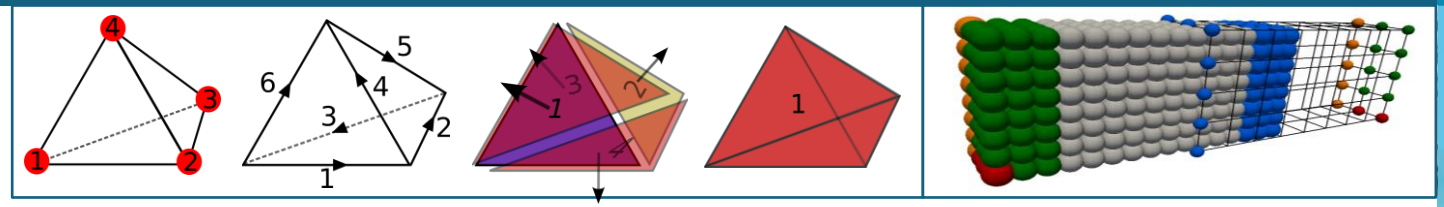
Discretizations and Analysis Product Update



Presenter: Mauro Perego

Contributors: B. Carnes, P. Kuberry, D. Noble, R. Pawlowski, E. Phipps, C. Ober, D. Ridzal, N. Roberts, A. Williams

Trilinos User Group meeting 2024

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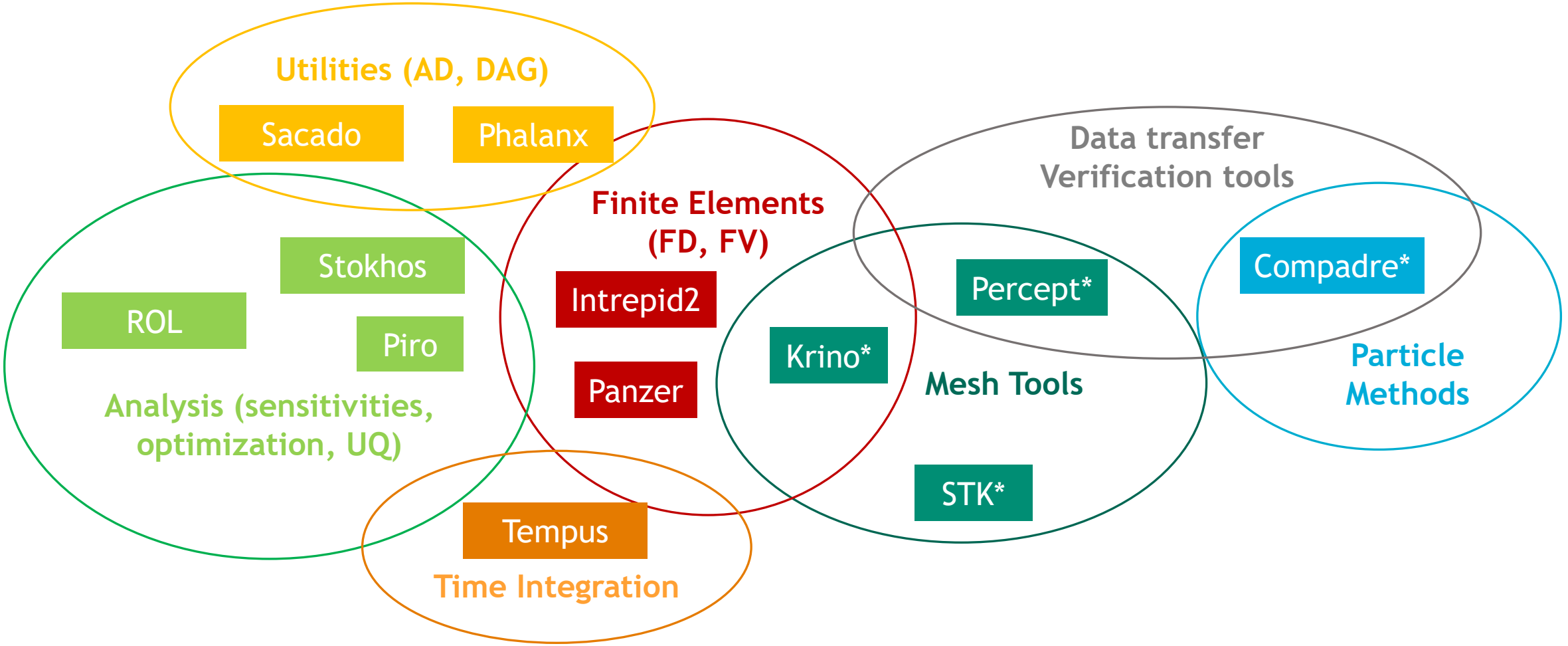
Discretizations and Analysis Product: overview



*Packages snapshotted into Trilinos

Discretizations and Analysis Product: update & plans

- **Epetra archival**. All the products can be built without Epetra.
  - Test coverage without Epetra is now good, but some Epetra tests need to be converted to Tpetra (Piro, Panzer, ROL)

- **Intrepid archival**
  - Percept and Krino to transitioned to Intrepid2
  - ROL tests still using Intrepid
  - No Sandia applications currently using Intrepid (?)

- **Ongoing efforts**
  - portable tools for efficient computation of operator action in a **matrix-free fashion**, for operators from high-order finite-element discretization on unstructured meshes.
  - Porting to SYCL

Discretizations and Analysis Product: update & plans

Sacado (POC: E Phipps)

- (In progress) Porting to SYCL – work by R. Pawlowski

Intrepid2 (POCs: M. Perego and N. Roberts)

- Publication: Roberts, Perego, Pawlowski, "Intrepid2: Structure preserving optimization for high-order discretizations", to appear in ICIAM proceedings book by Springer.
- Parallelization of `getValues` for evaluation of basis functions at different set of points in different regions (needed, e.g., by PIC codes)
- Work on passing execution space instances (see **talk by M. Arnst on Thu, 8:10am**).
- Ongoing work for providing tools for matrix-free high-order discretizations.

Phalanx (POC: R. Pawlowski)

- (In progress) Porting to SYCL
- Updated for C++20

Discretizations and Analysis Product: update & plans

Tempus (POC: C. Ober)

- Failing timestep will reset the initial guess of the timestep to the previous step and timestep reduced, instead of reusing the current solution. This avoids the situation when the current solution has Nans.
- Duplicated the Epetra tests with Tpetra versions. Ready for Epetra Deprecation!
- Started using Clang-Format.
- Split-up several tests that were running long when using debug mode and platform was loaded.
- Changed usage of `InArgs` to handle changes from other packages (e.g., NOX and LOCA)

Panzer (POC: R. Pawlowski)

- Many performance improvements: more code executing on device, on demand workset evaluations, improved caching, MiniEM assembly
- Updated for C++20
- Transitioning unit tests from Epetra to Tpetra (please let us know if there are capabilities missing in the Tpetra stack)
- Adding optional ROL dependency and examples

Discretizations and Analysis Product: update & plans

ROL (POC: D. Ridzal)

- Newish ROL website: rol.sandia.gov
- **PyROL** = Python interface for ROL
  - Interfaced PyTorch with ROL

Stokhos (POC: E. Phipps)

- (FY25) Deprecation and removal of PCE scalar.

Piro (POC: M. Perego)

- Improved support for transient simulation-constrained optimization using Tempus and ROL (work by Kim Liegeois)
- (FY25) Adding Tpetra tests to replace deprecated Epetra-based capability tests

Discretizations and Analysis Product: update & plans

STK (A. Williams)

- Recently added GPU search
- Sierra-developed Morton-LBVH implementation
- Optionally depends on ArborX
- (In progress) Support for ATS-4 (STK Search, STK Mesh)
- (In progress) Fixes to support HIP-Unified space, etc.

Compadre (POC: P. Kuberry)

- Added Cardinal Cubic splines Kernels