Discretization Capability Area

Overview

People: Pavel Bochev, Eric Cyr, Carter Edwards, Rob Kirby, Roger Pawlowski, Kara Peterson, Denis Ridzal, Alan Williams

SAND 2012-9588P
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?

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

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

Shards
definition of cell topology

Trilinos

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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

**Intrepid**
local PDE discretization

**Phalanx**
PDE expression trees

**FEI, Panzer**
global DOFs; linear systems
**Discretization Capability Area**

Which packages?

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**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 $L^2$ 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

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**Shards**
- cell topology

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**Intrepid**
- local PDE discretization

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**Phalanx**
- PDE expression trees

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**FEI, Panzer**
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**Trilinos**
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)
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*