



Discretization Capability Area

Overview

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Discretization Capability Area

What is it?

The Discretization Capability Area is a collection of **low-level software tools** that enable rapid development of application codes based on the numerical solution of partial differential equations (PDEs).

File input / output,
meshing, partitioning



PDE Discretization

The nitty-gritty that
takes you  from the
computational mesh to
your first linear system.



Linear / nonlinear
solvers, eigensolvers,
optimization, etc.



Discretization Capability Area

Which packages?

Shards

definition of cell topology

Intrepid

local (cell-based) FE/FV/FD basis definition;
numerical integration; cell geometry; etc.

Phalanx

decomposition of complex PDE systems into a number of
elementary user-defined expressions; efficient management
of expression dependencies; hooks to embedded tools, etc.

FEI, Panzer

user-defined assignment and management of global degrees of freedom;
assembly of local PDE discretization data into distributed linear systems; etc.



Discretization Capability Area

Which packages?

Shards

- a suite of common tools for topological data that facilitate interoperability between PDE software
- cell definitions (e.g., triangle, hexahedron, etc.)
- methods to manage and access information about cell topologies:
 - (1) query adjacencies of subcells
 - (2) find subcell permutation w. r. to global cell
 - (3) create user-defined custom cell topologies

Shards

cell topology

Intrepid

local PDE discretization

Phalanx

PDE expression trees

FEI, Panzer

global DOFs; linear systems



Discretization Capability Area

Which packages?

Intrepid

- physics-compatible cell-local PDE discretizations
- streamlined access to finite element, finite volume and finite difference methods
- support for a wide range of cell topologies
- compatible finite element spaces of arbitrary degree for $H(\text{grad})$, $H(\text{curl})$, $H(\text{div})$ and $L2$ spaces
- Lagrange-interpolating and modal FE bases
- prototype for polyhedral FE bases
- prototype for control-volume (CV) FEM
- numerical integration: spatial and stochastic
- cell geometry tools: volumes, normals, tangents, reference-to-physical maps

Shards

cell topology

Intrepid

local PDE discretization

Phalanx

PDE expression trees

FEI, Panzer

global DOFs; linear systems



Discretization Capability Area

Which packages?

Phalanx

- cell-local field (variable, data) evaluation kernel specifically designed for general PDE solvers
- decomposition of complex PDE systems into a number of elementary user-defined expressions
- management of expression dependencies
- enables rapid development of large PDE codes
- user-defined data types and evaluation types offer unprecedented flexibility for direct integration with user applications
- they also enable embedded technology such as automatic differentiation for sensitivity analysis, optimization and uncertainty quantification

Shards

cell topology

Intrepid

local PDE discretization

Phalanx

PDE expression trees

FEI, Panzer

global DOFs; linear systems



Discretization Capability Area

Which packages?

FEI, Panzer

- user-defined assignment and management of global degrees of freedom (DOFs)
- assembly of cell-local PDE discretization data into global, distributed linear systems
- insulate PDE application codes from linear-algebra issues such as sparse matrix storage and mappings of DOFs to distributed linear equations
- support multi-physics problems, allowing for arbitrarily complicated PDE discretizations with multiple DOFs per subcell (edge-based, face-based, node-based and mixed)

Shards

cell topology

Intrepid

local PDE discretization

Phalanx

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Discretization Capability Area

News

- Drekar (used in CASL) represents a superb demonstration of all tools in the Discretization Capability Area: talk to R. Pawlowski and E. Cyr
- Panzer is now officially available in Trilinos (still experimental – patience, please)

Two related presentations today:

- 3:45pm - 4:15pm, **E. Cyr: *A New Degree-of-Freedom Capability***
- 4:15pm – 4:30pm, **S. Gao: *Discretization Tool Use in Charon***