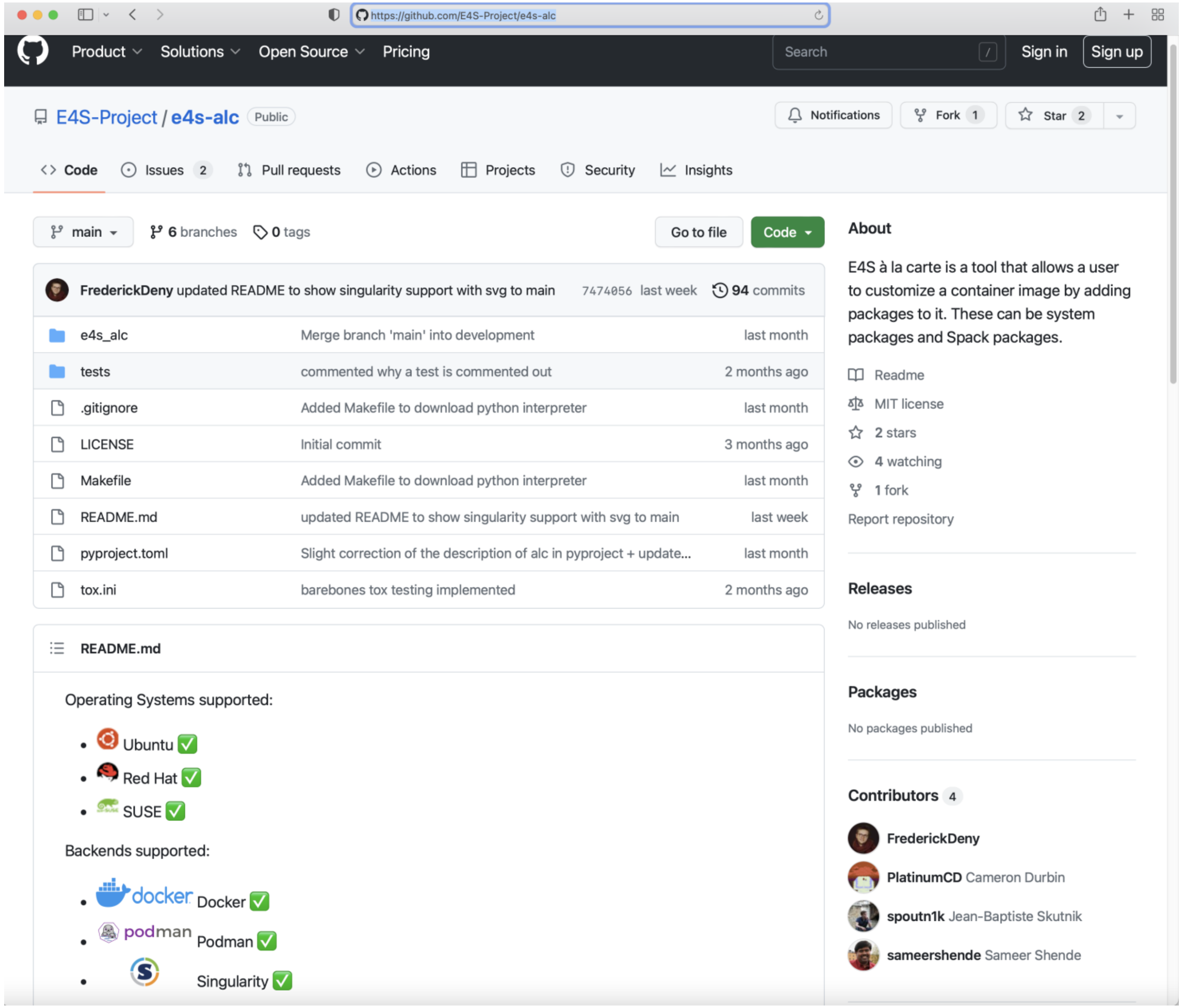
ecpe4s-ubuntu20.04-ppc64le-23.05.sif mirror 1

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



E4S-Project / e4s-alc Public

6 branches 0 tags

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

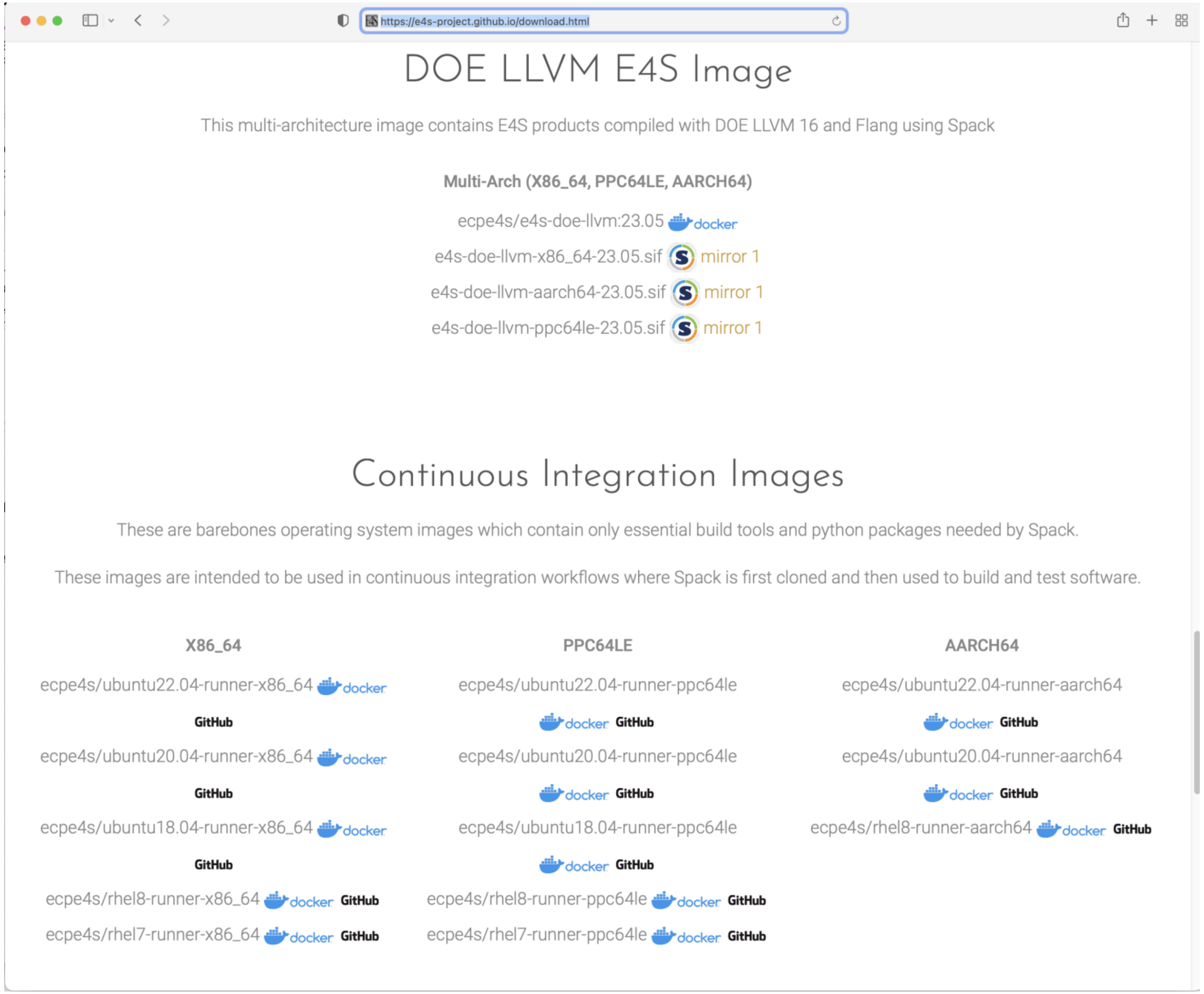
Add to a base image:

- Spack packages
- OS packages
- Tarballs

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

EXASCALE COMPUTING PROJECT

E4S 23.05 DOE LLVM and CI images



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

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

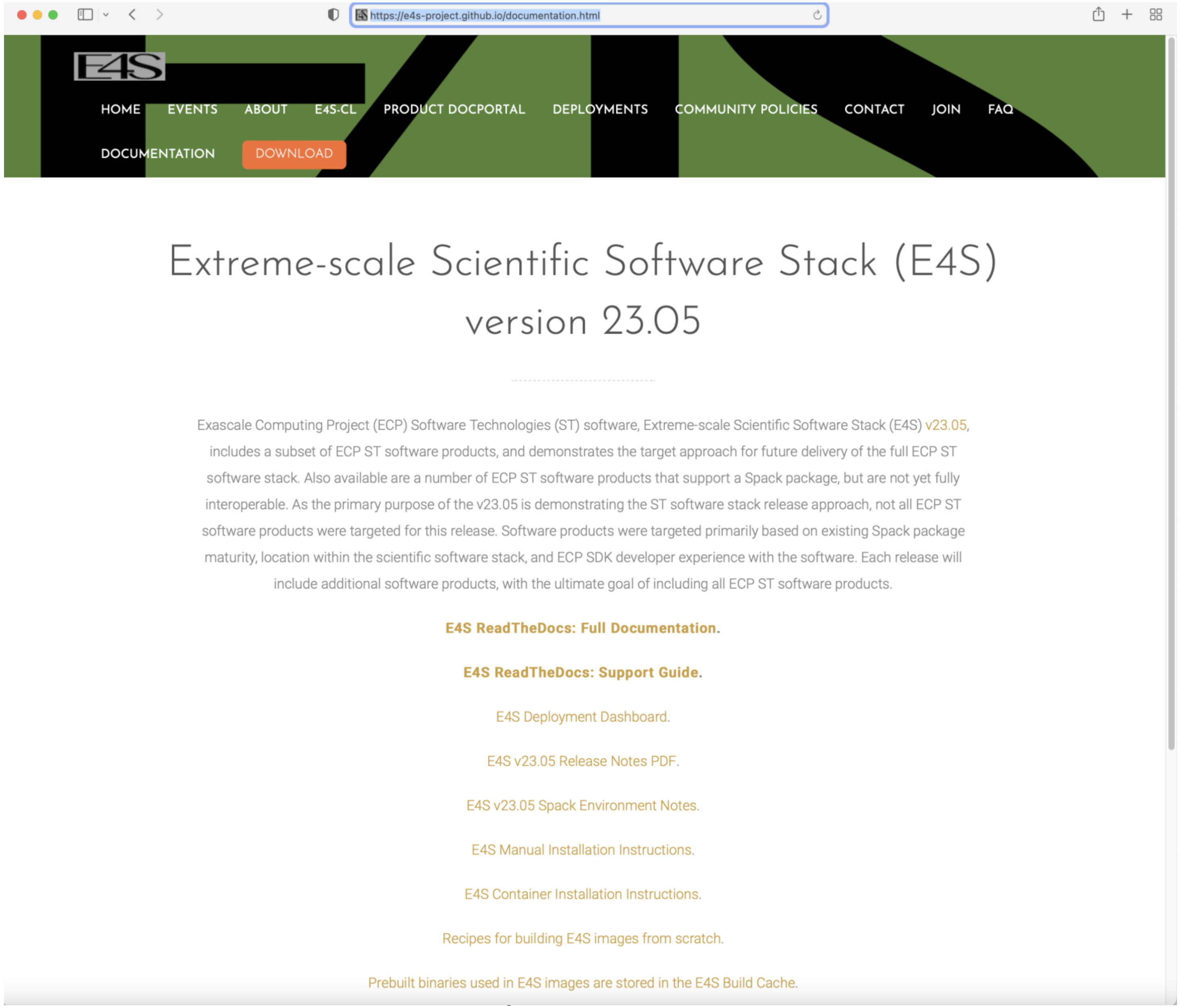
These are barebones operating system images which contain only essential build tools and python packages needed by Spack.

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



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.

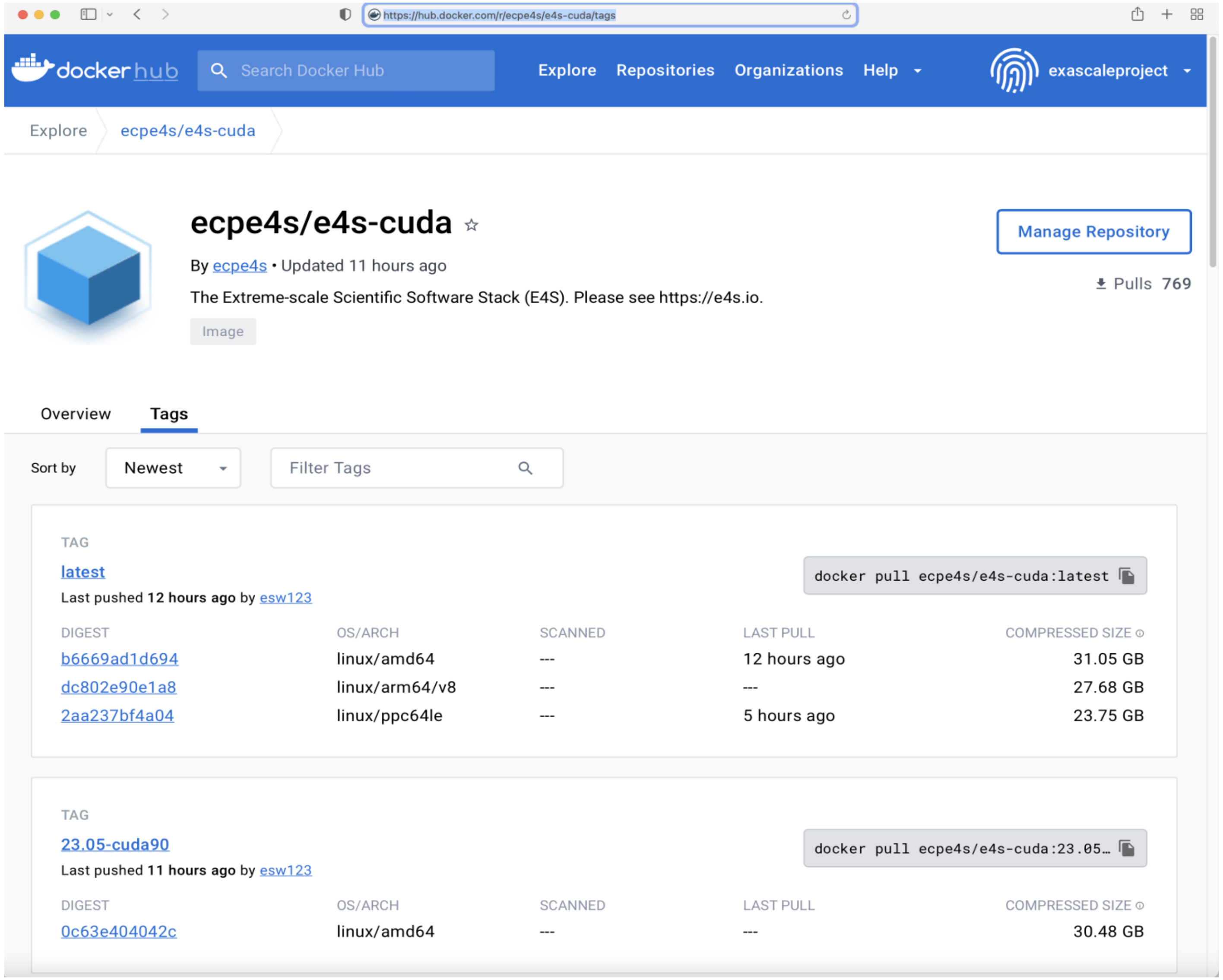
E4S Manual Installation Instructions.

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



ecpe4s/e4s-cuda ☆

By ecpe4s • Updated 11 hours ago

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

Image

Manage Repository

Pulls 769

Overview | Tags

Sort by: Newest | Filter Tags

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…
```

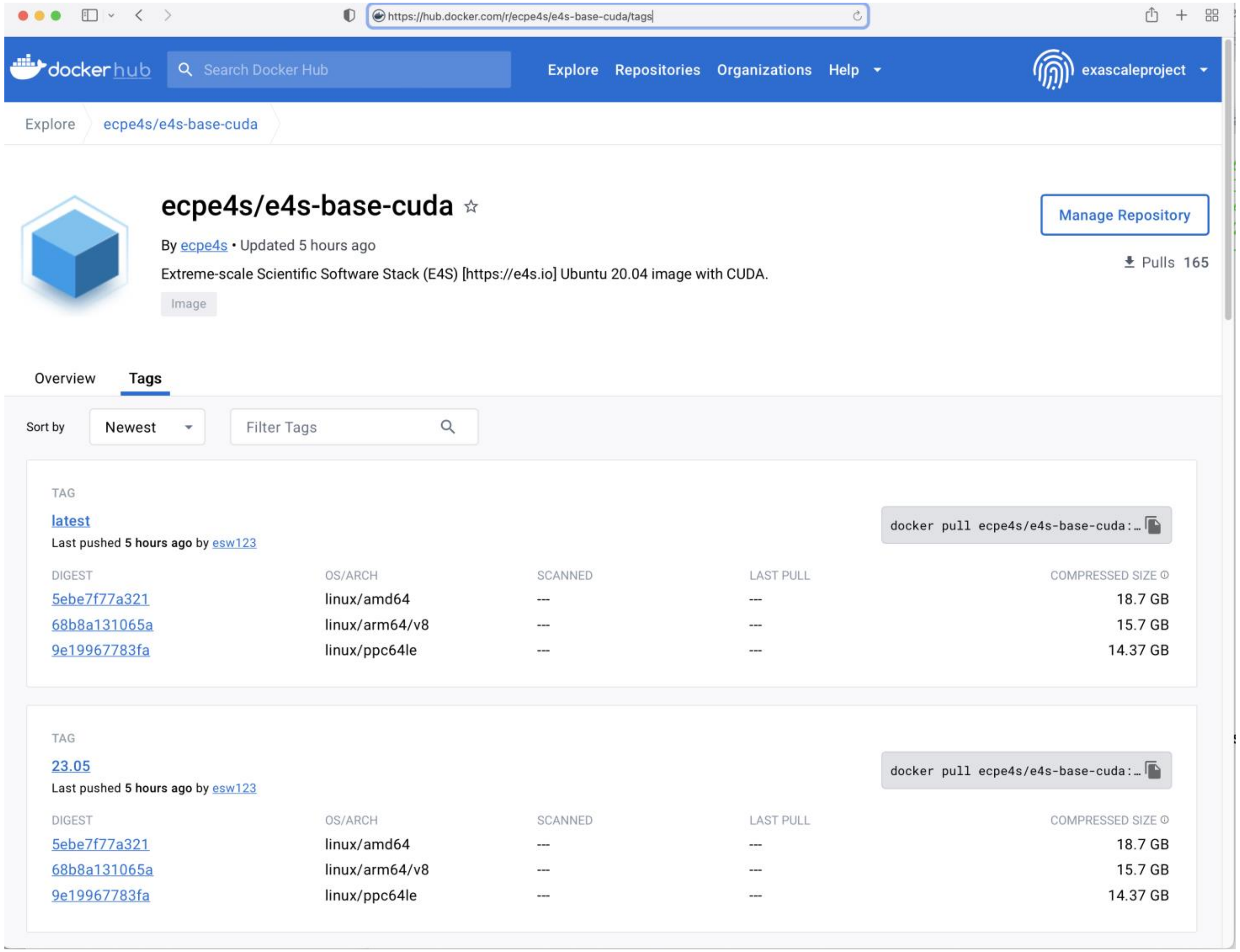
DIGEST	OS/ARCH	SCANNED	LAST PULL	COMPRESSED SIZE
0c63e404042c	linux/amd64	---	---	30.48 GB

```
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



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.

Pulls 165

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:…`

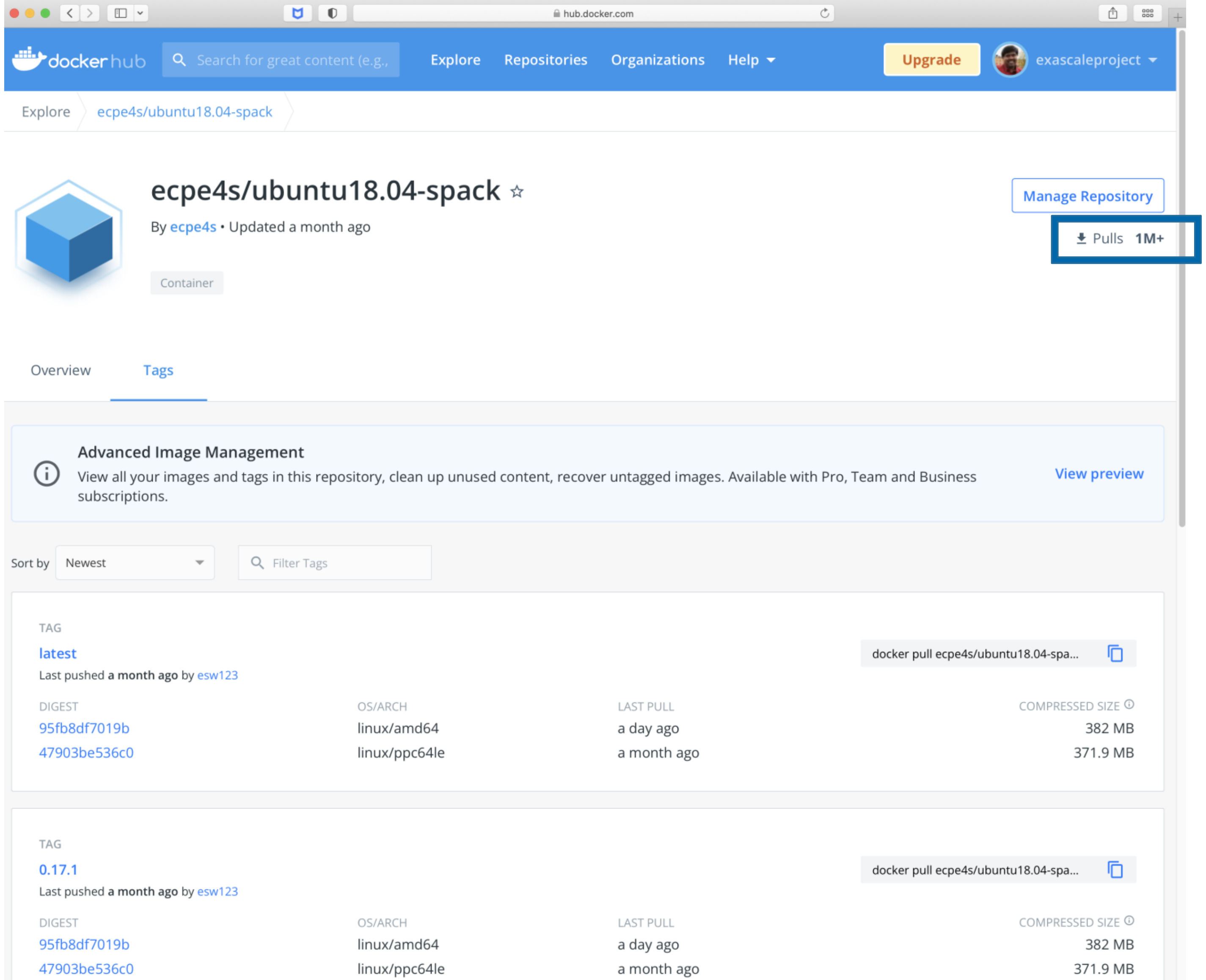
DIGEST	OS/ARCH	SCANNED	LAST PULL	COMPRESSED SIZE
5ebe7f77a321	linux/amd64	---	---	18.7 GB
68b8a131065a	linux/arm64/v8	---	---	15.7 GB
9e19967783fa	linux/ppc64le	---	---	14.37 GB

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



Explore › ecpe4s/ubuntu18.04-spack

ecpe4s/ubuntu18.04-spack ☆

By ecpe4s • Updated a month ago

Container

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`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...`

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95fb8df7019b	linux/amd64	a day ago	382 MB
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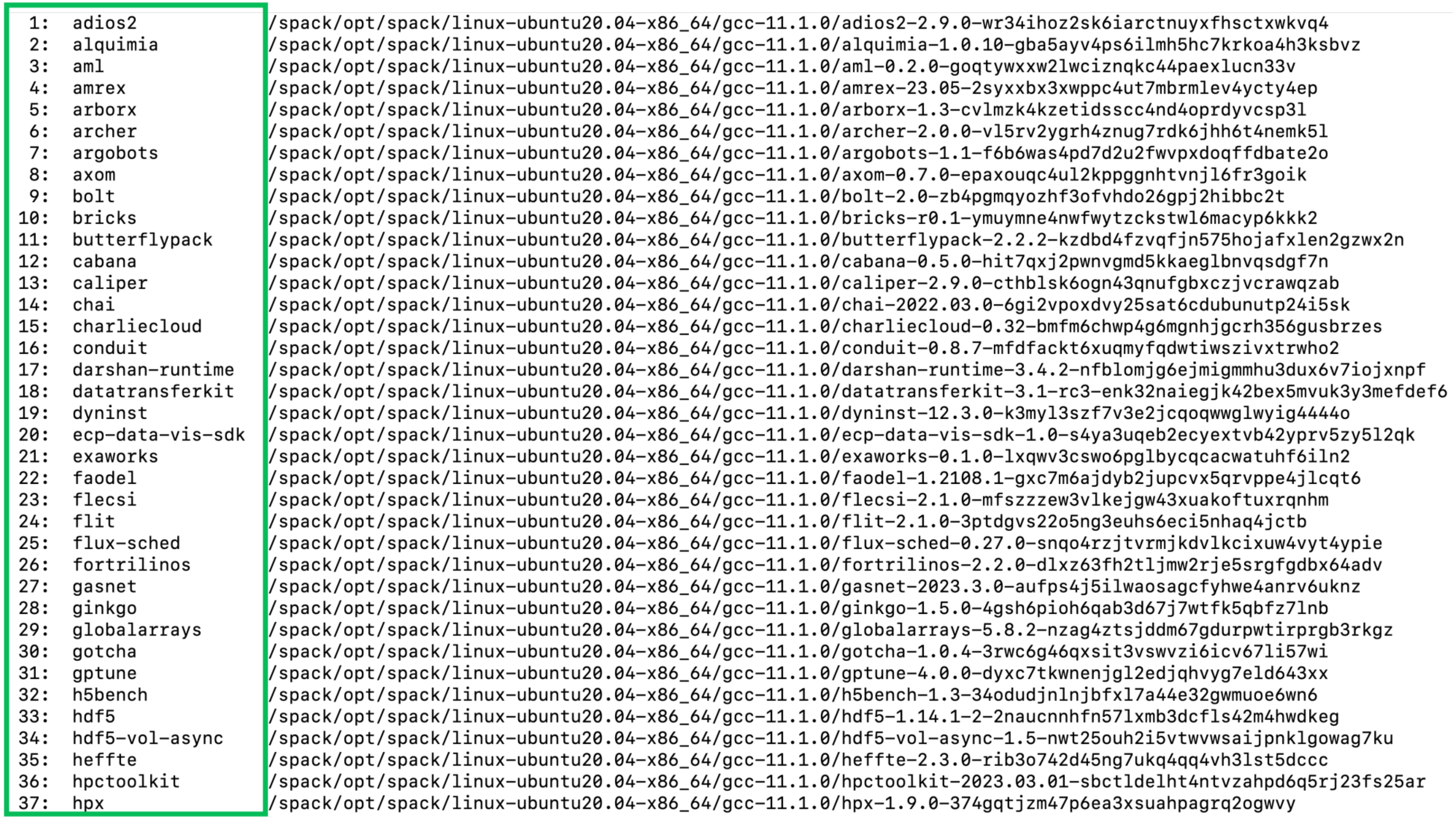
23.05 Release: 100+ Official Products + dependencies (gcc, x86_64)



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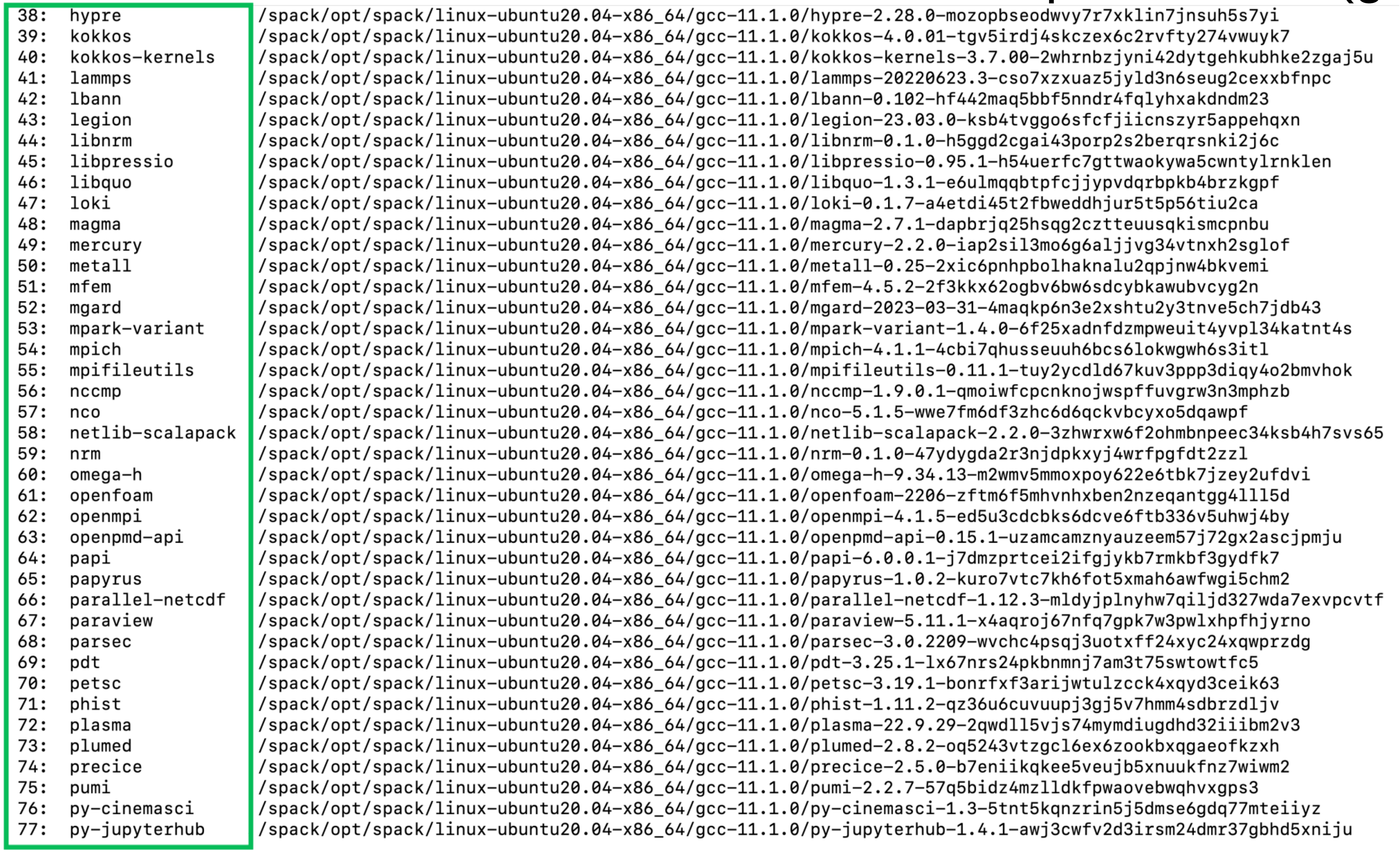
```

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)



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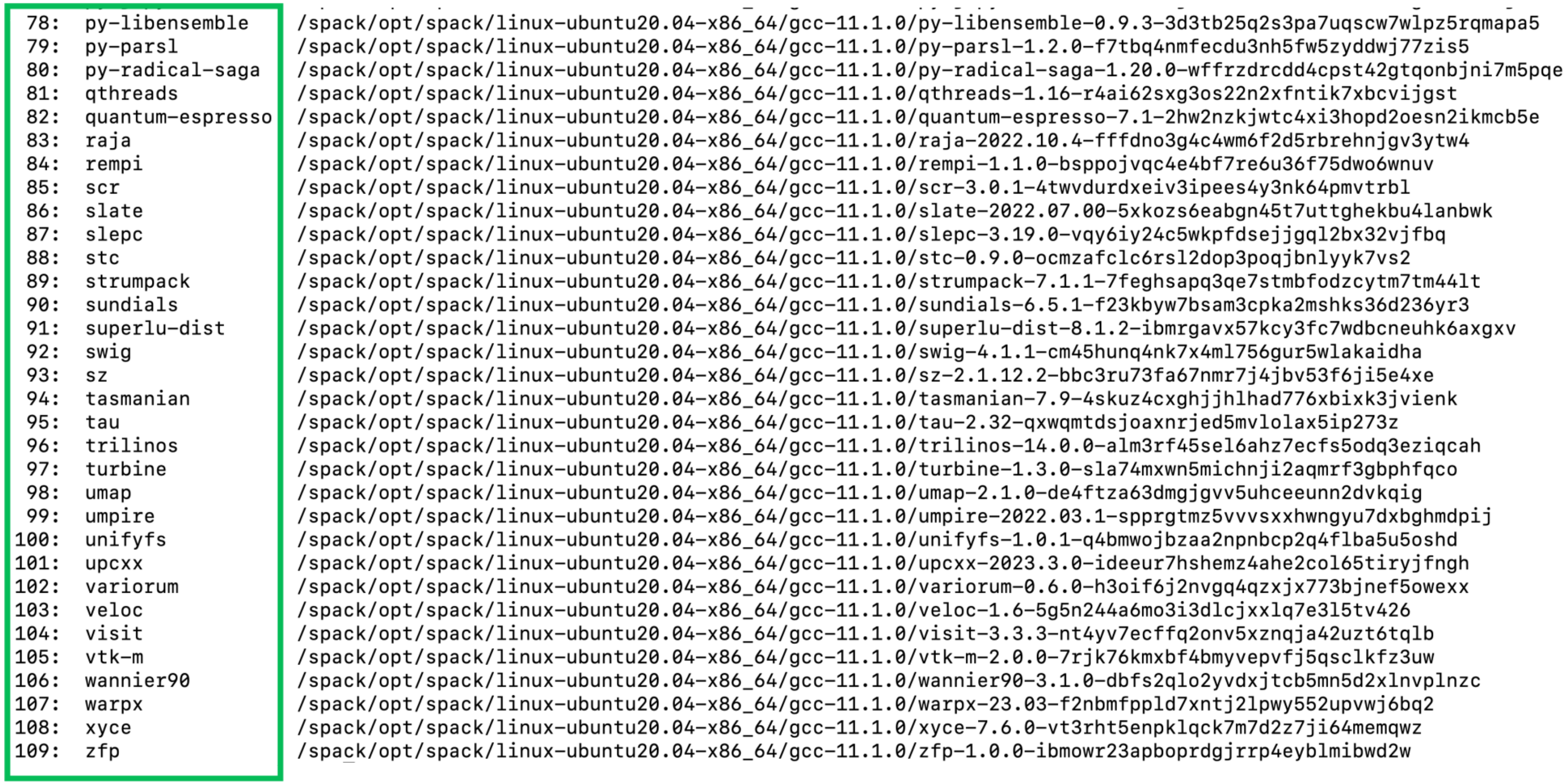
23.02 Release: 100 Official Products + dependencies (gcc, x86_64)



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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

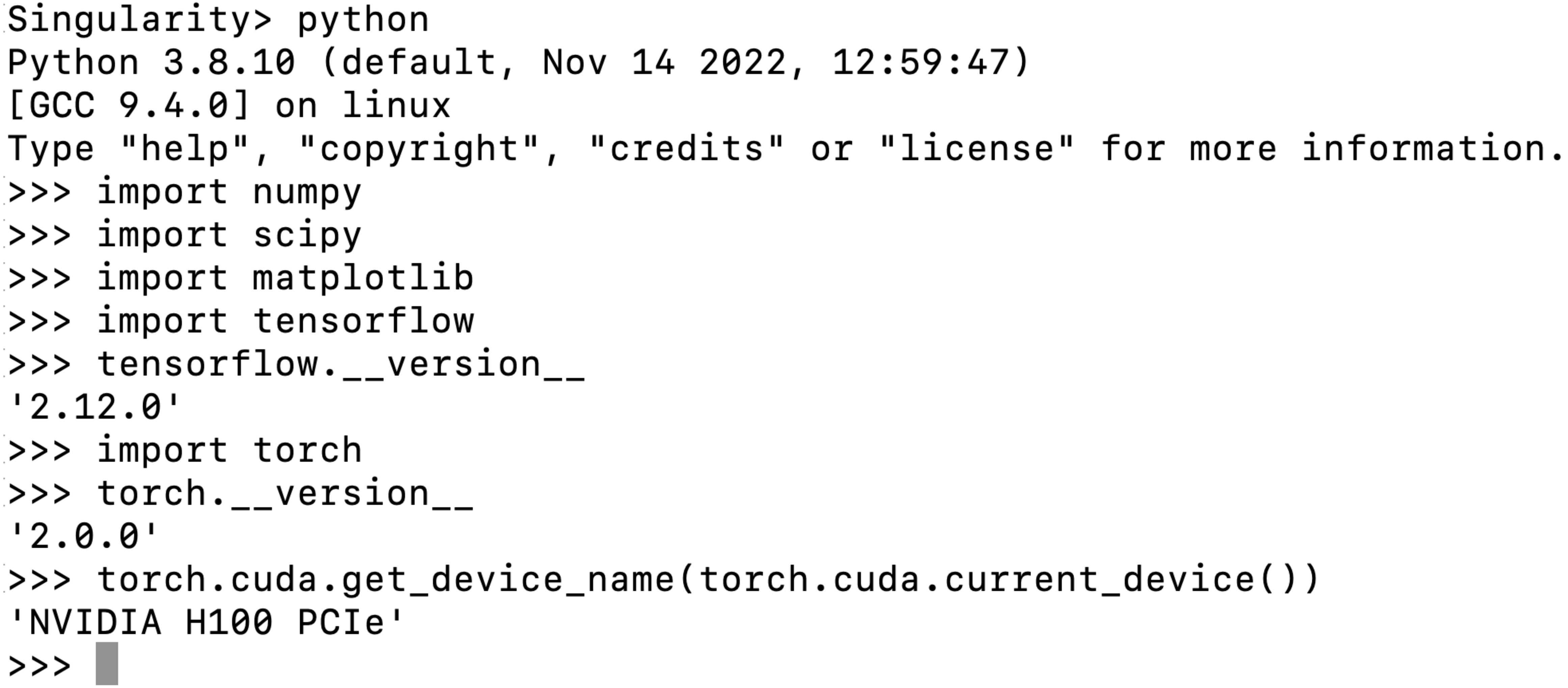
AI products with GPU support
- Tensorflow
- Pytorch

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

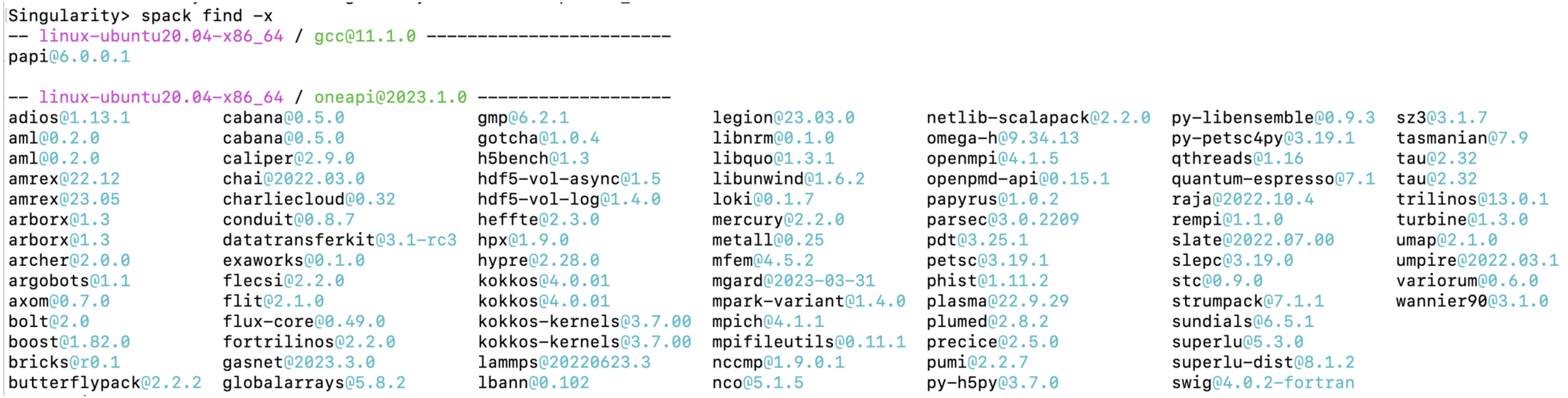
E4S Support for AI/ML frameworks with V100, A100, and H100 GPUs



```
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

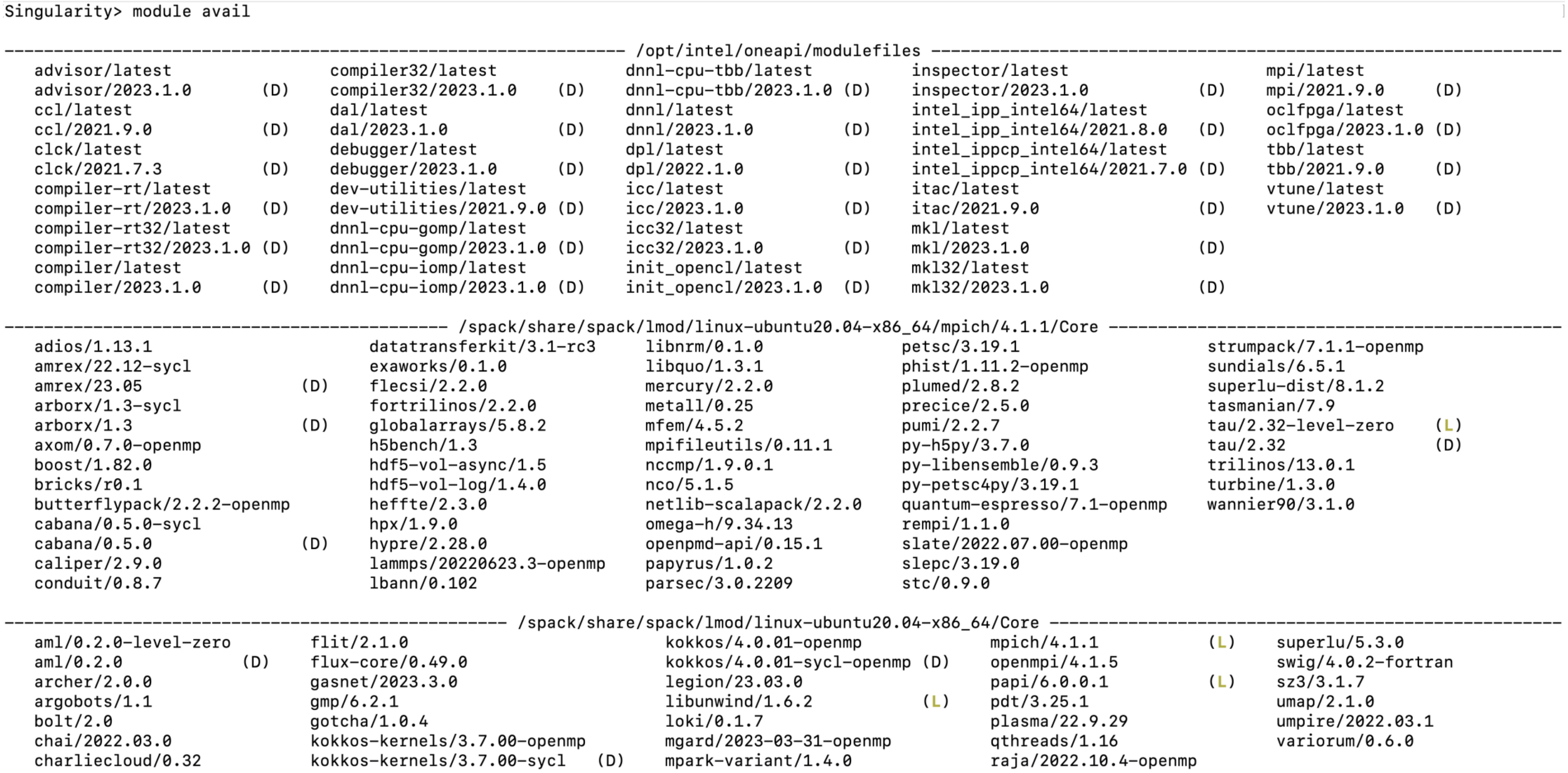
E4S 23.05 Intel oneAPI 2023.1: Packages built with Intel compilers



```
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

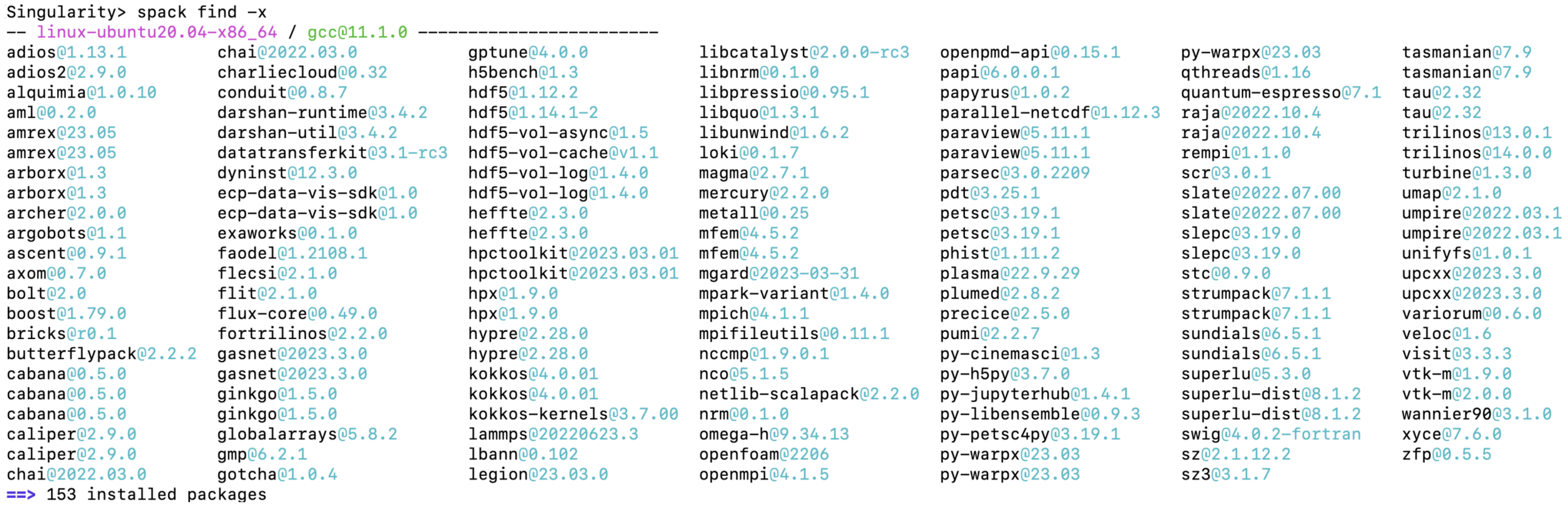
E4S 23.05 Intel oneAPI 2023.1: Packages built with Intel compilers



```
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

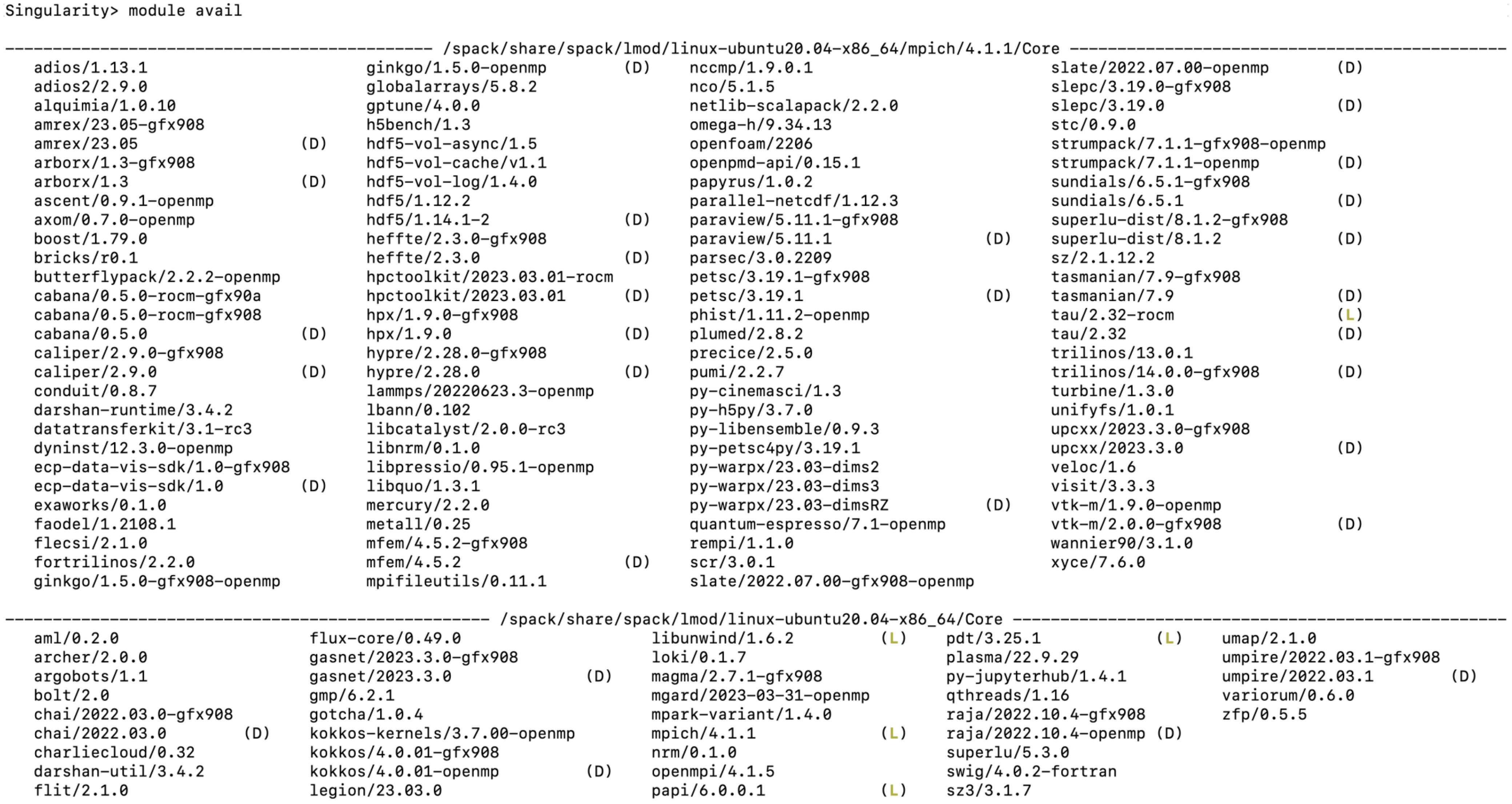
E4S Support for ROCm variants for MI250X (gfx90a) on x86_64



```
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

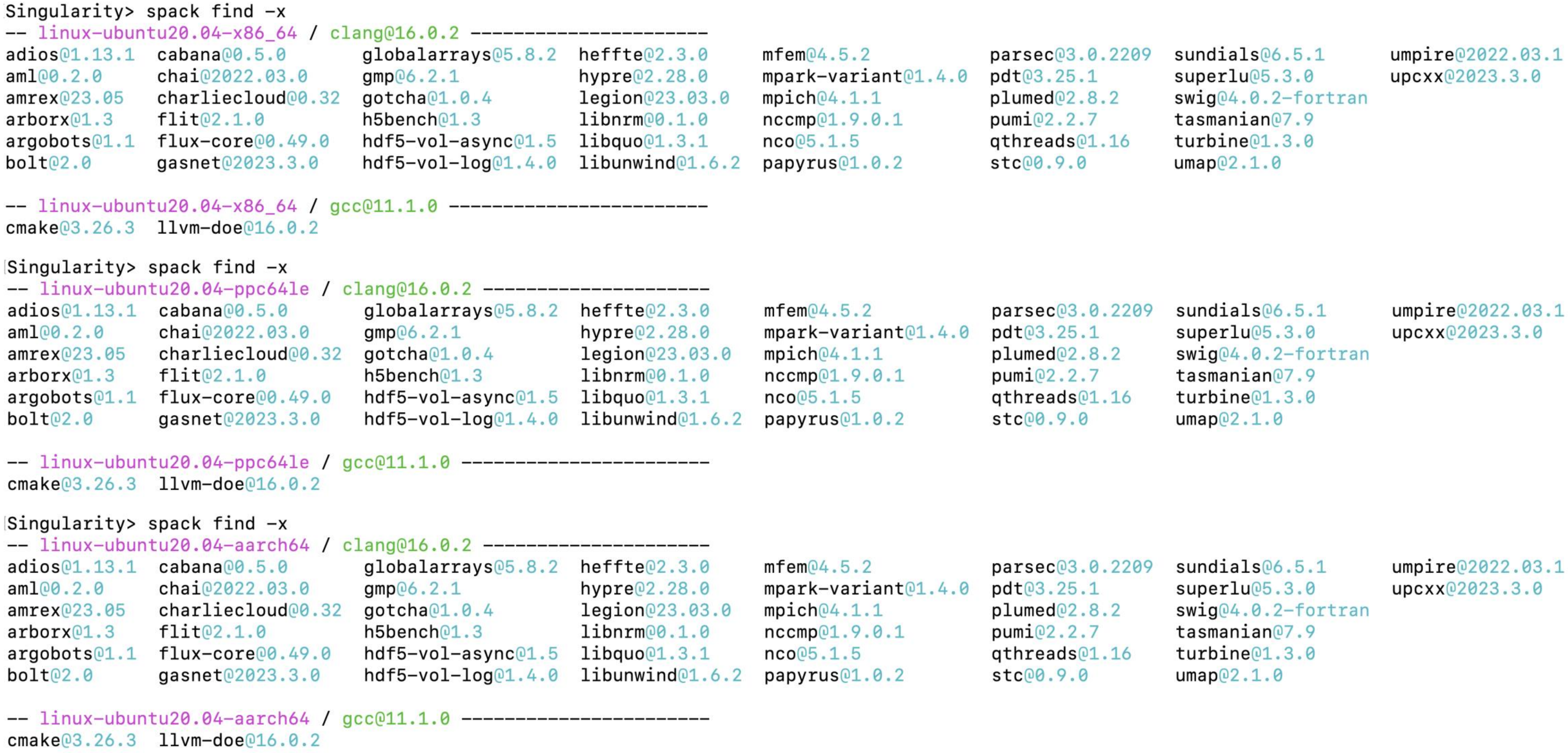
E4S Support for ROCm variants for MI250X (gfx90a) on x86_64



```
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
```

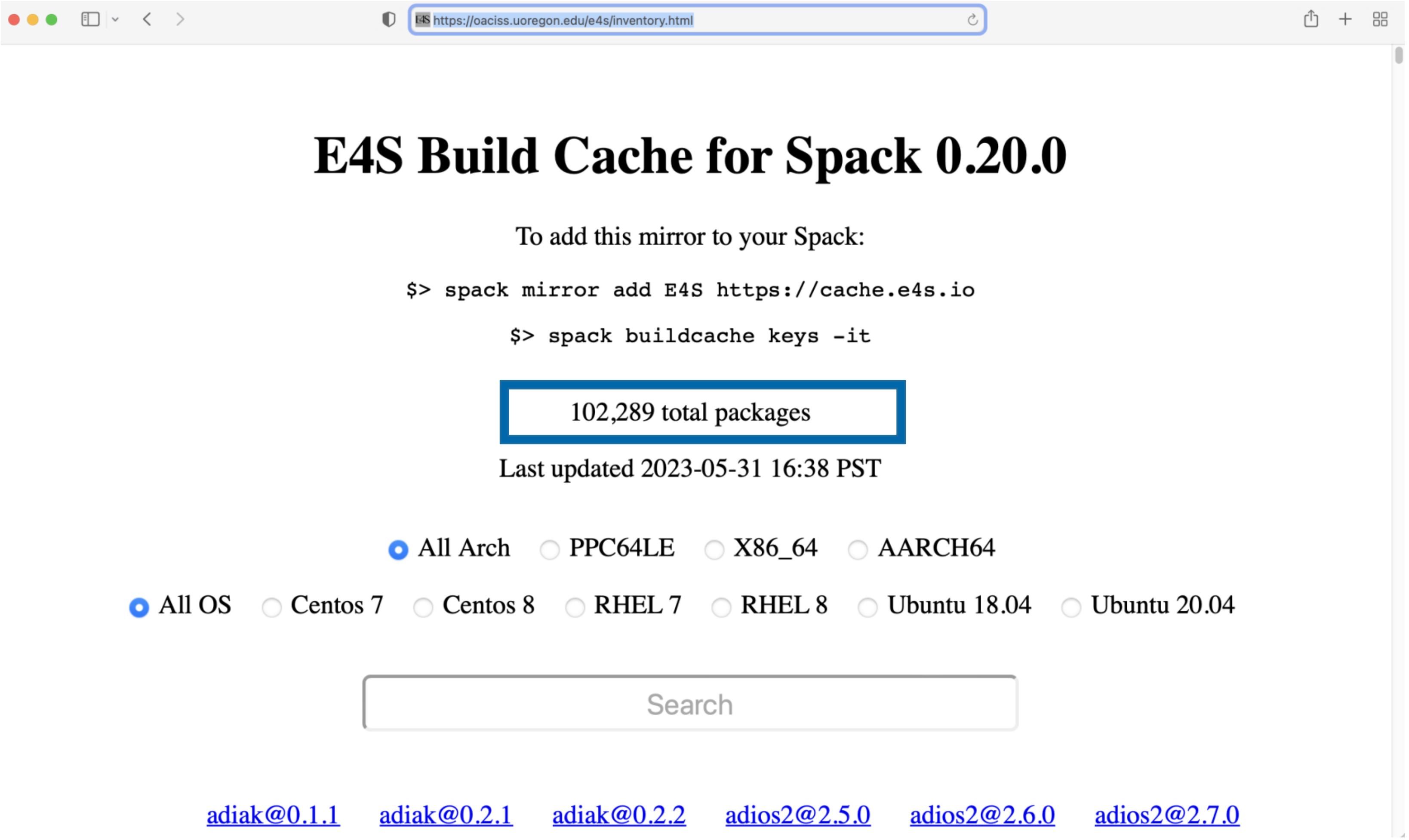
E4S 23.05 supports AMD MI100 (gfx908) as well as MI250X (gfx90a) GPUs

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

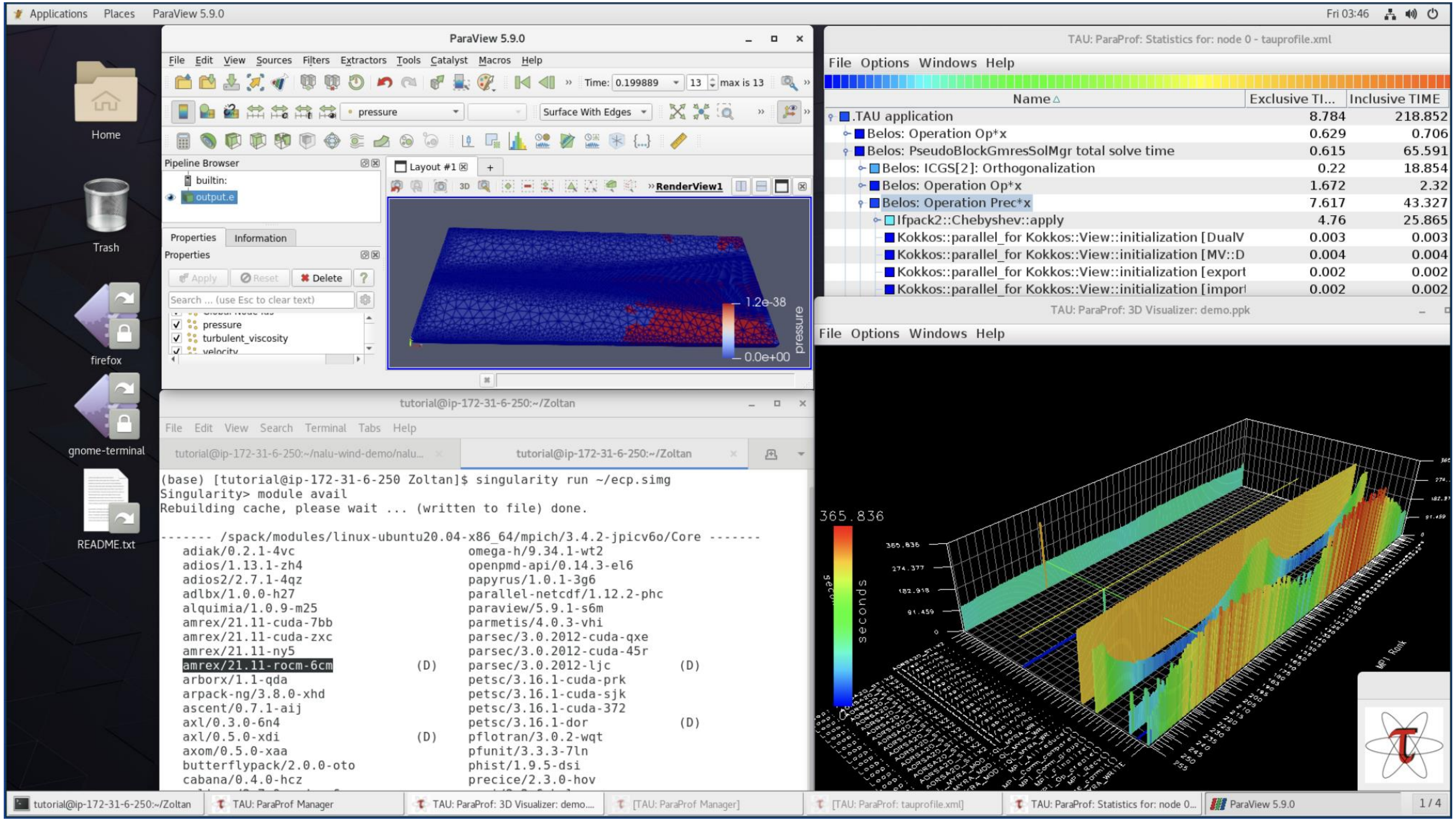
Search

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.

EXASCALE COMPUTING PROJECT

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
Layout #1
RenderView1
Properties
Information
Apply
Reset
Delete
Search ... (use Esc to clear text)
pressure
turbulent_viscosity
velocity
1.2e-38
0.0e+00
pressure
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
274.377
182.918
91.459
0
MPI Rank
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
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

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

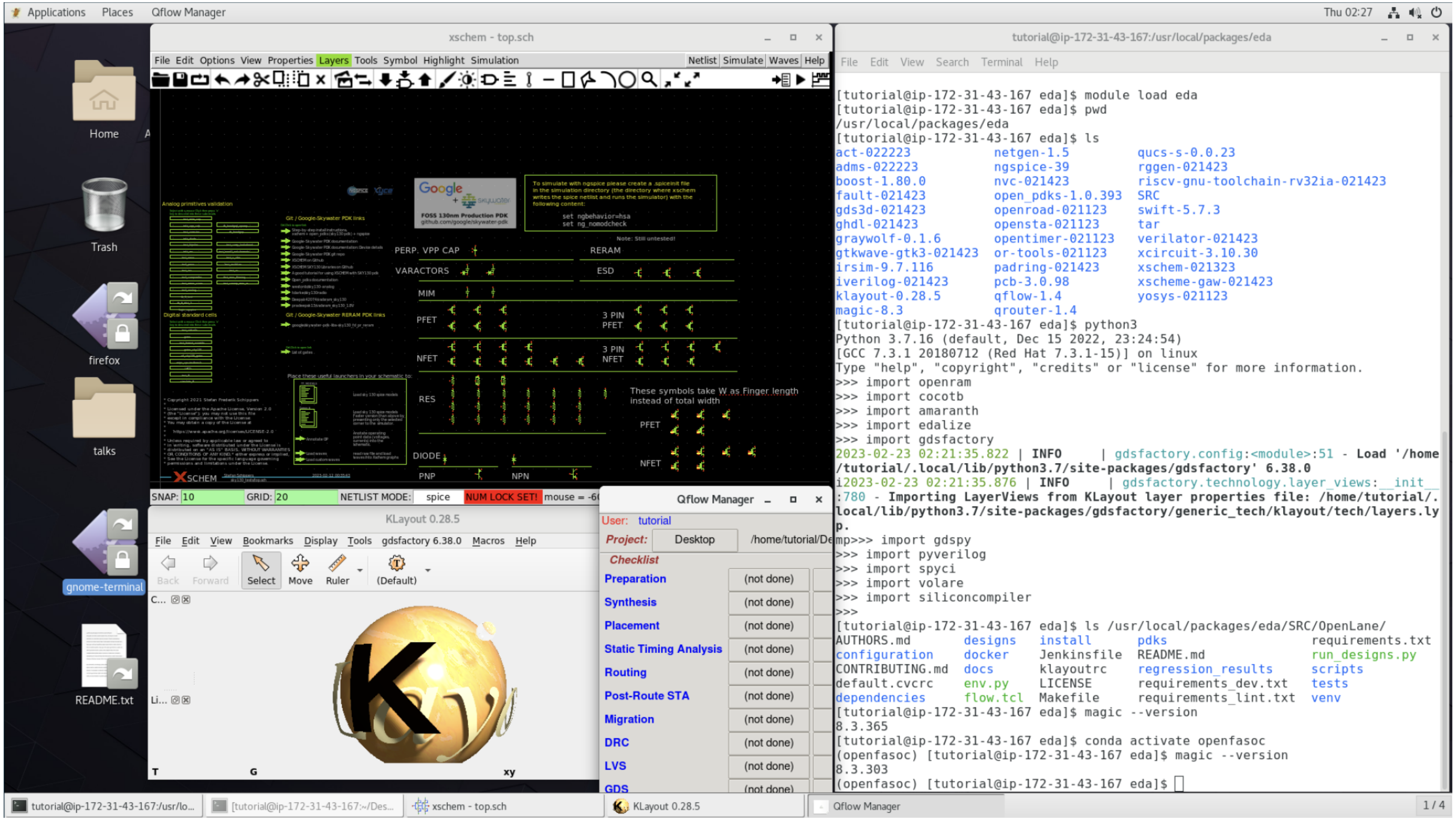
```
(base) [tutorial@ip-172-31-6-250 Zoltan]$ singularity run ~/ecp.simg
Singularity> module avail
Rebuilding cache, please wait ... (written to file) done.

------- /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
```

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



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
SNAP: 10 GRID: 20 NETLIST MODE: spice NUM LOCK SET! mouse = -6
KLayout 0.28.5
File Edit View Bookmarks Display Tools gdsfactory 6.38.0 Macros Help
Back Forward Select Move Ruler (Default)
tutorial@ip-172-31-43-167:/usr/local/packages/eda
File Edit View Search Terminal Help
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

```
[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]$
```

Qflow Manager

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)

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

https://e4s.io/eda

EXASCALE COMPUTING PROJECT

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

EXASCALE COMPUTING PROJECT

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
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

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.

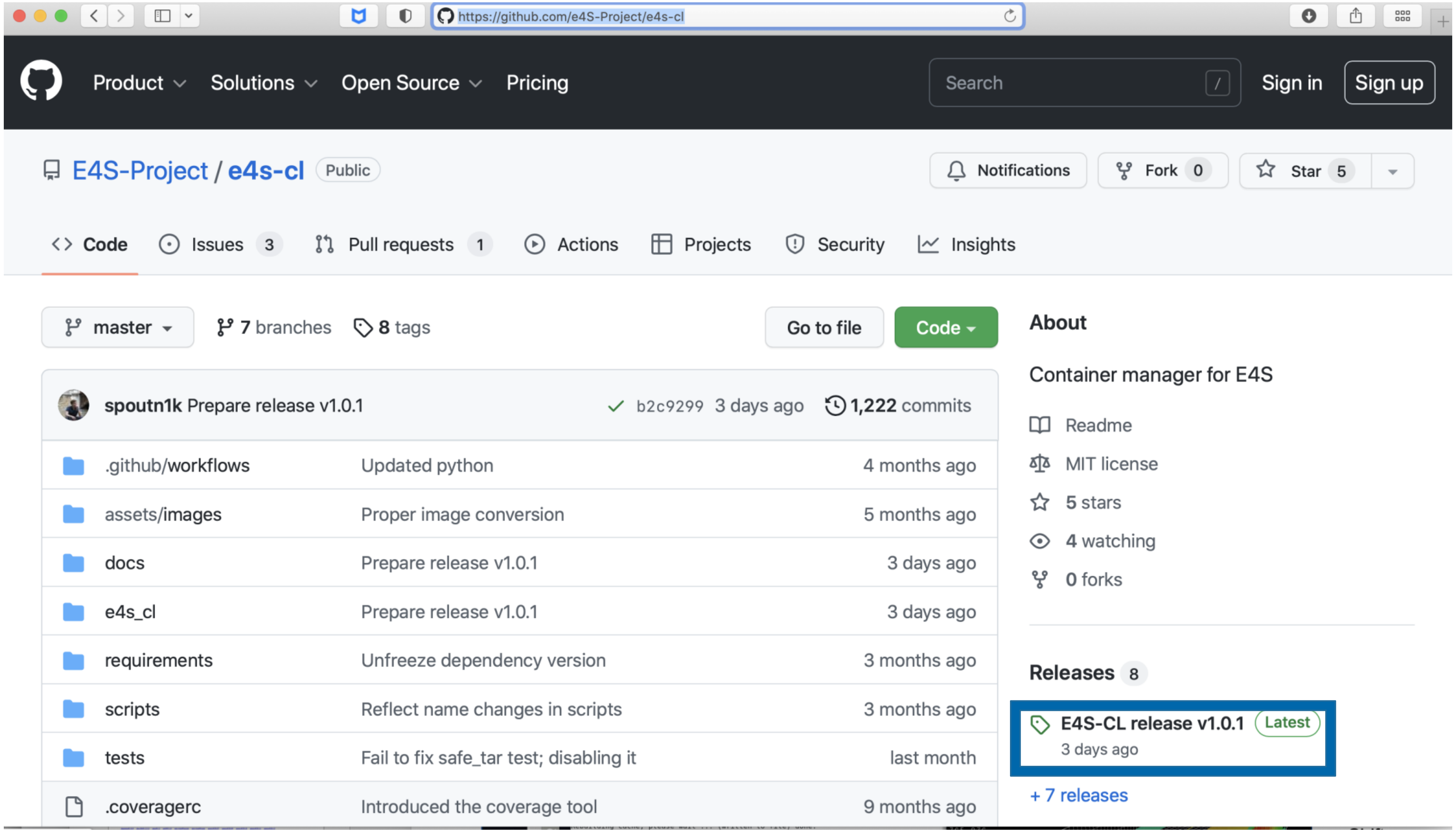
- e4s-cl is a new tool that simplifies the launch and MPI replacement.
  - e4s-cl init --backend [singularity|shifter|docker] --image <file> --source <startup_cmds.sh>
  - e4s-cl mpirun -np <N> <command>

- 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

New release of e4s-cl on GitHub



E4S-Project / e4s-cl Public

spoutn1k Prepare release v1.0.1 ✓ b2c9299 3 days ago 1,222 commits

.github/workflows	Updated python	4 months ago
assets/images	Proper image conversion	5 months ago
docs	Prepare release v1.0.1	3 days ago
e4s_cl	Prepare release v1.0.1	3 days ago
requirements	Unfreeze dependency version	3 months ago
scripts	Reflect name changes in scripts	3 months ago
tests	Fail to fix safe_tar test; disabling it	last month
.coveragerc	Introduced the coverage tool	9 months ago

About

Container manager for E4S

- Readme
- MIT license
- 5 stars
- 4 watching
- 0 forks

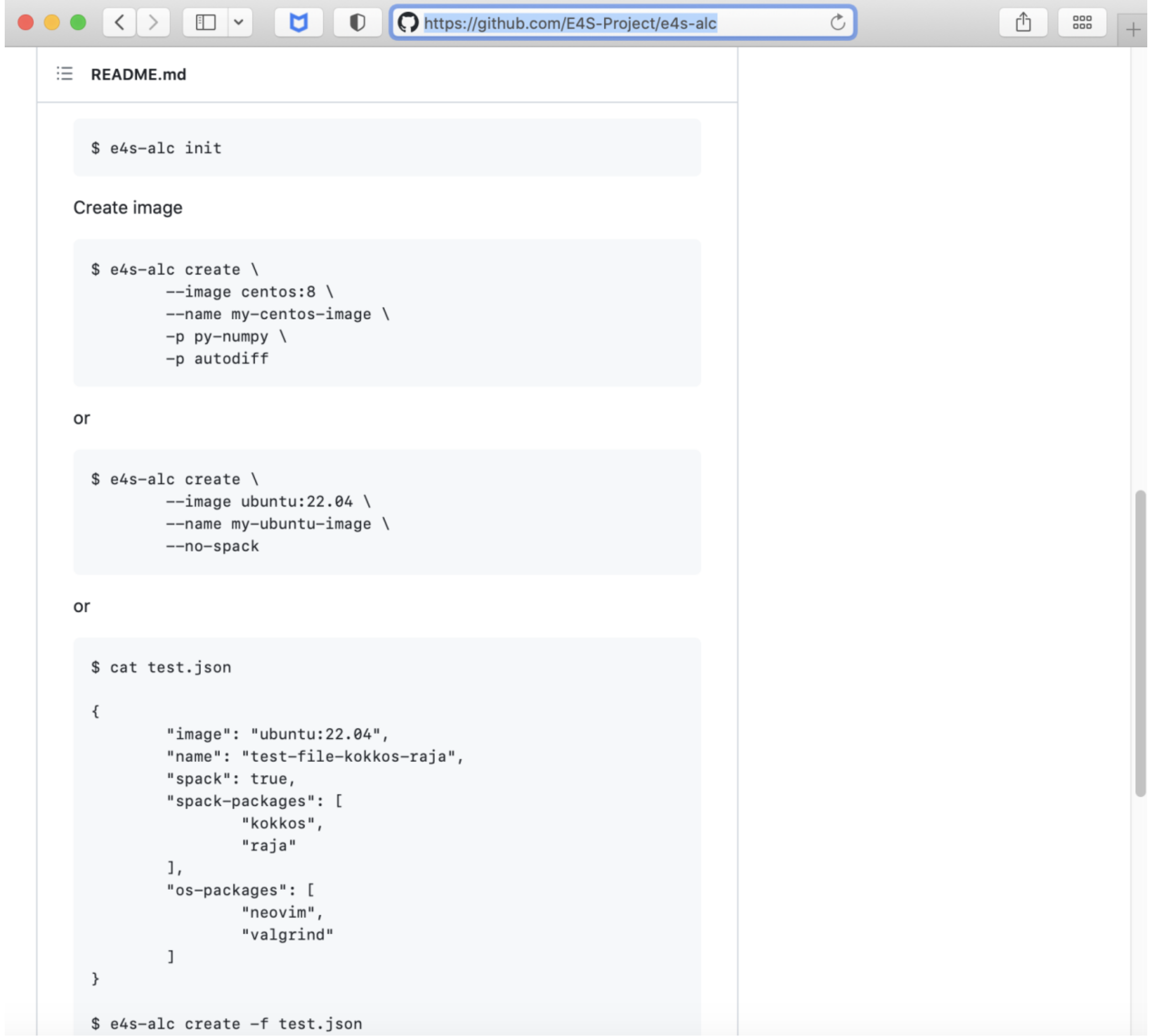
Releases 8

E4S-CL release v1.0.1 Latest
3 days ago

+ 7 releases

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

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



```
$ 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

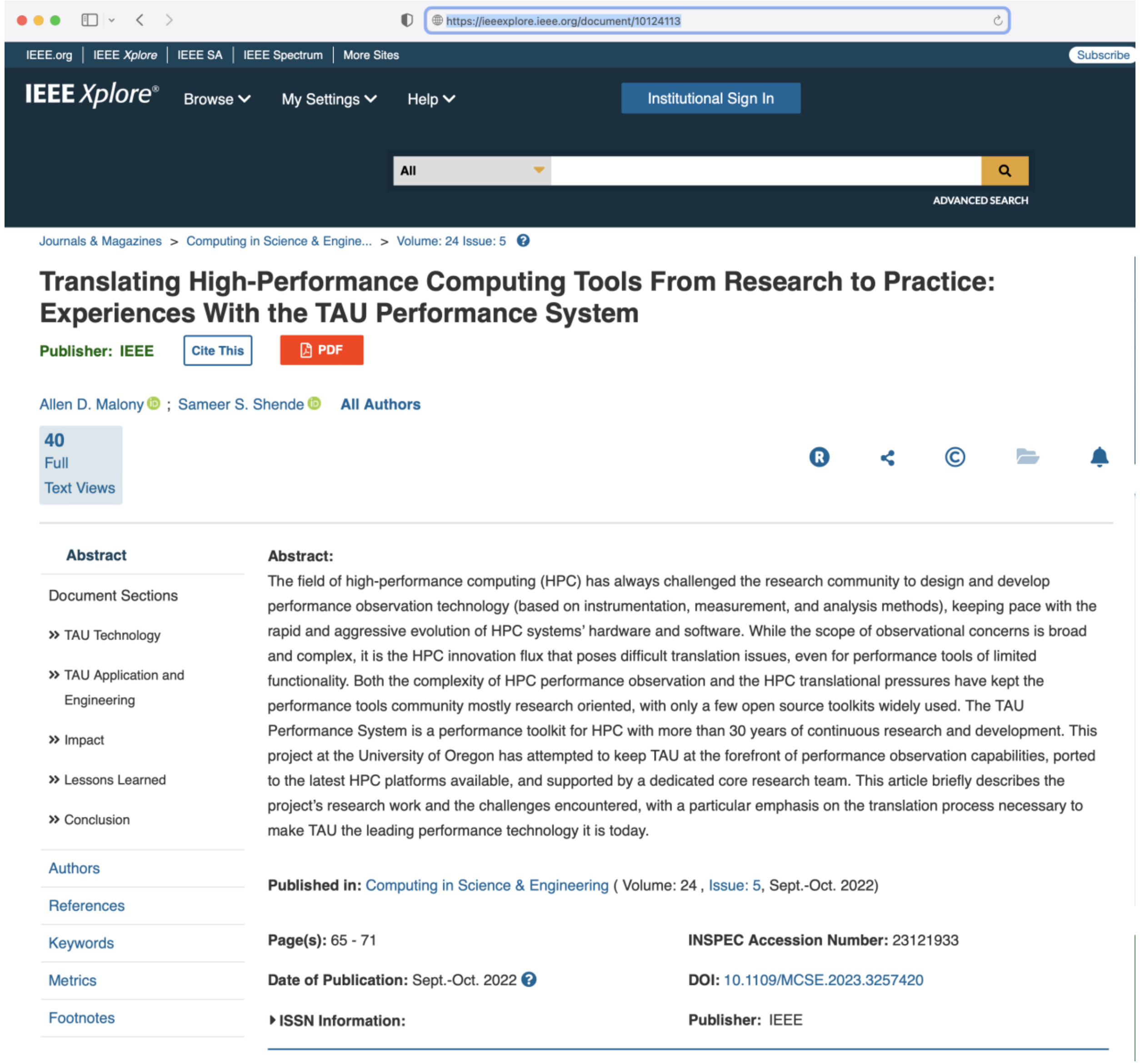
```
$ cat test.json

{
        "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
```

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

Add packages to a container image:

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

Translating HPC Tools from Research to Practice: TAU



Translating High-Performance Computing Tools From Research to Practice: Experiences With the TAU Performance System

Publisher: IEEE

Allen D. Malony ; Sameer S. Shende **All Authors**

Abstract:

The field of high-performance computing (HPC) has always challenged the research community to design and develop performance observation technology (based on instrumentation, measurement, and analysis methods), keeping pace with the rapid and aggressive evolution of HPC systems' hardware and software. While the scope of observational concerns is broad and complex, it is the HPC innovation flux that poses difficult translation issues, even for performance tools of limited functionality. Both the complexity of HPC performance observation and the HPC translational pressures have kept the performance tools community mostly research oriented, with only a few open source toolkits widely used. The TAU Performance System is a performance toolkit for HPC with more than 30 years of continuous research and development. This project at the University of Oregon has attempted to keep TAU at the forefront of performance observation capabilities, ported to the latest HPC platforms available, and supported by a dedicated core research team. This article briefly describes the project's research work and the challenges encountered, with a particular emphasis on the translation process necessary to make TAU the leading performance technology it is today.

Published in: Computing in Science & Engineering (Volume: 24 , Issue: 5, Sept.-Oct. 2022)

Page(s): 65 - 71

INSPEC Accession Number: 23121933

Date of Publication: Sept.-Oct. 2022

DOI: 10.1109/MCSE.2023.3257420

ISSN Information:

Publisher: IEEE

Questions?

Software Deployment at Facilities

EXASCALE COMPUTING PROJECT

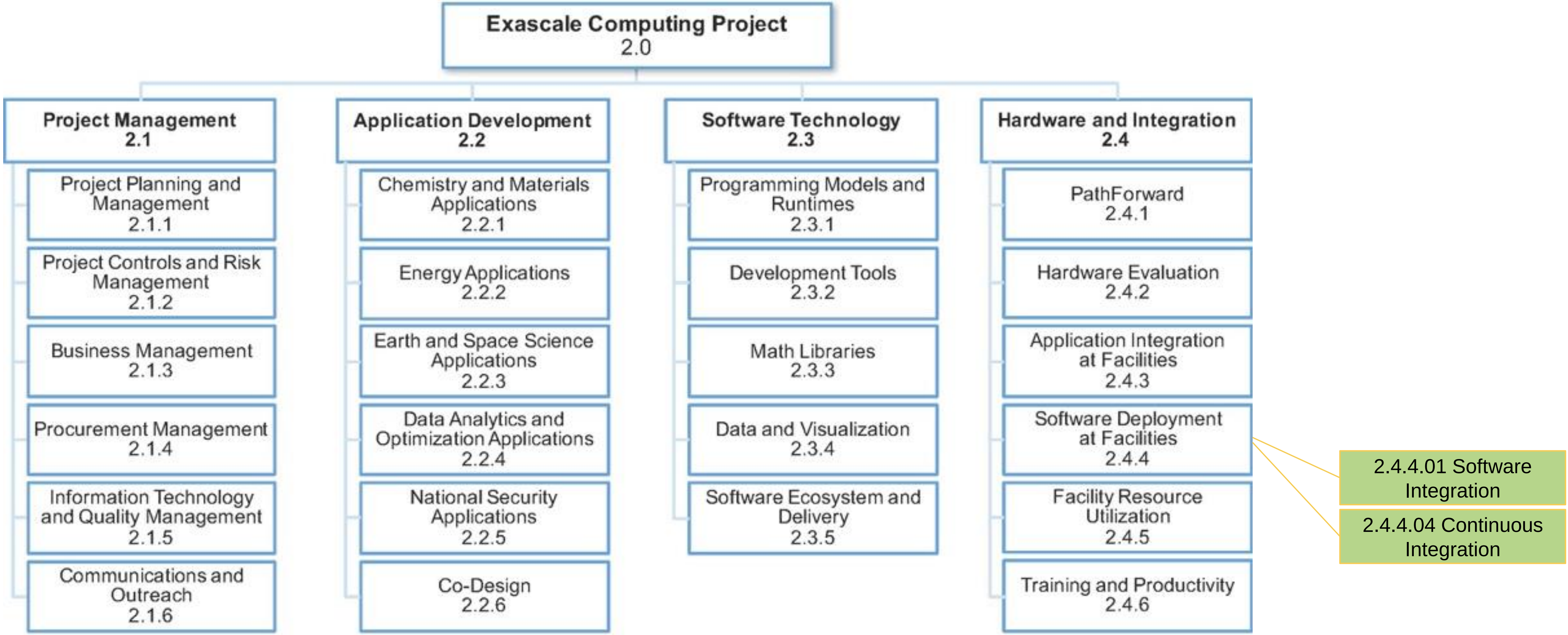
Ryan Prout

Continuous Integration and Software Integration

Points for today

- Cohesive software deployment community is important

- ECP has showcased how to provide common standards and infrastructure for packaging, testing, delivering, and integrating software across facilities

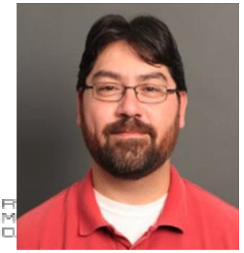


Exascale Computing Project 2.0

- **Project Management 2.1**
  - Project Planning and Management 2.1.1
  - Project Controls and Risk Management 2.1.2
  - Business Management 2.1.3
  - Procurement Management 2.1.4
  - Information Technology and Quality Management 2.1.5
  - Communications and Outreach 2.1.6
- **Application Development 2.2**
  - Chemistry and Materials Applications 2.2.1
  - Energy Applications 2.2.2
  - Earth and Space Science Applications 2.2.3
  - Data Analytics and Optimization Applications 2.2.4
  - National Security Applications 2.2.5
  - Co-Design 2.2.6
- **Software Technology 2.3**
  - Programming Models and Runtimes 2.3.1
  - Development Tools 2.3.2
  - Math Libraries 2.3.3
  - Data and Visualization 2.3.4
  - Software Ecosystem and Delivery 2.3.5
- **Hardware and Integration 2.4**
  - PathForward 2.4.1
  - Hardware Evaluation 2.4.2
  - Application Integration at Facilities 2.4.3
  - Software Deployment at Facilities 2.4.4
    - 2.4.4.01 Software Integration
    - 2.4.4.04 Continuous Integration
  - Facility Resource Utilization 2.4.5
  - Training and Productivity 2.4.6

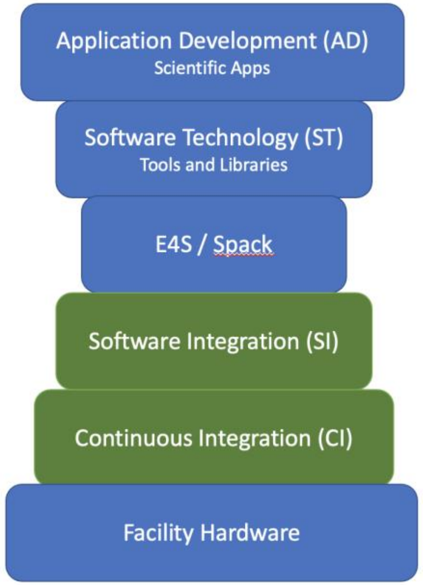
Software Deployment Focus Areas

Project Short Name	PI Name, Inst	Short Description/Objective
2.4.4.01 Software Integration	Shahzeb Siddiqui (LBL)	Build/Test/Deploy ST products at facilities
2.4.4.04 Continuous Integration	Paul Bryant (ORNL)	Develop and Deploy ECP CI infrastructure



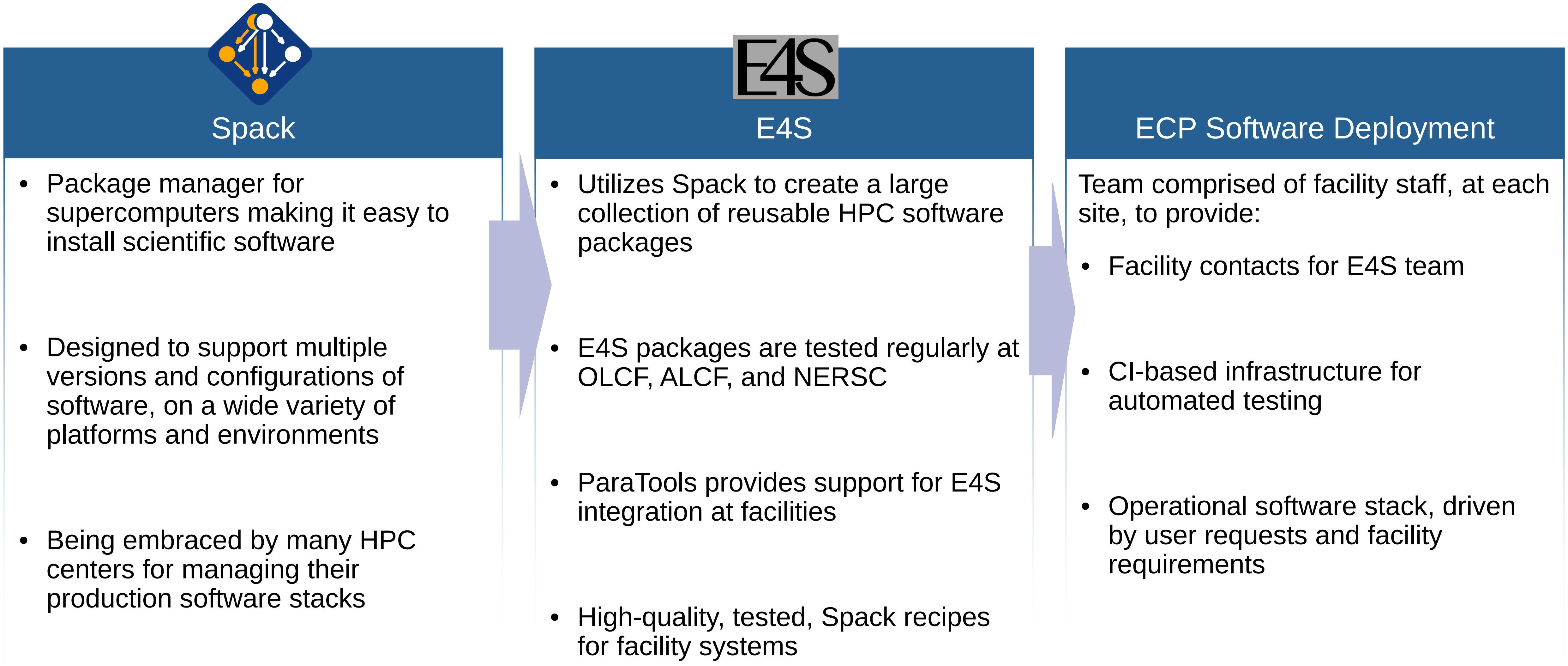
Combined Purpose:
Provide infrastructure and support for integrating software at facilities (*eye towards efficiency and automation*)

Tools and Infrastructure:
Spack
E4S
Gitlab



Ray Powell Not pictured

Emphasizing Relationships



Spack

- Package manager for supercomputers making it easy to install scientific software
- Designed to support multiple versions and configurations of software, on a wide variety of platforms and environments
- Being embraced by many HPC centers for managing their production software stacks

E4S

- Utilizes Spack to create a large collection of reusable HPC software packages
- E4S packages are tested regularly at OLCF, ALCF, and NERSC
- ParaTools provides support for E4S integration at facilities
- High-quality, tested, Spack recipes for facility systems

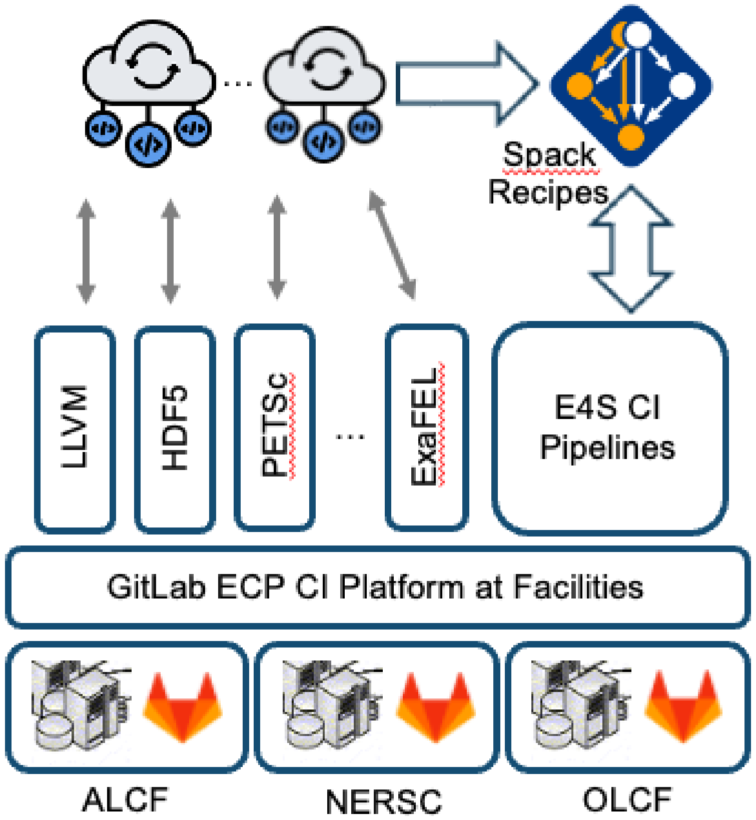
ECP Software Deployment

Team comprised of facility staff, at each site, to provide:

- Facility contacts for E4S team
- CI-based infrastructure for automated testing
- Operational software stack, driven by user requests and facility requirements

Facilitating Software Distribution (Spack, E4S, and CI Infrastructure)

- CI infrastructure at each facility enables automatic builds and testing directly on target systems.



Spack Recipes

LLVM

HDF5

PETSc

...

ExaFEL

E4S CI Pipelines

GitLab ECP CI Platform at Facilities

ALCF

NERSC

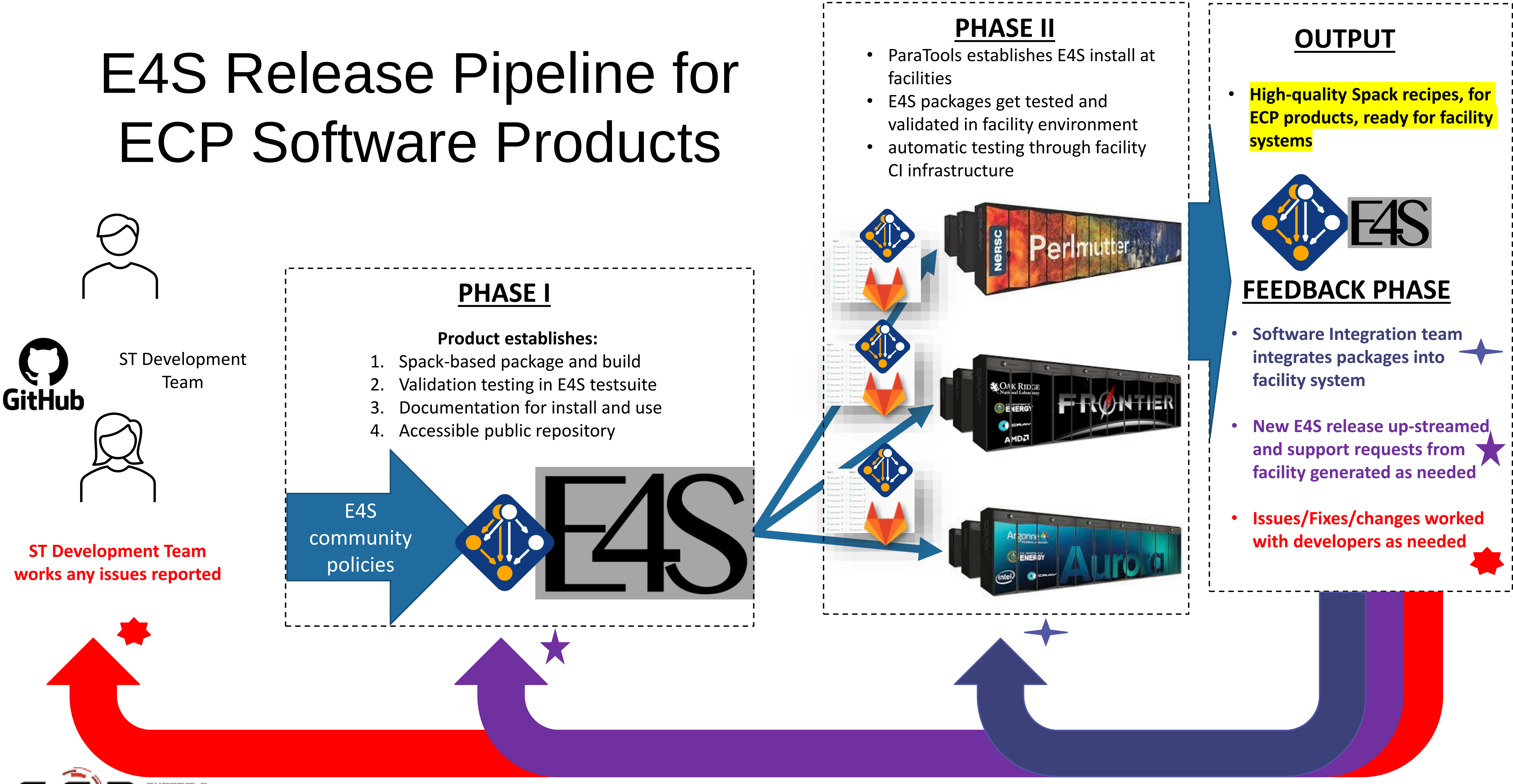
OLCF

- ParaTools establishes stable E4S Release for distribution

E4S

- E4S releases are shipped to facilities by ParaTools.
- Facilities manage and integrate software into their production environments (driven by their unique requirements)

E4S Release Pipeline for ECP Software Products



GitHub

ST Development Team

ST Development Team works any issues reported

PHASE I

Product establishes:

1. Spack-based package and build
2. Validation testing in E4S testsuite
3. Documentation for install and use
4. Accessible public repository

E4S community policies

PHASE II

- ParaTools establishes E4S install at facilities
- E4S packages get tested and validated in facility environment
- automatic testing through facility CI infrastructure

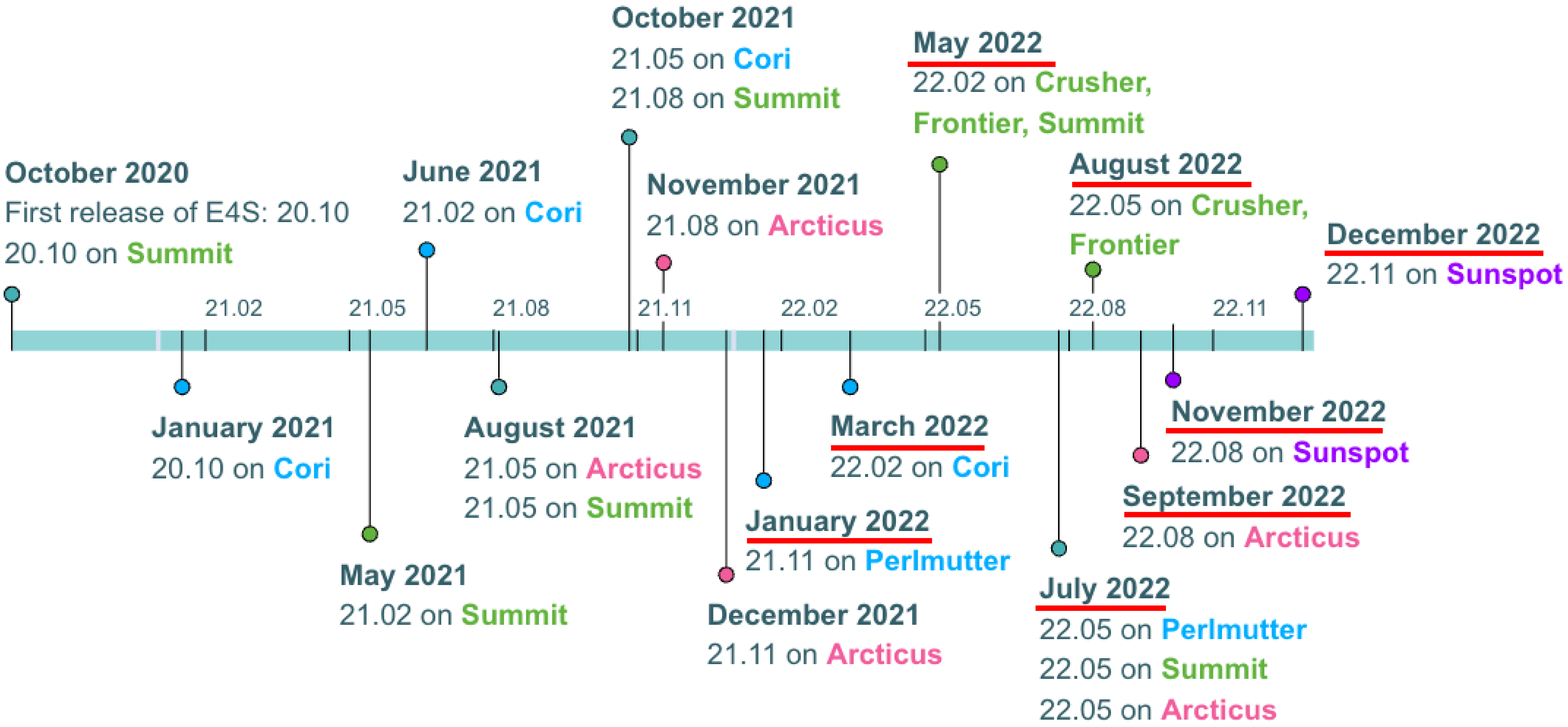
OUTPUT

- High-quality Spack recipes, for ECP products, ready for facility systems

FEEDBACK PHASE

- Software Integration team integrates packages into facility system
- New E4S release up-streamed and support requests from facility generated as needed
- Issues/Fixes/changes worked with developers as needed

E4S Release and Integration Timeline



October 2020
First release of E4S: 20.10
20.10 on Summit

January 2021
20.10 on Cori

May 2021
21.02 on Summit

June 2021
21.02 on Cori

August 2021
21.05 on Arcticus
21.05 on Summit

October 2021
21.05 on Cori
21.08 on Summit

November 2021
21.08 on Arcticus

December 2021
21.11 on Arcticus

January 2022
21.11 on Perlmutter

March 2022
22.02 on Cori

May 2022
22.02 on Crusher, Frontier, Summit

July 2022
22.05 on Perlmutter
22.05 on Summit
22.05 on Arcticus

August 2022
22.05 on Crusher, Frontier

September 2022
22.08 on Arcticus

November 2022
22.08 on Sunspot

December 2022
22.11 on Sunspot

Takeaways

- CI infrastructure, based on facility environments, is incredibly useful
  - Powers automatic testing and nightly builds
  - There are hurdles with regards to security/resources and providing *”true”* CI directly on production, multi-tenant, facility HPC systems

- Relationships are key
  - Enabling a sustainable ecosystem for teams to package, distribute, and manage software environments is important
  - E4S has shown how to create a vehicle for software, in collaboration with software and facility teams, by enabling targeted testing and releases to supported facilities
  - Important to work with facility staff to understand the unique needs and security constraints of their environments
  - ECP software deployment efforts are an excellent example for how to provide common standards and infrastructure to test and deliver software across facilities

Questions?

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https://www.exascaleproject.org

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ECP

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.