Sandia National Laboratories

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ASC DEVOPS TRILINOS PLANNING TEAM

Common Build Trilinos Products

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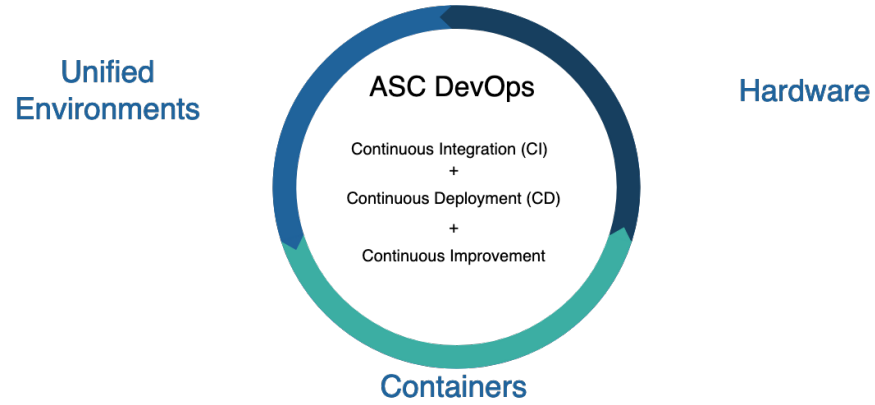
NNSA

ADVANCED SIMULATION AND COMPUTING (ASC) DEVOPS INITIATIVE

ASC DevOps Vision

ASC codes are developed, tested, deployed, and released quickly, efficiently, and robustly with established credibility on all key ASC platforms. Codes are efficiently coupled and integrated in the ASC DevOps ecosystem, which is governed by well-defined processes, practices, and standards. Ultimately, end-users will be able to seamlessly run recently released credible ASC code(s) on key ASC platforms.



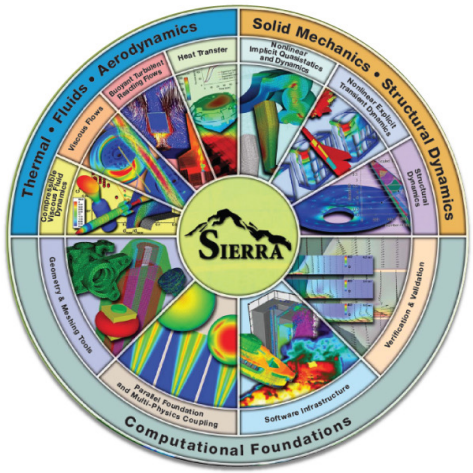
Complicated Effort

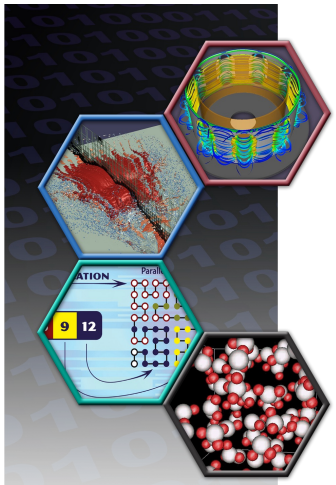
- Multiple prior attempts
- Required a new, different approach

Essentials to success

- Communication & Governance Structure
  - Broad consensus, from technical staff up to senior management
- Team Building & Managing Change
- Managing complexity & Effort
  - Software ecosystem and library dependencies

ASC AND A UNIFIED ENVIRONMENT AT SANDIA





RAMSES

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Sub-program Integration

- Codes + Models + Credibility
- + HPC Systems, Operations, & Software Stack

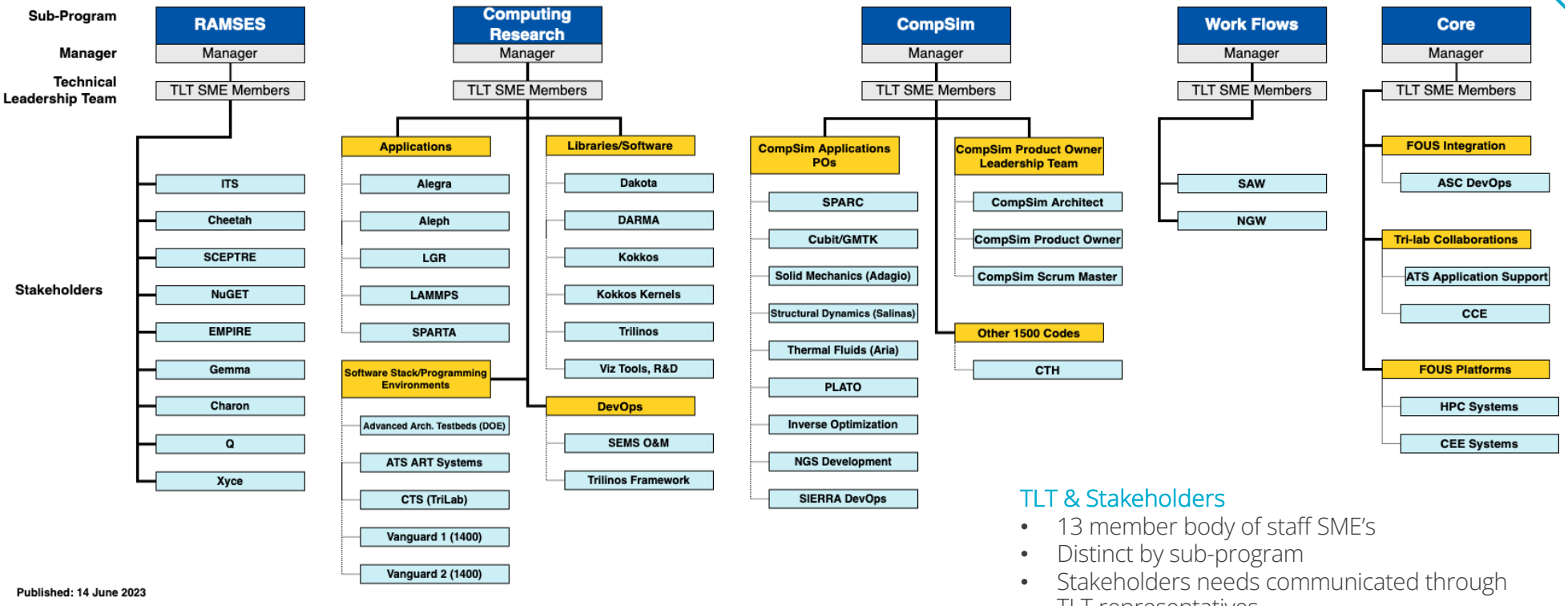
Scope

- 31 Scientific & Engineering Code Teams and multiple systems admin. teams
  - HPC: Prototype, Advanced, and Commodity
  - Desktop: Windows, Linux, Mac
- 200+ Developers
- Partner daily with users (designers & analysts)

History

- Some teams on build systems pre-date1995
- Multiple attempts at unified ASC DevOps

ASC TECHNICAL LEADERSHIP TEAM (TLT) AND STAKEHOLDERS



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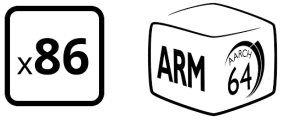
TLT & Stakeholders

- 13 member body of staff SME's
- Distinct by sub-program
- Stakeholders needs communicated through TLT representatives

ASC UNIFIED ENVIRONMENT

Continuous Integration

Heterogenous Architectures



Network Hierarchy

OPEN SECURE CLASSIFIED

The ASC Unified Environment Stack

Tooling, Profilers, & Debuggers
- 9 tooling products
- 5 profilers & debuggers

Compilers & MPI
- 5 compilers
- 2 flavors of MPI

TPLs
- 13 TPLs

34 products, multiple architectures, multiple networks, many combinatorics

TRILINOS PLANNING TEAM

Solver Library (Trilinos) Builds: Motivating down-select of configurations

Solver Package	Configuration Options (27 out of 326)	Code Teams *(none of which have the same configuration)*														
		alegra	aleph	charon	cubit_gmtk	dakota	empire	gemma	plato	sceptre	sierra	sparc	xyce	Conflict	Num. Of Code Teams Impacted
Amesos2	Amesos2_ENABLE_Epetra	ON					ON					OFF		C	3
EpetraExt	EpetraExt_BUILD_BTF	OFF					ON						ON	C	3
Galeri	Trilinos_ENABLE_Galeri						ON				OFF			C	2
Intrepid2	Trilinos_ENABLE_Intrepid2						ON				ON	OFF		C	3
Isorropia	Trilinos_ENABLE_Isorropia	ON					ON				OFF		ON	C	4
Kokkos	KokkosKernels_ENABLE_SUPERNODAL_SPTRSV						ON				OFF			C	2
Kokkos	Kokkos_ENABLE_CUDA_UVM						ON					OFF		C	2
Kokkos	Kokkos_ENABLE_DEPRECATED_CODE_3						ON					OFF		C	2
Kokkos	Kokkos_ENABLE_OPENMP			OFF			ON				OFF			C	3
Kokkos	Trilinos_ENABLE_Kokkos				OFF		ON			ON	ON		ON	C	5
MueLu	Trilinos_ENABLE_MueLu	ON	OFF				ON			ON	ON	ON		C	6
NOX	NOX_ENABLE_LOCA	ON	OFF				ON						ON	C	4
Pamgen	Trilinos_ENABLE_Pamgen	ON					ON				ON	OFF		C	4
Panzer	Panzer_ENABLE_TESTS			OFF			ON							C	2
Panzer	Trilinos_ENABLE_Panzer						ON					OFF		C	2
SEACAS	Trilinos_ENABLE_SEACAS		ON				ON	ON		ON	OFF			C	5
STK	Trilinos_ENABLE_STK		ON				ON				OFF			C	3
STK	Trilinos_ENABLE_STKCoupling	ON					OFF					ON		C	3
STK	Trilinos_ENABLE_STKSimd						OFF					ON		C	2
Stokhos	Trilinos_ENABLE_Stokhos						ON				OFF	OFF	ON	C	4
Teuchos	Trilinos_ENABLE_TeuchosKokkosComm					OFF	ON							C	2
Teuchos	Trilinos_ENABLE_TeuchosKokkosCompat					OFF	ON							C	2
Tpetra	Tpetra_ENABLE_DEPRECATED_CODE						ON					OFF		C	2
Tpetra	Trilinos_ENABLE_Tpetra	ON	OFF				ON	ON	ON	ON	ON	ON		C	8
TrilinosCouplings	Trilinos_ENABLE_TrilinosCouplings	ON					ON				OFF		ON	C	4
Zoltan2	Trilinos_ENABLE_Zoltan2		OFF							ON	ON	ON		C	4

STRATEGIES FOR THE COMMON BUILD

- Build a (or a set of) common Trilinos with all variants that any code team wants enabled
- Using Spack
- Concerns:
  - Will this impact runtime performance?
  - Build systems
    - Tribits vs CMake
  - Versions of the dependencies?
  - Are there conflicts by enabling certain packages will others need to be disabled?
    - Currently we don't see any conflicts

LIST OF VARIANTS ENABLED

44 of 51 Trilinos Packages

Adelus	Isorropia	Shards
Amesos	Kokkos	Stokhos
Amesos2	ML	Stratimikos
Anasazi	MueLu	Teko
AztecOO	NOX	Tempus
Belos	Pamgen	Teuchos
Epetra	Panzer	Thyra
EpetraExt	Percept	Tpetra
FEI	Phalanx	Trilinos
Galeri	Piro	TrilinosCouplings
Gtest	ROL	TrilinosSS
Ifpack	RTOp	Triutils
Ifpack2	SEACAS	Xpetra
Intrepid	STK	Zoltan
Intrepid2	Sacado	Zoltan2

PRODUCT DELIVERY

- Configuration of Trilinos
  - Codes still build Trilinos
  - Consistent build formula, which can reduce debugging time
- Build Cache
  - Reduces build time
  - Get Trilinos + dependencies
  - Code teams can selectively reuse certain software and customize others
  - Must use Spack
  - Offers the most time savings with the most flexibility
- Common Set of Builds
  - Modules
  - No need to build Trilinos
  - Challenge is to get the code teams on the same page or at least the same chapter
- Nightly Trilinos Integration Build
  - Several code teams build and integrate Trilinos into their code each night
  - Take over the responsibility of providing the latest Trilinos so multiple code teams are not rebuilding

SCOPE OF CHALLENGE/LANDSCAPE

- Compilers
  - GCC 10.3.0
  - GCC 12.1.0
  - Intel
  - Clang
- OpenMPI
  - Built on all the compilers
- Intel MPI

- Variants of the common build
  - Complex vs Noncomplex
  - Float vs Int
  - GPU's
    - Cuda
    - ROCM

AUE COMPILERS AND TPLS

- Ancillary benefit of this projects: we will be able to test the products released under AUE for suitability with Trilinos
- Reuse TPLs that are provided with the AUE environment

Shared Trilinos & AUE TPLs

- BLAS
- Boost
- CGNS
- HDF5
- Hypre
- LAPACK
- NetCDF
- METIS
- ParMetis
- SuperLU