PORTAGE - A Flexible Conservative Remapping Framework for Modern HPC Architectures

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1. Summary
We demonstrate the design and performance of Portage, a flexible, conservative, parallel remapping framework designed for modern HPC platforms.

2. Introduction
- **Remapping**: transfer of field data between two computational meshes (or point clouds)
- Remapping is used to transfer data between:
  - two computational codes and their meshes,
  - two physics modules of a single code, or
  - poor quality and good-quality meshes in Arbitrary-Lagrangian Eulerian (ALE) methods
- Conservative, Accurate, Bounds-preserving, Fast, Scalable

3. Schematic of Exact Intersection Remapping

4. Portage Framework Design
- Portage is templated on most components - mesh, state, search, interface and interpolate classes.
- Allows clients to use custom components or default ones
- Portage takes care of executing the algorithm with distributed, threaded and GPU parallelism
- Functional design will allow use task parallelism (e.g., FleCSI/Legion)

5. Supplied Component Classes
- **Mesh/State**: Simple Mesh (serial, cartesian mesh, scalar fields) Jal
- **Search**: kd-tree search
- **Intersect**: R2D-R3D (github.com/devompowell/r3d)
- **Interpolation**: 1st-, 2nd- and 3rd-order accurate interpolation with Barth-Jespersen gradient limiting for bounds-preservation

6. Handling Unstructured Polyhedral Meshes
- Default mesh interface assumes unstructured polyhedral meshes, possibly non-convex with curved faces
- Supplied search, intersect, interpolation handle such meshes
- Can replace with more efficient components for specialized meshes
- Some basic functionality expected from supplied mesh class (node coordinates, cell → nodes, node → cells, etc.)
- Rest can be constructed by Portage (if not supplied)

7. Distributed memory parallelism
- If source cells overlapping target cell are not on MPI rank, one has to fetch them
- Portage copies and transmits mesh/field data so that clients don't have to redistribute
- Check if bounding boxes of target mesh on rank i overlaps with source mesh from rank j
- If there is overlap, get source mesh and field data from rank i to rank j - no communication needed subsequently

8. On-node parallelism
- On-node parallelism achieved through NVidia Thrust parallel constructs like thrust::transform or thrust::for_each
- Similar constructs in Kokkos (Trilinos) and C++17 standard
- Abstracted out as Portage::transform so that we can call std::transform if Thrust not enabled
- Thrust can be directed to run the parallel constructs using OpenMP, Intel TBB or CUDA backends
- Requires search, intersect and interpolate to be written in functional style - be functors with no side effects
- Code is fully tested with OpenMP - early version of 1st order remap tested with CUDA

9. Test Machine - ASC Snow at Los Alamos National Lab

10. Handling Unstructured Polyhedral Meshes
- Peak performance: 445 TFlop/s
- Machine: Snow
- Specs: Based on Penguin Computing Inc.'s TundraES racks
  - 368 Intel Broadwell nodes, 2 sockets/node, 18 cores/socket (13248 cores)
- Memory/Node: 128GB
- Interconnect: Intel Omnipath

10.1 OpenMP scaling on single node

10.2 Results - MPI+OpenMP Strong, Weak Scaling
Standard partitioning refers to closely aligned partitioning for source and target mesh
Reverse partitioning reverses the MPI ranks for the source mesh to create a greater mismatch

11. Results - Mesh-Mesh Remapping

12. Remapping between Particle Swarms (Point Clouds)
- Portage can transfer data between two particle swarms
- Estimation of field at target particle from Local Regression Estimate (LRE)[Dilts, G.A.] on source swarm
- Currently only on-node parallelism. Distributed parallel implementation coming soon
- Lack of scaling on-node likely due to poor search scaling
- Portage can also remap from mesh-mesh using particles as an intermediary

13. Multi-material Remapping and Interface Reconstruction
- Remapping of quantities when source cells may have multiple materials
- Only material values of field and volume fractions of materials in each cell known on source mesh
- Need to temporarily subordinate source cells into pure material polyhedra by interface reconstruction
- Interface reconstruction package Tangram in the works

14. Tangram Results with XM0F2D Plugin

15. Other ongoing improvements
- Remapping of vector and tensor fields
- Improvement of intersection efficiency (most time spent here)
- Minimizing data exchange between processors
- Automatic data dependency resolution using FleCSI/Legion
- Automatic task parallelism through FleCSI/Legion
- Cartesian mesh, Spherical mesh and other specializations

16. Availability
- Open Source at http://www.github.com/laristra/portage

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