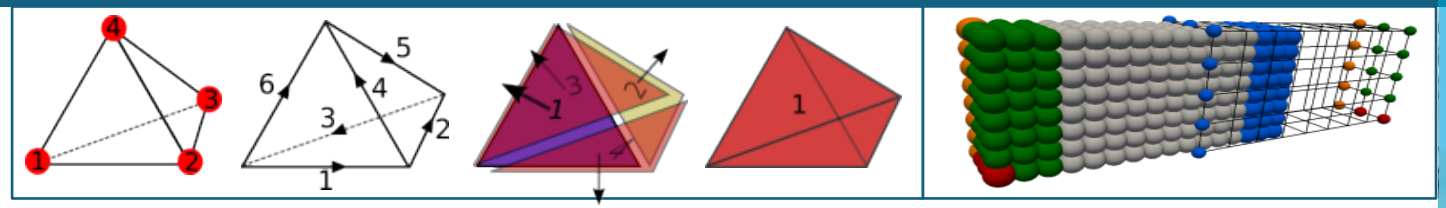
SAND2023-05419C

Sandia National Laboratories

Trilinos Discretizations Product Update

CCR Center for Computing Research



Presenter: Nate Roberts

Contributors: B. Carnes, K. Kim, P. Kuberry, D. Noble, R. Pawlowski, M. Perego, A. Williams

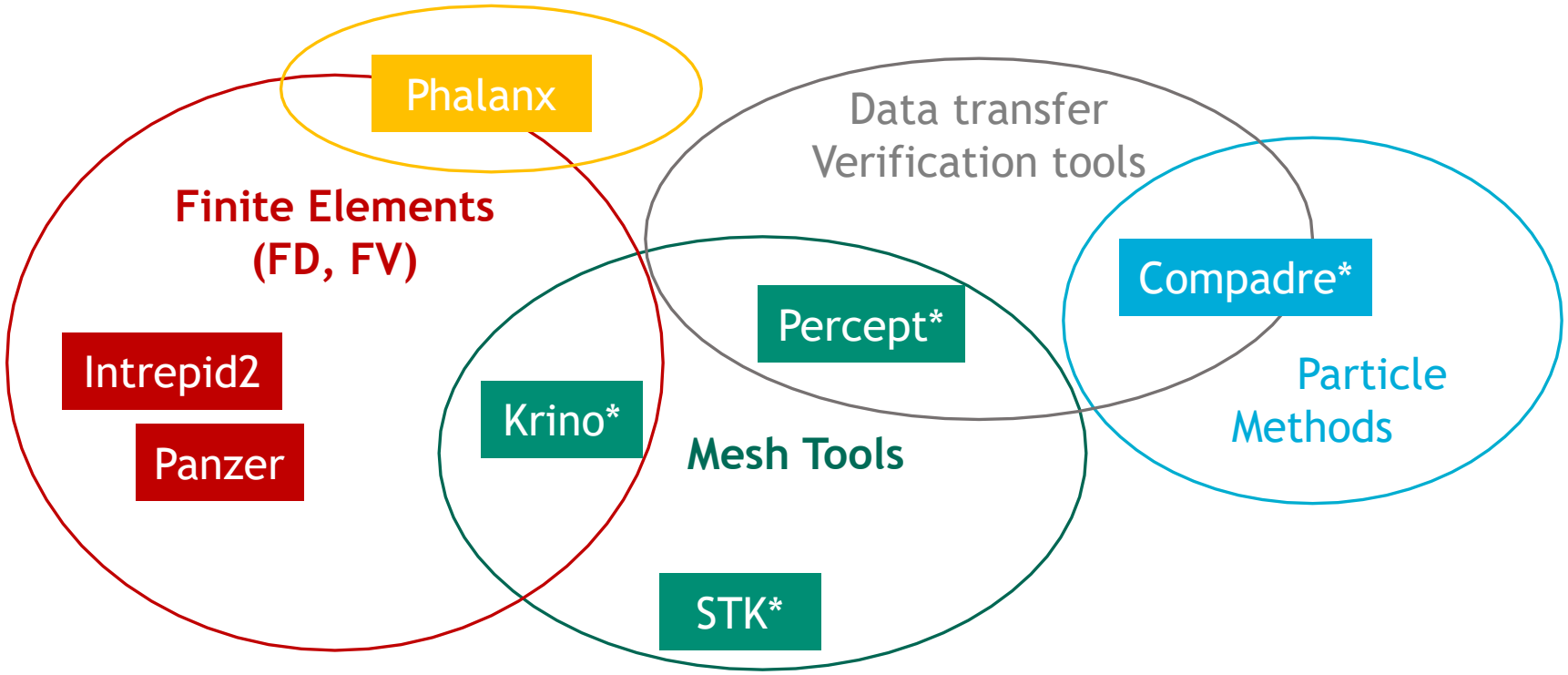
EuroTUG 2023

U.S. DEPARTMENT OF ENERGY NNSA

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

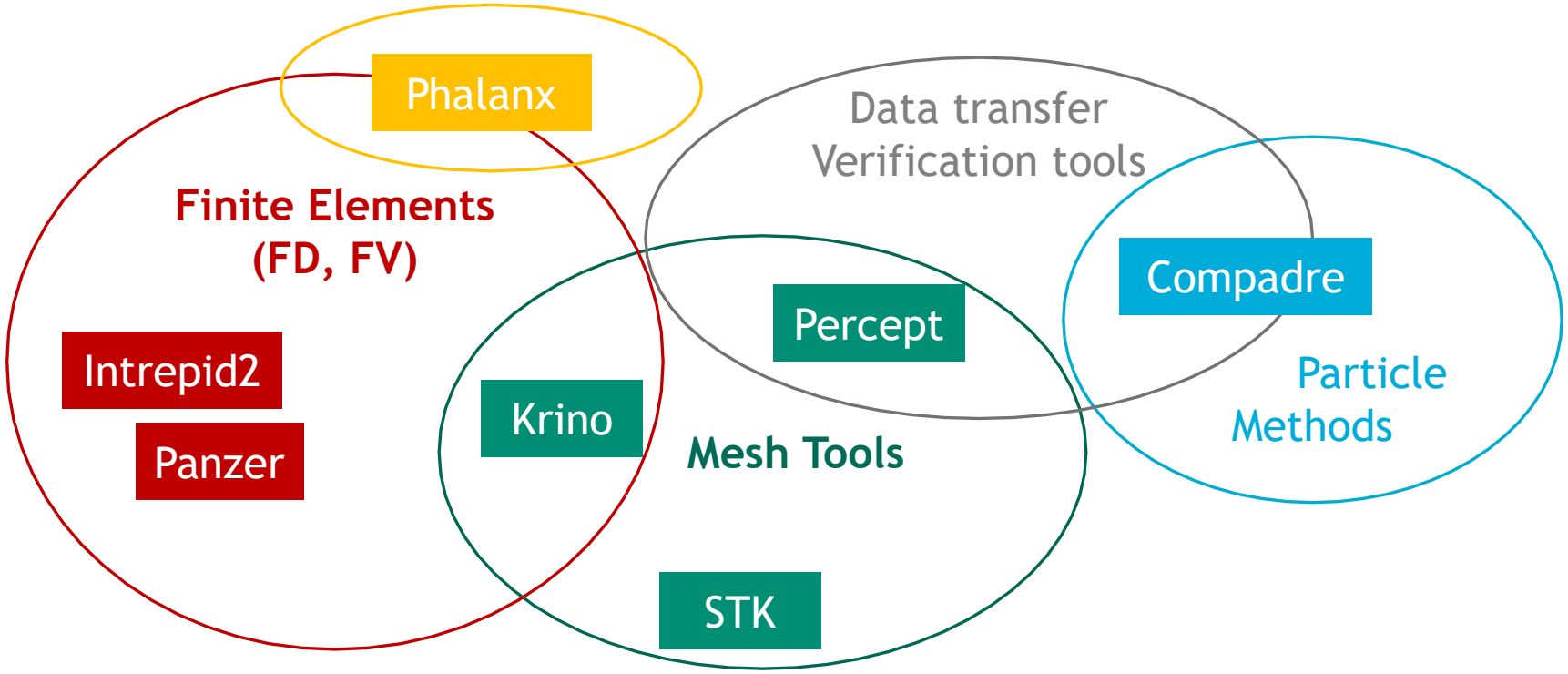
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

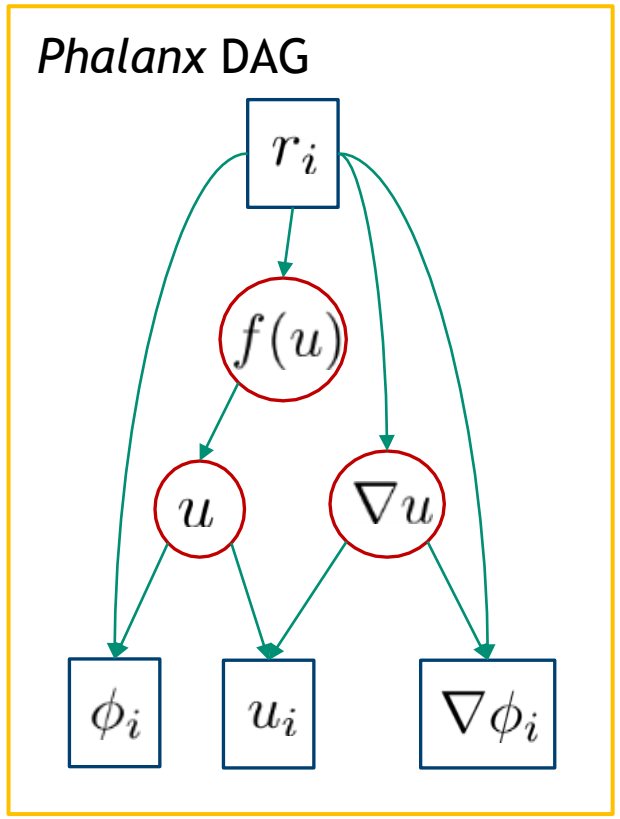
Discretizations Product: overview
(actively developed packages)



*Packages snapshotted into Trilinos

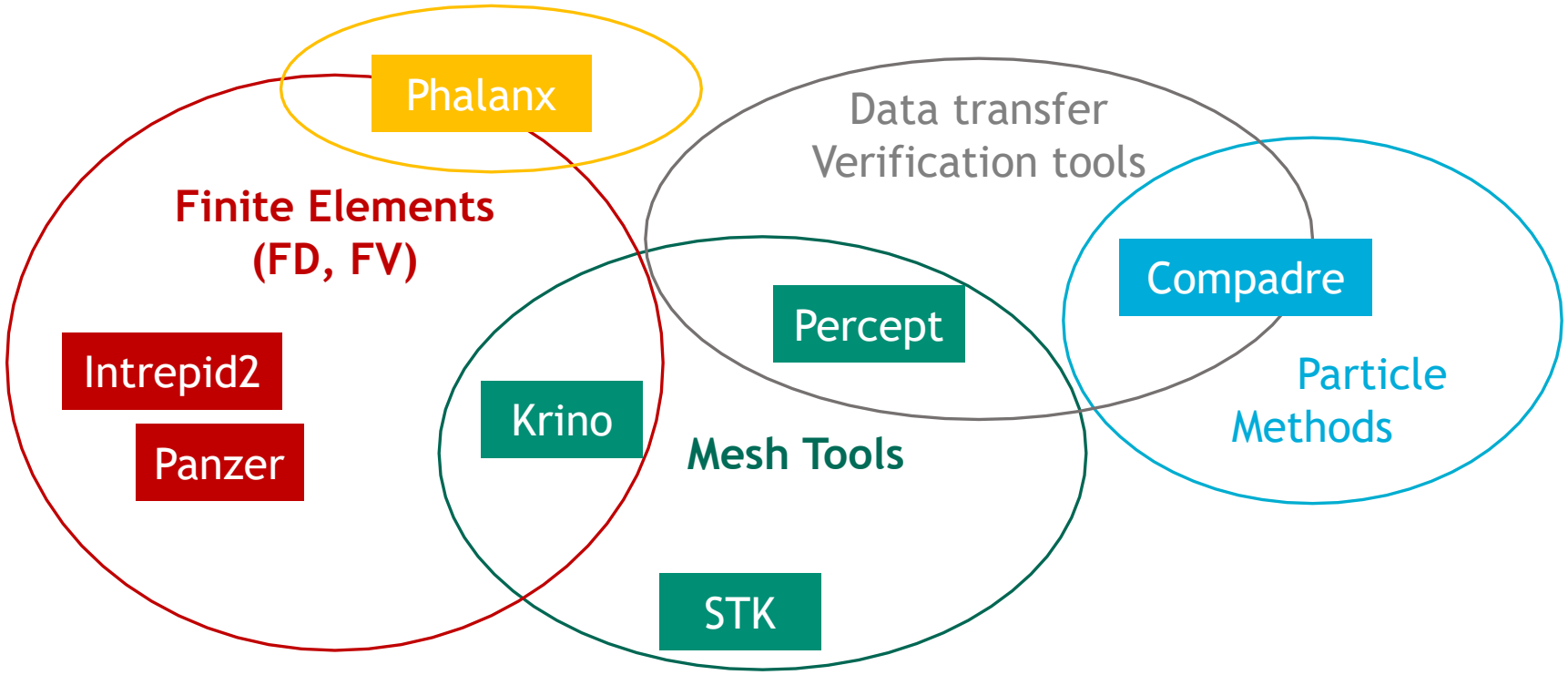
Discretizations Product: overview
(actively developed packages)



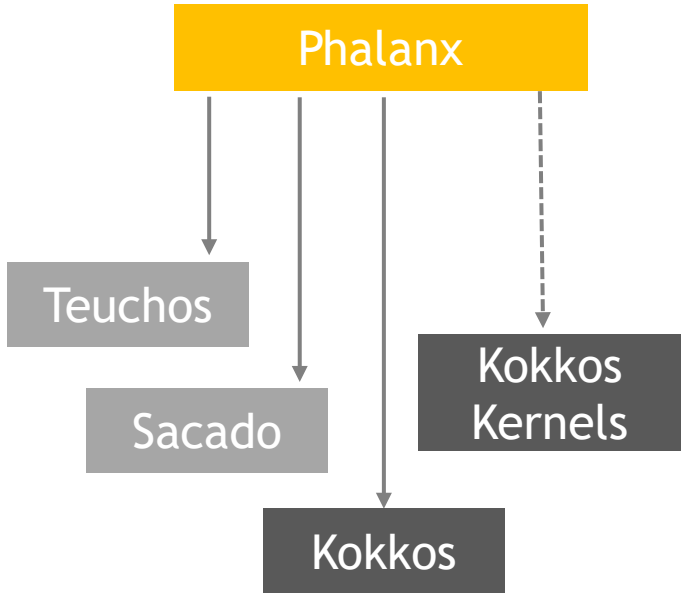


Phalanx: DAG-based expression evaluation – *R. Pawlowski*
used to decompose complex PDE systems into a number of elementary user-defined expression

Discretizations Product: overview
(actively developed packages)

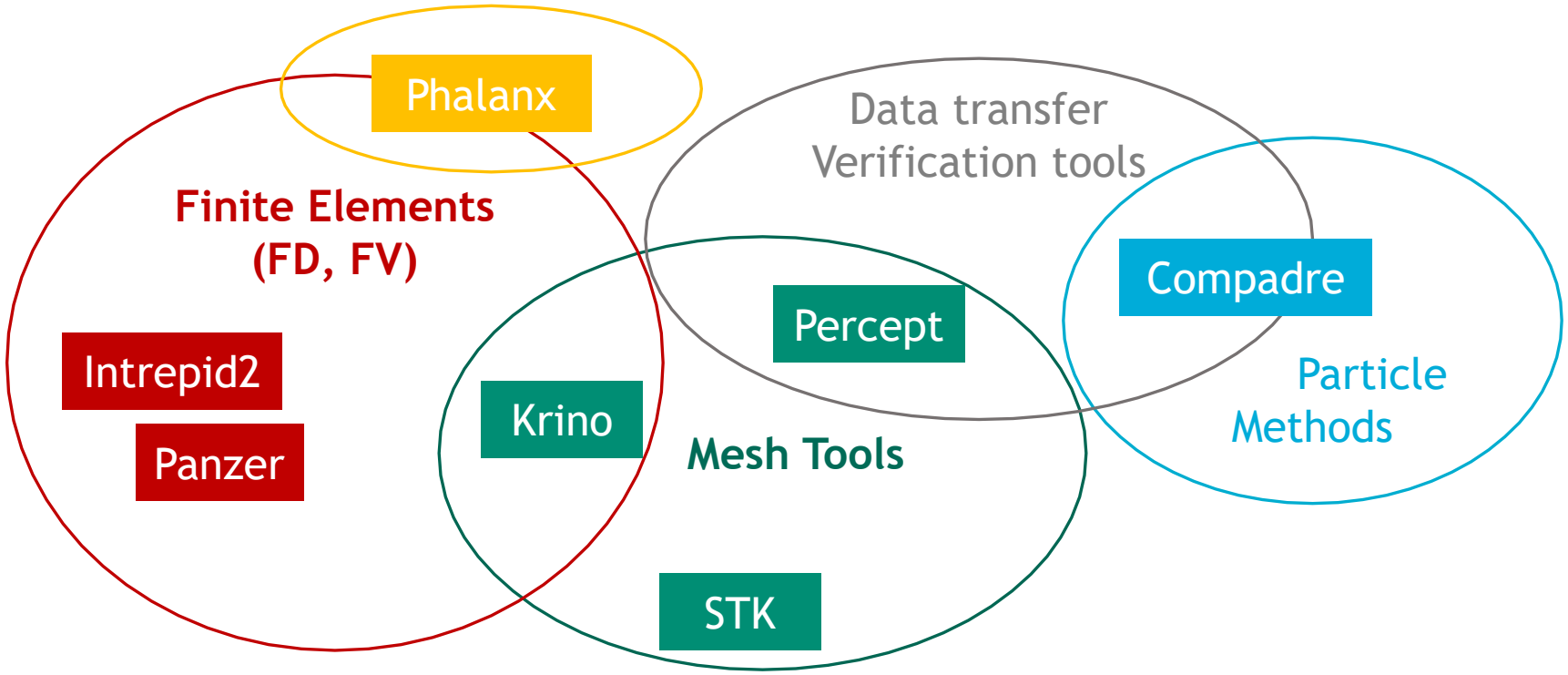


Dependencies:

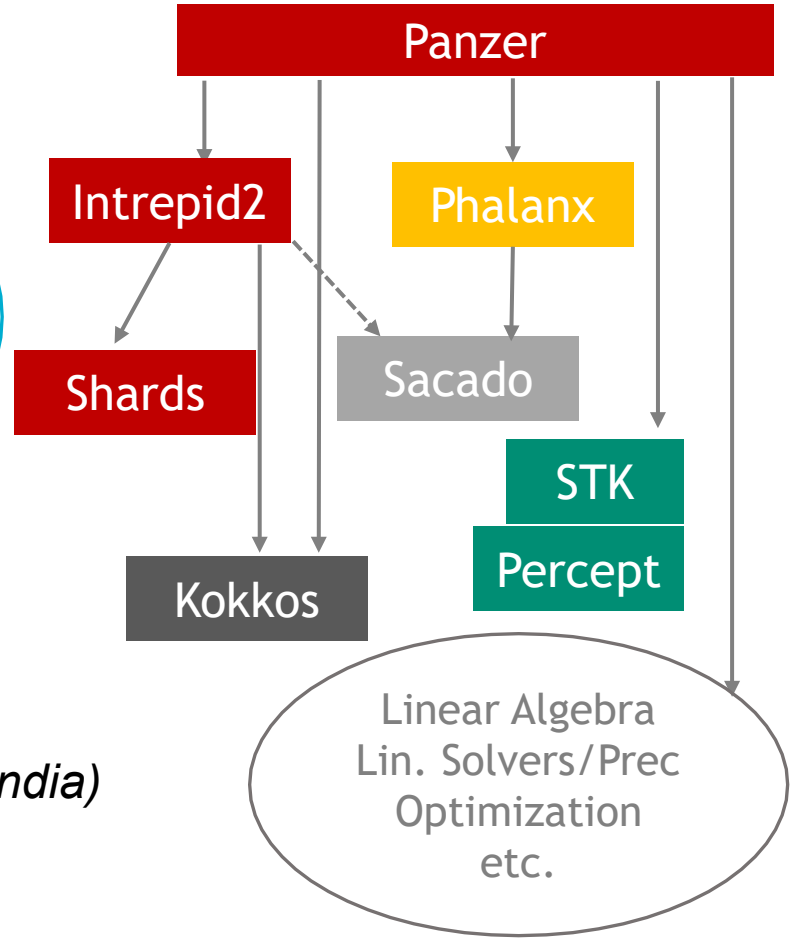


Phalanx: DAG-based expression evaluation – *R. Pawlowski*
used to decompose complex PDE systems into a number of elementary user-defined expression

Discretizations Product: overview
(actively developed packages)



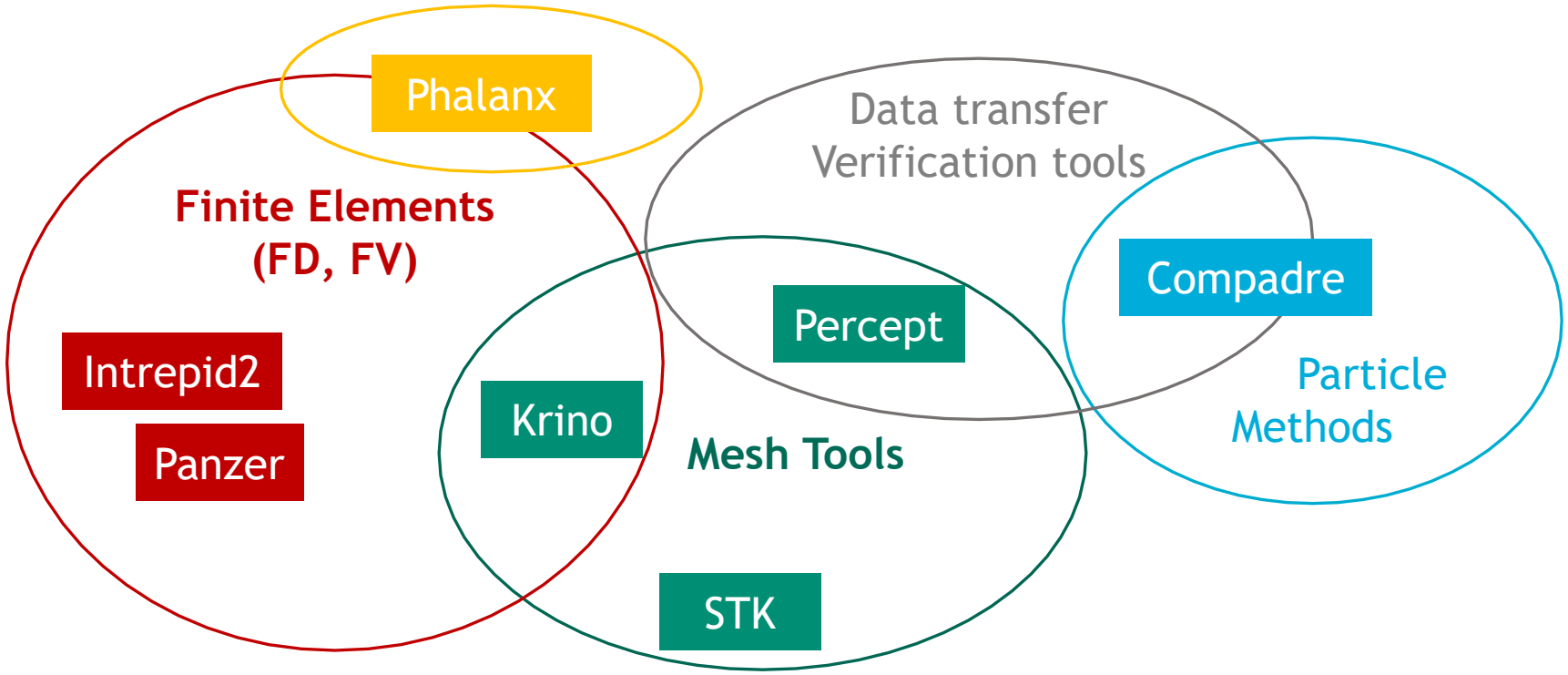
Dependencies:



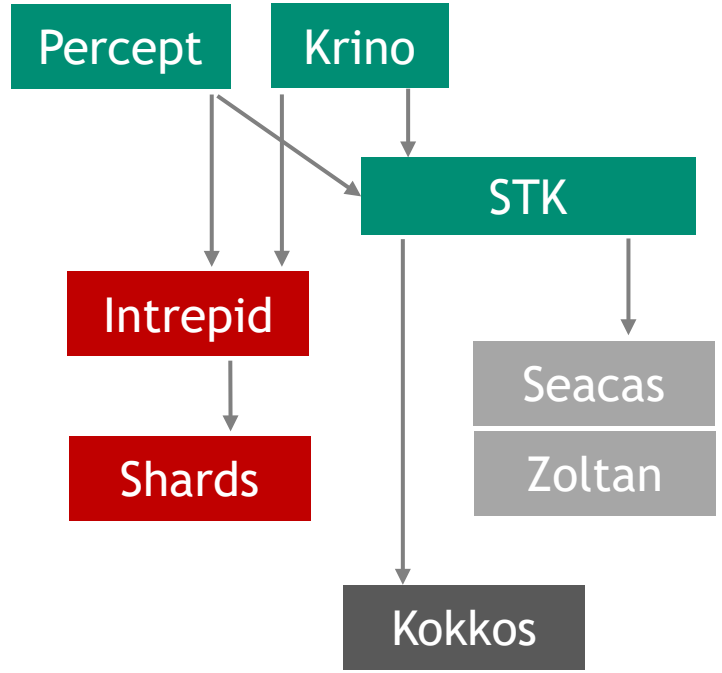
Intrepid2: Local FE assembly –*N. Roberts, M. Perego (K. Kim left Sandia)*
Basis functions definitions, quadrature rules, orientations, projections

Panzer: FE library – *R. Pawlowski*
DoF Management, FE global assembly into distributed nonlinear systems, handling of linear/nonlinear solvers, sensitivities and PDE-constrained optimization, Import/Export of meshes

Discretizations Product: overview
(actively developed packages)



Dependencies:



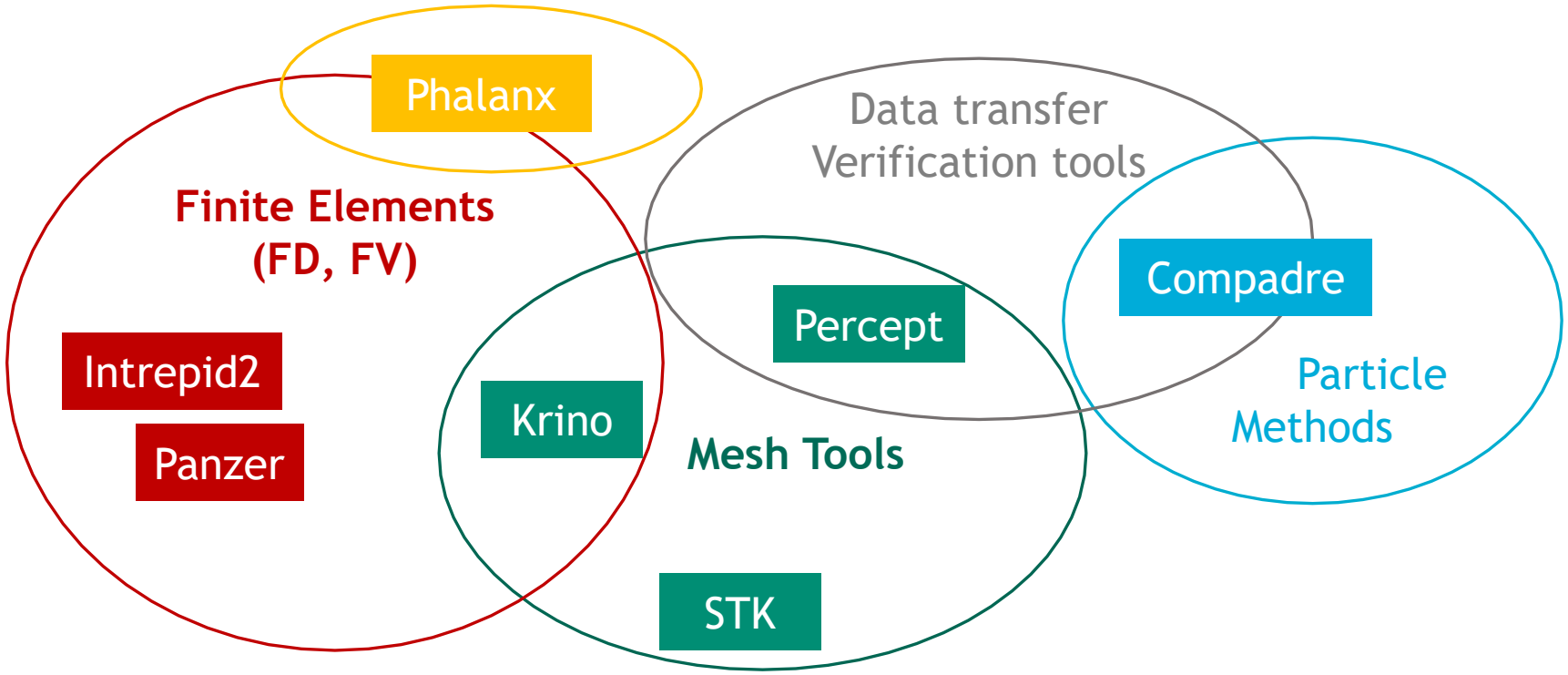
STK: unstructured mesh in-memory, parallel-distributed database – *A. Williams*

Mesh topology data structure, mesh subsetting, coefficient data, mesh field data, support for changing the mesh topology, and support for parallel operations on the mesh

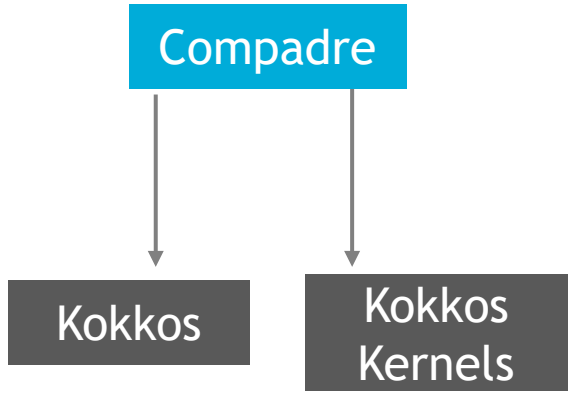
Krino: tools for level set fields – *D. Noble*

Percept: tools to enable solution verification, mesh adaptation and data transfer – *B. Carnes*

Discretizations Product: overview
(actively developed packages)



Dependencies:



Compadre: local tools for mesh-free approximation of linear operators – *P. Kuberry*

Applications: mesh-free discretizations and data-transfer

Discretizations Product: update

- The discretizations product is **UVM-free.**
- The Kokkos-based discretization packages can now run on **AMD/HIP.**
- The discretizations product can be built **without Epetra.**
- **Intrepid archival planned for FY24**
  - Krino and Percept will switch to Intrepid2 by FY23, Q2
  - **Please contact Mauro or me if you need help switching to Intrepid2**
- Short on funding this year, but we are working towards **matrix-free assembly** (more on this in the Intrepid2 deep-dive part of this talk)

Discretizations Product: update
(General Improvements/Planning)

Intrepid2 (more in the deep dive)

- Several optimizations relying on structured data (tensor basis, affine meshes, extruded meshes, etc.)
- Provided tools for FE projections tools on boundary side sets (for Dirichlet conditions)
- Almost-finalized implementation of high-order hierarchical basis functions (pyramids coming soon)
- (FY23) implementation of getValue() function for multiple cells
- (FY23) support for orientations with structured integration

Phalanx

- New tools for constructing and managing lifetimes of Kokkos View-Of-Views, specifically targeted to work with UVM free and HIP builds
  - Three implementations for different use cases: Recommend using PHX::ViewOfViews3. This will be the default moving forward and will probably be renamed
  - Darma/Maestro (checkpoint) serialization support available
  - Supports inner Kokkos::Views with Sacado FAD scalar types
  - (Coming soon) Extension to DynRankView is coming
- New utility for creating a vtable on device: designed to support UVM free and HIP builds
- Note: No plans/funding to port to SYCL backend

Discretizations Product: update
(General Improvements/Planning)

Panzer

- New search algorithm for point matching in periodic BC setup (uses stk_search). Order of magnitude improvements at scale. Not the default yet but can enable with plist value
- New examples that show how to use DOF manager with Intrepid2 projection utilities
- Epetra stack is now optional.
  - Need to merge Teko branch for full panzer functionality
  - Replicated most Epetra tests to Tpetra in anticipation of dropping the Epetra stack
- New tools to convert mesh data from 2nd to 1st order
- Support for UMR library: inline uniform refinement of STK meshes that snaps boundaries to geometry. Note, UMR is currently internal to Sandia, but may be open sourced in the future
- Moved more operations to device
- Note: No plans/funding to port to SYCL backend
- (FY23) DOF Manager: fix writing of tensor-based FE elements to STK mesh.

Discretizations Product: update
(General Improvements/Planning)

STK
- STK has been ported to the AMD/GPU platforms
- STK Balance has been optimized to produce better decompositions for cases involving contact
- (FY23) Enhancements to STK Transfer to provide moving-least-squares interpolation
- (FY23) Documentation/examples for STK Transfer
- (FY23) Conservative transfer capability

Krino
- Enhanced support for interface-conforming discretizations for analytic and faceted interfaces
- Improved CPU performance when generating interface-conforming discretizations
- Improved the capture of sharp mesh features (edges and vertices) when generating interface-conforming discretizations
- (FY23) Improve local volume conservation when renormalizing level set fields
- (FY23) Improve capability for refining a mesh in the vicinity of a level set interface

Compadre
- Improved remapping on a sphere (for climate application)
- Added option to use Bernstein polynomials as basis for the GMLS reconstruction space