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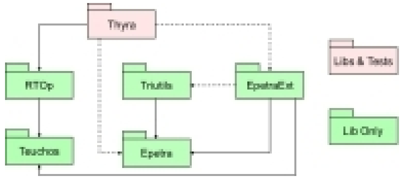
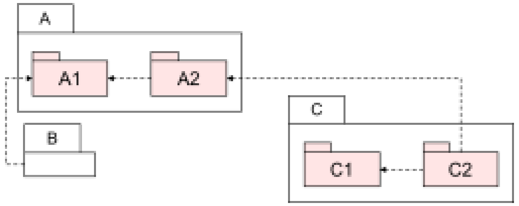
Sandia National Laboratories

Challenges and Suggested Solutions to Sustainable Build, Test, and Integration Processes in CSE Software Ecosystems





Roscoe A. Bartlett
Department 1424
Software Engineering and Research

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https://bartlettroscoe.github.io/

U.S. DEPARTMENT OF ENERGY
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Bartlett: Build, Test, and Integration Efforts in CSE Software

- **2001-2010**: Trilinos numerical algorithms development (https://trilinos.org)
  - Contributed to many Trilinos packages (5K+ commits)
  - Build and integrations with research and production application codes and Trilinos
- **2005:** Co-developed of Makefile.export.<package> system for Trilinos autotools build system
  - Scalable package-based architecture for Makefile-based build systems
- **2007**: Lead ASC Vertical Integration milestone (pioneered APP+Trilinos integration processes)
- **2008-present**: Took over transition and maintenance of Trilinos build system to CMake
  - Scalable architecture for large CMake projects 8 years before well supported by modern CMake 3.7
- **2008-present:** Lead numerous contracts with Kitware to extend CMake, CTest and CDash
  - CMake: e.g.: Ninja support for Fortran, improved parallel build performance for Ninja
  - CTest: e.g. Parallel running of tests, test resource allocation control (for GPUs)
  - CTest, CDash: e.g. Asynchronous submits and processing, subproject support, improved query filters
- **2010-2016**: Infrastructure team lead and integration architect for DOE CASL project (Consortium for the Advanced Simulation of Light-water reactors) (https://casl.gov/)
  - Multi-institution, multi-team, multi-repository development and integration workflows
- **2015**: Initial co-author of Exascale Computing Project xSDK Community Package Policies
- **2016-2020:** Tool and Development Environment Lead for SNL ATDM project
  - Lead stabilization of Trilinos on pre-exascale platforms (largest in Trilinos history)
  - Developed integration plans for Trilinos and ATDM application codes
- **2019:** Developed prototype for tools and third-party library installation system using Spack => SNL SEMS Spack-CM
- **2021-present**: Refactoring Trilinos/CMake build system to modern CMake
  - Initial goal: Maintain backward compatibility for thousands CMakeLists.txt files and thousands of user configure scripts in all environments!

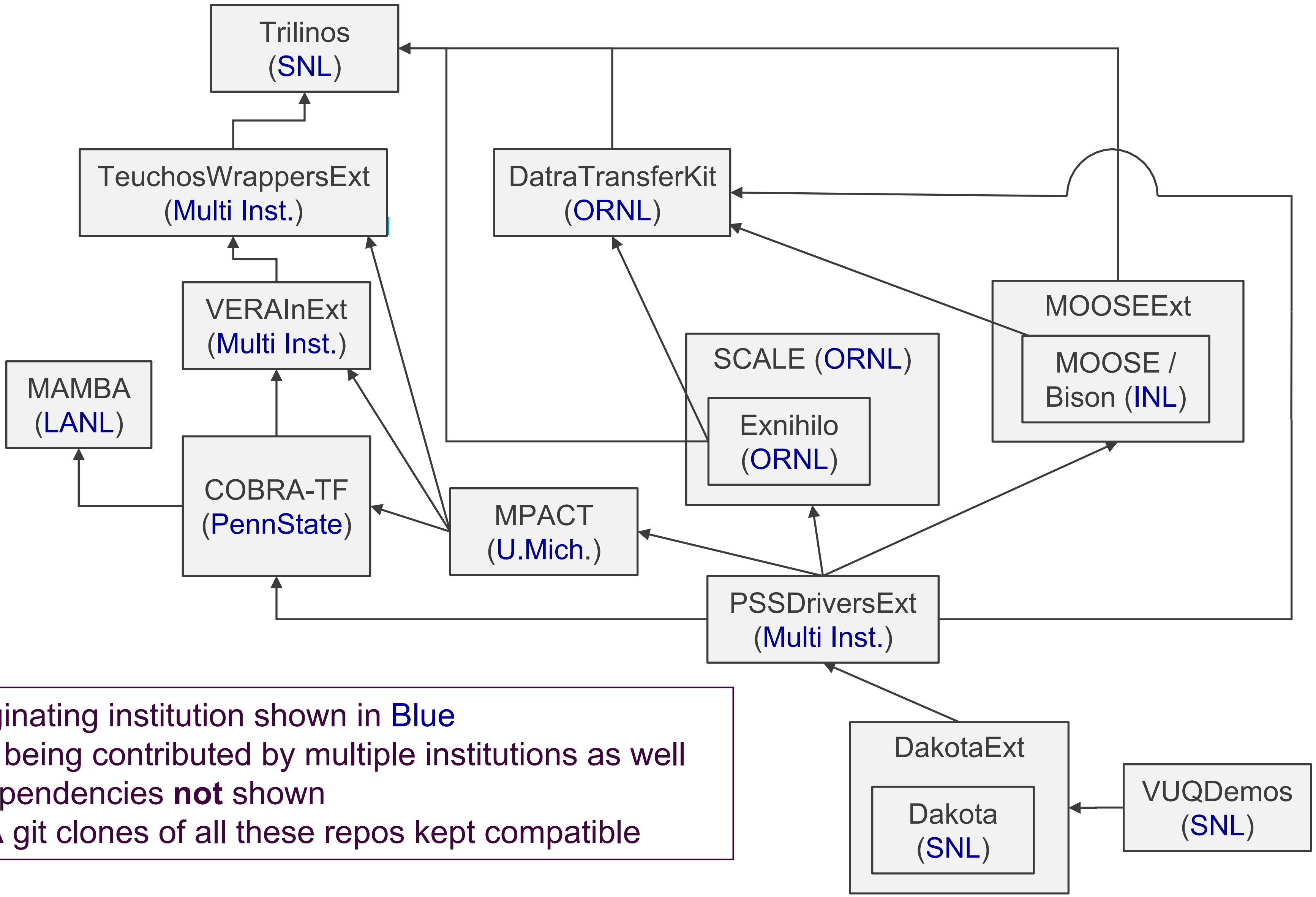
Overview of CASL

- **CASL: C**onsortium for the **A**dvanced **S**imulation of **L**ightwater reactors
- DOE Innovation Hub including DOE labs, universities, and industry partners
- Goals:
  - Advance modeling and simulation of lightwater nuclear reactors
  - Produce a set of simulation tools to model lightwater nuclear reactor cores to provide to the nuclear industry: **VERA: Virtual Environment for Reactor Applications**.
- Phase 1: July 2010 – June 2015
- Phase 2: July 2015 – June 2020
- Organization and management:
  - ORNL is the hub of the Hub
  - Milestone driven (6 month plan-of-records (PoRs))
  - Focus areas: **Physics Integration (PHI)**, Thermal Hydraulic Methods (THM), Radiation Transport Methods (RTM), Advanced Modeling Applications (AMA), Materials Performance and Optimization (MPO), Validation and Uncertainty Quantification (VUQ)

CASL VERA Development Overview (2016)

- VERA development was complicated in almost every way ☹
- VERA composed of:
  - 21 different Git repositories (clones of other repos)
  - Different access lists for each Git repository (NDAs, Export Control, IP, etc.)
  - Integrating development efforts from many teams from 9+ institutions
- Single large CMake build system using TriBITS CMake Framework:
  - Very large full source code base:
    - 55K source and script files
    - 12M lines of code (not comments)
    - 2,700 CMakeLists.txt files
  - 229 packages + subpackages enabled (out of 496 total) ≈ **46% of full code base**
  - Most CMake developer reconfigures take place in less than 30 seconds!
- VERA Software Development Process:
  - VERA integration maintained by continuous and nightly testing:
    - Pre-push CI testing: checkin-test-vera.sh, cloned VERA git repos
    - Post-push CI testing: CTest/CDash, all VERA git repos
    - Nightly testing: MPI and Serial builds, Debug and Release builds, …
    - Main 100% passing builds and tests most days!
  - Many internal and external repository integrations on daily basis
  - VERA releases are taken off of stable 'master' branches on casl-dev git repos.
  - Very low maintenance cost of the infrastructure

Dependences Between Selected CASL VERA Repositories (2016)



- Primary/originating institution shown in Blue
- Most codes being contributed by multiple institutions as well
- All direct dependencies **not** shown
- Local VERA git clones of all these repos kept compatible

Layers of Build Tools and Build Systems

Package dependency handling and build/install/test orchestration

- Listing of different packages (each with their own meta-build system tool) and dependencies and version information.
- Acquires (and patches) source code for each package for the correct version, consistent configure, builds, and installs
- Examples (popular) tools/approaches: Spack, CMake External Project, SNL CApp, home grown scripts
- Arguably the most popular approach: Home-grown scripts

Meta-build system / Build file generator

- Uses higher-level description of the build targets in platform independent way
- Rules for each compiler and platform to generate detailed compiler and linker command-line options
- Automatically computes dependencies specification in generated Makefiles, Ninja files, or other tools
- Example (popular) tools/approaches: CMake, GNU Autotools, home-grown Makefiles (with thing configure scripts)
- Arguably the most popular approach: CMake

Build driver with low-level dependencies

- Given dependencies between different input and output files, runs low -level compile commands
- Only builds output targets that are out of date given the time stamps of their upstream dependencies (files).
- Example (popular) tools: (GNU) Makefiles, Google Ninja
- Arguably the most popular approach: GNU Makefiles

Raw compile and link commands

```
$ g++ -I<dir1> -I<dir2> … -isystem <dirn> … -fopenmp -O3 -DNDEBUG -fPIC -std=c++14 -MD -MT … -o
  <object_file>.o -c <source_file>.cpp
$ g++ … <object1>.o <object2>.o … -Wl,-rpath,<dir1>:<dir2> … -L<dir3> … -l<lib1> -l<lib2> … -o <exec>
```

Why CMake?

Open-source tools maintained and used by a large community and supported by a profession software development company (Kitware).

CMake:

- Simplified build system, easier maintenance
- Improved mechanism for extending capabilities (CMake language)
- Support for all major C, C++, and Fortran compilers.
- Automatic full dependency tracking (headers, src, mod, obj, libs, exec)
- Good Fortran support (parallel builds with modules with src => mod => object tracking, C/Fortran interoperability, etc.)
- Shared libraries on all platforms and compilers (support for RPATH)
- Faster configure times (e.g. > 10x faster than autotools)
- Generates different backend builds: Makefiles, Google **Ninja**, Visual Studio, Eclipse, XCode, …
- Portable support for cross-compiling

CTest:

- Parallel running and scheduling of tests and test time-outs, resource (GPU) allocation
- Memory testing (Valgrind)
- Line coverage testing (GCC GCOV)
- Better integration between test system and build system

CDash:

- Web server for display, query, and archive of build, test, memory, and coverage results
- Flexible query and filtering of build and test results
- REST API to extra data to develop various tools

Recent news:

- There has been significant growth in CMake adoption, maturation and feature development in recent years.
- CMake is now most popular build system for C++ code in the world
- Improved documentation: Book "Professional CMake"

Major obstacles to build, test, and integration of CSE Software

Package dependency handling and build/install/test orchestration
e.g. Spack, homegrown scripts

↓

Meta-build system / Build file generator
e.g. CMake, GNU Autotools, homegrown Makefiles

↓

Build driver with low-level dependencies
e.g.: Makefiles, Google Ninja

↓

Raw compile and link commands

```
$  g++ … -o <object_file>.o -c
   <source_file>.cpp
$  g++ <object1>.o … -o <exec>
```

- **Heterogeneity in the build file generators (CMake, Autotools, home-grown tools that generate Makefiles, etc.)**
- Inconsistent and incompatible usages of CMake (mix of old and modern CMake approaches with different packages)
- Inability to tweak generation of low-level compile and link lines to address difficult cases on some builds and platforms (i.e. **CMake**)
- Compatible upgrades of dependent packages (i.e. "Dependency hell")
- Lack of robust portable test suites to drive packages integration processes (e.g. fragile randomly failing tests).
- Difficulties debugging through all of the different layers down to low-level compiler and linker command-lines (i.e. Spack => CMake => Makefiles/Nina => Raw compile and linke commands)

Suggested solutions to major obstacles to build, test, and integration

Package dependency handling and build/install/test orchestration
e.g. Spack, homegrown scripts

↓

Meta-build system / Build file generator
e.g. CMake, GNU Autotools, homegrown Makefiles

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Build driver with low-level dependencies
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Raw compile and link commands

```
$ g++ … -o <object_file>.o -c
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$ g++ <object1>.o … -o <exec>
```
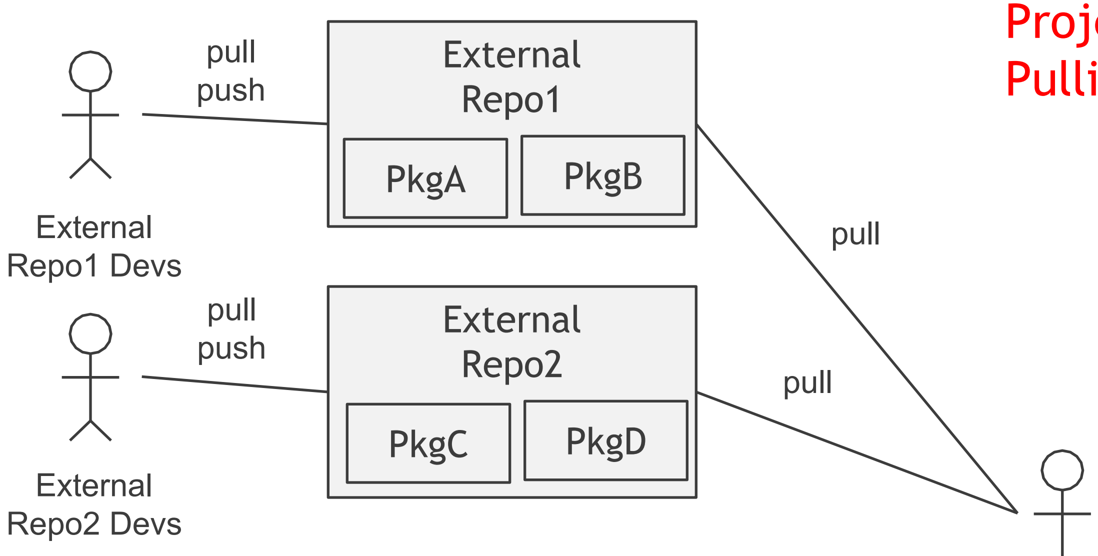
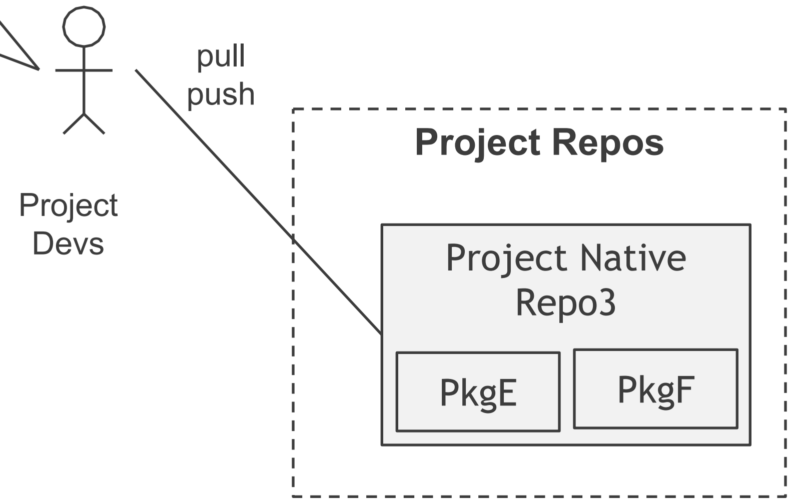

- **Heterogeneity in the build file generators (CMake, Autotools, home-grown tools that generate Makefiles, etc.)**
  - ⇒ **Use CMake as the meta-build system for all packages!**
- Inconsistent and incompatible usages of CMake (mix of old and modern CMake approaches with different packages)
  - ⇒ Develop and adopt minimal standards for the usage of CMake and the interoperability of modern CMake-based packages.
- Inability to tweak generation of low-level compile and link lines to address difficult cases on some builds and platforms (i.e. **CMake**)
  - ⇒ Continue to develop CMake to allow finer-grained control when needed of the include directory handling and other options.
- Compatible upgrades of dependent packages (i.e. "Dependency hell")
  - ⇒ Adopt Semantic Versioning Standard (semver.org) and policies for transitioning package ecosystems for breaks in compatibility.
- Lack of robust portable test suites to drive packages integration processes (e.g. fragile randomly failing tests).
  - ⇒ Invest in the development and maintenance of test suites!
- Difficulties debugging through all of the different layers down to low-level compiler and linker command-lines
  - ⇒ Standardize on usage of Spack and simplify/streamline usage
  - ⇒ But, support configuration and development with just CMake

Package/Repository Integration: What Not to Do

Project Developers Directly Pulling from the External Repos

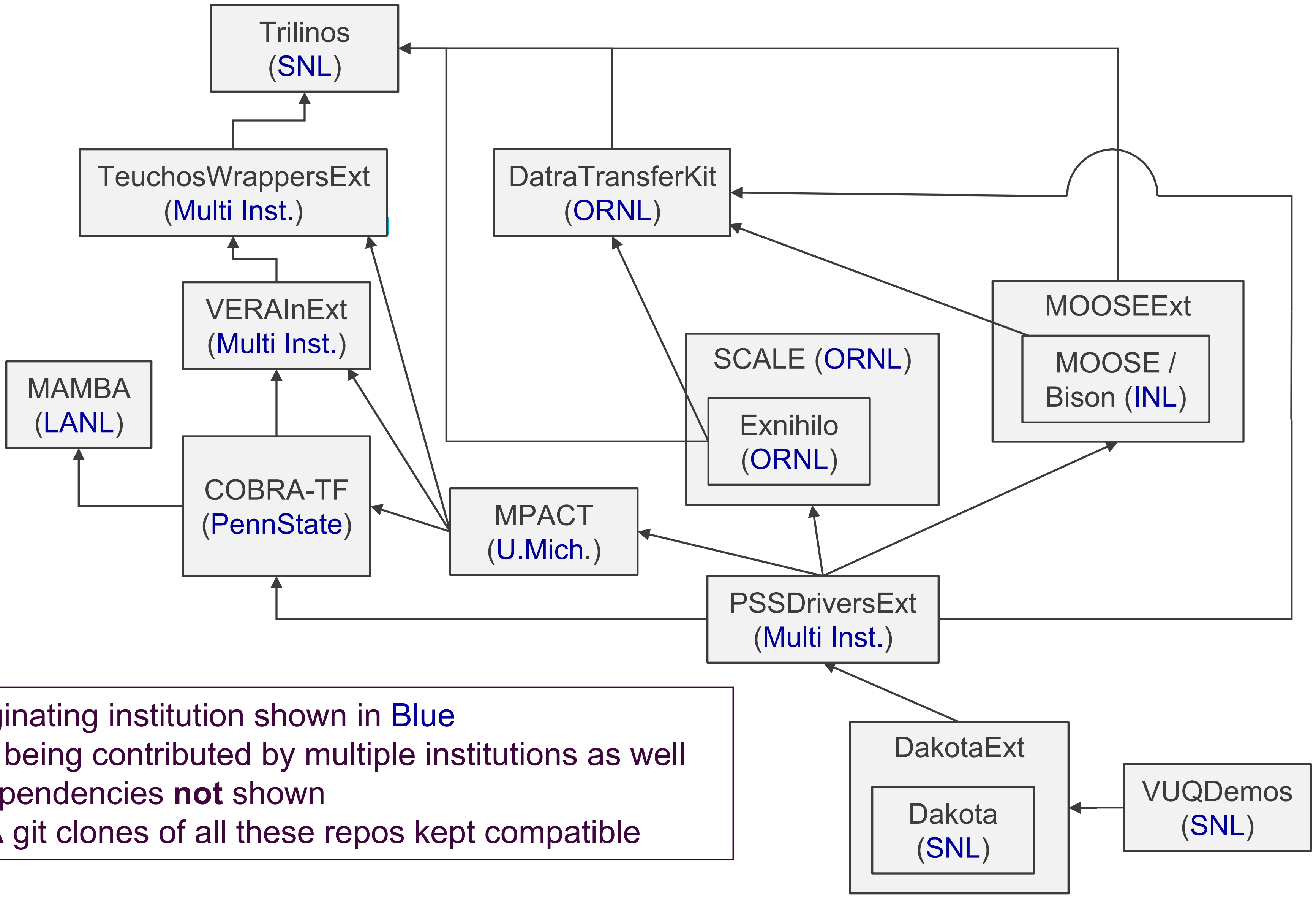




Why is this so bad?

- Lack of test coverage in the external repo's native test suite to cover project's needs.
- External repo developers not testing against the project's code and tests.
- External repo may be broken w.r.t. to the project for long periods of time.
- Project developers frequently pull code that does not even configure or build.
- Broken code frequently interrupting the work of project developers.

Dependences Between Selected CASL VERA Repositories (2016)



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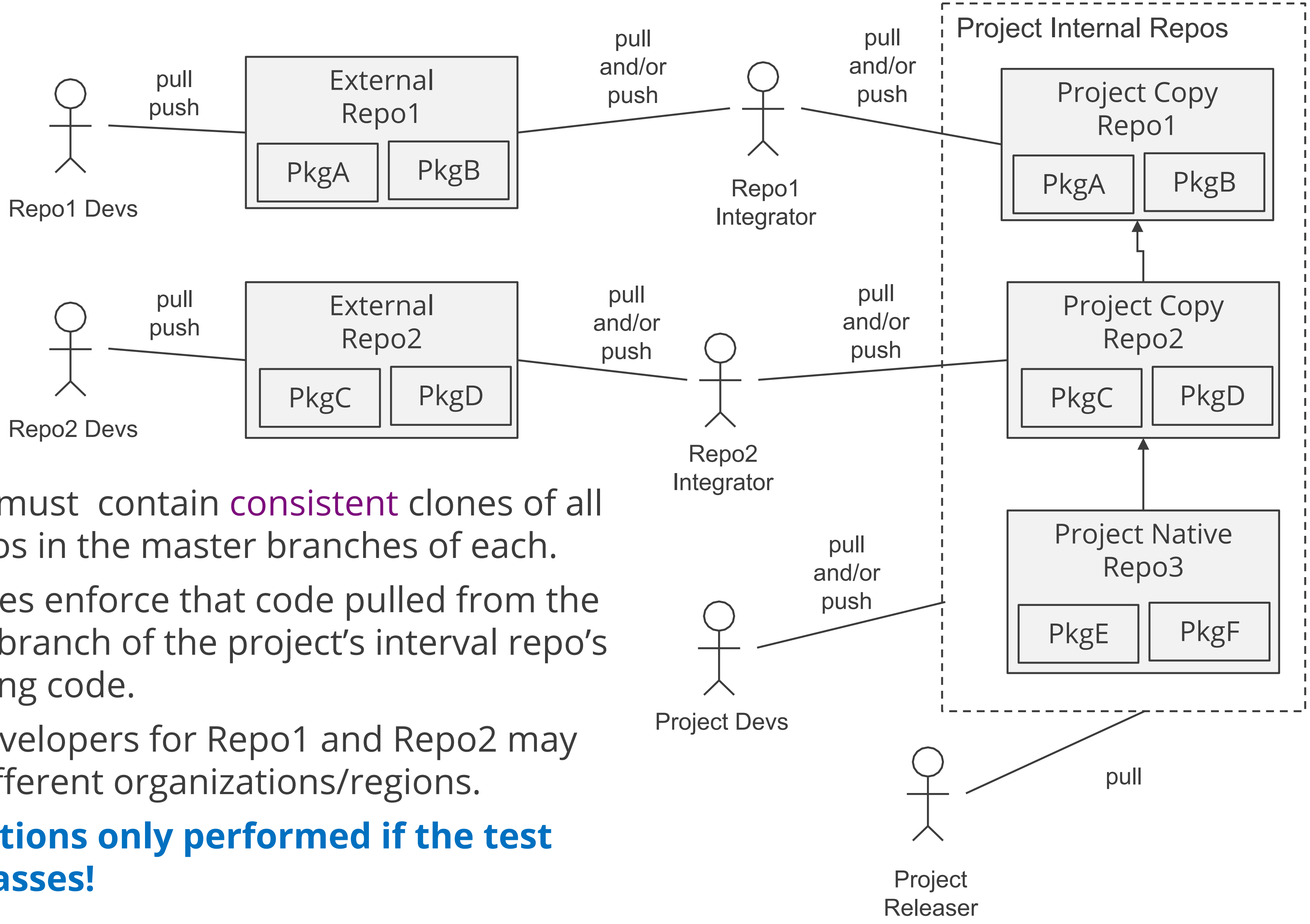
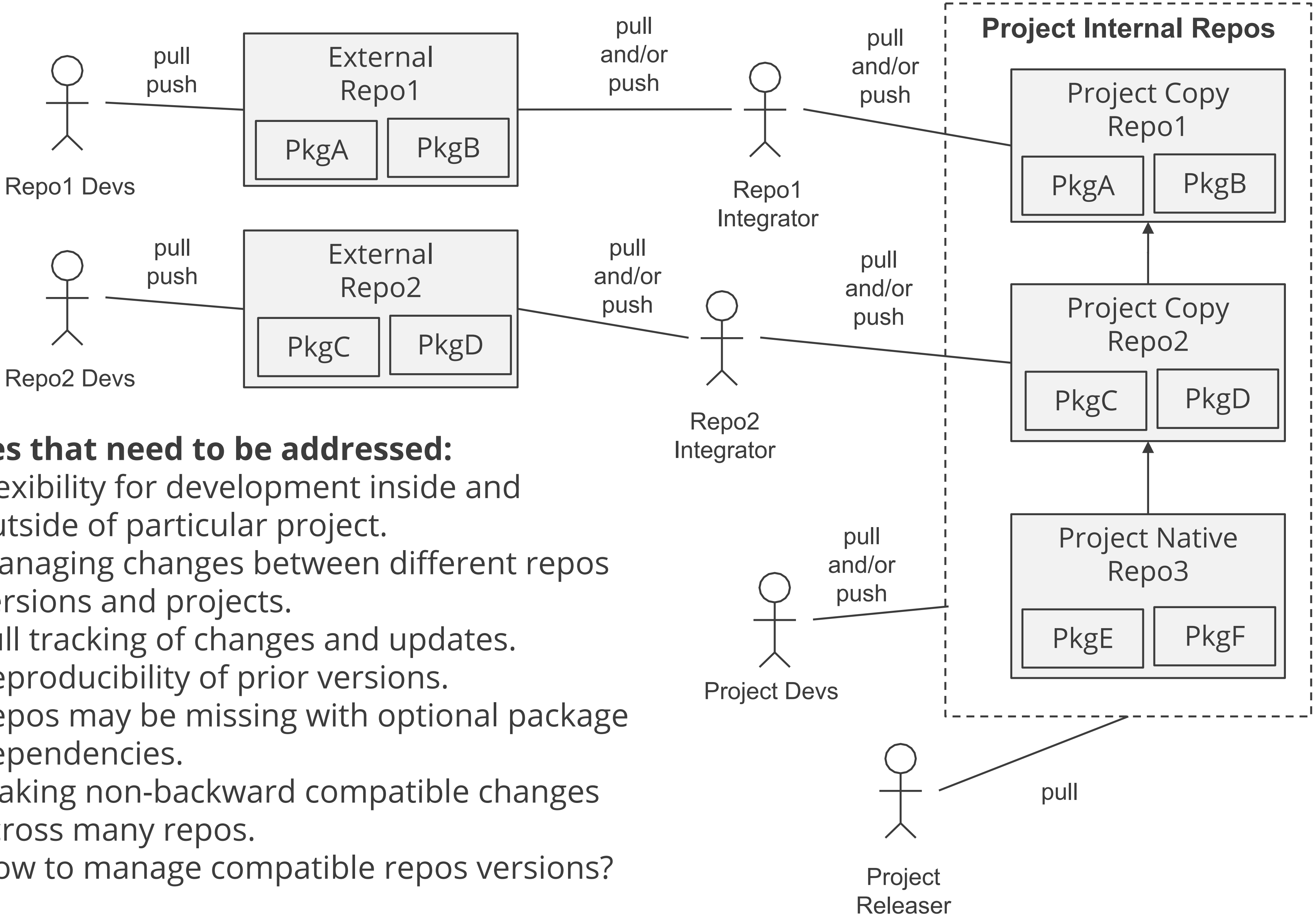
Integration of Packages/Repositories into Project (CASL VERA)



- Project must contain consistent clones of all the repos in the master branches of each.
- Processes enforce that code pulled from the master branch of the project's interval repo's is working code.
- Core developers for Repo1 and Repo2 may be in different organizations/regions.
- **Integrations only performed if the test suite passes!**

Managing Compatible Repos and Repo Versions



Issues that need to be addressed:

- Flexibility for development inside and outside of particular project.
- Managing changes between different repos versions and projects.
- Full tracking of changes and updates.
- Reproducibility of prior versions.
- Repos may be missing with optional package dependencies.
- Making non-backward compatible changes across many repos.
- How to manage compatible repos versions?

Build, Test, and Integration: Final Recommendations

Package dependency handling and build/install/test orchestration
e.g. Spack, homegrown scripts

↓

Meta-build system / Build file generator
e.g. CMake, GNU Autotools, homegrown Makefiles

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Build driver with low-level dependencies
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Raw compile and link commands

```
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$  g++ <object1>.o … -o <exec>
```

- **Standardize on the usage of CMake** for generating build files (i.e. Makefiles or Ninja files, it does not matter which)
- **Extend/refine/improve CMake and the usage of CMake** to handle all portability aspects in generating low-level compile and link options
- **Develop and refine minimal standards for usage of CMake** to improve package portability and package interoperability.
- **Train package development teams on modern CMake** and accepted minimal standards for usage of CMake.
- **Fund early CMake porting work and interactions with venders** to new HPC platforms along with early test packages
- **Quickly push out binaries for new CMake releases** to all HPC and support platforms as soon as they are released.
  - Example: We need CMake 3.23 to address backward compatibility for transition of TriBITS and Trilinos to modern CMake.
- **Keep higher-level package build/orchestration software out of the low-level details** of architectures, compiler options etc. (I.e. **Let CMake handle all low-level compiler and linker details**).
  - Example: Avoid drilling low-level compiler options through compiler wrappers to underlying CMake builds.

Questions and Comments?