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Zoltan2: A new toolkit of combinatorial algorithms addressing the needs of parallel applications on emerging architectures

Zoltan2 Overview and Goals

Algorithms needed by applications on emerging architectures

- Partitioning and task placement for hierarchical memory systems
- Node-level coloring for multi-threaded parallelism

Multi-threaded implementations that run on emerging architectures

Support for very large application problem sizes

- Templated data types for local and global indices

Application-focused interface supporting meshes, matrices, vectors, particles, coordinates, graphs

Open-source software in Trilinos' next-generation solver stack



Successor to the Widely Used Zoltan Toolkit

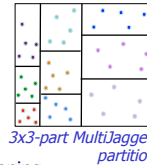
	Zoltan	Zoltan2
Parallelism	MPI-only	MPI+X
API	Application builds model (e.g., graph, hypergraph) for algorithm	Application describes its data (matrix, mesh); algorithm builds model
Capabilities	Parallel partitioning Parallel coloring Global and local ordering	Parallel partitioning Architecture-aware task placement On-node coloring On-node ordering
Optional TPLs	PT-Scotch (INRIA/LaBRI) ParMETIS (U. Minnesota) PaToH (Ohio St. U.)	PT-Scotch (INRIA/LaBRI) ParMETIS (U. Minnesota) ParMA (Rensselaer) AMD (U. Florida) LDMS: Lightweight Distributed Metric Service (Sandia)
Maturity	Highly mature; maintenance only	Research platform for emerging architectures
Integration	No dependence on Trilinos	Integrated with Trilinos next-generation software stack
Language	C (with F90 & C++ APIs)	Templated C++11
Distribution	Stand-alone or in Trilinos	In Trilinos

Scalable Partitioning

Assign data/work to processors so that processor idle time and interprocessor communication are minimized

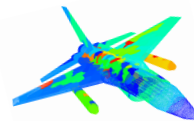
MultiJagged: Multi-threaded geometric (coordinate) partitioning

- MPI+OpenMP implementation
- Multisection has less data movement, greater scalability than Recursive Coordinate Bisection
- Fast; scalable; enforces geometric locality
- Good for adaptivity, particles, contact detection



Topology-based (graph, hypergraph, mesh) partitioning

- Explicitly models communication costs through data dependencies
- Good for mesh-, matrix- and network-based applications



Unstructured mesh partitioning; image courtesy of Bhardwaj (Sandia)

Integrated with

- Graph partitioning: PT-Scotch; ParMETIS
- Hypergraph partitioning: Zoltan
- Mesh partitioning & partition improvement: ParMA (Rensselaer)

Architecture-Aware Task Placement

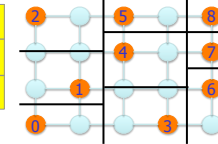
Given a (possibly non-contiguous) node allocation in a parallel computer, reduce application communication costs and runtime by placing interdependent MPI tasks on "nearby" cores

Important in extreme-scale systems:

- Allocations can be sparse and spread far across the network
- Messages can travel long routes
- Increasing locality reduces congestion and communication time

Tasks with stencil-like communication pattern

2	5	8
1	4	7
0	3	6



Geometric task placement on allocated nodes in torus network

Approach:

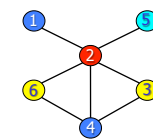
- Use *geometric proximity* of tasks' data as a proxy for communication costs between tasks
- Apply *MultiJagged* partitioner to order both tasks' data and nodes' coordinates
- Map a task to the core with the same part number

On-Node Balanced Graph Coloring

Coloring: Label graph vertices so that adjacent vertices have different labels and the number of labels is small

- Good for on-node parallelism: Each label is an independent set that can be computed in parallel

	1	2	3	4	5	6
1	X	X	X	X	X	X
2	X	X	X	X	X	X
3	X	X	X	X	X	X
4	X	X	X	X	X	X
5	X	X	X	X	X	X
6	X	X	X	X	X	X



Balanced coloring of matrix columns

Balanced coloring: Label roughly the same number of vertices with each label, at the possible expense of using slightly more labels

- Important for GPUs: labels with too few vertices cause idle time

On-Node Matrix Ordering

Find permutation of local matrix that reduces fill during factorization

- Reverse Cuthill-McKee
- Sorted Degree
- Approximate Minimum Degree, via AMD

Used, e.g., in Trilinos' IFPACK2 sparse-matrix preconditioners

Ongoing and Future Work

- Integration of Kokkos performance-portable programming model (Edwards, Trott; Sandia) into Zoltan2 interface and algorithms
- KokkosKernels: New toolkit of on-node Kokkos-based graph algorithms
- Task placement for new network topologies (e.g., Dragonfly)
- Interface to PULP (Slota, Madduri, Rajamanickam; PSU, Sandia) for partitions that minimize multiple constraints & objectives

More Information: <http://www.fastmath-scidac.org> or contact Karen Devine, kddevin@sandia.gov