VI. Recent Developments & Future Trends in Trilinos

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What to expect?

Trilinos updates:

- Updates from the **Trilinos leadership** as well as for the **DevOps pipeline** and the **different product areas**:
  - What has changed / been added recently?
  - Work-in-progress
  - Future trends and plans for TRILINOS
- Selected aspects are being discussed (non-exhaustive!)

Breaking change in 2024 & 2025:

- Deprecation of the EPETRA stack

Later today: Hackathon

To help with the transition to TPETRA, we will have a hackathon w/ TPETRA developers. Ask your questions. Work on your code. Together.

Disclaimer

The following slides are based on the slide decks of presentations given by *Curt Ober*, *Sam Browne*, *Roger Pawlowksi*, *Christian Glusa*, and *Mauro Perego* at the TRILINOS User Group Meeting 2023 (TUG '23); please see the website for more details.

Trilinos DevOps Pipeline (TDOP) Planning

Trilinos Philosophy

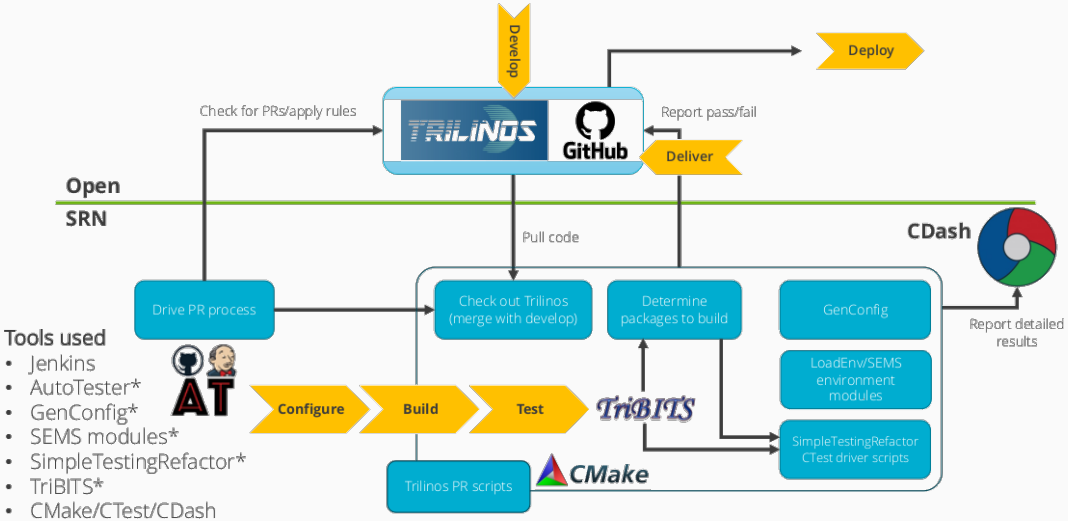
> *"The* Trilinos *Project is an effort to facilitate the design, development, integration and ongoing support of mathematical software libraries within an object-oriented framework for the solution of large-scale, complex multi-physics engineering and scientific problems.* Trilinos *addresses two fundamental issues of developing software for these problems: (i)* ***Providing a streamlined process and set of tools for development of new algorithmic implementations*** *and (ii)* ***promoting interoperability of independently developed software****."*

Heroux et al., "An Overview of the Trilinos *Project", ACM Transactions on Mathematical Software, Vol. V, No. N, December 2004, Pages 1–27*

> *"The* Trilinos *project was established to address two important needs: (1) bringing teams of library developers together in order to* ***leverage commonalities and produce compatible software components****, formally called packages and (2) to* ***amortize the cost and efforts associated with more formal software engineering requirements****. With a modest level of coordination and without unduly compromising package team autonomy,* Trilinos *project members could leverage each other's efforts, consolidate commonly needed tools, make packages compatible, and define a common set of software engineering tools and processes.."*

Heroux and Willenbring, "A new overview of the Trilinos *project", Scientific Programming 20 (2012), p. 83–88*

Overview of Current Trilinos DevOps Pipeline



Executive Summary – Trilinos Plans to . . .

DEVELOP

- Remain single repository to maintain developer productivity
- Retain key capabilities of TriBITS and form a support team

CONFIGURE

- Utilize ASC DevOps common Trilinos configurations (e.g., RAMSES and CompSim)
- Provide/maintain a Spack recipe that others can use (e.g., ASC stakeholders and Spack)

BUILD

- Maintain/support CMake & TriBITS and Spack builds
- Incorporate Containers and GitHub Actions to catch build errors and keep builds clean

TEST

- Add Integration testing for Trilinos packages (e.g., Kokkos and KokkosKernels)
- Support application's integration testing of Trilinos to mitigate integration issues

DELIVER & DEPLOY

- Support both delivery (Trilinos GitHub) and deployment (Spack)
- Steward Trilinos's Spack recipe with support from Framework and Trilinos developers

Trilinos remains a single repository, retaining the capabilities of TriBITS

- What are the **complaints and perceived issues**?
  - *"*Trilinos *is too big.* Trilinos *is too complex."* → Too many packages/dependencies
  - Should Trilinos be *"partitioned"*?
  - Why do we have TriBITS?
- **Points to consider**
  - Survey says . . . 76% favored single Trilinos repository
    - Large loss of productivity with multiple repos for developers and applications
  - TriBITS provides CMake layer of common/consistent functionality across Trilinos packages
    - Most large software projects have some CMake layer (e.g., LNLL's BLT and VTK modules)
  - Recent and ongoing TriBITS improvements (e.g., modern CMake and external builds)
- **Planned solution/response**
  - **Single Trilinos repository** to maintain developer productivity
  - Retain **key capabilities of TriBITS** and form a **support team**
  - **Review packages/dependencies** to ensure we have the **minimum set**
  - Consider **not using (and removing) subpackages capability** of TriBITS/Trilinos

Simplify Trilinos configurations and provide Spack recipe

- What are the **complaints and perceived issues**?
  - Too many configuration options to get the build you would like
  - Not easy to configure/build for a single/few package(s)
- **Points to consider**
  - Survey says . . .
    - Configuration preference - CMake/TriBITS (35%), CMake/Scripting (32%), CMake/Package Manager/Scripting (23%)
    - **Documentation on configuring/building needs improvement. New users have difficulty.**
- **Planned solution/response**
  - Improve documentation for configuration options and provide examples
  - Provide **"recommended" configure defaults** based on PR testing
  - Utilize ASC DevOps common Trilinos configurations (e.g., RAMSES and CompSim)
  - Review dependencies to **ensure required and optional dependencies are correctly defined**
  - **Provide/maintain a Spack recipe that others can use** (e.g., ASC stakeholders and Spack)
  - Generate intra-package/TPL dependencies with TriBITS for CMake & TriBITS and Spack recipe

Maintain CMake+TriBITS and Spack builds, incorporate Containers and GitHub Actions

- What are the **complaints and perceived issues**?
  - Build times are long
- **Points to consider**
  - Survey says ...
    - Trilinos build times are not long compared to application build times. (21 to 9 respondents)
    - **>90% build times less than an hour**
  - Container usage is dependent on CEE LAN RHEL 8
- **Planned solution/response**
  - Continue CMake & TriBITS builds (more for developers/power users)
  - Expand support for Spack & CMake builds (more for stakeholders/future usage/sysadmins)
  - Add a **Spack PR build** (meaning a Spack build must pass to commit)
  - Incorporate Containers and GitHub Actions to catch build errors and keep builds clean
  - Utilize **build caches (ccache) to increase speed**

Add integration testing for Trilinos and support integration testing of Trilinos

- What are the **complaints and perceived issues**?
  - **PR testing results not visible to foreign nationals and external developers**
  - Trilinos needs **better performance testing**
  - Lengthy process to snapshot packages like Kokkos → integration takes too long
- **Points to consider**
  - Trilinos testing covers CTS/testbed (SRN) platforms
  - There are gaps in PR testing due to **hardware availability** (e.g., AMD GPUs)
  - Integration testing between
    - Trilinos packages would introduce additional overhead
    - Upstream packages/Trilinos/applications can reduce turn-around time
  - Trilinos has **internal "performance" dashboard**
- **Planned solution/response**
  - Add integration testing for Trilinos packages (e.g., Kokkos and KokkosKernels)
  - Support application's integration testing of Trilinos to mitigate integration issues
  - **Add application use cases for performance monitoring**
  - Expand performance testing and memory monitoring (e.g., Watchr)
  - Move PR and nightlies to SON/OHPC for foreign nationals and external collaborators

Support both Trilinos GitHub and Spack and steward Trilinos's Spack recipe

- What are the **complaints and perceived issues**?
  - "Need to deliver code changes more quickly to applications."
  - Difficult to use Spack's recipe for Trilinos
- **Points to consider**
  - Survey says ...
    - **Preference is to use CMake installation over package manager** (20 to 6 respondents)
    - **Package manager (e.g., Spack) is path forward** for the future
  - In the past, primarily only delivered Trilinos and applications deployed.
- **Planned solution/response**
  - Support both delivery (Trilinos GitHub) and deployment (Spack)
  - Steward Trilinos's Spack recipe with support from Framework and Trilinos developers

Next Steps . . .

FY24

- Epetra → Tpetra Transition for Trilinos packages
- Current planned tasks
  - Test/support CompSim and RAMSES Trilinos configurations (coordinating with ASC DevOps)
  - **Ownership/support of Spack-based Trilinos build added to nightly/PR testing**
  - **Transition from SEMS Autotester to GitHub Actions & Containers**
  - **Transition from GenConfig to Spack for configuration management**
- Continued planning of TDOP

FY25

- Epetra → Tpetra transition for stakeholders
- Start other planned TDOP responses

Introduction of New Strategic and Operational Leadership

New Leadership Structure

Strategic Leadership

- Should cover broad research areas
  - Algorithms research
  - Big picture – vision for possible new areas
  - Software Sustainability
  - Long-term application needs
- Current Strategic Leaders
  - *Mike Heroux*
  - *Eric Phipps*
  - *Siva Rajamanickam*
  - *Heidi Thornquist*
  - *Jim Willenbring*





Operational Leadership

- Should cover operational areas
  - Product manager
  - Framework lead
  - New area leads
    - Representation for every package
    - Need to balance packages/effort
- Current Operational Leaders
  - *Sam Browne* – **Framework**
  - *Christian Glusa* – **Solvers**
  - *Curt Ober* – **Product manager**
  - *Roger Pawlowski* – **Trilinos Core**
  - *Mauro Perego* – **Discretizations and Analysis**





Current Trilinos Product Areas and Packages

Framework	Data Services	Discretizations	Linear Solvers	Nonlinear Solvers	Product Manager
• PyTrilinos • Teuchos • TrilinosCouplings • ~~TriUtils~~	• ~~Epetra~~ • ~~EpetraExt~~ • Galeri • ~~Isorropia~~ • Kokkos • Kokkos Kernels • Pamgen • SEACAS • Tpetra • Xpetra • Zoltan/Zoltan2	• Compadre • ~~Domi~~ • ~~FEI~~ • ~~Intrepid~~/Intrepid 2 • MiniTensor • Panzer • Percept • Phalanx • Shards • Krino • STK	• Adelus • ~~Amesos~~/Amesos2 • Anasazi • ~~AztecOO~~ • Belos • ~~Ifpack~~/Ifpack2 • ~~Komplex~~ • ~~ML~~ • MueLu • Pliris • ShyLU/ShyLU-DD/ShyLU-Node • Stratimikos • Teko	• ~~Moertel~~ • NOX • ~~Pike~~ • Piro • ROL • RTOp • ~~Rythmos~~ • Sacado • Stokhos • Tempus • Thyra	• N/A

• ~~Package~~ – Slated for Archival in FY23-FY25

Package – Snapshotted package

Proposed Trilinos Areas and Packages

Framework	Core	Solvers	Discretizations and Analysis	Product Manager
• N/A	• Galeri • Kokkos • Kokkos Kernels • Pamgen • SEACAS • Tpetra • Zoltan/Zoltan2 • PyTrilinos • Teuchos • RTOp • Thyra	• Adelus • Amesos2 • Anasazi • Belos • Ifpack2 • MueLu • Pliris • ShyLU/ShyLU-DD/ShyLU-Node • Stratimikos • Teko • NOX • Xpetra	• Compadre • Intrepid2 • MiniTensor • Panzer • Percept • Phalanx • Shards • Krino • STK • Sacado • Stokhos • Tempus • TrilinosCouplings • Piro • ROL	• N/A

Trilinos Framework Updates

Current Trilinos Product Areas and Packages

Selected updates (FY23)

- **7 TRILINOS packages deprecated and removed from repository**
- PR builds
  - CCACHE tooling to accelerate PR builds
  - Expanded warning flags
  - Turned off EPETRA and other packages in CUDA build
- Nightly builds
  - Added Clang & OPENMP, C++20 builds
  - Added KOKKOS/KOKKOSKERNELS develop -> TRILINOS develop build

Selected plans for FY24

- Promote C++20 build to PR status
- **Add at least one Spack-based PR build**
- **Migrate from SEMS Autotester to GitHub Actions for CI/PR builds**
- Stretch goal: use **Spack to manage configurations** of TRILINOS for PR testing (as opposed to current GenConfig system)
- **Add advanced hardware builds** as hardware becomes available (e.g., AMD GPU hardware)

Trilinos Core Product Area Update

Teuchos updates

- Mostly in **maintenance mode**
- **Improved YAML parser support**
- TRILINOS leadership: discussions on what we can clean up and remove

Tpetra updates

- FY23
  - Performance, Performance Testing/Monitoring, software quality improvements
  - **Epetra → Tpetra transition**
- FY24
  - **Application transition support: Epetra → Tpetra**
  - Cleanup unnecessary D2H (device-to-host) and H2D (host-to-device) transfers

Epetra depracation

- **Deprecation of Epetra from Trilinos (End of FY24; Deadline Sept. 2024)**
  - All Trilinos packages compile and function without Epetra
    - Nightly testing without Epetra ✓
  - **All "needed" Epetra testing has equivalent Tpetra testing**
  - Packages consult with stakeholders to determine any missing Tpetra functionality
    - Try to assess performance impacts
  - **Epetra still available and tested during FY24**
- **Deprecation of Epetra from stakeholder applications (End of FY25; Deadline Sept. 2025)**
  - Applications transition to Tpetra
  - Packages handle any new issues and performance problems
- **Epetra stack archival to separate repository (Beginning of FY25; Oct. 2025)**

Zoltan2 updates

- Two new graph partitioners in (coming to) Zoltan2:
  - **Sphynx**: Spectral partitioner, multi-GPU
    - Speedup from randomized eigensolver
  - **Jet**: Multilevel, KOKKOS-based partitioner (CPU and GPU)
    - High quality. Beats Metis by 6-10% in edge cuts. Coming soon.
    - Currently limited to single GPU, multi-GPU in progress.

See the TUG' 23 slides for more details

PyTrilinos2 updates

- **New package**
- Auto-generation of Python interface using PyBind11 and binder

PyTrilinos updates

- Plan to deprecate and remove due to PYTRILINOS2 (no timeline at this point)
  PyTrilinos implementation based on SWIG wrappers

RTOp, Thyra, and Xpetra updates

- **Maintenance mode**
- Leadership: Is XPETRA a potential candidate for deprecation with EPETRA removal?

Kokkos-related update

- TRILINOS can now build TRILINOS against an external install of Kokkos
  - TRILINOS SPACK builds do this by default

See KOKKOS *talks (Monday) and TUG' 23 for more details*

Trilinos Solver Updates

Many algorithmic developments

Amesos2 update

- Updates to STRUMPACK, SuperLU_dist, MUMPS and LAPACK adapters

Belos & Anasazi update

• Randomized eigensolver	*Switzer, Boman, Loe*
• Improved testing with Tpetra	*Thornquist, NGA*
• Extend GCRO-DR linear solver to use Kokkos linear algebra for GEMMA	*Dang, Loe*
• **(WIP)** Integration of serial dense matrix traits in Belos to enable use of Teuchos/Kokkos objects	*Loe, Thornquist*

Ifpack2 update

- 4th kind Chebyshev smoother — *Phillips*
- Algorithmic and performance improvements for BlockTriDiag and BlockJacobi — *Liegeois*

  (WIP) Schur complement approach
- Stream based RILU(k) and triangular solves — *Dang*
- Optimize Kokkos Kernels MDF ILU(0) solver and expose it in IFPACK2 — *Ransegnola*
- Patch solver with data compression — *Harper*
- **(Upcoming)** block version of traditional ILU(0) — *Foucar*

MueLu update

• Better ML/MueLu compatibility (parameter translation, aggregation algorithms, ..)	*Siefert, Tuminaro*
• Reitzinger-Schöberl type multigrid for Maxwell problems	*Siefert, Tuminaro*
• BlockCRS support	Siefert
• Improved setup performance on device (TAFC Tpetra changes)	*Berger-Vergiat, Hu, Ren*
• Reformulated Darcy solver	*Glusa*
• Matrix-free multigrid with user-specified operators	*Glusa*
• AMG for hierarchical matrices	*Glusa*
• **(WIP)** Refactor of host-only and Kokkos code paths	*Glusa, Harper*
• **(WIP)** MueLu tutorial overhaul	*Harper, Mayr*
• **(Upcoming)** Matrix-free AMG	*Harper*

NOX update

- Refactored internal use of model evaluators — *Ober, Pawlowski*
- LOCA Householder constraint solver can now be nested within a Tempus transient problem (Tpetra version) — *Pawlowski*

ShyLU update

- FastILU algorithmic improvements and testing, new block version — *Foucar*
- Transpose solve with Basker — *Ellingwood*
- Tacho: runs with HIP. WIP: performance for solves on streams — *Yamazaki*

ShyLU/FROSch update

• Fully recursive multi-level implementation	*Heinlein, Röver*
• Monolithic coarse spaces via partition-of-unity approach	*Heinlein, Knepper, Saßmannshausen*
• GPU capabilities	*Heinlein, Yamazaki*
• **(WIP)** Spectral coarse spaces	*Heinlein, Knepper, Yamazaki*

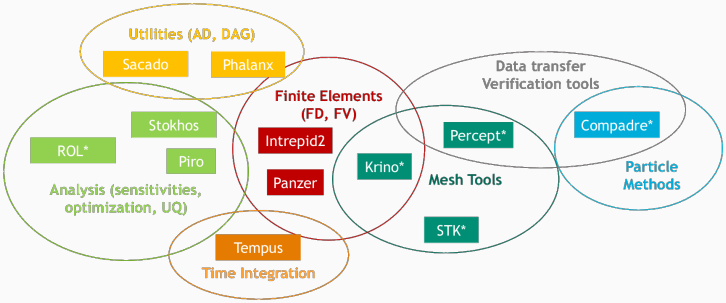
Stratimikos update

• Use of half precision preconditioners (IFPACK2, MUELU, SHYLU/FROSCH)	*Glusa, Loe, Yamazaki*

Teko update

• EPETRA dependency is now optional	NGA, Pawlowski

Trilinos Discretizations and Analysis Product Update



Epetra archival

All the packages can be built without Epetra

- **Good test coverage without Epetra**
- Some Epetra tests still need to be converted to Tpetra

Intrepid archival

- Working on transition of Krino and Percept to Intrepid2
- ROL still need to transition to Intrepid2 (ROL uses Intrepid for testing)

New effort

Develop portable tools for **efficient computation** of operator actions in a **matrix-free** fashion for **high-order finite-element discretization on unstructured meshes**.

Thank you for your attention!

Questions?