E4S: The Extreme-scale Scientific Software Stack for Collaborative Open Source Software

Michael A. Heroux, Sandia National Laboratories Director of Software Technology, US Exascale Computing Project

The 2nd E4S Forum September 24, 2020



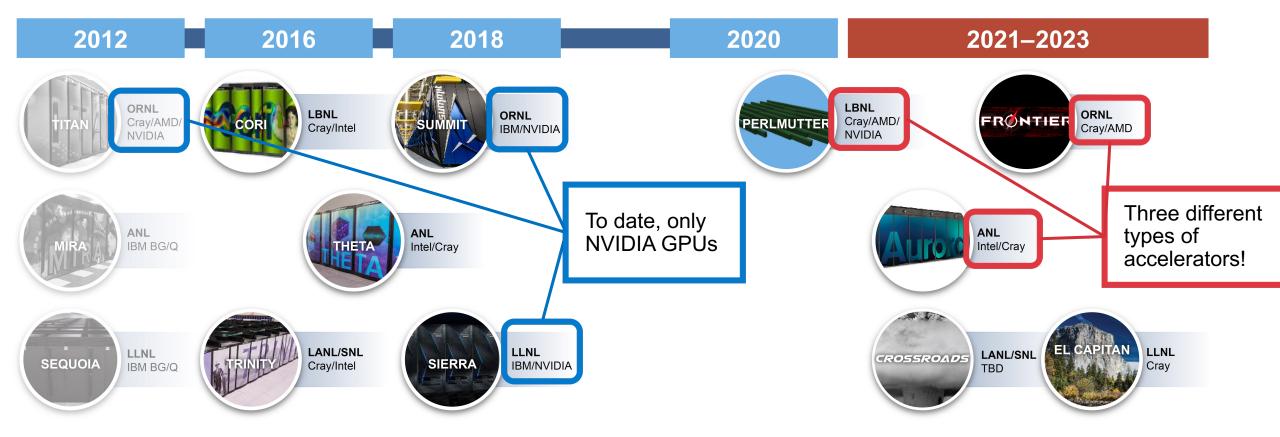


Department of Energy (DOE) Roadmap to Exascale Systems

An impressive, productive lineup of *accelerated node* systems supporting DOE's mission

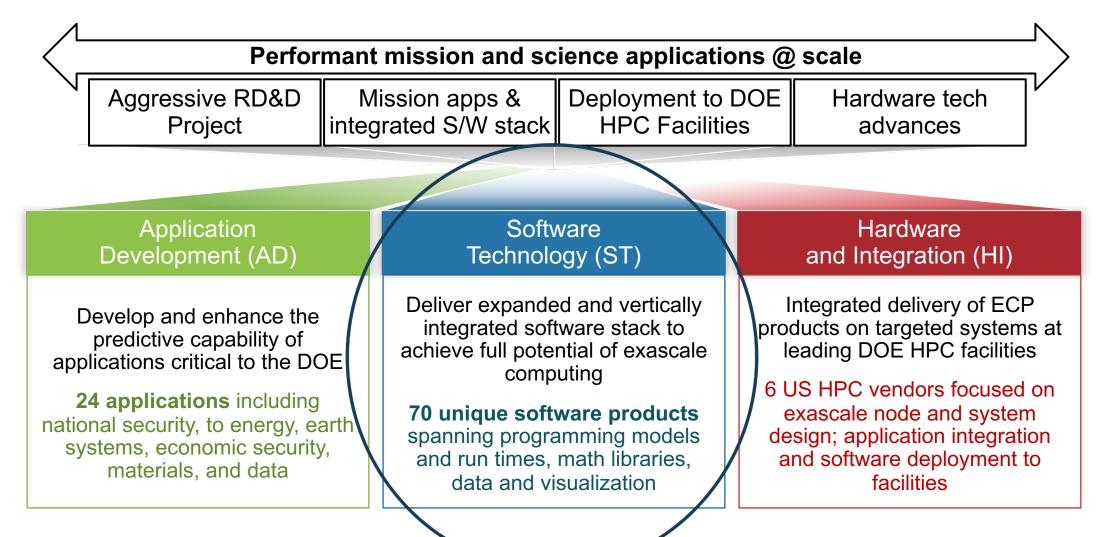
Pre-Exascale Systems

Future Exascale Systems





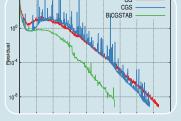
ECP Software Technology (ST) is one of three focus areas

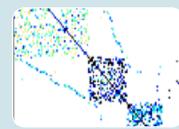




ECP ST has six technical areas











National Nuclear Security Administration

Programming Models & Runtimes

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

Development Tools

Continued, multifaceted capabilities in portable, opensource LLVM compiler ecosystem to support expected ECP architectures, including support for F18 Performance

analysis tools that accommodate new architectures, programming models, e.g., PAPI, Tau

Math Libraries

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

Data and Visualization

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

Software Ecosystem

Develop features in Spack necessary to support all ST products in E4S, and the AD projects that adopt it
Development of Spack stacks for reproducible turnkey deployment of large collections of software

Optimization and interoperability of containers on HPC systems
Regular E4S releases of the ST software stack and SDKs with regular

integration of new

ST products

NNSA ST

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

We work on products and applications needed now and into the future

Key themes:

- Exploration/development of new algorithms/software for emerging HPC capabilities:
- High-concurrency node architectures and advanced memory & storage technologies.
- Enabling access and use via standard APIs.

Software categories:

- The next generation of well-known and widely used HPC products (e.g., MPICH, OpenMPI, PETSc)
- Some lesser used but known products that address key new requirements (e.g., Kokkos, RAJA, Spack)
- New products that enable exploration of emerging HPC requirements (e.g., SICM, zfp, UnifyCR)

Example Products	Engagement
MPI – Backbone of HPC apps	Explore/develop MPICH and OpenMPI new features & standards.
OpenMP/OpenACC –On-node parallelism	Explore/develop new features and standards.
Performance Portability Libs: Kokkos, RAJA	Lightweight APIs for compile-time polymorphisms.
LLVM/Vendor compilers	Injecting HPC features, testing/feedback to vendors.
Perf Tools - PAPI, TAU, HPCToolkit	Explore/develop new features.
Math Libraries: BLAS, sparse solvers, etc.	Scalable algorithms and software, critical enabling technologies.
IO: HDF5, MPI-IO, ADIOS	Standard and next-gen IO, leveraging non-volatile storage.
Viz/Data Analysis	ParaView-related product development, node concurrency.

The Extreme-Scale Scientific Software Stack (E4S):



A collaborative HPC Linux Ecosystem

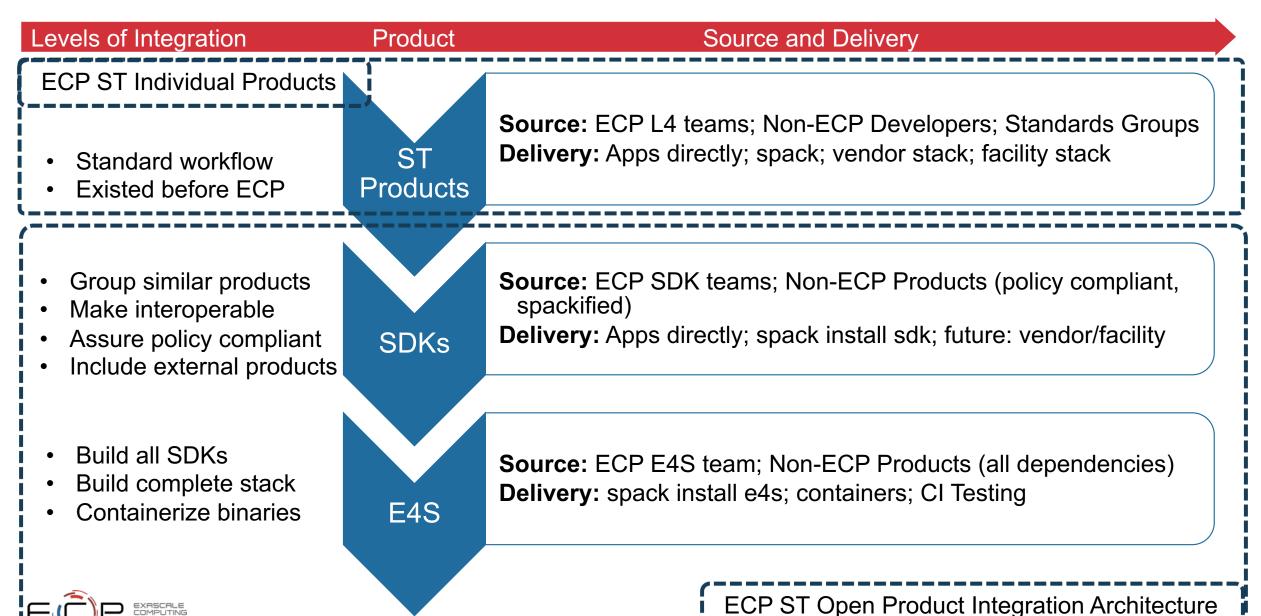




Delivering an open, hierarchical software ecosystem



Delivering an open, hierarchical software ecosystem



E4S Components

- E4S is a curated release of ECP ST products based on Spack [http://spack.io].
- E4S Spack cache to support bare-metal installs at facilities and custom container builds:
 - x86_64, ppc64le, and aarch64
- Container images on DockerHub and E4S website of pre-built binaries of ECP ST products.
- Base images and full featured containers (GPU support).
- GitHub recipes for creating custom images from base images.
- e4s-cl for container launch and for replacing MPI in application with system MPI libraries.
- Validation test suite on GitHub provides automated build and run tests.
- Automates build process via GitLab Continuous Integration to ensure packages can be built.
- E4S Doc Portal aggregates and summarizes documentation and metadata by raking product repos.
- E4S VirtualBox image with support for Docker, Shifter, Singularity, and Charliecloud runtimes.
- AWS image to deploy E4S on EC2.

https://e4s.io



Extreme-scale Scientific Software Stack (E4S)

- <u>E4S</u>: A Spack-based distribution of ECP ST and related and dependent software tested for interoperability and portability to multiple architectures
- Provides distinction between SDK usability / general quality / community and deployment / testing goals
- Will leverage and enhance SDK interoperability thrust
- Oct 2018: E4S 0.1 24 full, 24 partial release products
- Jan 2019: E4S 0.2 37 full, 10 partial release products
- Nov 2019: E4S 1.0 <u>50 full</u>, 5 partial release products
- Feb 2020: E4S 1.1 50 full, 10 partial release products



<u>e4s.io</u>

Lead: Sameer Shende (U Oregon)



E4S 1.1 Full Release: 50 ECP Packages and all dependencies

- Adios
- AML
- Argobots
- Bolt
- Caliper
- Darshan
- Dyninst
- Faodel
- Flecsi
- Gasnet
- GEOPM
- Gotcha
- HDF5
- HPCToolkit
- Hypre

- Kokkos
- Legion
- Libnrm
- Libquo
- Magma
- Mercury
- MFEM
- MPICH
- MPIFileUtils
- Ninja
- OpenMPI
- PAPI
- Papyrus
- Parallel
 netCDF

- PDT
- PETSc
- Qthreads
- Raja
- Rempi
- SCR
- Spack
- Strumpack
- Sundials
- SuperLU
- SZ
- Tasmanian
- TAU
- Trilinos
- Turbine

				3. ssh				
linux-centos7-	x86_64 / gcc@4.8.	5						
	cuda@9.1.85	gmp@6.1.2	kokkos@2.03.00	libxml2@2.9.4		openssl@1.0.2n	readline@7.0	
automakee1.15.1	flex@2.6.4	help2man@1.47.4	libpciaccess@0.13.5	m4@1.4.18	ncurses86.0	papi@5.5.1	tar@1.29	
bison@3.0.4	gcc@7.3.0	hwloc@1.11.9	libsigsegv@2.11	magma@2.4.0	numactl@2.0.1	1 pdt@3.25	util-macros@1.19.1	
bzip2@1.0.6	adbm@1.14.1	hwloc@2.0.1	libtool@2.4.6	mpc@1.1.0	openblase0.2.	20 perl@5.24.1	xz@5.2.3	
cmake@3.11.1	gettext@0.19.8.1	isl@0.19	libunwind@1.1	mpfr@4.0.1	openmpi@3.0.1	pkgconf@1.4.0	zlib@1.2.11	
linux-centos7-	x86_64 / acc@7.3.	0						
adios@1.13.1	freetypee2.	7.1	ison-c@0.13.1	libxfixes@5.	0.2 p	api@5.5.1	pv-mccabe@0.6.1	salite@3.22.0
adlbxe0.8.0	gasnete1.30	.0	kbprotoe1.0.7	libxml202.9	4 0	apyrus@develop	py-mocke2.0.0	stc 0.7.3
adlbxe0.8.0	gasnet@1.30	.0	kokkos@2,03,00	libxshmfence		araview@5.4.1	py-mpi4py@3.0.0	strumpack@3.1.
ant@1.9.9	qdb@8.0.1		kytree@1.0.2	libxt@1.1.5	p	armetis@4.0.3	py-natsort@5.2.0	suite-sparse@5
autoconf@2.69	adbm@1.14.1		lcms@2.8	libxv@1.0.10	, r	atch@2.7.6	py-nose@1.3.7	sundials@3.1.0
automakee1.14	geopm@0.4.0		legion@17.10.0	libxvmc@1.0	9 p	cre@8.41	py-numexpr@2.6.1	superlu85.2.1
automakee1.15.1	gettext@0.1		leveldb@1.20	libyogrt@1.2	0-6 0	cre@8.41	py-numpy@1.13.3	superlu-dist@5
ax180.1.1	git@2.15.1		libarchive@3.3.2	1mod@7.7.13		dsh@2.31	py-pandas@0.21.1	swig@3.0.12
binutils@2.27	alib@2.56.0		libbsd@0.8.6	lug@5.3.4		dt@3.25	py-pbr@3.1.1	sz@1.4.12.3
binutils@2.29.1	alm@0.9.7.1		libcircle@0.2.1-rc.	lua-luafiles	vstem®1 6 3 n	erl@5.24.1	py-pillow@3.2.0	tor@1.29
bison@3.0.4	globalarray		libedit@3.1-20170329			etsc@3.8.4	py-pkgconfig@1.2.2	tasmanian86.0
bolt@1.0b1	alproto@1.4		libffi@3.2.1	lwarp@1.0.2		flotran@xsdk-0.3.0	py-py@1.4.33	tau@2.28
boost@1.66.0	amp86.1.2		libice@1.0.9	lz4@1.8.1.2	, p	ixman@0.34.0	py-pycodestyle@2.3.1	tcl@8.6.8
boost@1.66.0	gobject-int	rospection@1.49.2	libiconv@1.15	lzma@4.32.7	, 1	kaconf@1.4.0	py-pyflakes@1.6.0	texinfo@6.5
boost@1.68.0	gotchae0.0.	2	libjpeg-turbo@1.5.3	1zo@2.09	, p	resentproto@1.0	py-pyparsing@2.2.0	tk@8.6.8
bzip2@1.0.6	got chaedeve		libmna@2.0.3	m4@1.4.18		rotobuf@3.5.1.1	py-pytables@3.3.0	trilinos@12.12
c-blosc@1.12.1	aperf@3.0.4		libpciaccess@0.13.5			v-araparse@1.4.0	py-pytest@3.6.0	turbine@1.0.0
cairo@1.14.12	harfbuzzel.		libpfm484.8.0	metis@5.1.0		y-babel@2.4.0	py-pytz@2017.2	turbine 1.0.0
caliper@1.8.0	hdf5@1.8.19		libpng@1.6.34	mfem@3.3.2		v-bottleneck@1.0.0	py-scipy@1.0.0	umpire@master
cmake@3.11.1	hdf5@1.8.19		libpthread-stubse0.4	miniconda2		y-configparser@3.5.0		unifvcremaster
conduitemaster	hdf5@1.10.1		libauo@1.3	miniconda3		v-cvcler@0.10.0	py-six@1.11.0	util-macrose1.
curl@7.59.0	hdf5@1.10.1		libsigsegv@2.11	mpich@3.2.1		v-cvthon@0.28.1	py-subprocess32@3.2.7	veloce1.0
damageproto@1.2.1	hdf5@1.10.1		libsm@1.2.2	mumps@5.1.1	, 1	v-dateutil@2.5.2	python@2.7.14	videoproto@2.3
darshan-runtime@3			libtiff@4.0.6	nasm@2.13.03		v-enum34@1.1.6	ghull@2015.2	vtkm@master
darshan-util@3.1.	6 help2man@1.	47.4	libtiff@4.0.8	ncurses@6.0		v-flake8@3.5.0	athreads@1.12	vtkm@1.1.0
doxygen@1.8.12	hpctoolkit		libtool@2.4	netcdf@4.4.1		v-funcsias®0.4	r@3.4.3	xcb-proto@1.13
dtcmp@1.1.0	hpctoolkit-	externalse2017.06	libtool@2.4.2	netlib-scald		y-functools3283.2.3	-2 raja@0.5.3	xextproto@7.3.
er@0.0.3	hwloc@1.11.		libtool@2.4.6	nettle@3.3		v-h5pv@2.7.1	ronkstr@0.0.2	xproto@7.0.31
exmcutils@0.5.3	hwloc@2.0.1		libunwind@1.1	ninja@1.8.2		y-hypothesis@3.7.0	readline@7.0	xtrans@1.3.5
expat@2.2.2	hypre@2.13.		libx11@1.6.5	numactl@2.0		y-jinja2@2.9.6	redset@0.0.3	xz@5.2.3
fftw@3.3.7	hypre@2.13.		libxqu@1.0.8	openblase0.2		v-kiwisolver@1.0.1	ruby@2.2.0	zfp@0.5.0
fixesproto@5.0	icu4c@60.1		libxcb@1.13	openmpi@3.0		v-lit@0.5.0	ruby-ronn@0.7.3	zlib@1.2.11
flex@2.6.4	inputproto	2.3.2	libxdamage@1.1.4	openssl@1.0		v-mako@1.0.4	scr@1.2.2	zsh@5.4.2
font-util@1.3.1	intel-tbb@2		libxdmcp@1.1.2	otf202.1		v-markupsafe@1.0	shuffile@0.0.3	zstd@1.3.0

Packages installed using Spack

- Umpire
- UnifyFS
- UPC++ Veloc
- Zfp

All ST products will be released through E4S



Partial (in-progress) Release: ASCENT, Catalyst, Flang, libEnsemble, LLVM, Visit, others

E4S Software Development Kits (SDKs):

Collaborative community development of complementary software capabilities





Software Development Kits (SDKs): Key delivery vehicle for ECP

A collection of related software products (packages) where coordination across package teams improves usability and practices, and foster community growth among teams that develop similar and complementary capabilities

- **Domain scope** Collection makes functional sense
- Interaction model How packages interact; compatible, complementary, interoperable
- **Community policies** Value statements; serve as criteria for membership
- Meta-infrastructure

Invokes build of all packages (Spack), shared test suites

Coordinated plans
 Inter-package planning. Augments autonomous package planning

• **Community outreach** Coordinated, combined tutorials, documentation, best practices

ECP ST SDKs: Grouping similar products for collaboration & usability

Programming Models & Runtimes Core

Tools & Technologies

Compilers & Support



Math Libraries (xSDK)

Viz Analysis and Reduction

Data mgmt., I/O Services & Checkpoint/ Restart

"Unity in essentials, otherwise diversity"



xSDK version 0.5: November 2019 (21 math libs, 2 domain-specific packages)

- AMReX
- ButterflyPACK
- DTK
- deal.ii
- Ginkgo
- hypre
- libEnsemble
- MAGMA
- MFEM
- Omega_h

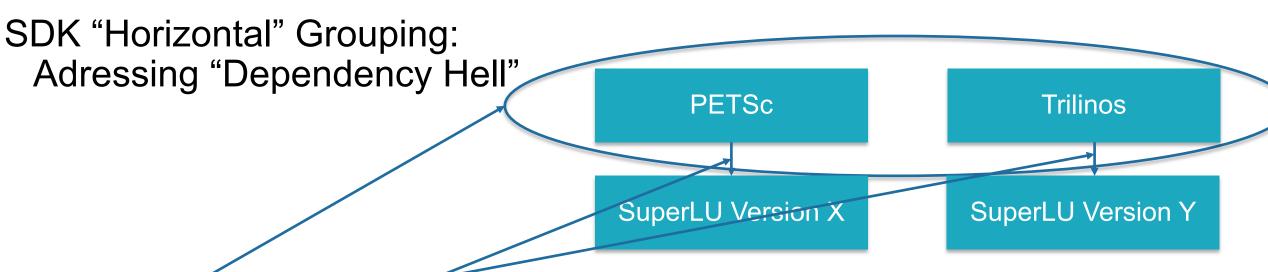
- PETSc/TAO
- PHIST
- PLASMA
- preCICE
- PUMI
- SLEPc
- STRUMPACK
- SUNDIALS
- SuperLU
- Tasmanian

- Trilinos
- Pflotran
- Alquimia

Notes:

- Growth:
 - 5 in release 0.1.
 - 7 in 0.2
 - 9 in 0.3
 - 19 in 0.4
 - 23 in 0.5
- You do not need to build all packages.
- We build and test all packages.
- Any subset is guaranteed to build if using the same build parameters, platforms.
- Similar builds should work or require less effort for success.





Horizonal (vs Vertical) Coupling

- Common substrate
- Similar function and purpose
 - •e.g., compiler frameworks, math libraries

Horizontal grouping:

- Assures X=Y.
- Protects against regressions.
- Transforms code coupling from heroic effort to turnkey.
- Potential benefit from common Community Policies
 - •Best practices in software design and development and customer support
- Used together, but not in the long vertical dependency chain sense
- Support for (and design of) common interfaces
 - Commonly an aspiration, not yet reality



xSDK compatible package: Must satisfy mandatory xSDK policies:

- M1. Support xSDK community GNU Autoconf or CMake options.
- M2. Provide a comprehensive test suite.
- M3. Employ user-provided MPI communicator.
- **M4**. Give best effort at portability to key architectures.
- **M5.** Provide a documented, reliable way to contact the development team.
- **M6.** Respect system resources and settings made by other previously called packages.
- M7. Come with an open source license.

M8. Provide a runtime API to return the current version number of the software.

 $\ensuremath{\textbf{M9.}}$ Use a limited and well-defined symbol, macro, library, and include file name space.

- M10. Provide an accessible repository (not necessarily publicly available).
- M11. Have no hardwired print or IO statements that cannot be turned off.

M12. For external dependencies, allow installing, building, and linking against an outside copy of external software.

- M13. Install headers and libraries under <prefix>/include/ and <prefix>/lib/.
- M14. Be buildable using 64 bit pointers. 32 bit is optional.
- **M15.** All xSDK compatibility changes should be sustainable.

M16. The package must support production-quality installation compatible with the xSDK install tool and xSDK metapackage.

Also **recommended policies**, which currently are encouraged but not required:

R1. Have a public repository.

R2. Possible to run test suite under valgrind in order to test for memory corruption issues.

R3. Adopt and document consistent system for error conditions/exceptions.

R4. Free all system resources it has acquired as soon as they are no longer needed.

R5. Provide a mechanism to export ordered list of library dependencies.

R6. Document versions of packages that it works with or depends on, preferably in machine-readable form

R7. Have README, SUPPORT, LICENSE, and CHANGELOG files in top directory.

xSDK member package: Must be an xSDK-compatible package, *and* it uses or can be used by another package in the xSDK, and the connecting interface is regularly tested for regressions.



BSSw blog article: P. Luszczek and U. Yang, Aug 2019,

https://bssw.io/blog_posts/building-community-through-software-policies

ECP ST SDKs will span all technology areas

Motivation: Properly chosen cross-team interactions will build relationships that support interoperability, usability, sustainability, quality, and productivity within ECP ST.

Action Plan: Identify product groupings where coordination across development teams will improve usability and practices and foster community growth among teams that develop similar and complementary capabilities

	Compilers and Support (7)	Tools and Technology (11)	xSDK (16)	Visualization Analysis and Reduction (9)	Data mgmt, I/O Services, Checkpoint restart (12)	Ecosystem/E4S at-large (12)
	openarc	TAU	hypre	ParaView	SCR	mpiFileUtils
Papyrus	Kitsune	HPCToolkit	FleSCI	Catalyst	FAODEL	TriBITS
SICM	LLVM	Dyninst Binary Tools	MFEM	VTK-m	ROMIO	MarFS
Legion	CHiLL autotuning comp	Gotcha	Kokkoskernels	SZ	Mercury (Mochi suite)	GUFI
Kokkos (support)	LLVM openMP comp	Caliper	Trilinos	zfp	HDF5	Intel GEOPM
RAJA	OpenMP V & V	PAPI	SUNDIALS	Vislt	Parallel netCDF	BEE
CHAI	Flang/LLVM Fortran comp	Program Database Toolkit	PETSc/TAO	ASCENT	ADIOS	FSEFI
PaRSEC*		Search (random forests)	libEnsemble	Cinema	Darshan	Kitten Lightweight Kernel
DARMA		Siboka	STRUMPACK	ROVER	UnifyCR	COOLR
GASNet-EX		C2C	SuperLU		VeloC	NRM
Qthreads		Sonar	ForTrilinos		IOSS	ArgoContainers
BOLT			SLATE		HXHIM	Spack
UPC++			MAGMA			
MPICH			DTK	PMR Tools		
Open MPI			Tasmanian		Legend	
Umpire			TuckerMPI	Data a	and Vis	
AML				Ecosy	stems and delivery	

E4S Community Candidate Policies V 1.0 Beta

Spack-based Build and Installation

Each E4S member package supports a scriptable Spack build and production-quality installation in a way that is compatible with other E4S member packages in the same environment. When E4S build, test, or installation issues arise, there is an expectation that teams will collaboratively resolve those issues.

• Minimal Validation Testing

Each E4S member package has at least one test that is executable through the E4S validation test suite (<u>https://github.com/E4S-Project/testsuite</u>). This will be a post-installation test that validates the usability of the package. The E4S validation test suite provides basic confidence that a user can compile, install and run every E4S member package. The E4S team can actively participate in the addition of new packages to the suite upon request.

Sustainability

All E4S compatibility changes will be sustainable in that the changes go into the regular development and release versions of the package and should not be in a private release/branch that is provided only for E4S releases.

Product Metadata

Each E4S member package team will provide key product information via metadata that is organized in the E4S DocPortal format. Depending on the filenames where the metadata is located, this may require minimal setup.

Public Repository

Each E4S member package will have a public repository, for example at GitHub or Bitbucket, where the development version of the package is available and pull requests can be submitted.

Imported Software

If an E4S member package imports software that is externally developed and maintained, then it must allow installing, building, and linking against a functionally equivalent outside copy of that software. Acceptable ways to accomplish this include (1) forsaking the internal copied version and using an externally-provided implementation or (2) changing the file names and namespaces of all global symbols to allow the internal copy and the external copy to coexist in the same downstream libraries and programs.

• Error Handling

Each E4S member package will adopt and document a consistent system for signifying error conditions as appropriate for the language and application. For e.g., returning an error condition or throwing an exception. In the case of a command line tool, it should return a sensible exit status on success/failure, so the package can be safely run from within a script.

Test Suite

Each E4S member package will provide a test suite that does not require special system privileges or the purchase of commercial software. This test suite should grow in its comprehensiveness over time. That is, new and modified features should be included in the suite.



E4S/SDK Policy Initiative Status

- Community policies are important for several reasons:
 - Commitment to quality
 - Membership criteria for the future
 - Community discussion
- Each SDK community developing policies like Math Libs (xSDK).
- Policies common to all SDKs will be promoted to E4S level
- Policies will determine:
 - Quality label
 - Membership in E4S and the SDKs
- Version 1.0 of policies due by end of 2020

		t-2 E4S Edit Vie		mmunity Format To			A G	Last edit		
	-	A, 🗗	100% 👻	Normal tex	t 👻	Calibri			‡≡ ≟≡ • 7 • • • •	• ⊟ • ₫
→ DK).			scriptable Spack bui member packages in expectation that tes executable through post-installation tes basic confidence th actively participate Promote to E45 list changes go into the private release/bran Circle back: P4 <u>Port</u> common platforms. operating systems, configurations shou including standard 1 accelerators. Consid	nbership Criteria P1 Spack-based Build a Iid and production-quail iid and production-quail ms will collaboratively P2 Minimal Validation test the 454 validation test that validates the usal at a user can compile, ir in the addition of new p P3 Sustainability All E44 regular development a hich that is provided only ability Each E4S membe Depending on the func compiler toolchains, are Iid be denoted in approg inux distributions, com er self asseed portat P5 Product Metadata 1	ty installation in . When EAS but sesolve those is <u>festing Each E4</u> uiting the the <u>pace</u> stall and run exackages to the S compatibility d release versi for EAS releaso r package team tion of the men- hitectures and riate Spack pace.	n a way that is iiid, test, or inst issues. IS member paci thub.com/EAS- kage. The EAS very EAS memb suite upon req changes will bl ions of the paci es. n will make a be mber package, accelerators. Li ckages when pu colchains, and ric - OS, GPU, e	compatible will allattion issues kage has at lea Project/testsu alldation test er package. Th uest. e sustainable in cage and shoul est effort at poo considerations ack of support sostible. different archi tc?	h other E4S arise, there is an stone test that is te). This will be a uite provides e E4S team can that the d not be in a tability to may include for tectures and		Jin 12: For some run exclus services a this is not the run exclus services a this is not 12: David Bee testsuite r the tests ; sprovided t Spack har since t its



E4S DocPortal

A Single Portal with Redirect to Product Documentation





Product Documentation Challenges: User Perspective



What it does License Support Contact info More ...



Finding new products What can solve my problem

Trusting accuracy of information

Up to date Complete

Hierarchical

Summary to deep dive



Product Documentation Challenges: Developer Perspective



Efficient and Effective generation and maintenance



Getting noticed by new users



Conveying summary information *and* details



E4S DocPortal Requirements



Provide a single online location for *accurate* product descriptions for ECP software products.



Derived requirements

Sustainable: Must be integrated into software team workflows.

Incremental: Must build on community approaches to providing this information.

Extensible: Must be usable by any open source software team.



E4S Documentation Portal Strategy



All content resides in product repositories

Use open source community approach of speciallyname files in software repositories. Adopt commonly used file names when available. ID new information items not already being requested.



Documentation portal provides single point of access

Web-based raking tool capture information from product repositories and present in summary form.

Aggregates and summarizes documentation and metadata for E4S products

Regularly updates information directly from product repositories

Location: <u>https://e4s-project.github.io/DocPortal.html</u>



E4S DocPortal Status



- Completed DocPortal Prototype and Design Document
- Reviewed prototype/design with Facilities and ST developers
- Version 1.0 available now:
 - https://e4s-project.github.io/DocPortal.html
 - Available from <u>e4s.io</u>
- Next steps:
 - Work with ECP ST teams to improve amount and quality of raked content
 - Develop policy and acceptance criteria for E4S DocPortal membership



E4S Products

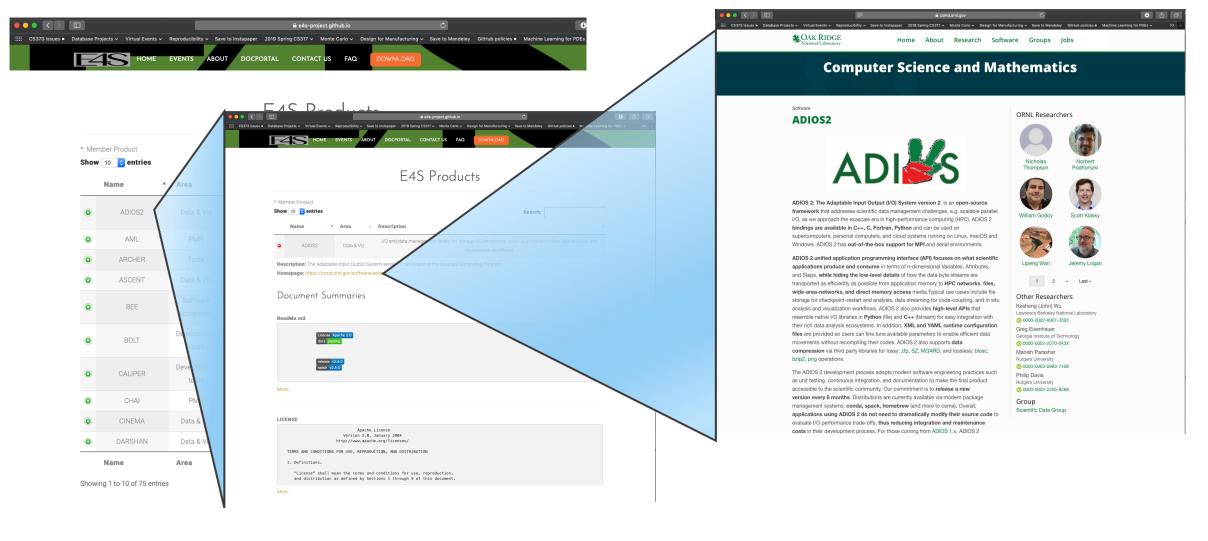
- Summary Info
 - Name
 - Functional Area
 - Description
 - License
- Searchable
- Sortable

Naı	ne	Area	Description Search:		
0	ADIOS2	Data & Viz	I/O and data management library for storage I/O, in-memory code coupling and online acta analysis and visualization workflows.		
0	AML	PMR	Hierarchical memory management library from Argo.		
0	ARCHER	Tools	Data race detection tool for OpenMP applications		
0	ASCENT	Data & Viz	Flyweight in situ visualization and analysis runtime for multi-physics HPC simulations		
0	BEE	Software Ecosystem	Container-based solution for portable build and execution across HPC systems and cloud resources		
0	BOLT	Development Tools	OpenMP over lightweight threads.		
0	CALIPER	Development tools	Performance analysis library.		
0	CHAI	PMR	A library that handles automatic data migration to different memory spaces behind an array-style interface.		
0	CINEMA	Data & Viz	Data analysis and visualization tool suite.		
0	DARSHAN	Data & Viz	I/O characterization tool.		



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

Goal: All E4S Product Documentation Accessible from single portal on E4S.io (Working Mock Webpage below)





Q: What do we need for adding a product to the DocPortal? A: A repo URL + up-to-date meta-data files

<u> </u>						_		6	github.com	_	
	CS373 Issu	es∎ Dat	tabase Projects 💊	 Virtual Events 	Reproducibility	 Save to Inst 	tapaper 20	019 Spring CS317	7 ∽ Monte Carlo	 Design for Manu 	ufacturing 🗸 S
		arah ar i			D						
	Se Se	arch or j	ump to		Pull requests	issues r	Marketpla	ce Explore			
1	"∃ E4S-F	Project	/ E4S-Do	cumenter							
						_					
	<> Code	(!)	Issues 2	 Pull reques 	sts 🕞 Actio	ons 凹 P	Projects	🕮 Wiki	Security	✓ Insights	Settir
		۲2 m	naster 👻	E4S-Documen	nter / data / e4	s products	s.vaml				
		\$ 11			,, .		.,				
			Wyatt Spear	Added more pro	ducts.						
		શ્ર 0	contributors								
		127	lines (127 s)	loc) 5.79 KB							
		1	- version:	. 0 1 0							
	<	2		l: https://gith	ub.com/ornladi	os/ADIOS2/b	lob/maste	r	>		
		3	#AID								
		4	 repo_url 	l: https://gith	ub.com/LLNL/ST	AT/blob/dev	elop				
		5	 repo_url 	l: https://gith	ub.com/PRUNERS	/archer/blo	b/master				
		6	 repo_url 	l: https://gith	ub.com/PRUNERS	/FLiT/blob/	devel				
		7	 repo_url 	l: https://gith	ub.com/PRUNERS	/ReMPI/blob	/master				
		8	 repo_url 	l: https://gith	ub.com/LLNL/FP	Checker/blo	b/master				
		9	#/AID								
		10	 repo_url 	l: https://xgit	lab.cels.anl.g	ov/argo/aml,	/blob/mas	ter			
		11	#ALPINE								
		12	 repo_url 	l: https://gith	ub.com/Alpine-	DAV/ascent/l	blob/deve	lop			
		13	 repo_url 	l: https://gitl	ab.kitware.com	/paraview/pa	araview/-	/blob/master			
		1.4	#_catalvet	Part of ParaVi	02						
		14	#-catatyst	Fart OF Faravi	ewr						

0007015500	E4S-Documenter/e4s_products.yaml at mast	roducibility - Save to Instapaper 2019 Spring CS317 - Monte Carlo - Desig er - E4S-Project/E4S-Documenter or		endeley GitHub policies = Machine Learning for PDEs ~ I ADIOS developed in the Exascale Computing Program
Sea	arch or jump to 7 Pul	l requests Issues Marketplace Explore		4 · ·
ornlad	lios / ADIOS2			⊘ Watch + 25 ☆ Star 101 ♀ Fork
<> Code	Issues 127 Issues 127	13 🕟 Actions 🛄 Projects 🛄 Wiki 😲 Security	└── Insights	
	🐉 master 👻 🐉 6 branches 🛇 11	tags Go to file Ad	d file - 🗠 Code -	About
	log eisenhauer Merge pull request #24	68 from eisenhauer/SendWarn × 571d695 4 days	ago 🕚 6,741 commits	Next generation of ADIOS developed in the Exascale Computing Program
	.circleci	Re-enable asan builds	3 months ago	\mathscr{O} adios2.readthedocs.io/en/latest/ind
	github	Merge pull request #2193 from chuckatkins/add-spack-ci-image	last month	adios cmake exascale-computing
	gitlab	ci: Move GitHub PR -> GitLab sync to gitlab.com	4 months ago	hdf5 hpc io ecp exascale
	bindings	bindings: Help C++11 clients avoid calling serial constructor with	MP last month	🛱 Readme
	Cmake	Fix typos in adios2-config generation script	last month	赴 View license
	docs	Merge pull request #2397 from pnorbert/bp4-stream-reader-mo	de 2 months ago	
	examples	examples: Fix helloSstWriter to avoid MPI constructor in serial bu	ild last month	Releases 11
	scripts	Bump minimum cmake versions in scripts as appropriate	last month	ADIOS v2.6.0 Production R (Latest) on May 30
	source	Merge pull request #2468 from eisenhauer/SendWarn	4 days ago	+ 10 releases
	testing	check read results	10 days ago	
	thirdparty	Merge branch 'upstream-EVPath' into Mismatch	12 days ago	Packages
	🗅 .clang-format	Update the clang-format config file	2 years ago	No packages published
	Clang-tidy	Reinstate the use of reinterpret_cast	4 years ago	
		Ignore files generated by readthedocs.	7 months ago	Contributors 32
1	Contributing.md	Restore CentOS 8 travis build	last month	🚱 🕲 🔕 🚱 🕂 🕆 🚷
_	ů.	superfluous check on CMake version.	3 months ago	
7	O any might to t		2 years ago	+ 21 contributors
	Copyright.txt	arnings	2 months ago	
		edocs warnings	15 months ago	Languages
٩	LICENSE	d BZIP2 64-bit	16 months ago	
_	2.02.102	se text	15 months ago	 C++ 70.7% CMake 9.0% Fortran 8.1% C 7.9%
		oftware X paper in README.	2 months ago	 Python 2.1% Shell 0.9% Other 1.3%
٩	ReadMe.md	Resurrect macOS builds on Azure Pipelines	last month	- • • • • • • • • • • • • • • • • • • •
		tell codacy / bandit to accept assert in python	2 years ago	

E4S DocPortal Initiative Status: Fall 2020

- Completed DocPortal Prototype and Design Document
- Reviewed prototype/design with Facilities and ST developers
- Version 1.0 available now: <u>https://e4s-project.github.io/DocPortal.html</u>
- Next steps:
 - Work with ECP ST teams to improve amount and quality of raked content
 - Develop policy and acceptance criteria for E4S DocPortal membership



How to Access E4S Software

From Source and Many Other Ways





E4S v1.1 Access

- From e4s-project.github.io
 - Source via Spack
 - E4S v1.1 GPU image
 - Docker, Singularity (ppc64le, x86_64) ...
- E4S v1.1 Release Available at DockerHub
 - 40+ ECP ST Products
 - Support for GPUs
 - NVIDIA
 - (CUDA 10.1.243)
 - ppc64le and x86_64
- Visit https://e4s.io for more details

		0		
	Ubuntu 18.04	CentOS 7		
ocker GitHub 🛓	E4S v1.1 GPU IMAGE ecpe4s/ubuntu1804-e4s-gpu (x86_64 with 	BASE IMAGES ecpe4s/centos7_x86_64_base 📥 doc	ter.	
locker GitHub 🚣	ROCm and CUDA)	GitHub	xer	
	• ecpe4s/ubuntu1804-e4s-gpu (ppc64le with	pe4s/centos7_ppc64le_base 🕁 do	cker	
MAGE	CUDA) 👉 docker GitHub 🛓	GitHub 🕂		
ker GitHub 🛓	BASE IMAGES	E4S COMPREHENSIVE IMAGE		
	ecpe4s/ubuntu1804_x86_64_base 👉 docker	exascaleproject/e4s_x86_64	GitHub	
$\bullet \bullet \checkmark$		roject.github.io/download.html	o Anno 1997 format an E40 ann ann	• • • +
			compressed XZ format on E4S servers.	
	Recipes for building ima	ges from scratch are availab	le on the E4S GitHub repository.	
	Our recipes make use of Spa	ck packages available as pre	-built binaries in the E4S build cache.	
	L Container		From source with	
	Releases		Caral	
	Keleases		Spack	
	• Docker Dowr	lload	☑ Visit the Spack Project	I
	Gingularity v		Spack contains packages for all of	
	● Singularity xt	36_64 Download		
			Spack contains packages for all of	
	Singularity p	36_64 Download	Spack contains packages for all of the products listed in the E4S 1.0	
		36_64 Download	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above	
	 Singularity p CharlieCloud 	36_64 Download bc64le Download Download	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the	
	Singularity p	36_64 Download bc64le Download Download	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more	
	 Singularity p CharlieCloud 	36_64 Download bc64le Download Download	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see	
	 Singularity p CharlieCloud OVA Downlost 	36_64 Download Doc64le Download Download	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the	
	 Singularity p CharlieCloud 	36_64 Download Doc64le Download Download	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see	(à.
	 Singularity p CharlieCloud OVA Downloa 	36_64 Download Doc64le Download Download ad	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the	is Get Help 👻 exascaleproject 👻 鑀
	 Singularity p CharlieCloud OVA Downloa 	36_64 Download Doc64le Download Download ad	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the	
	 Singularity p CharlieCloud OVA Downloa 	36_64 Download boc64le Download Download ad erhub • reselutionmut 804-ets-gpu expets/ubuntut 804-ets-gpu	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the returned at the sector of t	is Get Help 👻 exascaleproject 👻 鑀
	 Singularity p CharlieCloud OVA Downloa 	36_64 Download Doc64le Download Download ad er hub	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the weare the second se	s Get Help • exascaleproject • 😜 Using 0 of 1 private repositories. <u>Get more</u>
	 Singularity p CharlieCloud OVA Downloa 	36_64 Download Doc64le Download Download ad er hub	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the returned at the sector of t	s Get Help • exacularproject • 💽 Using 0 of 1 private repositories. Get more Manage Repository
	 Singularity p CharlieCloud OVA Downloa 	36_64 Download bc64le Download Download ad (© @ reserved erycuty (@ coesevidentuit 8.64-eks geu ecyce4s/ubuntuit 8.64-eks geu) ecpce4s/ubuntuit 8.64-eks geu) ecpce4s/ubuntuit 8.64-eks geu)	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the weare the second se	s Get Help • exacularproject • 💽 Using 0 of 1 private repositories. Get more Manage Repository
	 Singularity p CharlieCloud OVA Downloa 	36_64 Download Download ad e nut	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the weare the second se	s Get Help • exacularproject • 💽 Using 0 of 1 private repositories. Get more Manage Repository
	Singularity p CharlieCloud OVA Downlor	36_64 Download Download ad ad certus cert	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the weare the second se	 Get Help • exascaleproject •
	Singularity p CharlieCloud OVA Downlor	36_64 Download Download ad	Spack contains packages for all of the products listed in the E4S 1.0 Full Release category (see above 1.0 Release Notes). General instructions for building software with Spack can be found at the Spack website. For more information, see /usr/local/packages/ecp in the weare the second se	s Get Help • exacutalization exact • exact of the second s

UB BASE IN ecpe4s/ubi7_x86_64_b; ecpe4s/ubi7_ppc64le_b; E4S COMPREHI ecpe4s/ubi7_x86_64_e;

CUSTOM

ecpe4s/superlu_sc







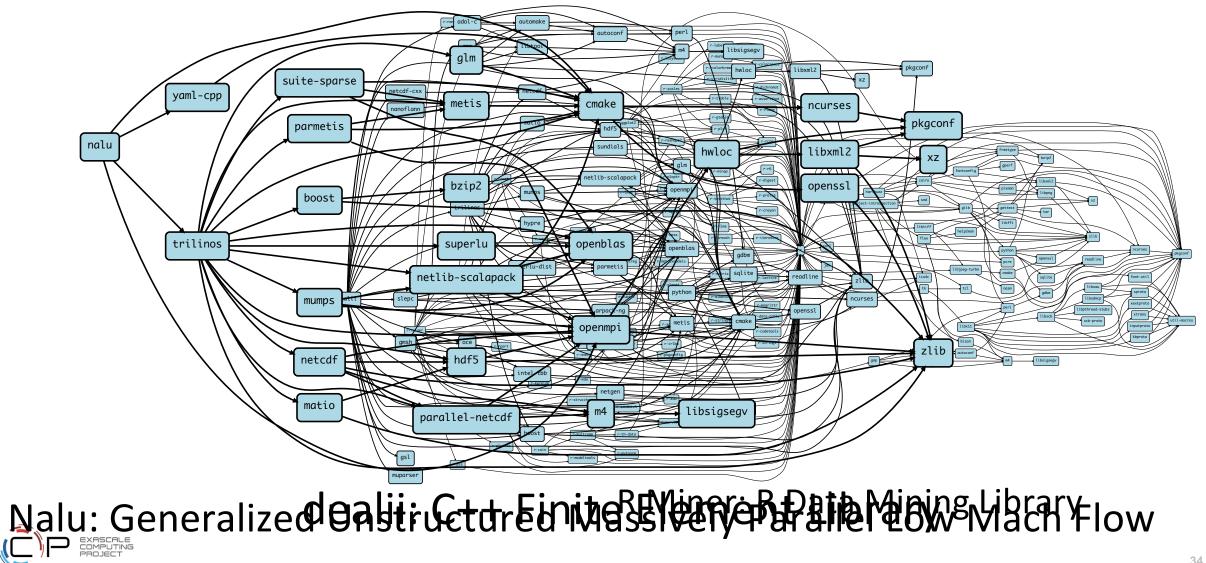




- E4S uses the Spack package manager for software delivery
- Spack provides the ability to specify versions of software packages that are and are not interoperable.
- Spack is a build layer for not only E4S software, but also a large collection of software tools and libraries outside of ECP ST.
- Spack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



Scientific software is becoming extremely complex



E4S Spack Build Cache and Container Build Pipeline

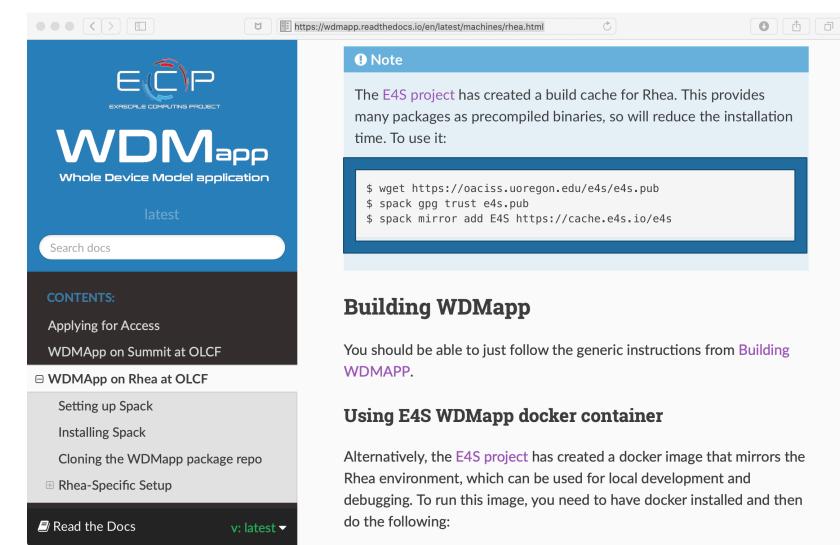




E4S: Spack Build Cache at U. Oregon

•••		aciss.uoregon.edu	C	• ± 0 +	
	E4S	Build Cache for Spac	k 0.15.0		
		To use this build cache, just add it to your Spack buildcache keystrustinstall	back		
		spack mirror add E4S https://cache.e4s.io/e4s			
	Click on c	 one of the packages below to see a list of all av All Architectures PPC64LE X Centos 7 Centos 8 RHEL 7 Last updated: 06-25-2020 19:30 PDT 11370 Spack packages 	36_64	ntu 18.04	 10,000+ binaries S3 mirror No need to build from source code!
		Search			
	adiak@0.1.1 adios2@2.5.0 adios2@ argobots@1.0 argobots@1.0rc1 arg axl@0.1.1 axl@0.3.0 axom@0.3.3	gobots@1.0rc2 arpack-ng@3.7.0 autocom	1@0.1.0 ant@1.10.0 f@2.69 automake@1 ils@2.32 binutils@2		
	• https:	//oaciss.uoregon.edu/e4s/	nventory.htm		

WDMApp: Speeding up bare-metal installs using E4S build cache



- E4S Spack build cache
- Adding E4S mirror
- WDMApp install speeds up!



https://wdmapp.readthedocs.io/en/latest/machines/rhea.html

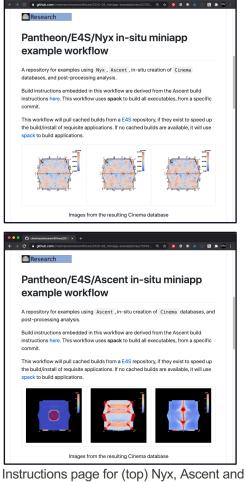
Pantheon and E4S support end-to-end ECP examples

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

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

Contributions

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



Instructions page for (top) Nyx, Ascent and Cinema workflow repository, and (bottom) Cloverleaf3d, Ascent, Cinema workflow. These curated workflows use Pantheon, E4S and spack to provide curated workflows for ECP.

LA-UR-20-27327 9/29/20

E4S: Building on top of previous efforts

- E4S did not emerge from nothing
- Leveraging the work of many others
- HPC Linux: Work done at U. of Oregon, and at ParaTools, Inc
- IDEAS-Classic: xSDK the original SDK continuing under ECP
- Spack Pre-dates E4S
- All the useful open source software created by the scientific community



E4S Summary

What E4S is not	What E4S is
 A closed system taking contributions only from DOE software development teams. 	 Extensible, open architecture software ecosystem accepting contributions from US and international teams. Framework for collaborative open-source product integration.
 A monolithic, take-it-or-leave-it software behemoth. 	 A full collection if compatible software capabilities and A manifest of a la carte selectable software capabilities.
A commercial product.	 Vehicle for delivering high-quality reusable software products in collaboration with others.
 A simple packaging of existing software. 	 The conduit for future leading edge HPC software targeting scalable next-generation computing platforms. A hierarchical software framework to enhance (via SDKs) software interoperability and quality expectations.

Some E4S Collaboration Models

Approach	Comments/Potential
Use E4S containers for tutorials and webinars	Many ST technologies offer tutorial/webex forums to learn more; range from introductory to advanced
Evaluate new capabilities using E4S software products	Accelerator-enabled software stack (compilers, programming environments, tools, math libraries, in situ), next-generation IO (HDF5, ADIOS, PNetCDF)
Install E4S	A goal for us: Want to explore how to make this possible. Collaboration can help us improve our product development and delivery.
Contribute to E4S and SDKs	 E4S and SDKs are open architectures enabling light-weight integration of similar products. Contributions already exist from NSF and European funded projects Talk with us about contributing your product to the DocPortal Assess your product against our community policies
Overall	Full collaborative interactions benefit everyone.



E4S/SDK Summary

- E4S/SDK Software: Curated release of complete production-quality HPC Linux software stack:
 - Latest ECP-developed features for 50+ products.
 - Ported and validated regularly on all common and emerging HPC platforms.
 - **Single DocPortal access** to all product documentation.
 - Collaborative development communities around SDKs to build culture of quality.
 - **Policies** for SW and user experience quality.
 - **Containers, build caches** for (dramatic) reduction in build time and complexity.
- E4S: A new member of the HPC ecosystem:
 - A managed portfolio of HPC software teams and products.
 - Enabling first-of-a-kind collaboration: vendors, facilities, US agencies, industry and internationally.
 - Extensible to new domains: AI/ML.
 - A new way of delivering reusable HPC software with ever-improving quality and functionality.







ECP Software Technology Capability Assessment Report (CAR) Version 2.0

- Comprehensive document about ECP ST structure, progress and planning
- Version 2.0:
 - E4S/SDK details
 - 2-page writeups for each product
 - Released February 1, 2020
- Version 2.5:
 - Refresh of 2-page writeups
 - Foreshadowing of next ECP features in E4S
 - Scheduled for November 15, 2020

