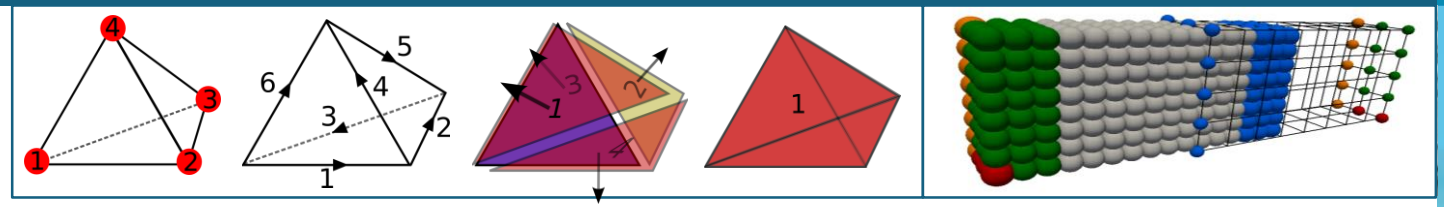
Discretizations and Analysis Product Update



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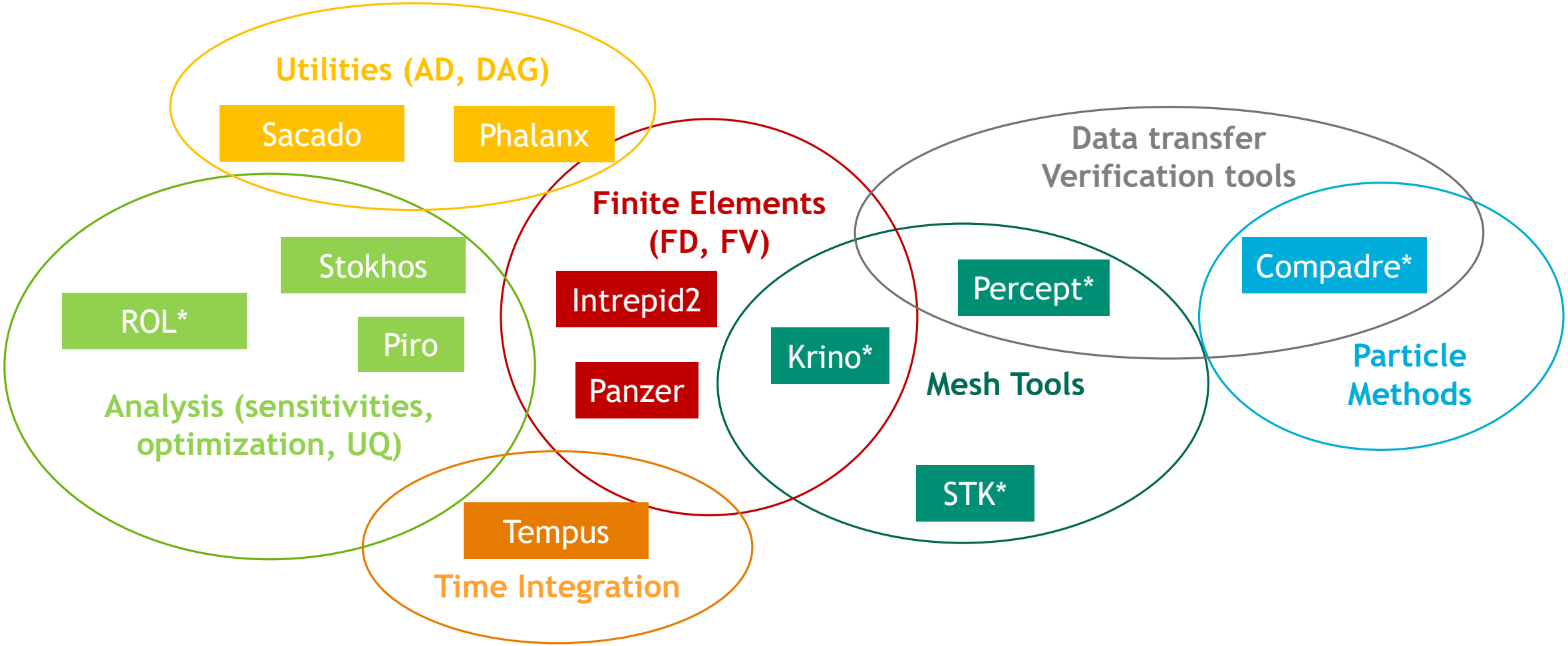
Trilinos User Group meeting 2023

SAND2023-11783PE

Discretizations and Analysis Product: overview
(actively developed packages)



*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

- **Intrepid archival**
  - Working on transition of Krino and Percept to Intrepid2
  - ROL still need to transition to Intrepid2 (ROL uses Intrepid for testing)
  - Sierra SM team is also working on transitioning to Intrepid2

- New effort: develop portable tools for efficient computation of operator action in a **matrix-free fashion**, for operators from high-order finite-element discretization on unstructured meshes.

Discretizations and Analysis Product: update & plans

Sacado (POC: Eric Phipps)

- **(FY 24)** exploration of source transformation-based reverse AD to potentially replace RAD and provide reverse AD capabilities on the device – by Kim Liegeois

Intrepid2 (POC: Mauro Perego, Nathan Roberts)

- optimization of projections: use of symmetric quadrature rules and inverse orientation mappings to work at the nonoriented reference level to avoid expensive loop overs cells to get values of basis functions and orient them.
- finalized sum-factorization work for assembly of high-order tensor-product elements accounting for orientation
- completed implementation of (hierarchical) high-order basis functions including Wedges and Pyramids for H(grad), H(div), H(curl) and H(vol) spaces.
- **(FY 24)** parallelize getValue for evaluation of basis functions at different set of points in different regions (needed, e.g., by PIC codes)
- **(FY24)** tools for matrix-free high-order discretizations

Phalanx (POC: Roger Pawlowski)

- Refactored some phalanx objects to accept execution space instances
- Tools to check which cuda streams are being used (enforce default stream not used)
- Examples for online standard deviation algorithm on device

Discretizations and Analysis Product: update & plans

Tempus (POC: Curt Ober)

- Split some tests to reduce timeouts of debug testing on loaded platforms.
- Added a few example problems.
- Minor bug and warning fixes.

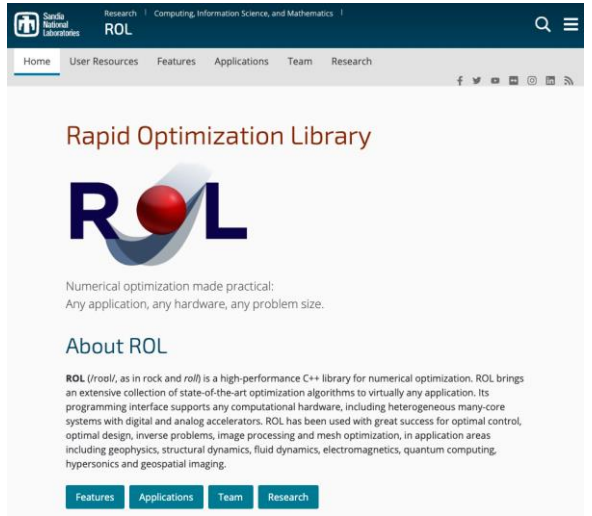
Panzer (POC: Roger Pawlowski)

- Curvilinear mesh support in I/O layers (currently restricted to Q2)
- Epetra requirement removed. Can now build with Epetra stack disabled
- Darcy problem added to MiniEM
- Response_SolutionWriter now supports user defined scaling of all exodus variables
- **(FY24)** Add Tpetra testing to replace deprecated Epetra-based capability tests
- **(FY24)** Potential restructure of subpackages to build less code for certain use cases (AdaptersSTK and Worksets without requiring assembly code in DiscFE)
- **(FY24)** Moving more DOFManager initialization to device

Discretizations and Analysis Product: update & plans

ROL (POC: Denis Ridzal)

- New ROL website: rol.sandia.gov
- New capabilities for nonsmooth optimization (Type-P formulation = proximable), to minimize the sum of a smooth nonconvex function and nonsmooth convex function.
- **(FY 24) PyROL** = Python interface for ROL, in collaboration with Kim Liegeois and Christian Glusa.



Stokhos (POC: Eric Phipps)

- (**FY 24**) Considering deprecating and removing the problematic PCE scalar type (Sacado::UQ::PCE<>), or at least its Kokkos/Tpetra integration.

Piro (POC: Mauro Perego)

- Removed dependency from archived packages Trikota and Rythmos
- Improved support for simulation-constrained optimization using ROL
- Added support for transient simulation-constrained optimization using Tempus and ROL (work by Kim Liegeois)
- (**TODO**) Add Tpetra testing to replace deprecated Epetra-based capability tests

Discretizations and Analysis Product: update & plans

STK (POC: Alan Williams)

- Enhancements to STK Transfer to provide moving-least-squares interpolation
- Documentation/examples for STK Transfer
- Conservative transfer capability
- **(FY 24)** STK Search (geometric proximity search) for GPU
- **(FY 24)** STK I/O for simulations with dynamic mesh topology (avoid creating new exodus files every time the mesh changes)
- **(FY 24)** Standalone Cmake build support (ability to build STK libraries with cmake outside of Trilinos)

Krino (POC: David Noble)

- Fully replaced Percept adaptivity with Krino adaptivity leading to much better parallel load balancing and more than an order of magnitude better performance
- Replaced Intrepid with Intrepid2
- **(FY 24)** Low dissipation, high quality, interface conforming discretizations for moving level set interfaces

Compadre (POC: Paul Kuberry)

- Update to tangent plane calculations, setting, and retrieving with accompanying tests
- **(FY 24)** possible implementation of Radial Basis Function evaluation