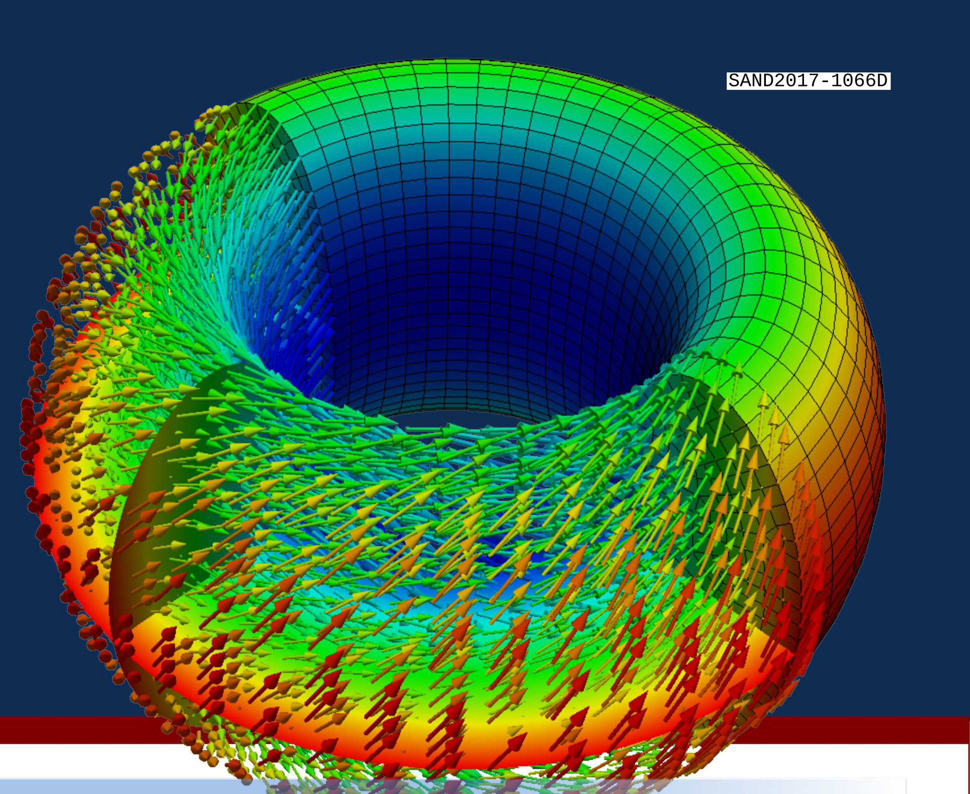
SAND2017-1066D

ECP 1.3.3.03a Develop General CS Components for ATDM Applications



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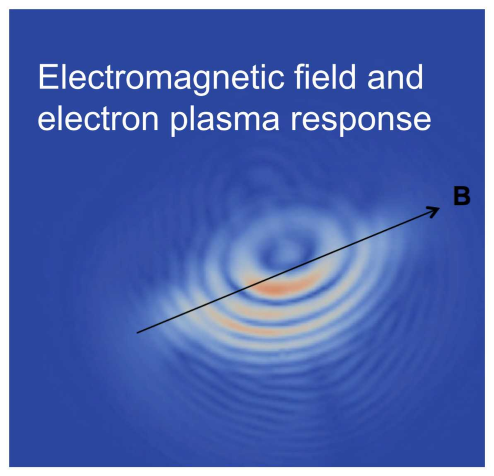
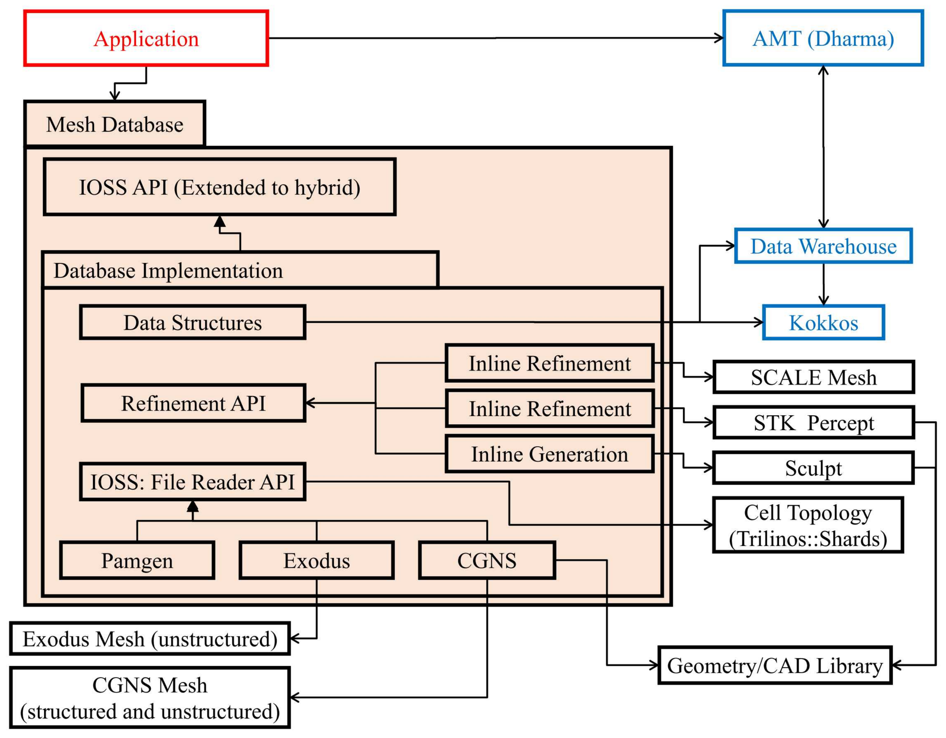
Project Description

- Develops general computer-science components required by ATDM applications:
  - **Mesh database** for structured, unstructured and hybrid meshes
  - Finite element **discretization tools**
  - **Time integration** library that supports IMEX and adjoint sensitivity analysis
  - Performance portable linear and nonlinear **solver abstractions**
- Components use ATDM Core capabilities:
  - **Kokkos** performance portability
  - **DARMA** asynchronous many-tasking (AMT)
  - **DataWarehouse**
  - **Sacado/Stokhos** embedded technology.
- Released as open source software components via Trilinos



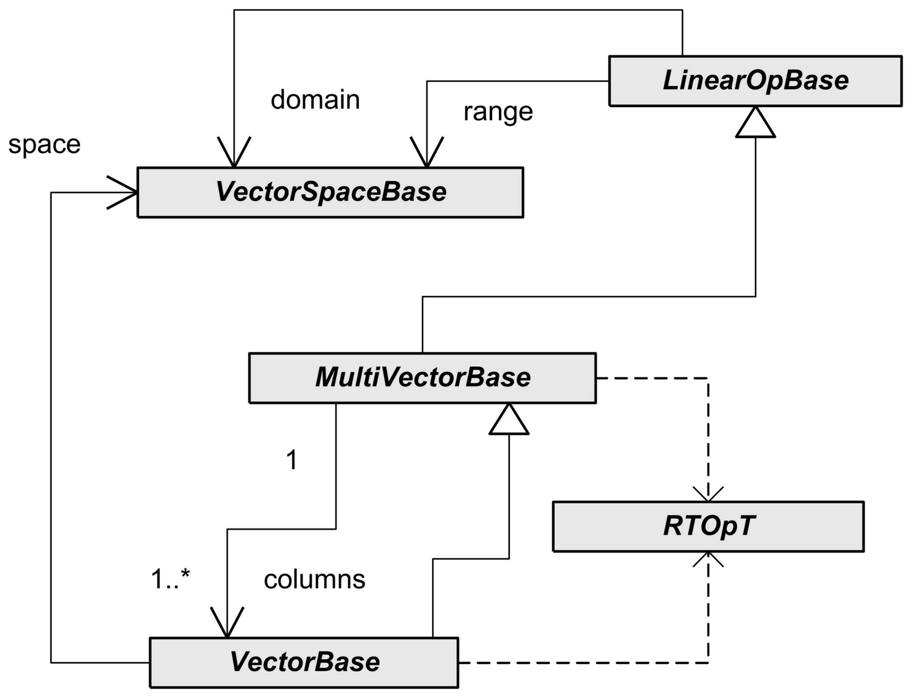
Mesh Database

- Rethink how application uses a mesh database
  - "Mesh as scaffolding"
  - I/O and simple tools
  - Application can define optimal structures
- Development (SEACAS/IOSS):
  - Structured, Unstructured and Hybrid
  - Kokkos and data warehouse integration
  - Burst buffer support
  - Inline refinement (Percept)
  - Structured mesh support (CGNS)



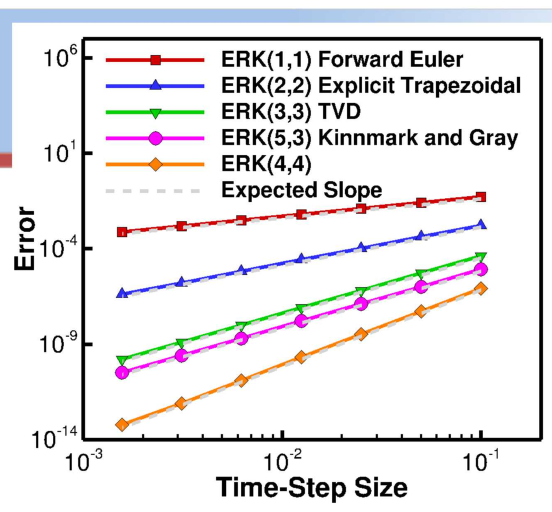
Performance Portable Solver Abstractions

- General interfaces for abstract numerical algorithms
  - Vector/Operator, Linear and nonlinear problem abstractions (Thyra)
  - Block Composition
  - User Defined Reduction/Transformation Operators (RTOps)
- Supports Trilinos solvers: Nonlinear, Optimization, Bifurcations analysis, Block Preconditioners and GMRES Solvers
- Development:
  - CUDA performant abstractions for Tpetra
  - Performance portable RTOps design



Time Integration

- Tempus: A new Time Integration package in Trilinos
- Built on Thyra solver Abstractions
- Design targets IMEX and adjoint sensitivity analysis
- Currently supports Euler (forward/backward), ERK (10 tableaus), DIRK (5 tableaus)



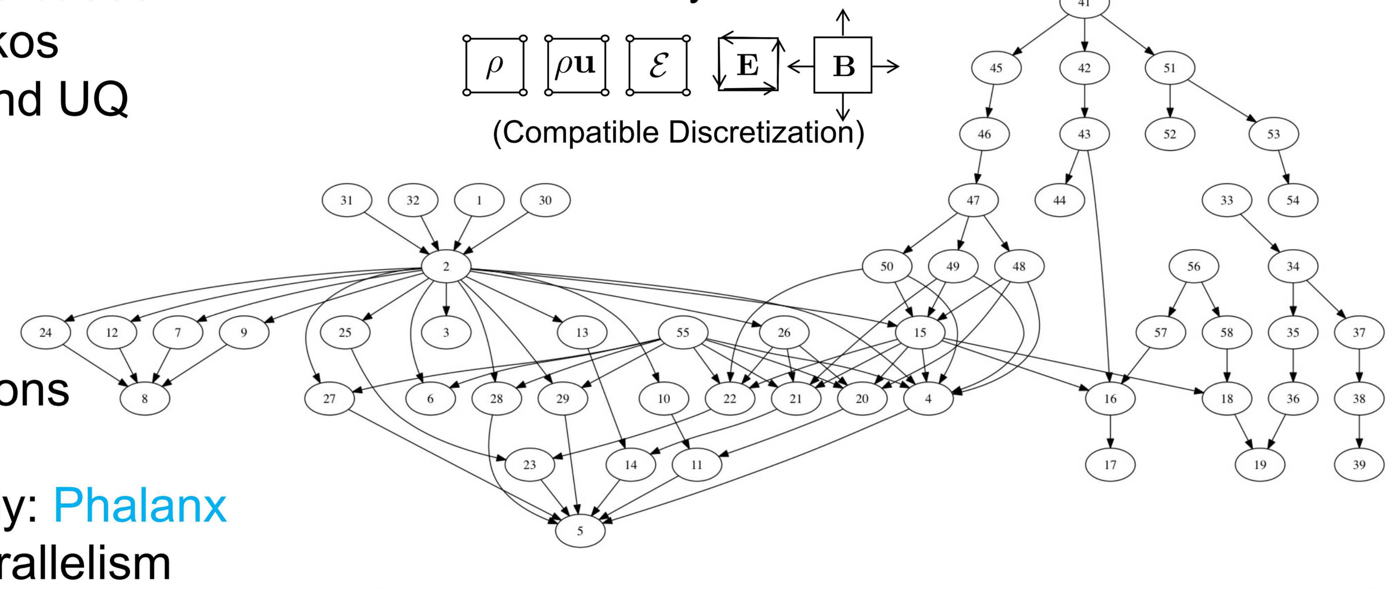
Discretization Tools

- General Tools
  - Stand-alone or integrated use cases
  - Performance portability: Kokkos
  - Embedded technology: AD and UQ
- Finite Element Tools: Intrepid2
  - Local assembly
  - High order bases
  - Nodal/Edge/Face discretizations
- DAG-based Multiphysics Assembly: Phalanx
  - Node local Task and Data parallelism
  - Experimental AMT via Kokkos
- Global Multiphysics Assembly Tools: Panzer
  - Degree of freedom indexer
  - Fully-coupled assembly
    - Mixed basis within element block (compatible discretizations)
    - Different equations across element blocks
    - Blocked or interleaved

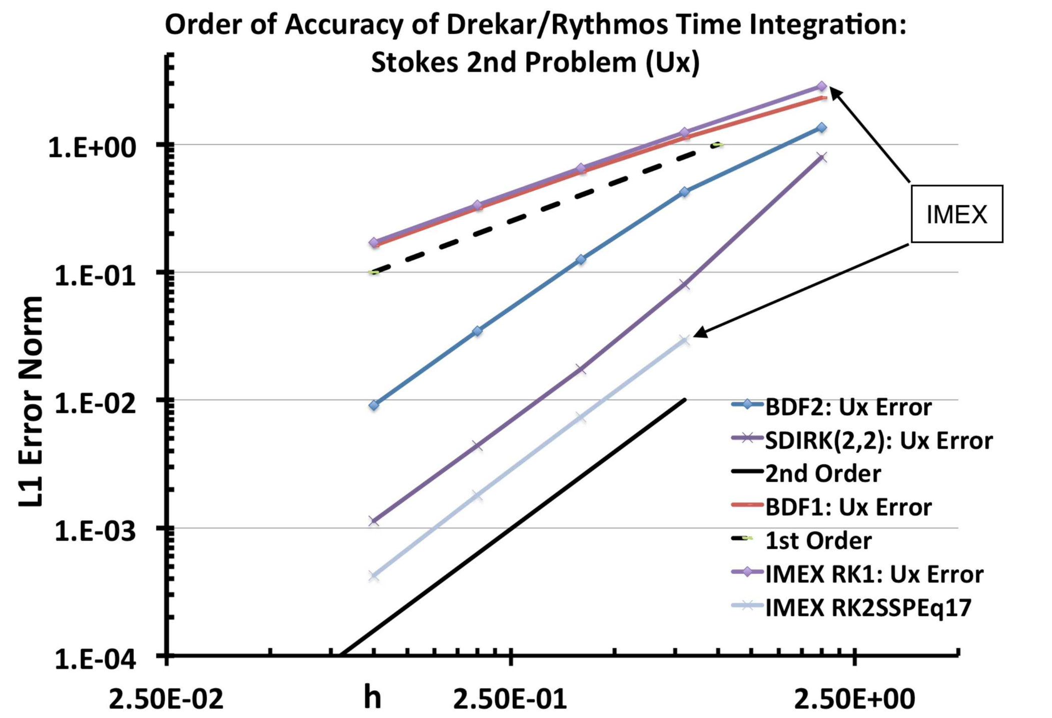
$$\mathcal{A}=\begin{bmatrix} I & \\ BF^{-1} & I\end{bmatrix}\begin{bmatrix} F & B^T \\ & S\end{bmatrix} \qquad S=C-BF^{-1}B^T$$

  - Workset builders
- Multiple applications built on tools: Drekar (Turbulent CFD/MHD/Multi-species plasma), EMPIRE (EM/PIC), Charon2 (Device), Albany (Quantum, Solid mech., Ice Sheet, …)

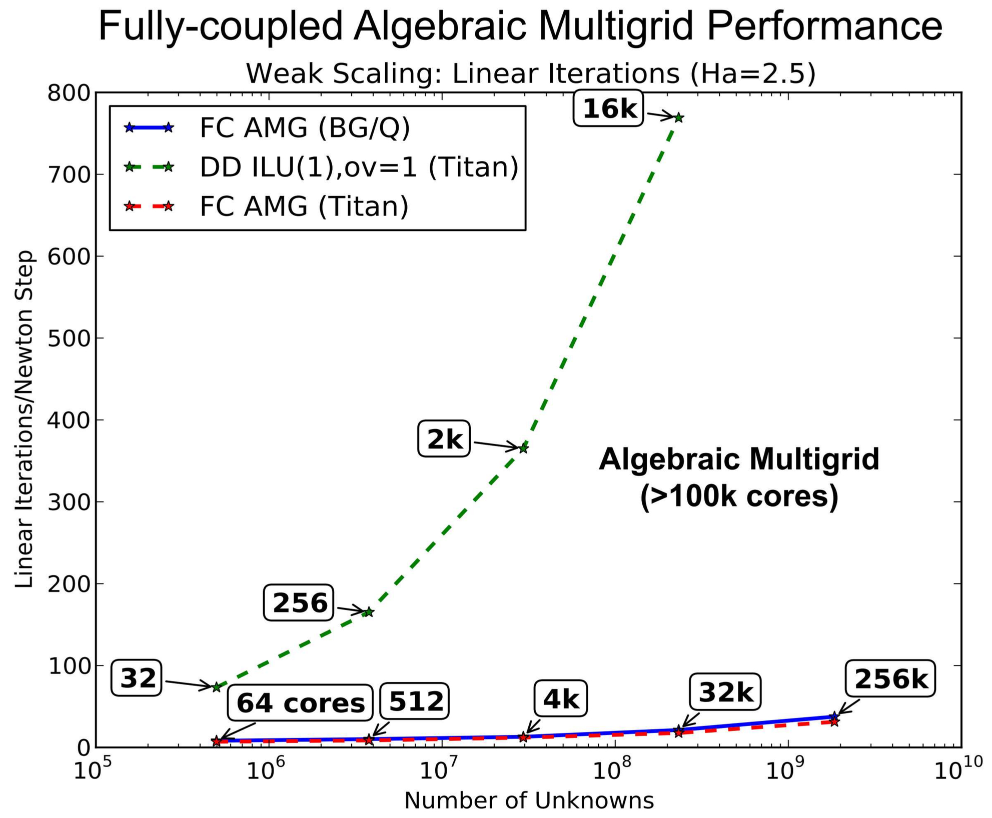
Drekar Multi-species Plasma Assembly DAG



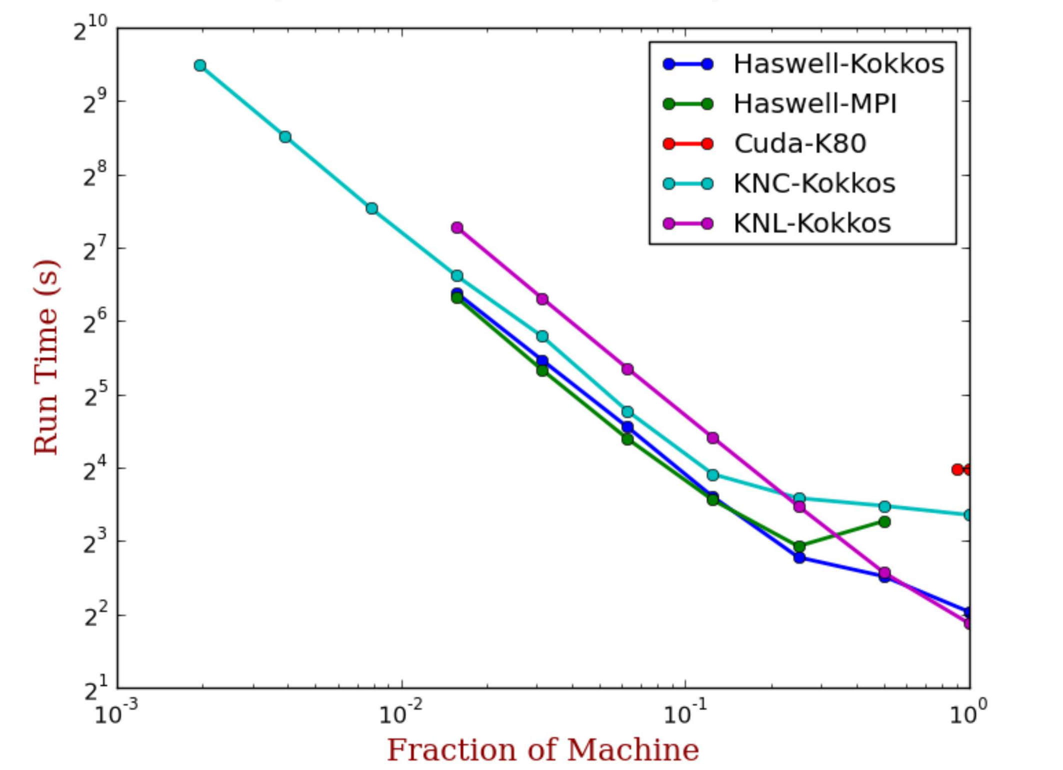
Evaluation Type	1 Thread/node	8 Threads/node	16 Threads/node
Residual	3.5	4.5	4.9
Jacobian	3.4	3.4	3.5



Fully-coupled Algebraic Multigrid Performance



Drekar Multi-species Plasma Assembly Performance



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