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Tutorial: The Zoltan Toolkit

Karen Devine and Cedric Chevalier
Sandia National Laboratories, NM

Umit Catalyurek
Ohio State University

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Outline

- High-level view of Zoltan
- Requirements, data models, and interface
- Dynamic Load Balancing and Partitioning
- Matrix Ordering
- Graph Coloring
- Utilities
- Alternate Interfaces
- Future Directions

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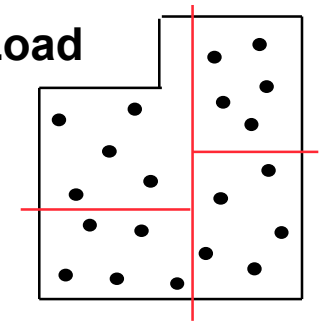
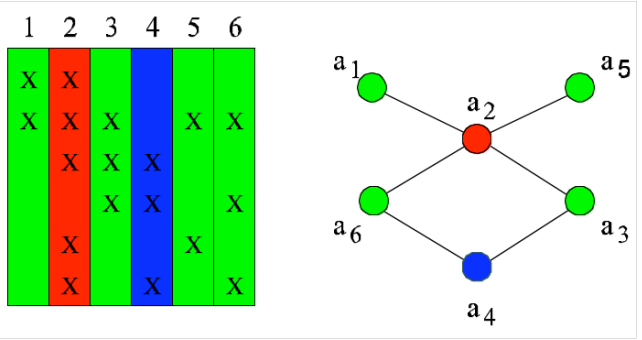
The Zoltan Toolkit

- **Library of data management services for unstructured, dynamic and/or adaptive computations.**

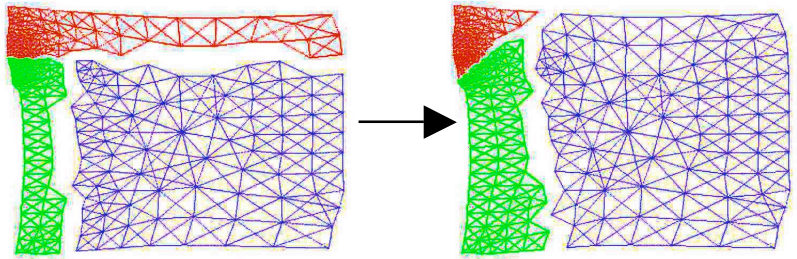
Dynamic Load Balancing



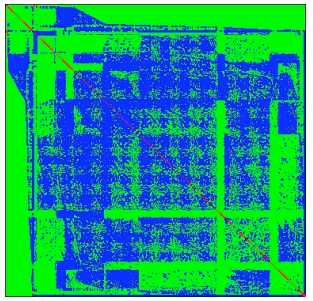
Graph Coloring



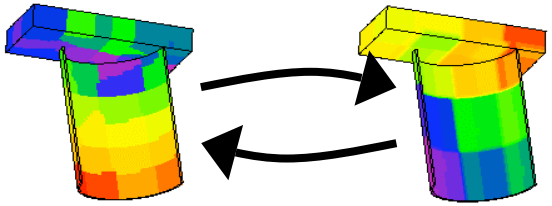
Data Migration



Matrix Ordering



Unstructured Communication



Distributed Data Directories

A	B	C	D	E	F	G	H	I
0	1	0	2	1	0	1	2	1

Zoltan System Assumptions

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- Assume distributed memory model.
- Data decomposition + “Owner computes”:
  - The data is distributed among the processors.
  - The owner performs all computation on its data.
  - Data distribution defines work assignment.
  - Data dependencies among data items owned by different processors incur communication.
- Requirements:
  - MPI
  - C compiler
  - GNU Make (gmake)

Zoltan Supports Many Applications

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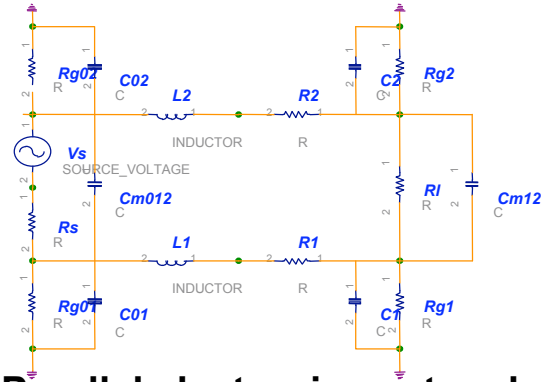
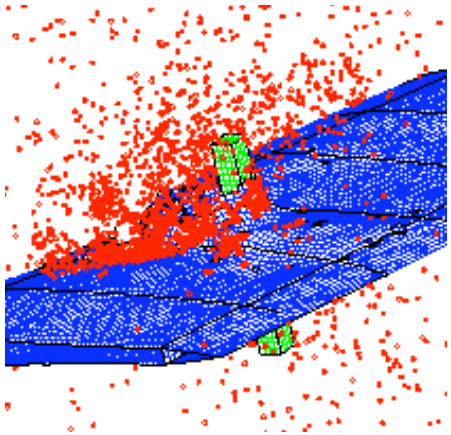
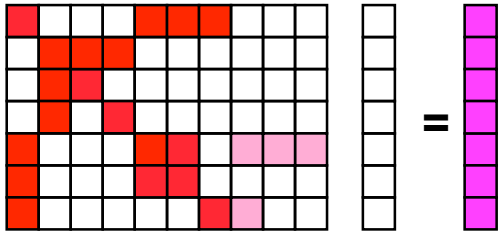
- **Different applications, requirements, data structures.**



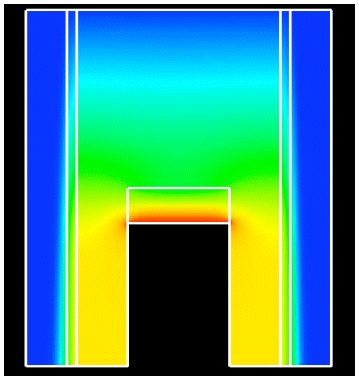
Parallel electronics networks



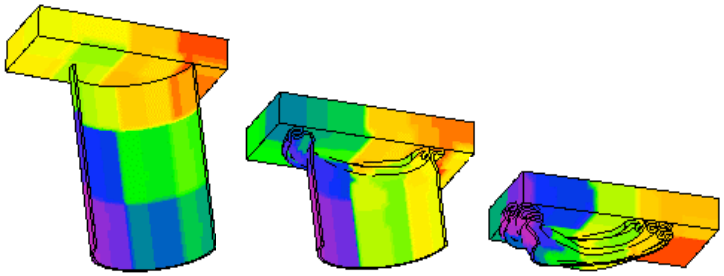
Particle methods



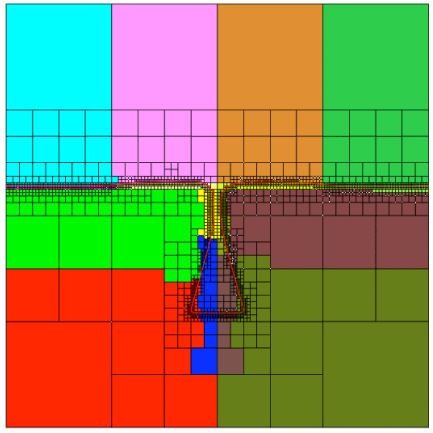
Linear solvers & preconditioners



Multiphysics simulations



Crash simulations



Adaptive mesh refinement

Zoltan Interface Design

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- Common interface to each class of tools.
- Tool/method specified with user parameters.

- Data-structure neutral design.
  - Supports wide range of applications and data structures.
  - Imposes no restrictions on application's data structures.
  - Application does not have to build Zoltan's data structures.

Zoltan Interface

- **Simple, easy-to-use interface.**
  - **Small number of callable Zoltan functions.**
  - **Callable from C, C++, Fortran.**

- **Requirement: Unique global IDs for objects to be partitioned/ordered/colored. For example:**
  - **Global element number.**
  - **Global matrix row number.**
  - **(Processor number, local element number)**
  - **(Processor number, local particle number)**

Zoltan Application Interface

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- **Application interface:**
  - **Zoltan queries the application for needed info.**
    - **IDs of objects, coordinates, relationships to other objects.**
  - **Application provides simple functions to answer queries.**
  - **Small extra costs in memory and function-call overhead.**
- **Query mechanism supports…**
  - **Geometric algorithms**
    - **Queries for dimensions, coordinates, etc.**
  - **Hypergraph- and graph-based algorithms**
    - **Queries for edge lists, edge weights, etc.**
  - **Tree-based algorithms**
    - **Queries for parent/child relationships, etc.**
- **Once query functions are implemented, application can access all Zoltan functionality.**
  - **Can switch between algorithms by setting parameters.**

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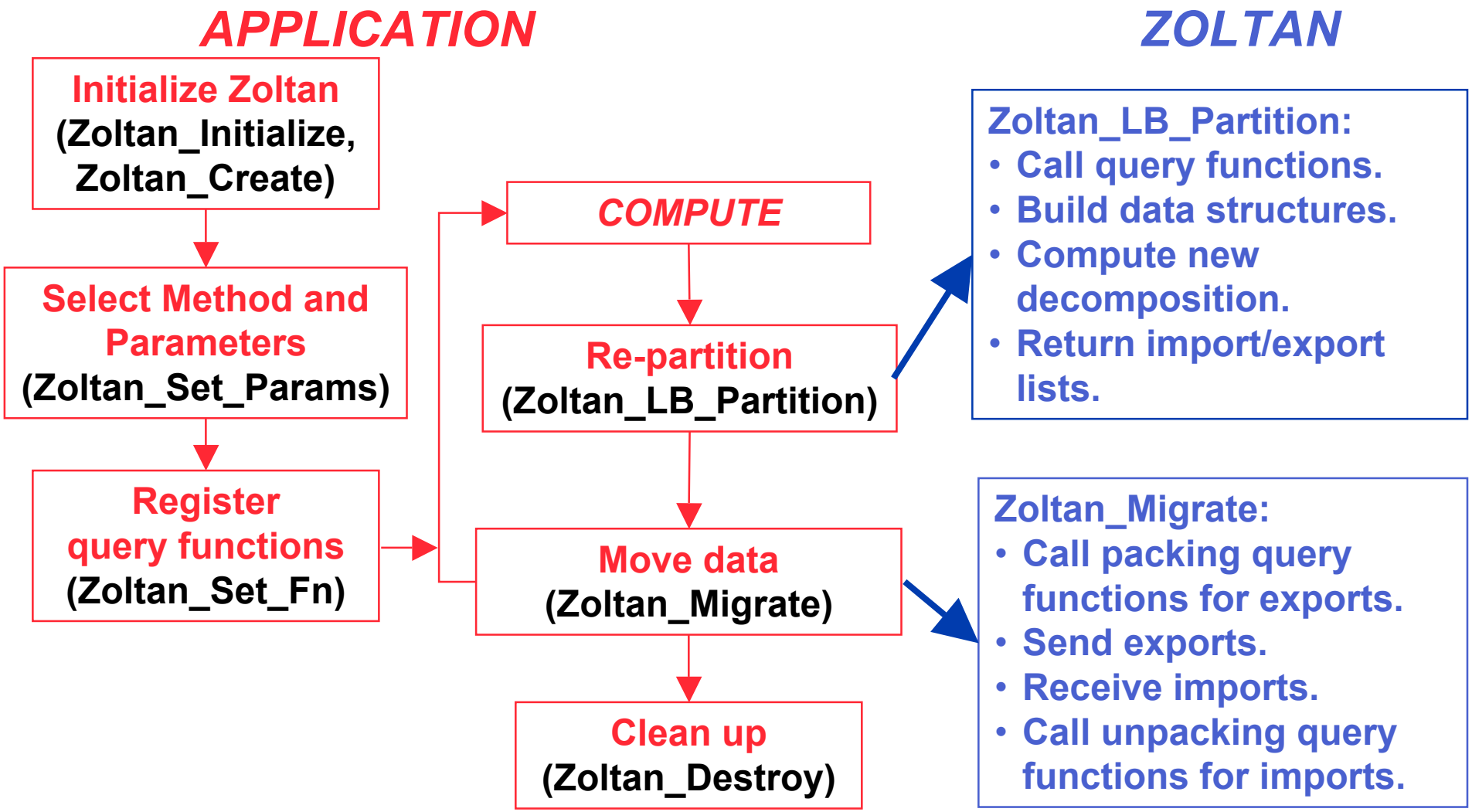
Zoltan Application Interface



Zoltan Query Functions

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General Query Functions	
`ZOLTAN_NUM_OBJ_FN`	Number of items on processor
`ZOLTAN_OBJ_LIST_FN`	List of item IDs and weights.
Geometric Query Functions	
`ZOLTAN_NUM_GEOM_FN`	Dimensionality of domain.
`ZOLTAN_GEOM_FN`	Coordinates of items.
Hypergraph Query Functions	
`ZOLTAN_HG_SIZE_CS_FN`	Number of hyperedge pins.
`ZOLTAN_HG_CS_FN`	List of hyperedge pins.
`ZOLTAN_HG_SIZE_EDGE_WTS_FN`	Number of hyperedge weights.
`ZOLTAN_HG_EDGE_WTS_FN`	List of hyperedge weights.
Graph Query Functions	
`ZOLTAN_NUM_EDGE_FN`	Number of graph edges.
`ZOLTAN_EDGE_LIST_FN`	List of graph edges and weights.

Example zoltanSimple.c: ZOLTAN_OBJ_LIST_FN

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```
void exGetObjectList(void *userDefinedData,
                     int numGlobalIds, int numLocalIds,
                     ZOLTAN_ID_PTR gids, ZOLTAN_ID_PTR lids,
                     int wgt_dim, float *obj_wgts,
                     int *err)
{
/* ZOLTAN_OBJ_LIST_FN callback function.
** Returns list of objects owned by this processor.
** lids[i] = local index of object in array.
*/
  int i;

  for (i=0; i<NumPoints; i++)
  {
    gids[i] = GlobalIds[i];
    lids[i] = i;
  }

  *err = 0;

  return;
}
```

Example zoltanSimple.c: ZOLTAN_GEOM_MULTI_FN

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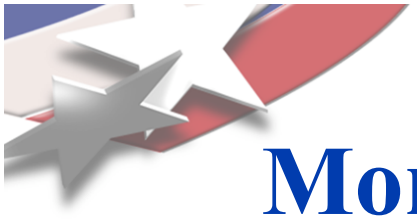
```
void exGetObjectCoords(void *userDefinedData,
                       int numGlobalIds, int numLocalIds, int numObjs,
                       ZOLTAN_ID_PTR gids, ZOLTAN_ID_PTR lids,
                       int numDim, double *pts, int *err)
{
/* ZOLTAN_GEOM_MULTI_FN callback.
** Returns coordinates of objects listed in gids and lids.
*/
  int i, id, id3, next = 0;
  if (numDim != 3) {
    *err = 1; return;
  }
  for (i=0; i<numObjs; i++){
    id = lids[i];
    if ((id < 0) || (id >= NumPoints)) {
      *err = 1; return;
    }
    id3 = lids[i] * 3;
    pts[next++] = (double)(Points[id3]);
    pts[next++] = (double)(Points[id3 + 1]);
    pts[next++] = (double)(Points[id3 + 2]);
  }
}
```



More Details on Query Functions

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- **void* data pointer allows user data structures to be used in all query functions.**
  - **To use, cast the pointer to the application data type.**
- **Local IDs provided by application are returned by Zoltan to simplify access of application data.**
  - **E.g. Indices into local arrays of coordinates.**
- **`ZOLTAN_ID_PTR` is pointer to array of unsigned integers, allowing IDs to be more than one integer long.**
  - **E.g., (processor number, local element number) pair.**
  - **`numGlobalIds` and `numLocalIds` are lengths of each ID.**
- **All memory for query-function arguments is allocated in Zoltan.**

```
void ZOLTAN_GET_GEOM_MULTI_FN(void *userDefinedData,
                              int numGlobalIds, int numLocalIds, int numObjs,
                              ZOLTAN_ID_PTR gids, ZOLTAN_ID_PTR lids,
                              int numDim, double *pts, int *err)
```

Using Zoltan in Your Application

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1. Decide what your objects are.
   - Elements? Grid points? Matrix rows? Particles?
2. Decide which tools (partitioning/ordering/coloring/utilities) and class of method (geometric/graph/hypergraph) to use.
3. Download Zoltan.
   - http://www.cs.sandia.gov/Zoltan
4. Write required query functions for your application.
   - Required functions are listed with each method in Zoltan User's Guide.
5. Call Zoltan from your application.
6. #include "zoltan.h" in files calling Zoltan.
7. Edit Zoltan configuration file and build Zoltan.
8. Compile application; link with libzoltan.a.
   - mpicc application.c -lzoltan

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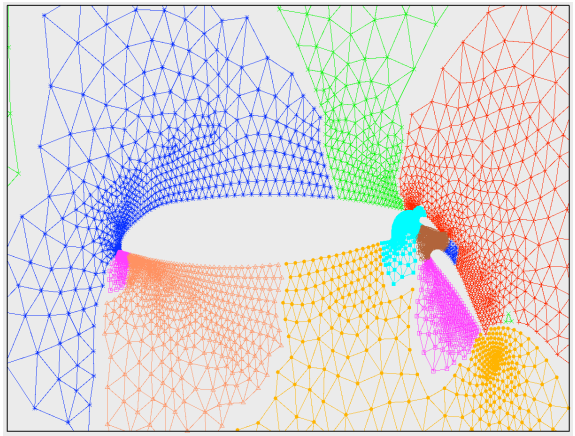
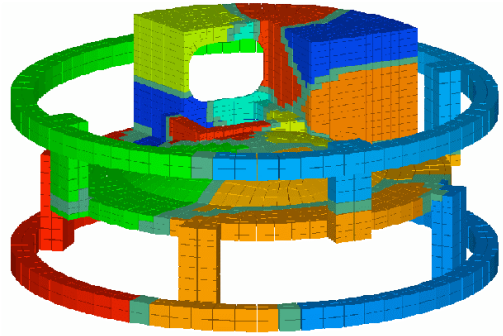
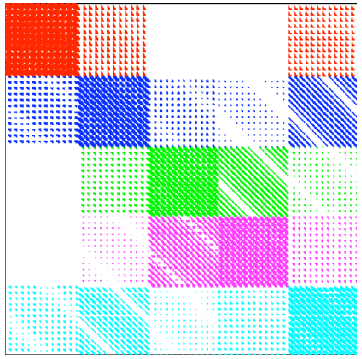
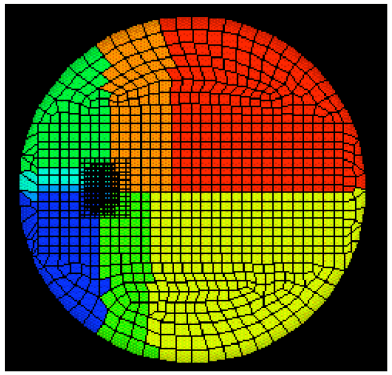
Partitioning and Load Balancing

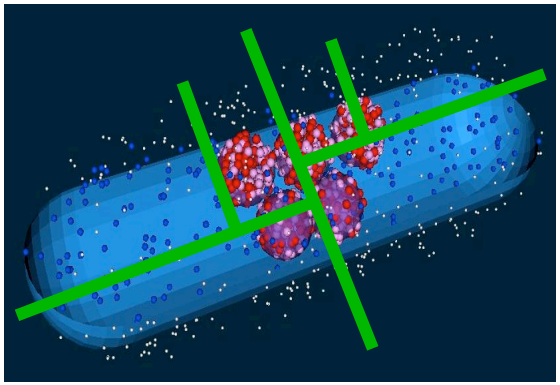
- Assignment of application data to processors for parallel computation.
- Applied to grid points, elements, matrix rows, particles, ….











Partitioning Interface

Zoltan computes the difference (Δ) from current distribution
Choose between:

a) Import lists (data to import from other procs)
b) Export lists (data to export to other procs)
c) Both (the default)

```
err = Zoltan_LB_Partition(zz,
    &changes, /* Flag indicating whether partition changed */
    &numGidEntries, &numLidEntries,
    &numImport, /* objects to be imported to new part */
    &importGlobalGids, &importLocalGids, &importProcs, &importToPart,
    &numExport, /* # objects to be exported from old part */
    &exportGlobalGids, &exportLocalGids, &exportProcs, &exportToPart);
```

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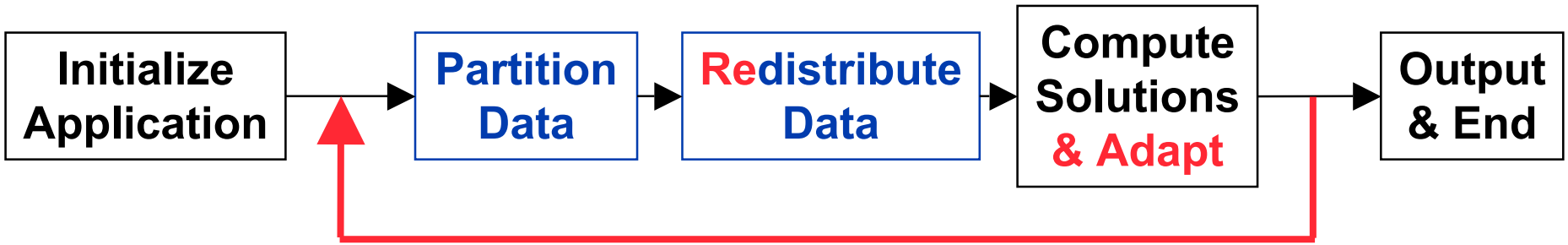
Static Partitioning

- Static partitioning in an application:
  - Data partition is computed.
  - Data are distributed according to partition map.
  - Application computes.
- Ideal partition:
  - Processor idle time is minimized.
  - Inter-processor communication costs are kept low.
- Zoltan_Set_Param(zz, “LB_APPROACH”, “PARTITION”);

Dynamic Repartitioning (a.k.a. Dynamic Load Balancing)



- Dynamic repartitioning (load balancing) in an application:
  - Data partition is computed.
  - Data are distributed according to partition map.
  - Application computes and, perhaps, adapts.
  - Process repeats until the application is done.

- Ideal partition:
  - Processor idle time is minimized.
  - Inter-processor communication costs are kept low.
  - Cost to redistribute data is also kept low.

- Zoltan_Set_Param(zz, "LB_APPROACH", "REPARTITION");

Zoltan Toolkit: Suite of Partitioners

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- No single partitioner works best for all applications.
  - Trade-offs:
    - Quality vs. speed.
    - Geometric locality vs. data dependencies.
    - High-data movement costs vs. tolerance for remapping.
- Application developers may not know which partitioner is best for application.

- Zoltan contains suite of partitioning methods.
  - Application changes only one parameter to switch methods.
    - Zoltan_Set_Param(zz, “LB_METHOD”, “new_method_name”);
  - Allows experimentation/comparisons to find most effective partitioner for application.

Partitioning Algorithms in the Zoltan Toolkit

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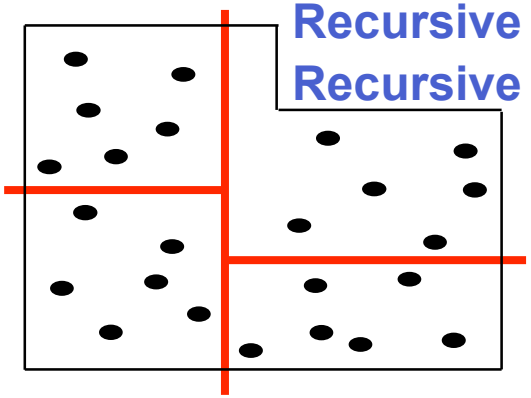
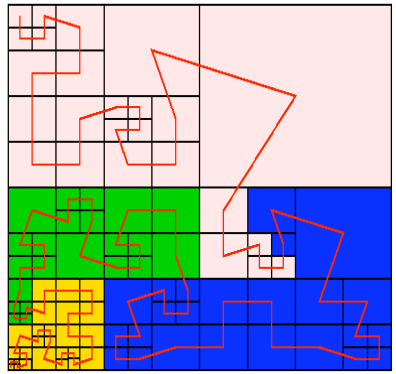
Geometric (coordinate-based) methods



Recursive Coordinate Bisection (Berger, Bokhari)

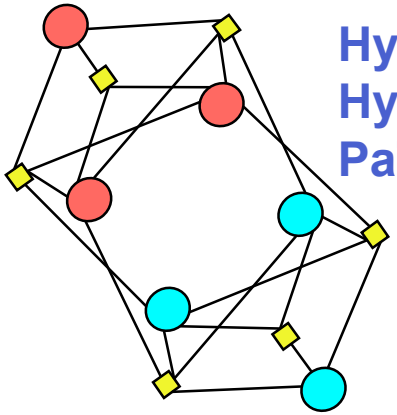
Recursive Inertial Bisection (Taylor, Nour-Omid)



Space Filling Curve Partitioning (Warren&Salmon, et al.)

Refinement-tree Partitioning (Mitchell)

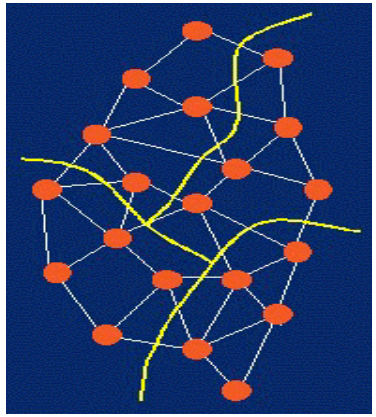
Combinatorial (topology-based) methods



Hypergraph Partitioning

Hypergraph Repartitioning

PaToH (Catalyurek & Aykanat)



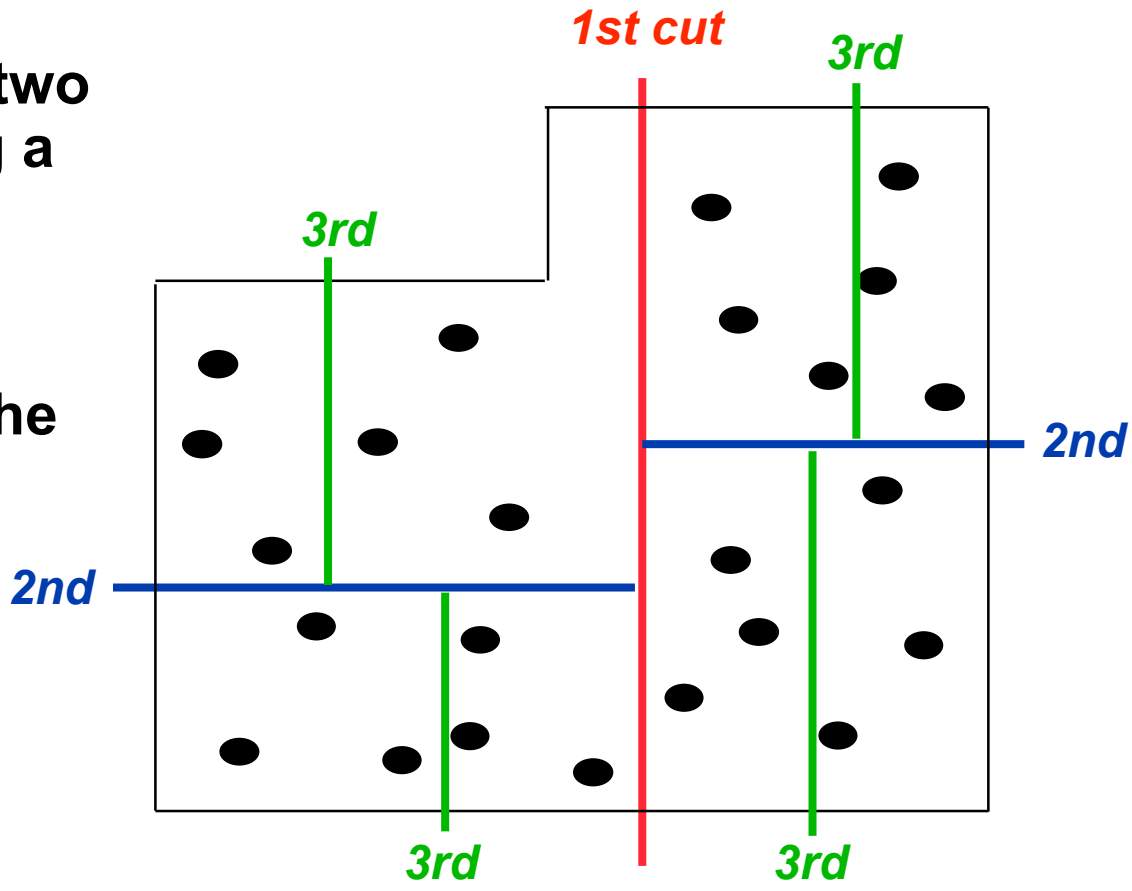
Zoltan Graph Partitioning

ParMETIS (U. Minnesota)

Jostle (U. Greenwich)

Recursive Coordinate Bisection

- Zoltan_Set_Param(zz, "LB_METHOD", "RCB");
- Berger & Bokhari (1987).
- Idea:
  - Divide work into two equal parts using a cutting plane orthogonal to a coordinate axis.
  - Recursively cut the resulting subdomains.



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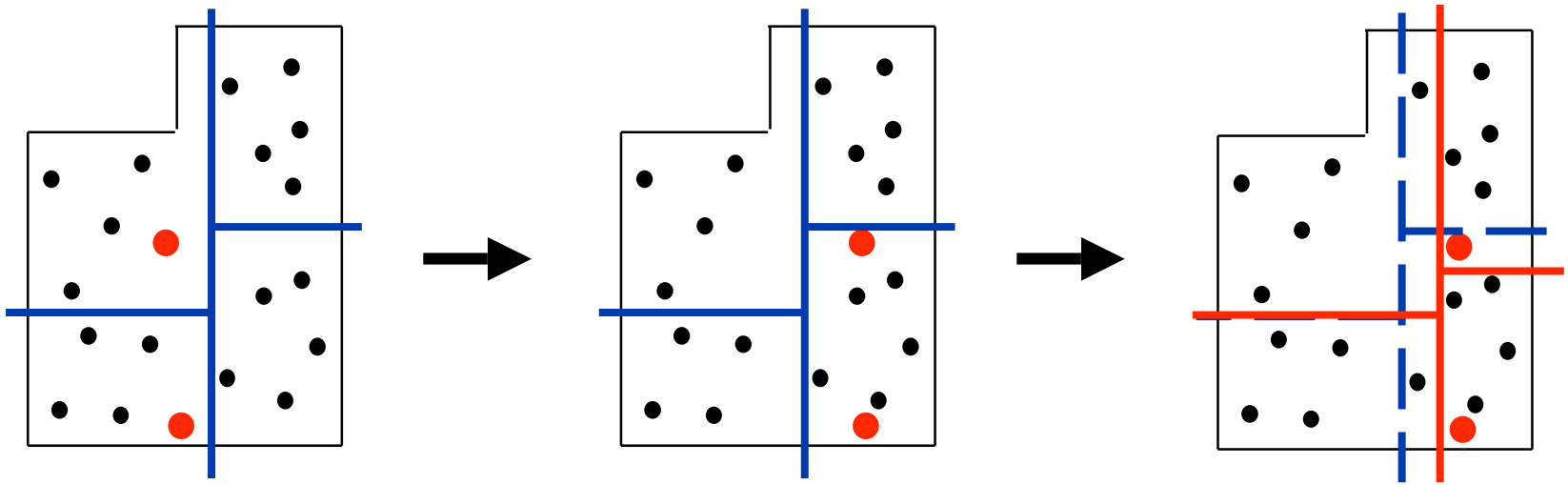
Geometric Repartitioning

- Implicitly achieves low data redistribution costs.
- For small changes in data, cuts move only slightly, resulting in little data redistribution.



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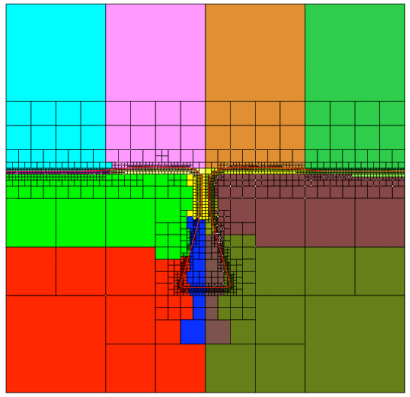
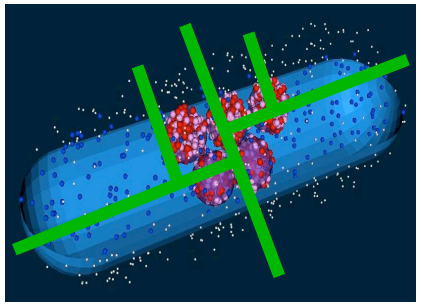
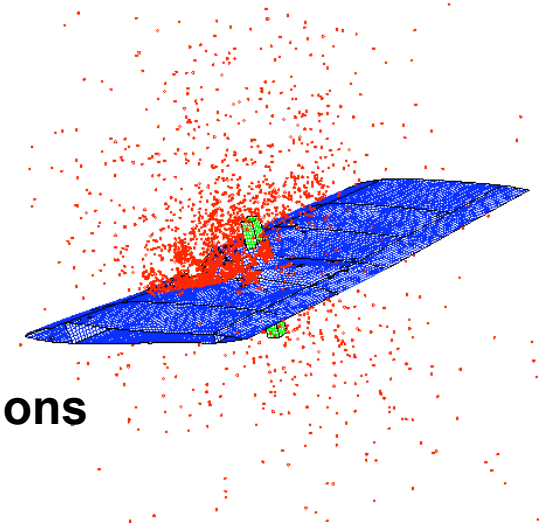
Applications of Geometric Methods

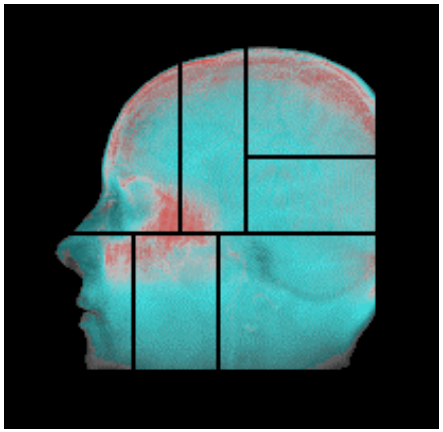


Adaptive Mesh Refinement

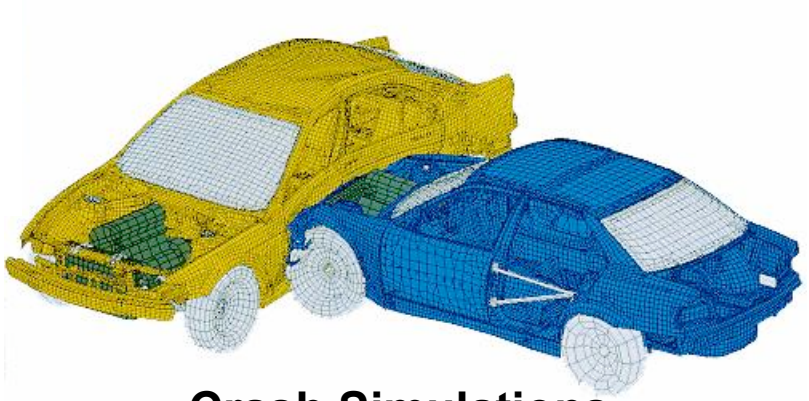




Particle Simulations



Parallel Volume Rendering



Crash Simulations
and Contact Detection

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RCB Advantages and Disadvantages

- **Advantages:**
  - **Conceptually simple; fast and inexpensive.**
  - **All processors can inexpensively know entire partition (e.g., for global search in contact detection).**
  - **No connectivity info needed (e.g., particle methods).**
  - **Good on specialized geometries.**

SLAC'S 55-cell Linear Accelerator with couplers: One-dimensional RCB partition reduced runtime up to 68% on 512 processor IBM SP3. (Wolf, Ko)

- **Disadvantages:**
  - **No explicit control of communication costs.**
  - **Mediocre partition quality.**
  - **Can generate disconnected subdomains for complex geometries.**
  - **Need coordinate information.**

Variations on RCB : Recursive Inertial Bisection

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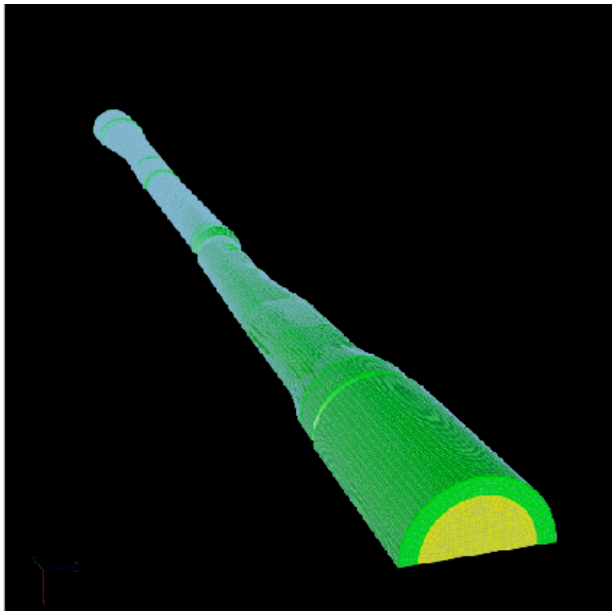
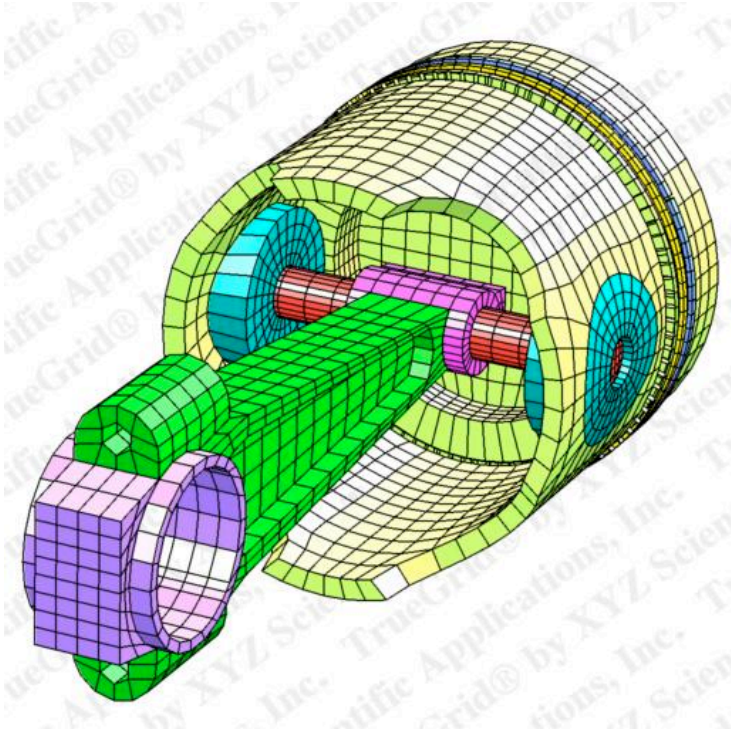
- Zoltan_Set_Param(zz, “LB_METHOD”, “RIB”);
- Simon, Taylor, et al., 1991
- Cutting planes orthogonal to principle axes of geometry.
- Not incremental.





Space-Filling Curve Partitioning (SFC)

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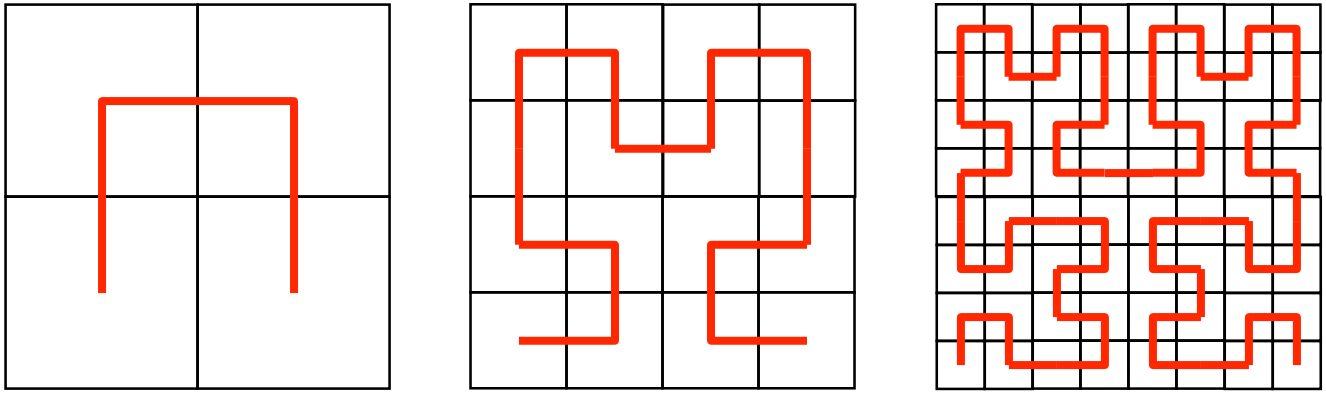
- Zoltan_Set_Param(zz, "LB_METHOD", "HSFC");
- Space-Filling Curve (Peano, 1890):
  - Mapping between R^3 to R^1 that completely fills a domain.
  - Applied recursively to obtain desired granularity.
- Used for partitioning by …
  - Warren and Salmon, 1993, gravitational simulations.
  - Pilkington and Baden, 1994, smoothed particle hydrodynamics.
  - Patra and Oden, 1995, adaptive mesh refinement.



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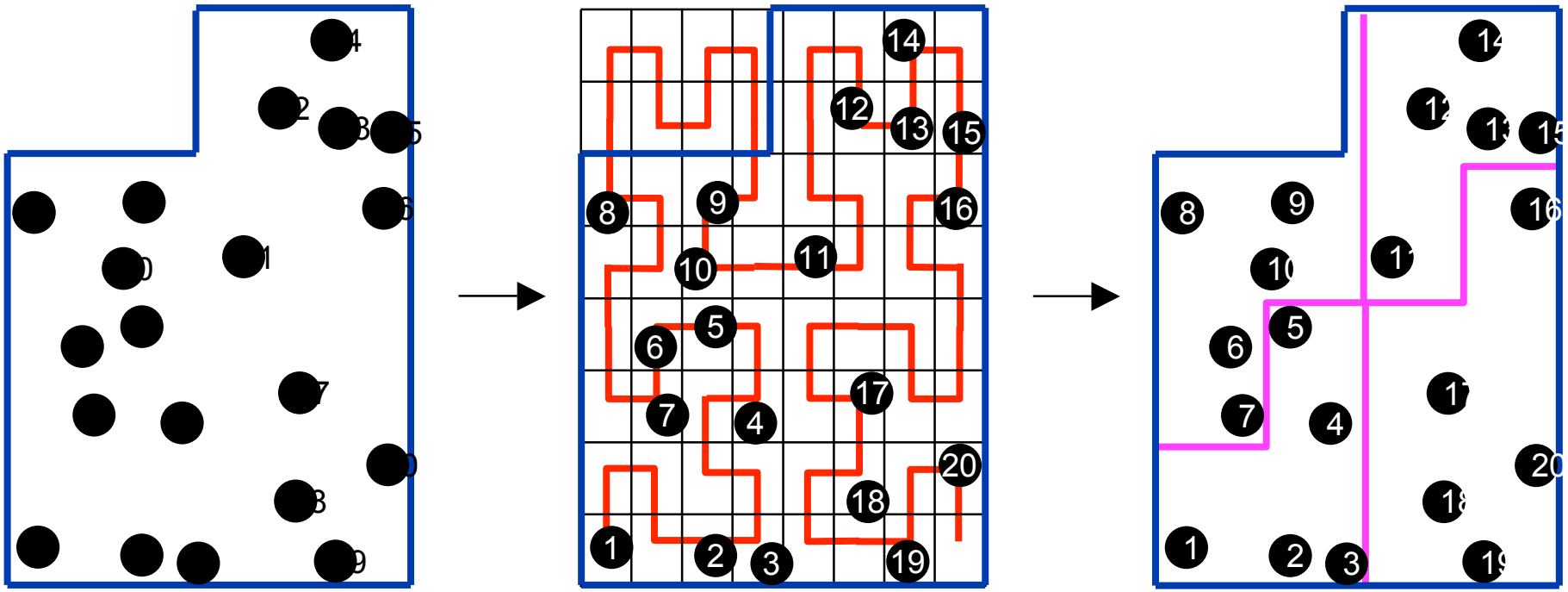
SFC Algorithm

- Run space-filling curve through domain.
- Order objects according to position on curve.
- Perform 1-D partition of curve.



SFC Advantages and Disadvantages

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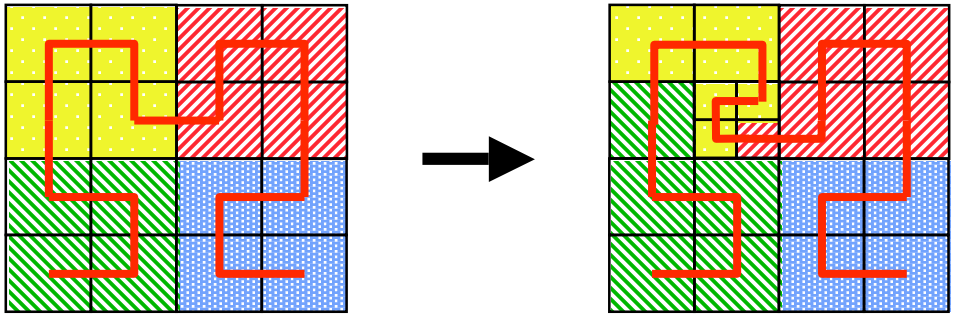
- **Advantages:**
  - **Simple, fast, inexpensive.**
  - **Maintains geometric locality of objects in processors.**
  - **Implicitly incremental for repartitioning.**



- **Disadvantages:**
  - **No explicit control of communication costs.**
  - **Can generate disconnected subdomains.**
  - **Often lower quality partitions than RCB.**
  - **Geometric coordinates needed.**

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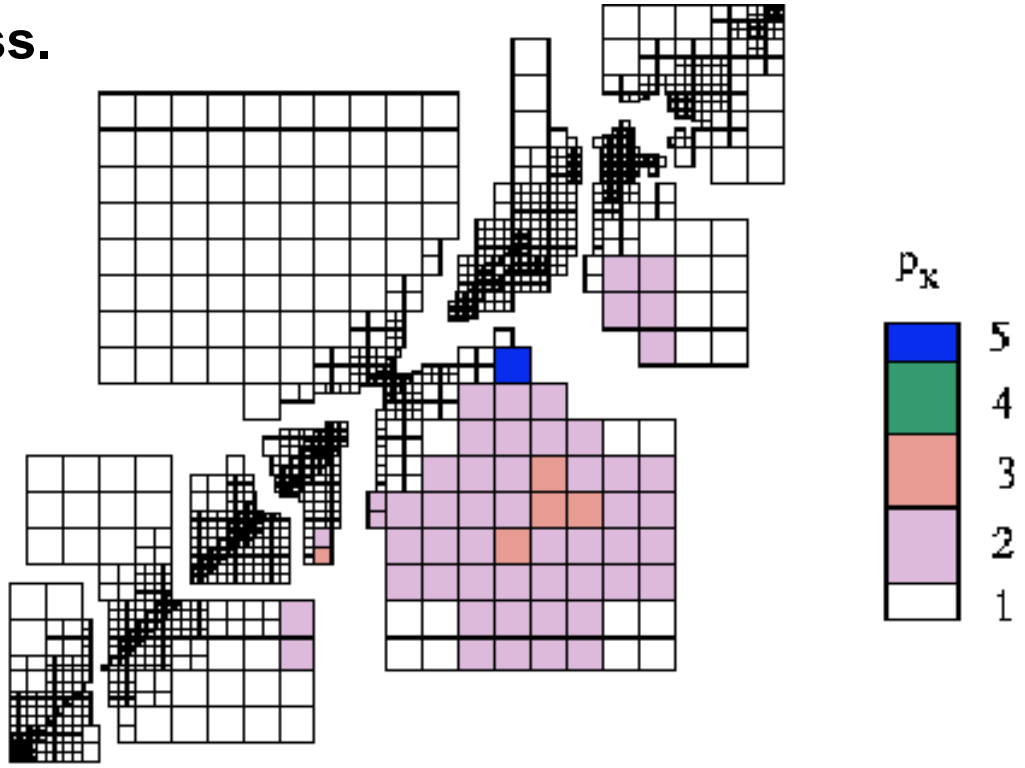
Applications using SFC

- **Adaptive hp-refinement finite element methods.**
  - **Assigns physically close elements to same processor.**
  - **Inexpensive; incremental; fast.**
  - **Linear ordering can be used to order elements for efficient memory access.**



hp-refinement mesh; 8 processors.
Patra, et al. (SUNY-Buffalo)

For geometric partitioning (RCB, RIB, HSFC), use …

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General Query Functions	
ZOLTAN_NUM_OBJ_FN	Number of items on processor
ZOLTAN_OBJ_LIST_FN	List of item IDs and weights.
Geometric Query Functions	
ZOLTAN_NUM_GEOM_FN	Dimensionality of domain.
ZOLTAN_GEOM_FN	Coordinates of items.
Hypergraph Query Functions	
ZOLTAN_HG_SIZE_CS_FN	Number of hyperedge pins.
ZOLTAN_HG_CS_FN	List of hyperedge pins.
ZOLTAN_HG_SIZE_EDGE_WTS_FN	Number of hyperedge weights.
ZOLTAN_HG_EDGE_WTS_FN	List of hyperedge weights.
Graph Query Functions	
ZOLTAN_NUM_EDGE_FN	Number of graph edges.
ZOLTAN_EDGE_LIST_FN	List of graph edges and weights.

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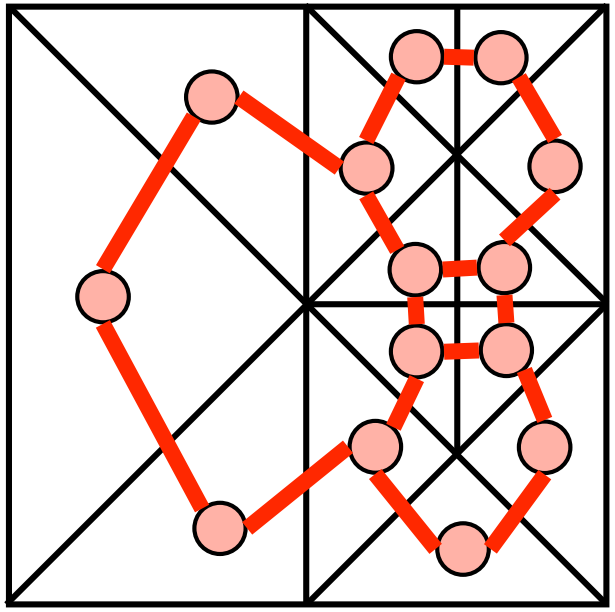
Graph Partitioning

- Zoltan_Set_Param(zz, "LB_METHOD", "GRAPH");
- Zoltan_Set_Param(zz, "GRAPH_PACKAGE", "ZOLTAN"); or
  Zoltan_Set_Param(zz, "GRAPH_PACKAGE", "PARMETIS");

- Kernighan, Lin, Schweikert, Fiduccia, Mattheyes, Simon, Hendrickson, Leland, Kumar, Karypis, et al.

- Represent problem as a weighted graph.
  - Vertices = objects to be partitioned.
  - Edges = dependencies between two objects.
  - Weights = work load or amount of dependency.
- Partition graph so that …
  - Parts have equal vertex weight.
  - Weight of edges cut by part boundaries is small.



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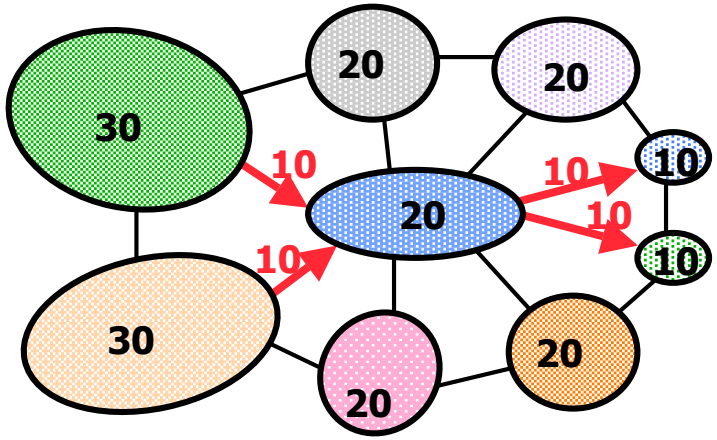
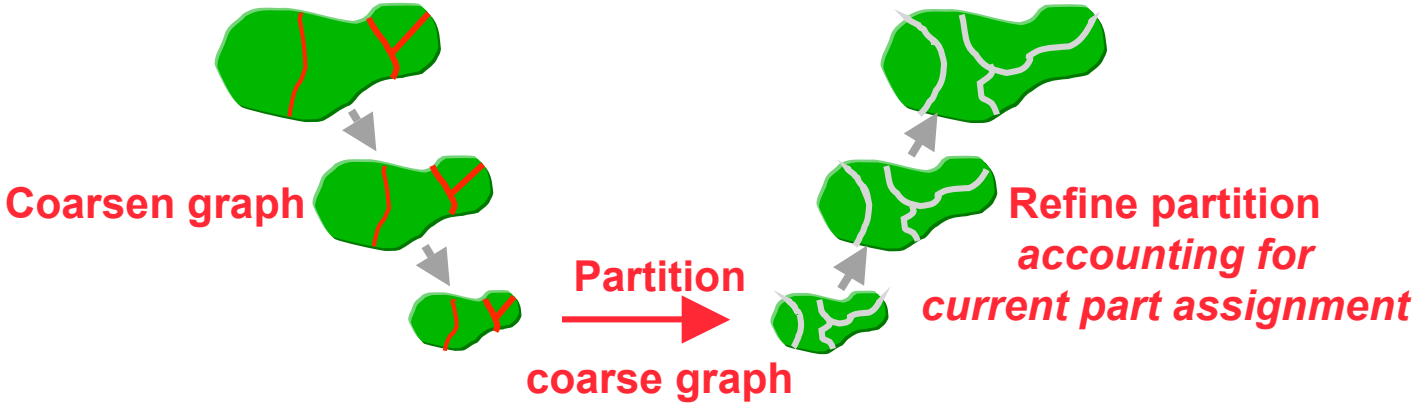
Graph Repartitioning

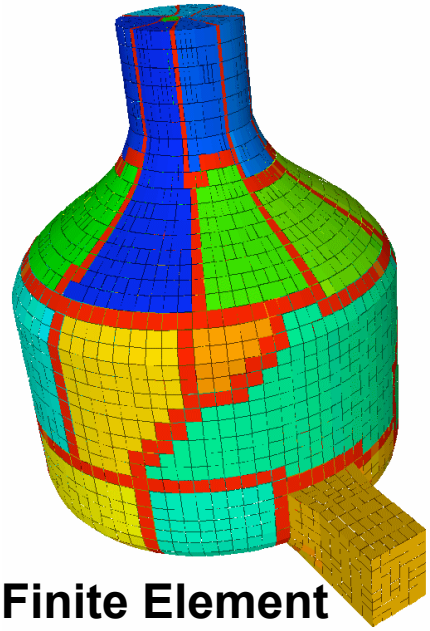
- **Diffusive strategies (Cybenko, Hu, Blake, Walshaw, Schloegel, et al.)**
  - **Shift work from highly loaded processors to less loaded neighbors.**
  - **Local communication keeps data redistribution costs low.**



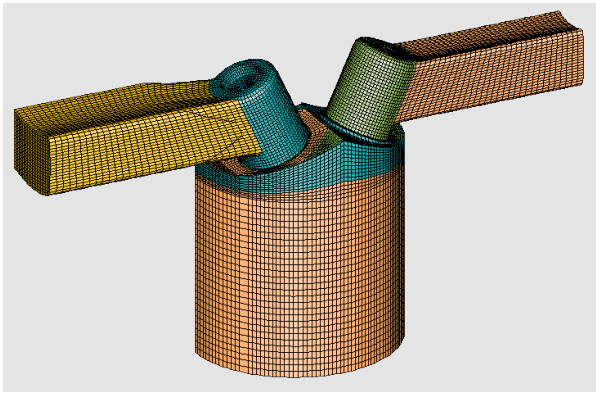
- **Multilevel partitioners that account for data redistribution costs in refining partitions (Schloegel, Karypis)**
  - **Parameter weights application communication vs. redistribution communication.**



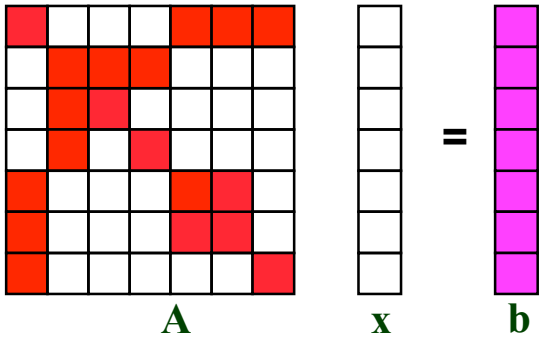
Applications using Graph Partitioning



Finite Element Analysis



Multiphysics and multiphase simulations



Linear solvers & preconditioners
(square, structurally symmetric systems)

Graph Partitioning: Advantages and Disadvantages

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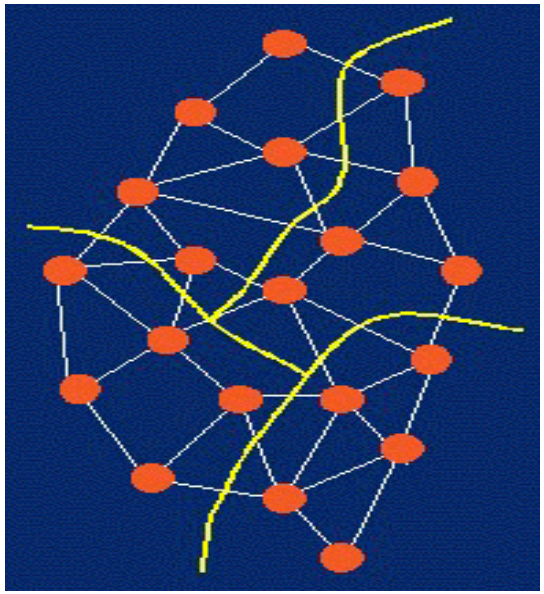
- **Advantages:**
  - **Highly successful model for mesh-based PDE problems.**
  - **Explicit control of communication volume gives higher partition quality than geometric methods.**
  - **Excellent software available.**
    - **Serial:** Chaco (SNL), Jostle (U. Greenwich), METIS (U. Minn.), Party (U. Paderborn), Scotch (U. Bordeaux)
    - **Parallel:** Zoltan (SNL), ParMETIS (U. Minn.), PJostle (U. Greenwich)



- **Disadvantages:**
  - **More expensive than geometric methods.**
  - **Edge-cut model only approximates communication volume.**

For graph partitioning, coloring & ordering, use …

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General Query Functions	
`ZOLTAN_NUM_OBJ_FN`	Number of items on processor
`ZOLTAN_OBJ_LIST_FN`	List of item IDs and weights.
Geometric Query Functions	
`ZOLTAN_NUM_GEOM_FN`	Dimensionality of domain.
`ZOLTAN_GEOM_FN`	Coordinates of items.
Hypergraph Query Functions	
`ZOLTAN_HG_SIZE_CS_FN`	Number of hyperedge pins.
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`ZOLTAN_HG_EDGE_WTS_FN`	List of hyperedge weights.
Graph Query Functions	
`ZOLTAN_NUM_EDGE_FN`	Number of graph edges.
`ZOLTAN_EDGE_LIST_FN`	List of graph edges and weights.

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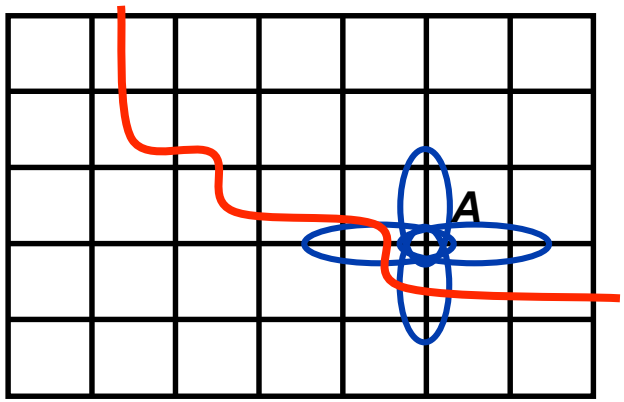
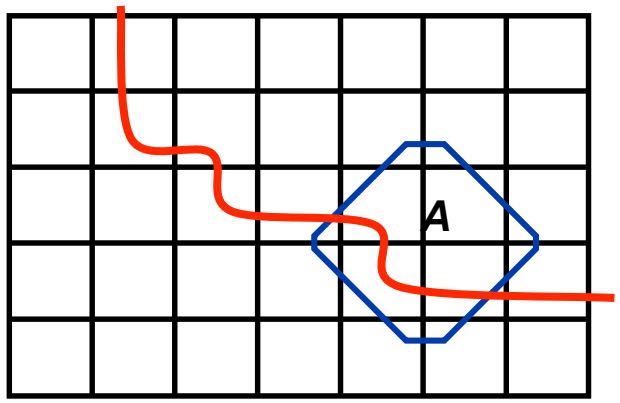
Hypergraph Partitioning

- Zoltan_Set_Param(zz, "LB_METHOD", "HYPERGRAPH");
- Zoltan_Set_Param(zz, "HYPERGRAPH_PACKAGE", "ZOLTAN"); or Zoltan_Set_Param(zz, "HYPERGRAPH_PACKAGE", "PATOH");

- Alpert, Kahng, Hauck, Borriello, Çatalyürek, Aykanat, Karypis, et al.
- Hypergraph model:
  - Vertices = objects to be partitioned.
  - Hyperedges = dependencies between two or more objects.
- Partitioning goal: Assign equal vertex weight while minimizing hyperedge cut weight.



Graph Partitioning Model



Hypergraph Partitioning Model

Hypergraph Repartitioning

- Augment hypergraph with data redistribution costs.
  - Account for data's current processor assignments.
  - Weight dependencies by their size and frequency of use.
- Partitioning then tries to minimize total communication volume:

  Data redistribution volume

  + Application communication volume

  Total communication volume
- Data redistribution volume: callback returns data sizes.
  - Zoltan_Set_Fn(zz, ZOLTAN_OBJ_SIZE_MULTI_FN, myObjSizeFn, 0);
- Application communication volume = Hyperedge cuts * Number of times the communication is done between repartitionings.
  - Zoltan_Set_Param(zz, "PHG_REPART_MULTIPLIER", "100");

Best Algorithms Paper Award at IPDPS07
"Hypergraph-based Dynamic Load Balancing for Adaptive Scientific Computations"
Catalyurek, Boman, Devine, Bozdag, Heaphy, & Riesen

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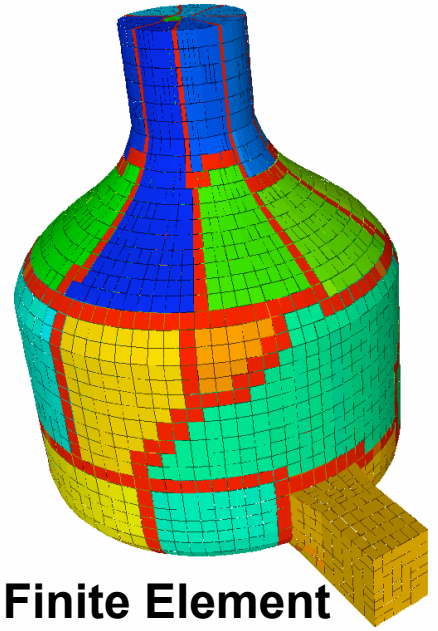
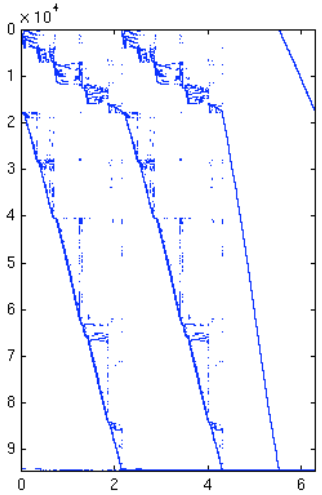
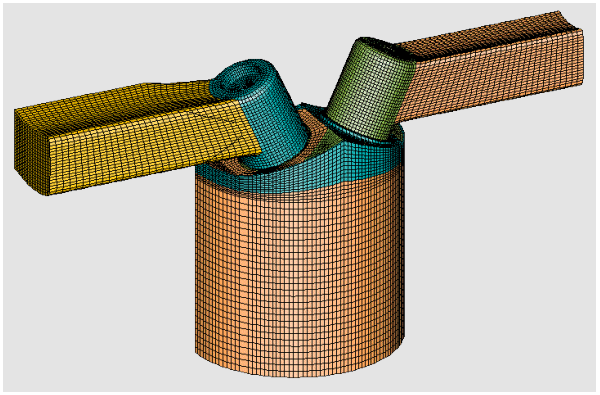
Hypergraph Applications



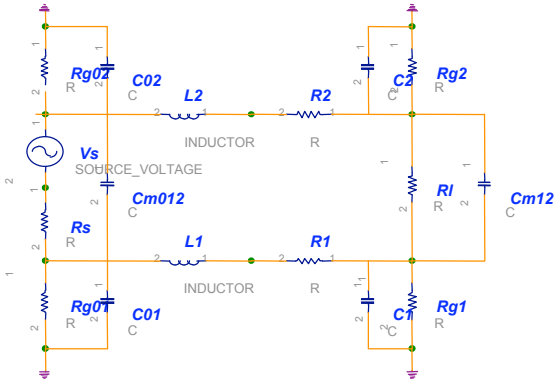
Finite Element Analysis



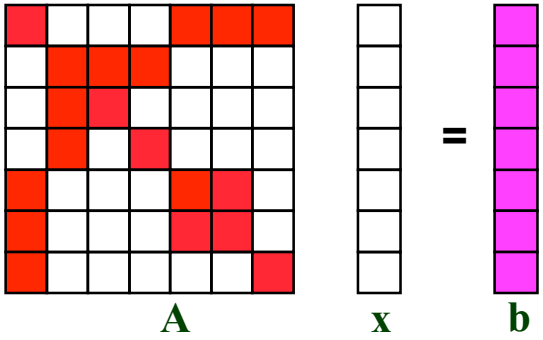
Linear programming for sensor placement



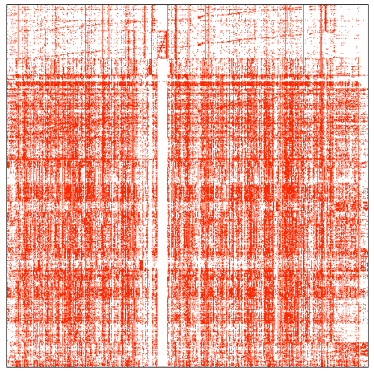
Multiphysics and multiphase simulations



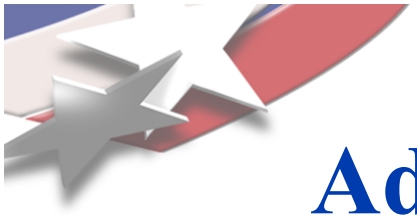
Circuit Simulations



Linear solvers & preconditioners
(no restrictions on matrix structure)



Data Mining



Hypergraph Partitioning: Advantages and Disadvantages

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- **Advantages:**
  - **Communication volume reduced 30-38% on average over graph partitioning (Catalyurek & Aykanat).**
    - **5-15% reduction for mesh-based applications.**
  - **More accurate communication model than graph partitioning.**
    - **Better representation of highly connected and/or non-homogeneous systems.**
  - **Greater applicability than graph model.**
    - **Can represent rectangular systems and non-symmetric dependencies.**
- **Disadvantages:**
  - **More expensive than graph partitioning.**

For hypergraph partitioning and repartitioning, use …

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General Query Functions	
`ZOLTAN_NUM_OBJ_FN`	Number of items on processor
`ZOLTAN_OBJ_LIST_FN`	List of item IDs and weights.
Geometric Query Functions	
`ZOLTAN_NUM_GEOM_FN`	Dimensionality of domain.
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`ZOLTAN_HG_EDGE_WTS_FN`	List of hyperedge weights.
Graph Query Functions	
`ZOLTAN_NUM_EDGE_FN`	Number of graph edges.
`ZOLTAN_EDGE_LIST_FN`	List of graph edges and weights.

Or can use graph queries to build hypergraph.

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General Query Functions	
ZOLTAN_NUM_OBJ_FN	Number of items on processor
ZOLTAN_OBJ_LIST_FN	List of item IDs and weights.
Geometric Query Functions	
ZOLTAN_NUM_GEOM_FN	Dimensionality of domain.
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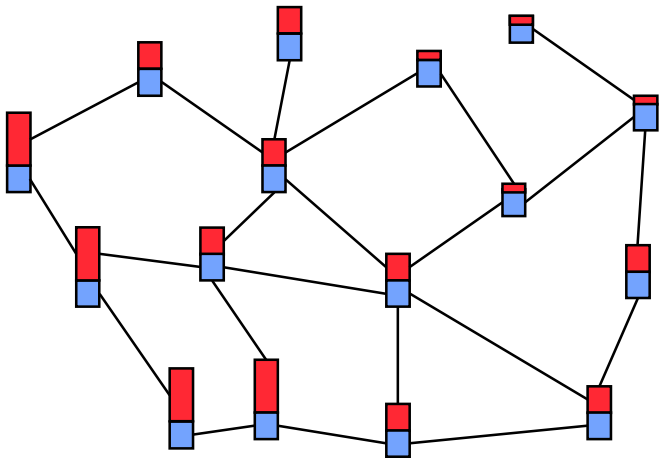
ZOLTAN_HG_SIZE_EDGE_WTS_FN	Number of hyperedge weights.
ZOLTAN_HG_EDGE_WTS_FN	List of hyperedge weights.
Graph Query Functions	
ZOLTAN_NUM_EDGE_FN	Number of graph edges.
ZOLTAN_EDGE_LIST_FN	List of graph edges and weights.

Multi-criteria Load-balancing

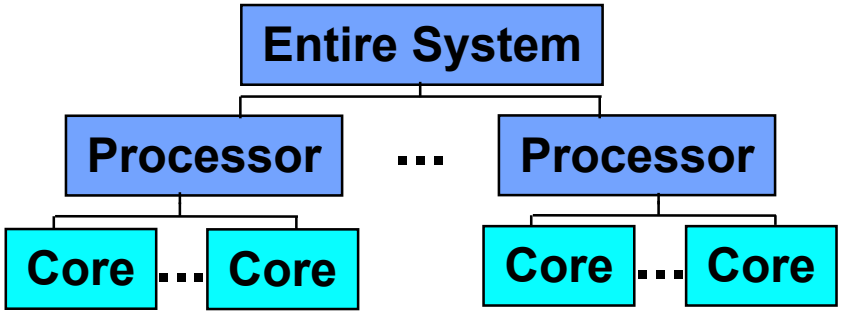
- Multiple constraints or objectives
  - Compute a single partition that is good with respect to multiple factors.
    - Balance both computation and memory.
    - Balance meshes in loosely coupled physics.
    - Balance multi-phase simulations.
  - Extend algorithms to multiple weights
    - Difficult. No guarantee good solution exists.
- Zoltan_Set_Param(zz, "OBJ_WEIGHT_DIM", "2");
  - With RCB, RIB and ParMETIS graph partitioning.



Heterogeneous Architectures

- Clusters may have different types of processors.
- Assign "capacity" weights to processors.
  - E.g., Compute power (speed).
  - Zoltan_LB_Set_Part_Sizes(…);
- Balance with respect to processor capacity.

- Hierarchical partitioning: Allows different partitioners at different architecture levels.
  - Zoltan_Set_Param(zz, "LB_METHOD", "HIER");



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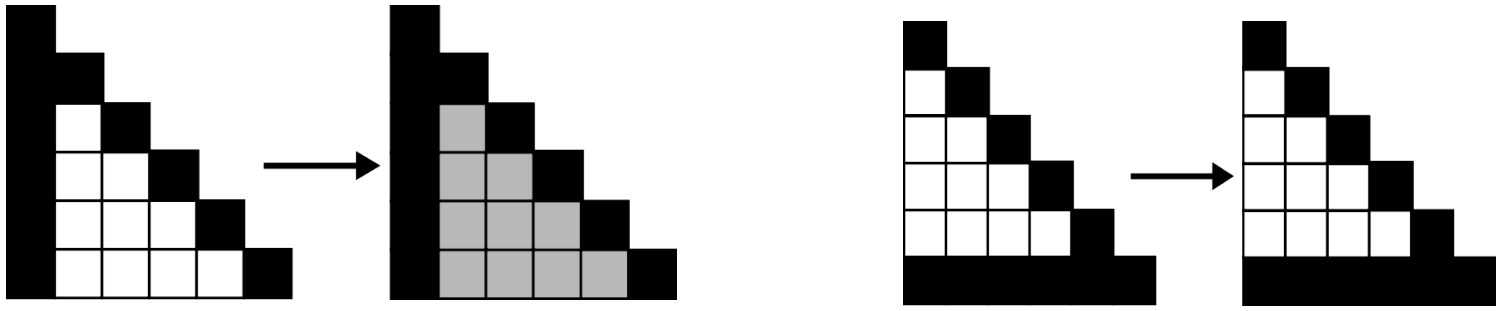
Sparse Matrix Ordering problem

- When solving sparse linear systems with direct methods, non-zero terms are created during the factorization process ($A \rightarrow LL^t$, $A \rightarrow LDL^t$ or $A \rightarrow LU$).
- Fill-in depends on the order of the unknowns.
  - Need to provide fill-reducing orderings.



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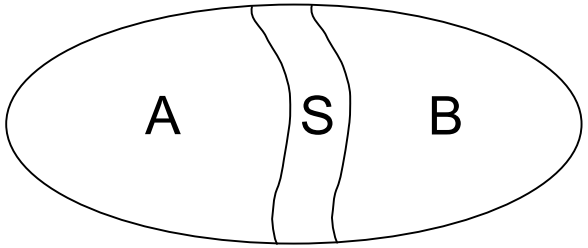
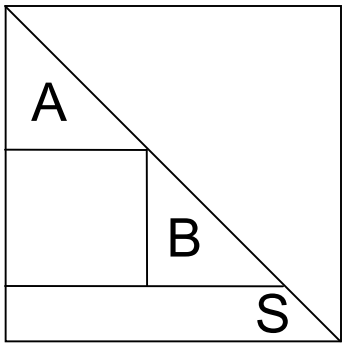
Fill Reducing ordering

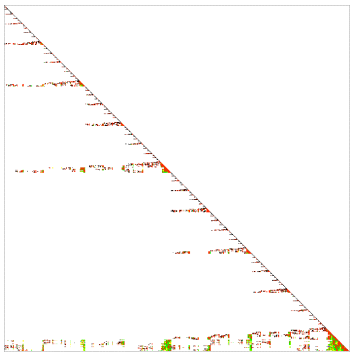
- **Combinatorial problem, depending on only the structure of the matrix *A*:**
  - **We can work on the graph associated with *A*.**
- **NP-Complete, thus we deal only with heuristics.**
- **Most popular heuristics:**
  - **Minimum Degree algorithms (AMD, MMD, AMF …)**
  - **Nested Dissection**

Nested dissection (1)

- **Principle [George 1973]**
  - **Find a vertex separator *S* in graph.**
  - **Order vertices of *S* with highest available indices.**
  - **Recursively apply the algorithm to the two separated subgraphs *A* and *B*.**







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Nested dissection (2)

- **Advantages:**
  - **Induces high quality block decompositions.**
    - **Suitable for block BLAS 3 computations.**
  - **Increases the concurrency of computations.**
    - **Compared to minimum degree algorithms.**
    - **Very suitable for parallel factorization.**
      - **It's the scope here: parallel ordering is for parallel factorization.**

Matrix ordering within Zoltan

- Computed by third party libraries:
  - ParMETIS
  - Scotch (more specifically PT-Scotch, the parallel part)
  - Easy to add another one.
- The calls to the external ordering library are transparent for the user, and thus Zoltan's call can be a standard way to compute ordering.

Zoltan ordering architecture

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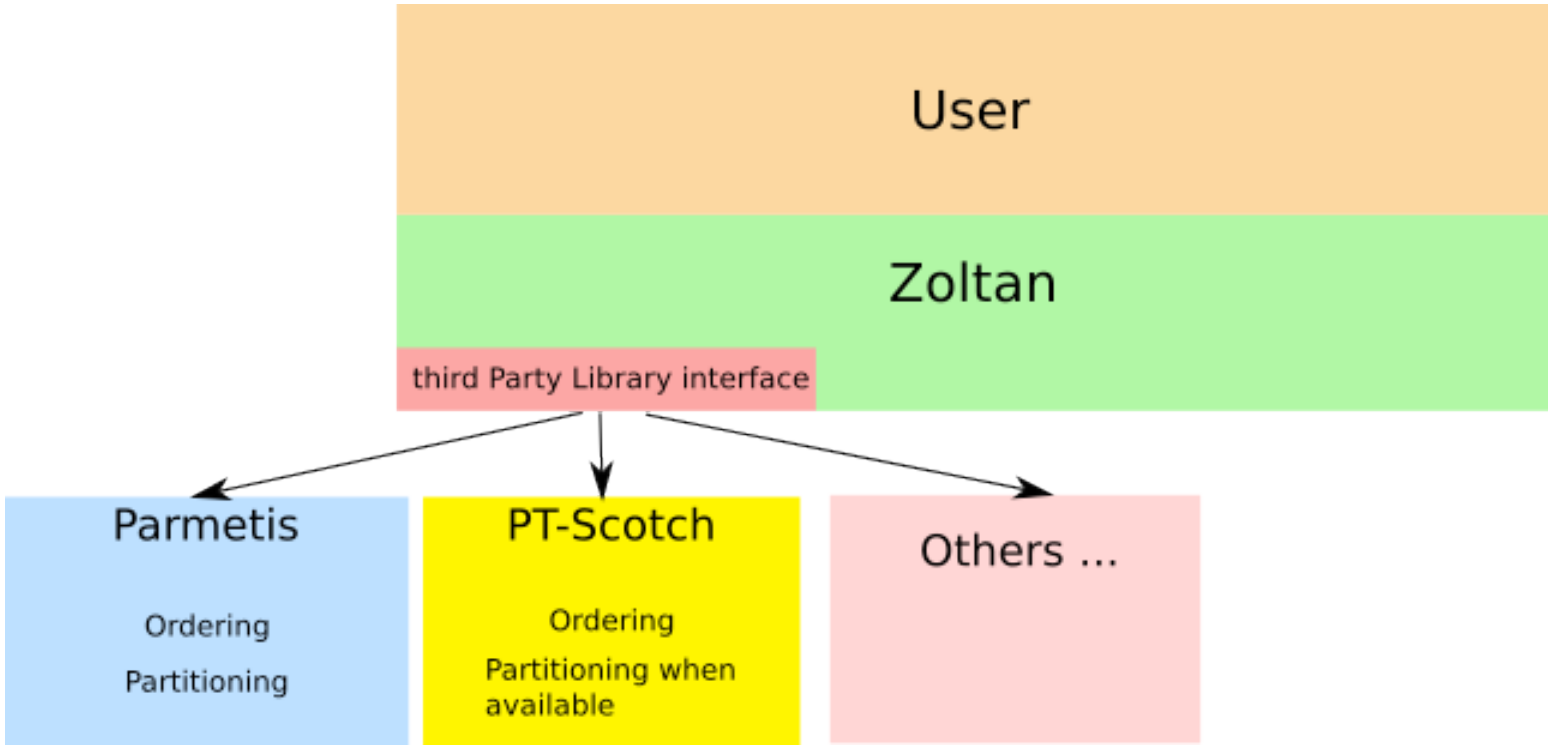

Ordering interface in Zoltan

- Compute ordering with one function:

  Zoltan_Order

- Output provided:
  - New order of the unknowns (direct permutation), available in two forms:
    - one is the new number in the interval [0,N-1];
    - the other is the new order of Global IDs.
  - Access to elimination tree, “block” view of the ordering.

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Experimental results (1)

- **Metric is OPC, the operation count of Cholesky factorization.**
- **Largest matrix ordered by PT-Scotch: 83 millions of unknowns on 256 processors (CEA/CESTA).**
- **Some of our largest test graphs.**

Graph	Size (10^6)		Average degree	O_{ss}	Description
	|V|	|E|			
audikw1	944	38354	81.2	5.48E+12	3D mechanics mesh, Par
cage15	5154	47022	18.2	4.06E+16	DNA electrophoresis,
quimonda07	8613	29143	6.7	6.92E+10	Circuit simulation, Quimor
23millions	23114	175686	7.6	1.29E+14	CEA/CESTA

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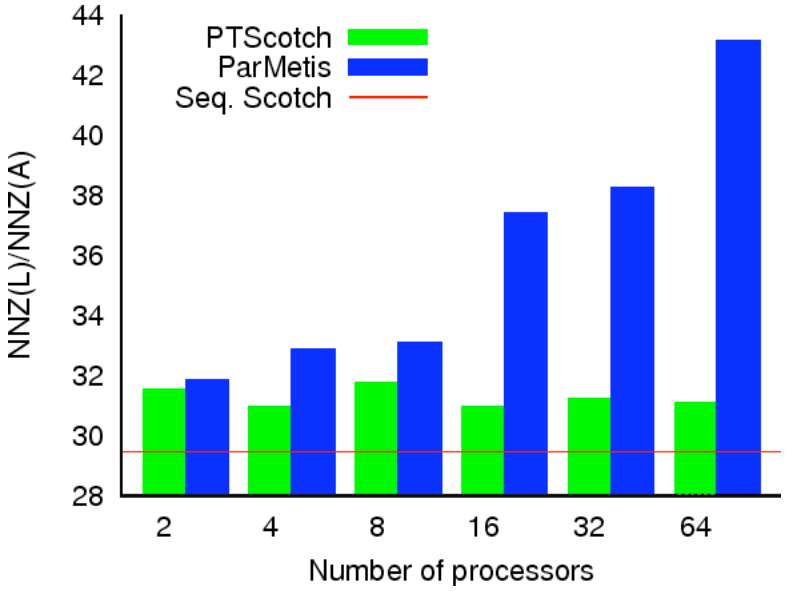
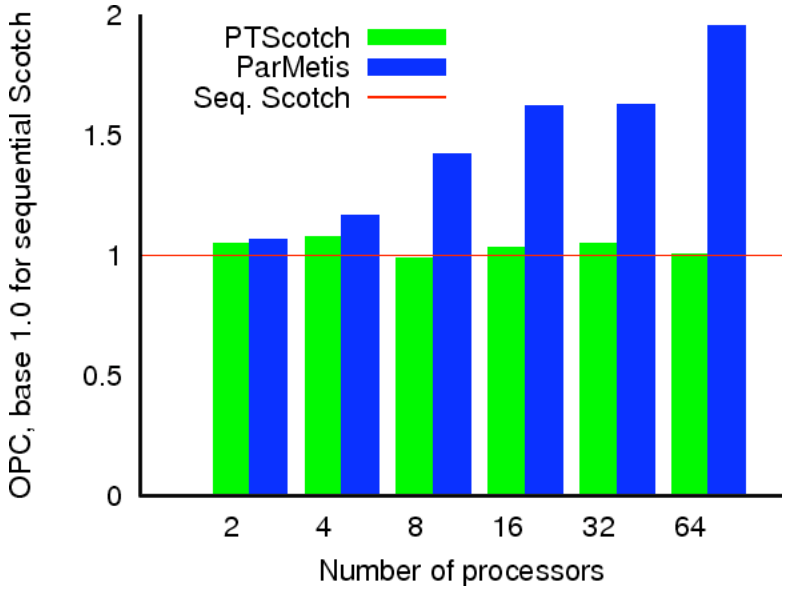
Experimental results (2)

Test case	Number of processes					
	2	4	8	16	32	64
audikw1						
O_{PTS}	5.73E+1	25.65E+1	25.54E+1	25.45E+1	25.45E+1	25.45E+1
O_{PM}	5.82E+1	26.37E+1	27.78E+1	28.88E+1	28.91E+1	21.07E+1
t_{PTS}	73.11	53.19	45.19	33.83	24.74	18.1





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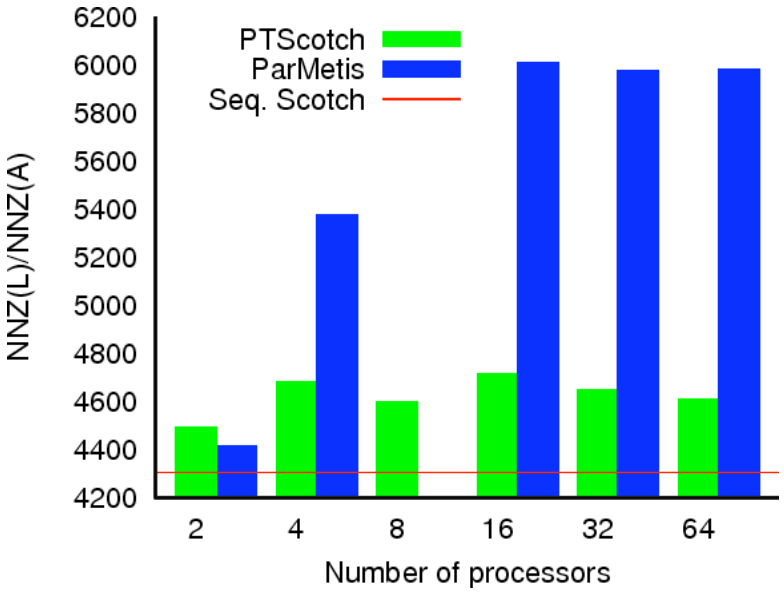
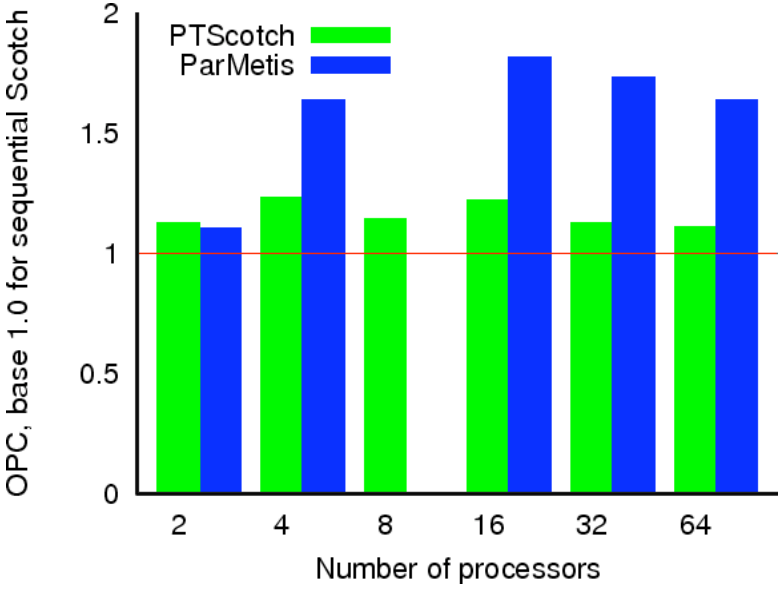
Experimental results (3)

Test case	Number of processes					
	2	4	8	16	32	64
cage15						
O_{PTS}	4.58E+16	5.01E+16	4.64E+16	4.94E+16	4.58E+16	4.50E+1
O_{PM}	4.47E+16	6.64E+16	†	7.36E+16	7.03E+16	6.64E+1
t_{PTS}	540.46	427.38	371.70	340.78	351.38	380.6
t_{PM}	195.93	117.77	†	40.30	22.56	17.8





Experimental results (4)

- **ParMETIS crashes for all other graphs.**

Test case	Number of processes					
	2	4	8	16	32	64
quimonda07						
O_{PTS}	-	-	5.80E+10	6.38E+10	6.94E+10	7.70E+1
t_{PTS}	-	-	34.68	22.23	17.30	16.62
23millions						
O_{PTS}	1.45E+14	2.91E+14	3.99E+14	2.71E+14	1.94E+14	2.45E+1
t_{PTS}	671.60	416.45	295.38	211.68	147.35	103.7

Summary of Matrix Ordering

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- Zoltan provides access to efficient parallel ordering for sparse matrices (especially with Scotch).
- Zoltan provides a standard way to call parallel ordering.
- Zoltan will provide also its own ordering tool in the future, dealing with ordering for non-symmetric problems.

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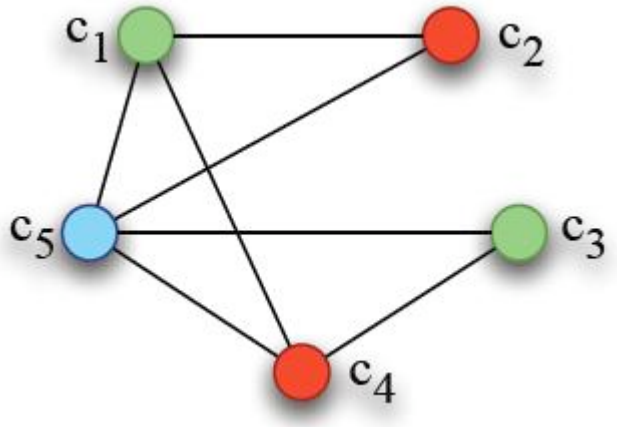
Zoltan Graph Coloring

- Parallel distance-1 and distance-2 graph coloring.
- Graph built using same application interface and code as graph partitioners.
- Generic coloring interface; easy to add new coloring algorithms.
- Algorithms
  - Distance-1 coloring: Bozdag, Gebremedhin, Manne, Boman, Catalyurek, *EuroPar'05, JPDC'08*.
  - Distance-2 coloring: Bozdag, Catalyurek, Gebremedhin, Manne, Boman, Ozguner, *HPCC'05, SISC'08* (in submission).

Distance-1 Graph Coloring

- **Problem (NP-hard)**
  Color the vertices of a graph with as few colors as possible such that no two adjacent vertices receive the same color.

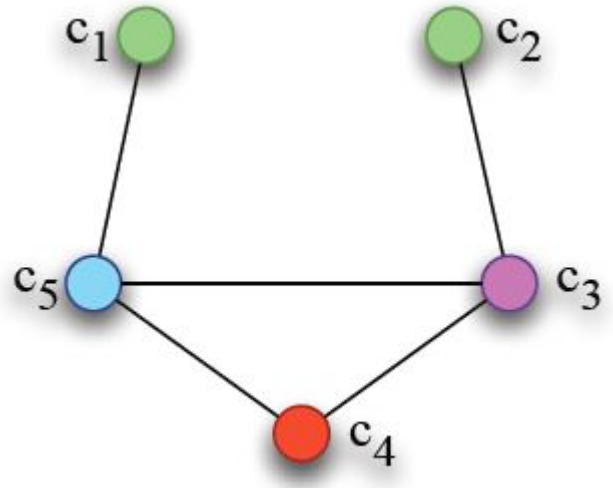
- **Applications**
  - **Iterative solution of sparse linear systems**
  - **Preconditioners**
  - **Sparse tiling**
  - **Eigenvalue computation**
  - **Parallel graph partitioning**



Distance-2 Graph Coloring

- **Problem (NP-hard)**
  Color the vertices of a graph with as few colors as possible such that a pair of vertices connected by a path on two or less edges receives different colors.

- **Applications**
  - **Derivative matrix computation in numerical optimization**
  - **Channel assignment**
  - **Facility location**
- **Related problems**
  - **Partial distance-2 coloring**
  - **Star coloring**



A Parallel Coloring Framework

- Color vertices iteratively in rounds using a first fit strategy
- Each round is broken into supersteps
  - Color a certain number of vertices
  - Exchange recent color information
- Detect conflicts at the end of each round
- Repeat until all vertices receive consistent colors

Coloring Interface in Zoltan

- Both distance-1 and distance-2 coloring routines can be invoked by Zoltan_Color function.
- The colors assigned to the objects are returned in an array.

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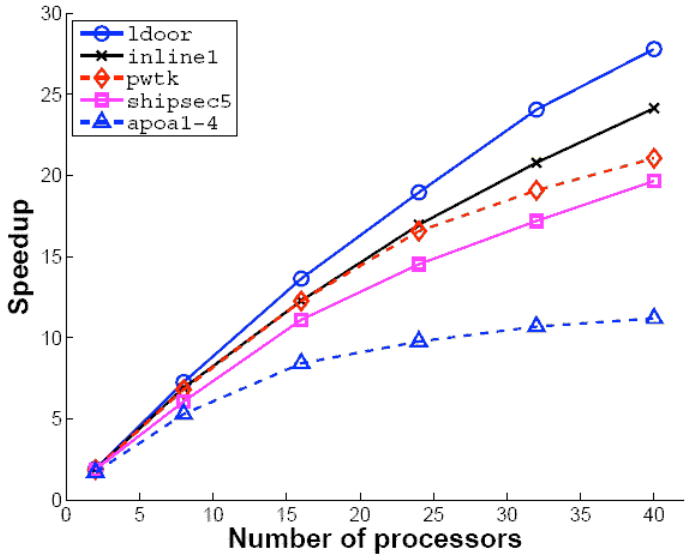
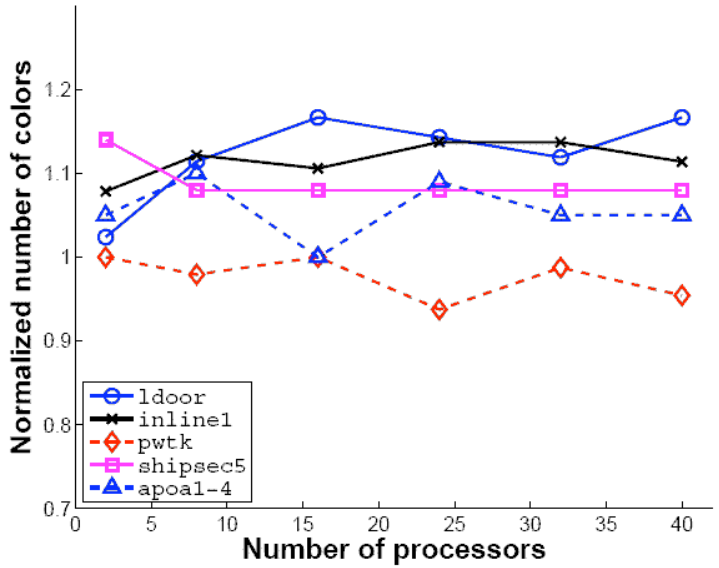
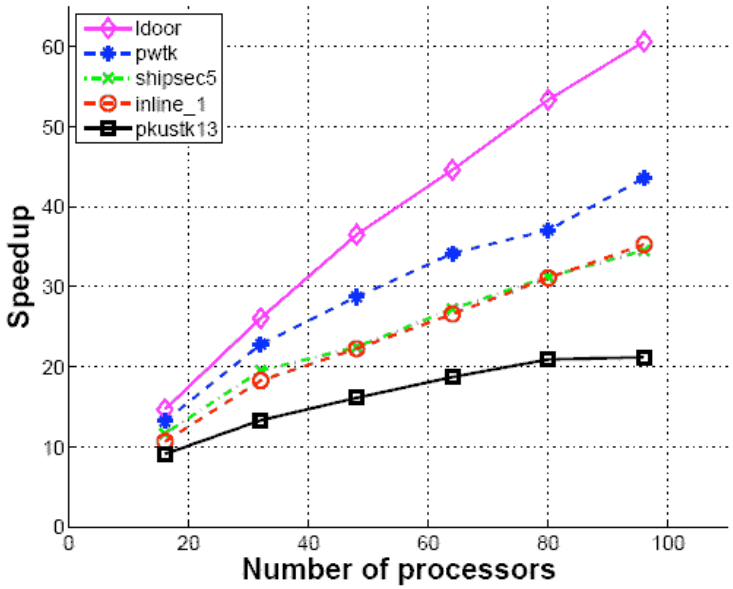
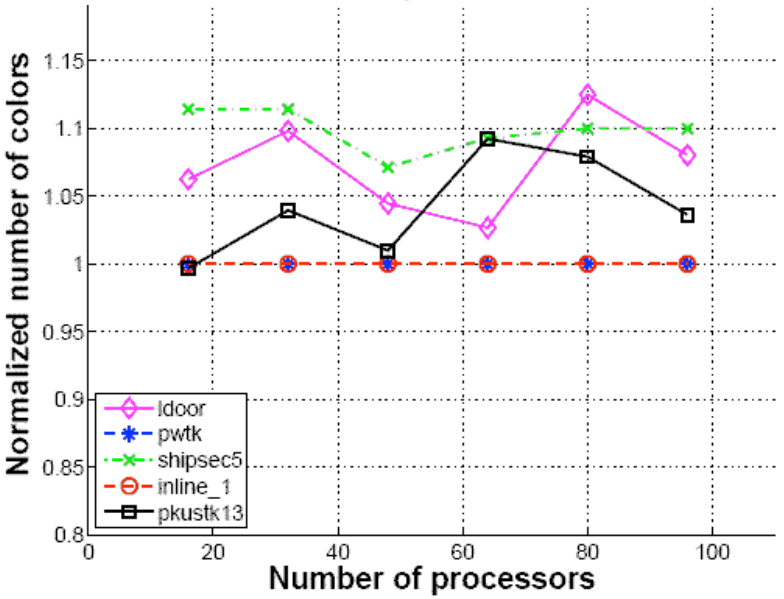
Experimental Results









Other Zoltan Functionality

- Tools needed when doing dynamic load balancing:
  - Data Migration
  - Unstructured Communication Primitives
  - Distributed Data Directories
- All functionality described in Zoltan User's Guide.
  - http://www.cs.sandia.gov/Zoltan/ug_html/ug.html

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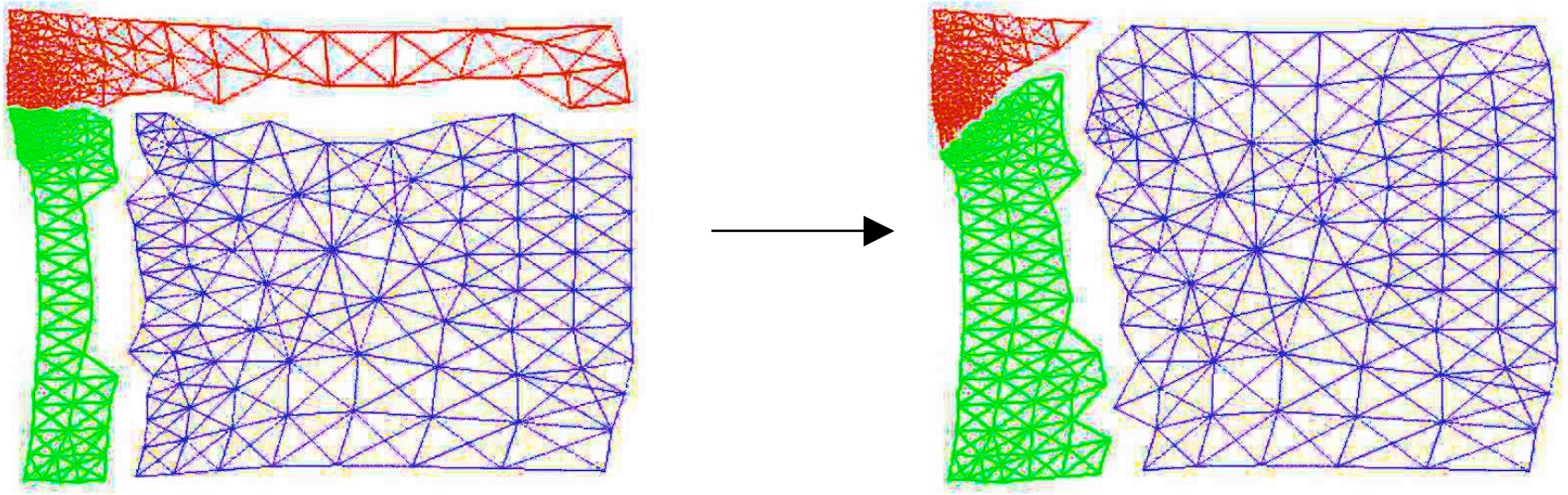
Zoltan Data Migration Tools

- **After partition is computed, data must be moved to new decomposition.**
  - **Depends strongly on application data structures.**
  - **Complicated communication patterns.**
- **Zoltan can help!**
  - **Application supplies query functions to pack/unpack data.**
  - **Zoltan does all communication to new processors.**



Using Zoltan's Data Migration Tools

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- **Required migration query functions:**
  - **ZOLTAN_OBJ_SIZE_MULTI_FN:**
    - Returns size of data (in bytes) for each object to be exported to a new processor.
  - **ZOLTAN_PACK_MULTI_FN:**
    - Remove data from application data structure on old processor;
    - Copy data to Zoltan communication buffer.
  - **ZOLTAN_UNPACK_MULTI_FN:**
    - Copy data from Zoltan communication buffer into data structure on new processor.

```
int Zoltan_Migrate(struct Zoltan_Struct *zz,
        int num_import, ZOLTAN_ID_PTR import_global_ids,
        ZOLTAN_ID_PTR import_local_ids, int *import_procs,
        int *import_to_part,
        int num_export, ZOLTAN_ID_PTR export_global_ids,
        ZOLTAN_ID_PTR export_local_ids, int *export_procs,
        int *export_to_part);
```

Zoltan Unstructured Communication Package

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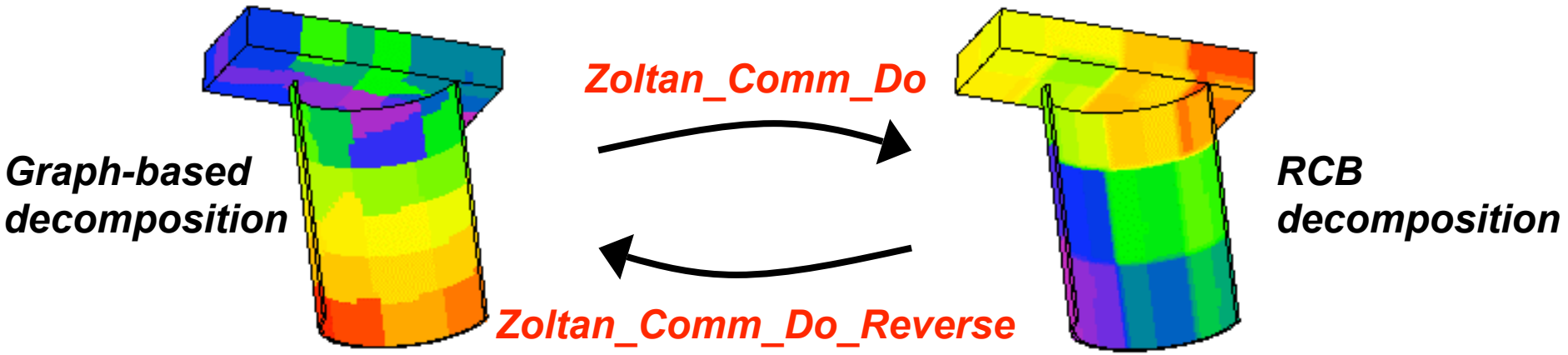
- **Simple primitives for efficient irregular communication.**
  - **Zoltan_Comm_Create: Generates communication plan.**
    - **Processors and amount of data to send and receive.**
  - **Zoltan_Comm_Do: Send data using plan.**
    - **Can reuse plan. (Same plan, different data.)**
  - **Zoltan_Comm_Do_Reverse: Inverse communication.**
- **Used for most communication in Zoltan.**



Example Application: Crash Simulations

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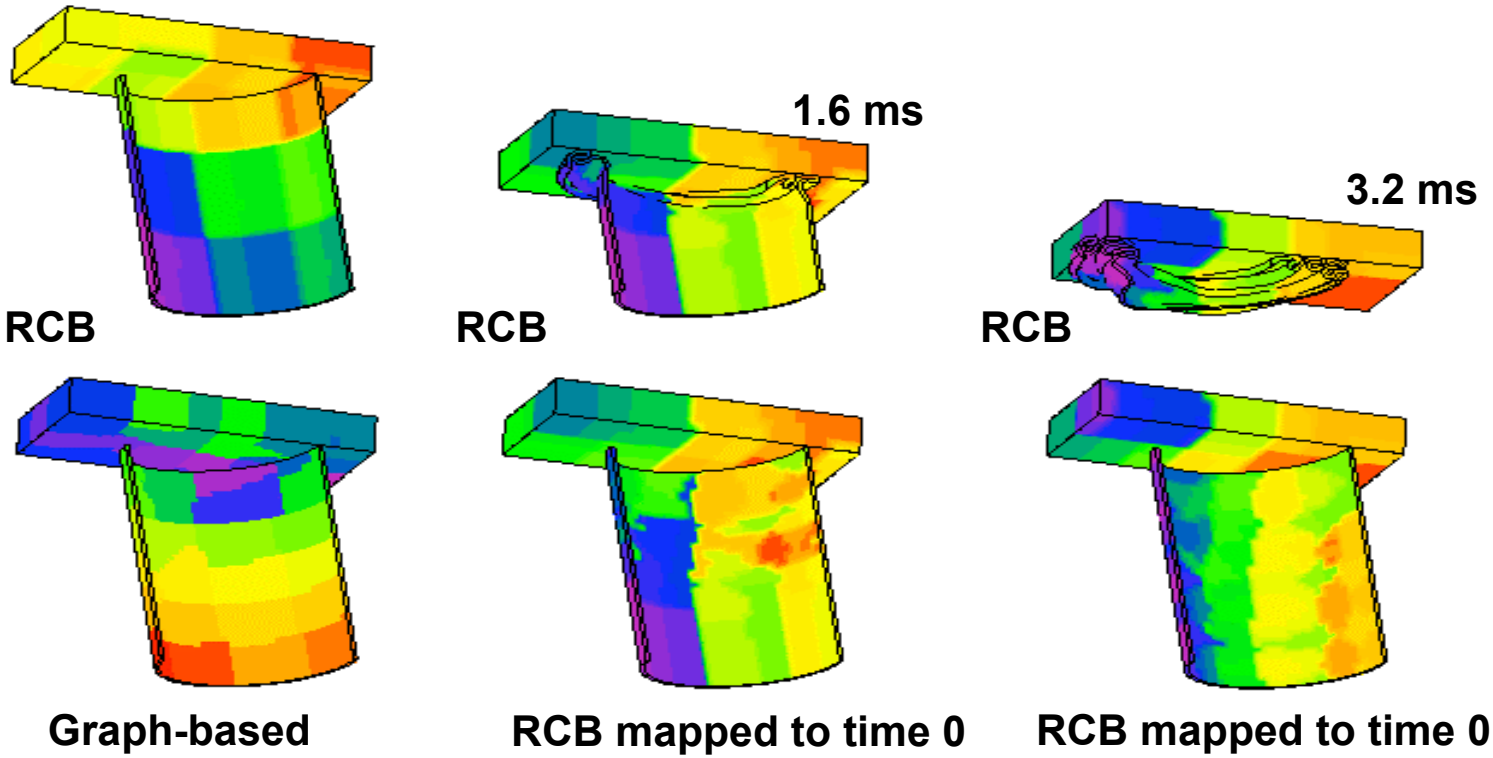
- **Multiphase simulation:**
  - **Graph-based decomposition of elements for finite element calculation.**
  - **Dynamic geometric decomposition of surfaces for contact detection.**
  - **Migration tools and Unstructured Communication package map between decompositions.**



Zoltan Distributed Data Directory

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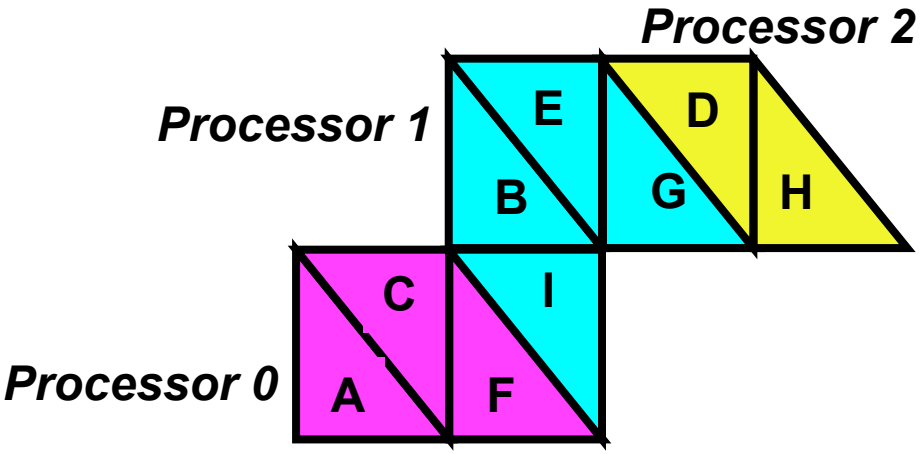
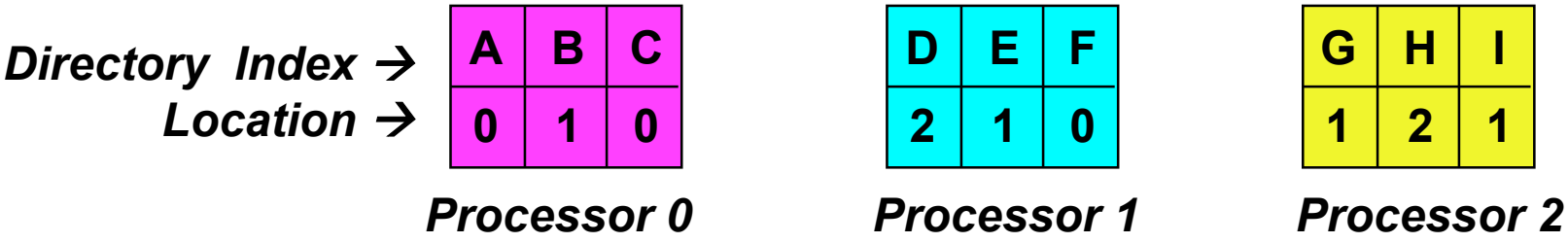
- **Helps applications locate off-processor data.**
- **Rendezvous algorithm (Pinar, 2001).**
  - **Directory distributed in known way (hashing) across processors.**
  - **Requests for object location sent to processor storing the object's directory entry.**





Alternate Interfaces to Zoltan

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- Isorropia package in Trilinos solver toolkit.
  - Epetra Matrix interface to Zoltan partitioning.
    - B = Isorropia::Epetra::create_balanced_copy(A, params);
  - Trilinos v9 will also include ordering and coloring interfaces in Isorropia.
  - SciDAC TOPS-2 CET.
- ITAPS iMesh interface to Zoltan.
  - New iMeshP parallel mesh interface to be incorporated in FY09.
  - SciDAC ITAPS CET.

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Future Work

- Two-dimensional matrix partitioning interfaces in Isorropia.
- Performance improvements for hypergraph partitioning.
- Multi-criteria hypergraph partitioning.
- Non-symmetric matrix ordering.

For More Information...

- **Zoltan Home Page**
  - http://www.cs.sandia.gov/Zoltan
  - User's and Developer's Guides
  - Download Zoltan software under GNU LGPL.

- **Email:**
  - {kddevin,ccheval,egboman}@sandia.gov
  - umit@bmi.osu.edu

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The End

Configuring and Building Zoltan

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- Create and enter the Zoltan directory:
  - gunzip zoltan_distrib_v3.0.tar.gz
  - tar xf zoltan_distrib_v3.0.tar
  - cd Zoltan
- Configure and make Zoltan library
  - Not autotooled; uses manual configuration file.
  - "make zoltan" attempts a generic build; library libzoltan.a is in directory Obj_generic.
  - To customize your build:
    - cd Utilities/Config; cp Config.linux Config.your_system
    - Edit Config.your_system
    - cd ../..
    - setenv ZOLTAN_ARCH your_system
    - make zoltan
    - Library libzoltan.a is in Obj_your_system

Config file

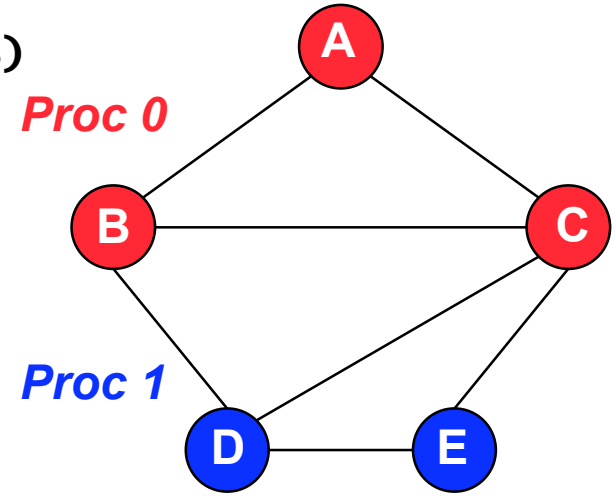

```
DEFS                    =
RANLIB                  = ranlib
AR                      = ar r

CC                      = mpicc -Wall
CPPC                    = mpic++
INCLUDE_PATH            =
DBG_FLAGS               = -g
OPT_FLAGS               = -O
CFLAGS                  = $(DBG_FLAGS)

F90                     = mpif90
LOCAL_F90               = f90
F90CFLAGS               = -DFMANGLE=UNDERSCORE -DNO_MPI2
FFLAGS                  =
SPPR_HEAD               = spprinc.most
F90_MODULE_PREFIX       = -I
FARG                    = farg_typical

MPI_LIB                 =
MPI_LIBPATH             =

PARMETIS_LIBPATH        = -L/Users/kddevin/code/ParMETIS3_1
PARMETIS_INCPATH        = -I/Users/kddevin/code/ParMETIS3_1
#PATOH_LIBPATH           = -L/Users/kddevin/code/PaToH
#PATOH_INCPATH           = -I/Users/kddevin/code/PaToH
```

Example Graph Callbacks

```
void ZOLTAN_NUM_EDGES_MULTI_FN(void *data,
  int num_gid_entries, int num_lid_entries,
  int num_obj, ZOLTAN_ID_PTR global_id, ZOLTAN_ID_PTR local_id,
  int *num_edges, int *ierr);
```

Proc 0 Input from Zoltan:
num_obj = 3
global_id = {A,C,B}
local_id = {0,1,2}

Output from Application on Proc 0:
num_edges = {2,4,3}
(i.e., degrees of vertices A, C, B)
ierr = ZOLTAN_OK



Example Graph Callbacks

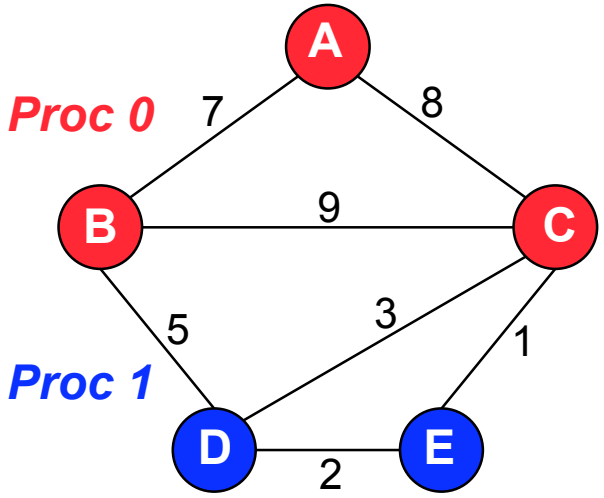
```
void ZOLTAN_EDGE_LIST_MULTI_FN(void *data,
  int num_gid_entries, int num_lid_entries,
  int num_obj, ZOLTAN_ID_PTR global_ids, ZOLTAN_ID_PTR local_ids,
  int *num_edges,
  ZOLTAN_ID_PTR nbor_global_id, int *nbor_procs,
  int wdim, float *nbor_ewgts,
  int *ierr);
```

Proc 0 Input from Zoltan:

```
num_obj = 3
global_ids = {A, C, B}
local_ids  = {0, 1, 2}
num_edges  = {2, 4, 3}
wdim = 0 or EDGE_WEIGHT_DIM parameter value
```

Output from Application on Proc 0:

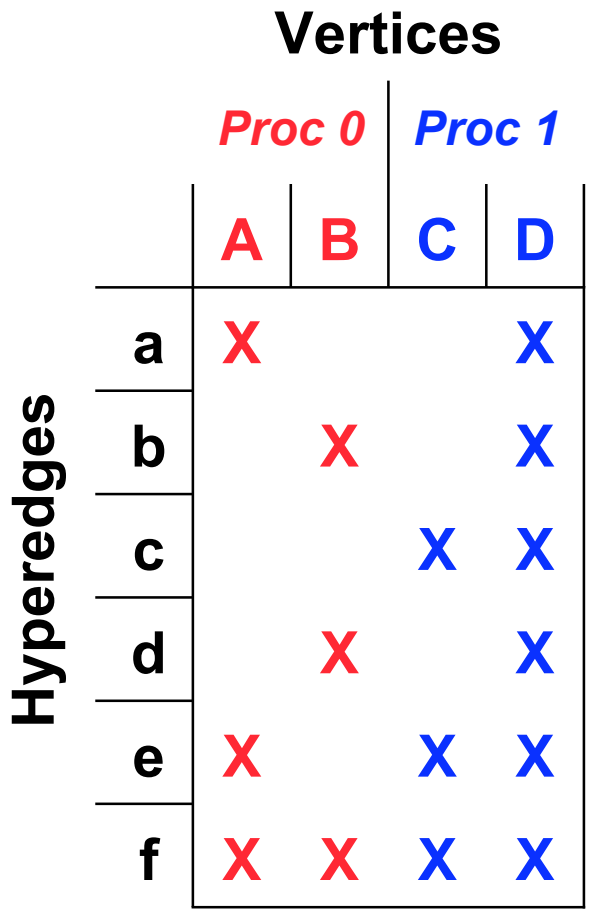
```
nbor_global_id = {B, C, A, B, E, D, A, C, D}
nbor_procs     = {0, 0, 0, 0, 1, 1, 0, 0, 1}
nbor_ewgts     = if wdim then
                   {7, 8, 8, 9, 1, 3, 7, 9, 5}
ierr = ZOLTAN_OK
```



Example Hypergraph Callbacks


```
void ZOLTAN_HG_SIZE_CS_FN(void *data, int *num_lists, int *num_pins,
  int *format, int *ierr);
```

```
Output from Application on Proc 0:
  num_lists = 2
  num_pins = 6
  format = ZOLTAN_COMPRESSED_VERTEX
           (owned non-zeros per vertex)
  ierr = ZOLTAN_OK

OR

Output from Application on Proc 0:
  num_lists = 5
  num_pins = 6
  format = ZOLTAN_COMPRESSED_EDGE
           (owned non-zeros per edge)
  ierr = ZOLTAN_OK
```



Example Hypergraph Callbacks

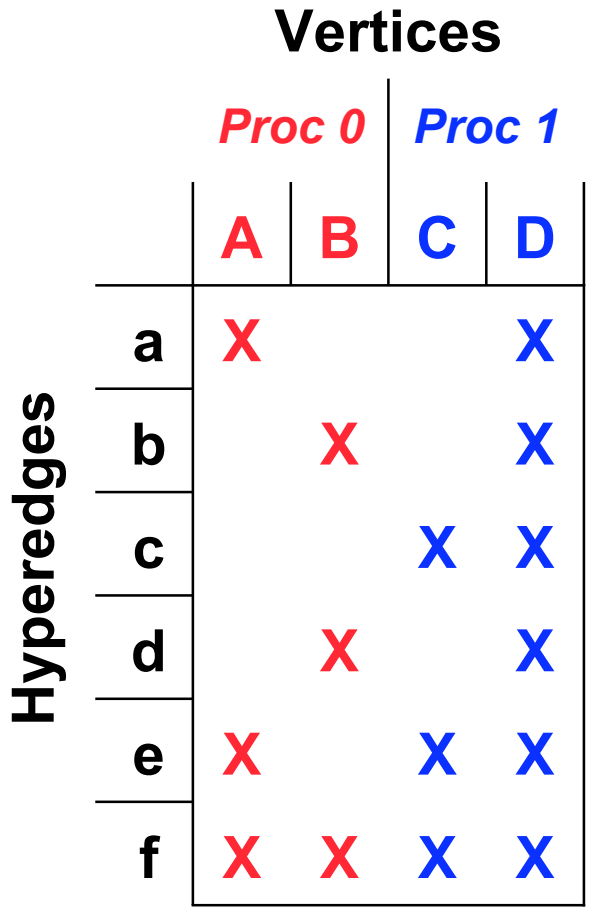

```
void ZOLTAN_HG_CS_FN(void *data, int num_gid_entries,
  int nvtxedge, int npins, int format,
  ZOLTAN_ID_PTR vtxedge_GID, int *vtxedge_ptr, ZOLTAN_ID_PTR pin_GID,
  int *ierr);
```

Proc 0 Input from Zoltan:

- nvtxedge = 2 or 5
- npins = 6
- format = ZOLTAN_COMPRESSED_VERTEX or ZOLTAN_COMPRESSED_EDGE

Output from Application on Proc 0:

- if (format = ZOLTAN_COMPRESSED_VERTEX)
  - vtxedge_GID = {A, B}
  - vtxedge_ptr = {0, 3}
  - pin_GID = {a, e, f, b, d, f}
- if (format = ZOLTAN_COMPRESSED_EDGE)
  - vtxedge_GID = {a, b, d, e, f}
  - vtxedge_ptr = {0, 1, 2, 3, 4}
  - pin_GID = {A, B, B, A, A, B}
- ierr = ZOLTAN_OK



Simple Example

- Zoltan/examples/C/zoltanSimple.c
- Application data structure:
  - int MyNumPts;
    - Number of points on processor.
  - int *Gids;
    - array of Global ID numbers of points on processor.
  - float *Pts;
    - Array of 3D coordinates of points on processor (in same order as Gids array).

Example zoltanSimple.c: Initialization

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```
/* Initialize MPI */
MPI_Init(&argc, &argv);
MPI_Comm_rank(MPI_COMM_WORLD, &me);
MPI_Comm_size(MPI_COMM_WORLD, &nprocs);

/*
** Initialize application data.  In this example,
** create a small test mesh and divide it across processors
*/

exSetDivisions(32);    /* rectilinear mesh is div X div X div */

MyNumPts = exInitializePoints(&Pts, &Gids, me, nprocs);

/*  Initialize Zoltan */
rc = Zoltan_Initialize(argc, argv, &ver);

if (rc != ZOLTAN_OK){
  printf("sorry...\n");
  free(Pts); free(Gids);
  exit(0);
}
```

Example zoltanSimple.c: Prepare for Partitioning

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```
/* Allocate and initialize memory for Zoltan structure */
zz = Zoltan_Create(MPI_COMM_WORLD);

/* Set general parameters */
Zoltan_Set_Param(zz, "DEBUG_LEVEL", "0");
Zoltan_Set_Param(zz, "LB_METHOD", "RCB");
Zoltan_Set_Param(zz, "NUM_GID_ENTRIES", "1");
Zoltan_Set_Param(zz, "NUM_LID_ENTRIES", "1");
Zoltan_Set_Param(zz, "RETURN_LISTS", "ALL");

/* Set RCB parameters */
Zoltan_Set_Param(zz, "KEEP_CUTS", "1");
Zoltan_Set_Param(zz, "RCB_OUTPUT_LEVEL", "0");
Zoltan_Set_Param(zz, "RCB_RECTILINEAR_BLOCKS", "1");

/* Register call-back query functions. */
Zoltan_Set_Num_Obj_Fn(zz, exGetNumberOfAssignedObjects, NULL);
Zoltan_Set_Obj_List_Fn(zz, exGetObjectList, NULL);
Zoltan_Set_Num_Geom_Fn(zz, exGetObjectSize, NULL);
Zoltan_Set_Geom_Multi_Fn(zz, exGetObject, NULL);
```

Example zoltanSimple.c: Partitioning

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Zoltan computes the difference (Δ) from current distribution
Choose between:

a) Import lists (data to import from other procs)
b) Export lists (data to export to other procs)
c) Both (the default)

```
/* Perform partitioning */
rc = Zoltan_LB_Partition(zz,
            &changes, /* Flag indicating whether partition changed */
            &numGidEntries, &numLidEntries,
            &numImport, /* objects to be imported to new part */
            &importGlobalGids, &importLocalGids,
            &importProcs, &importToPart,
            &numExport, /* # objects to be exported from old part */
             &exportGlobalGids, &exportLocalGids,
            &exportProcs, &exportToPart);
```

Example zoltanSimple.c: Use the Partition

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```
/* Process partitioning results;
** in this case, print information;
** in a "real" application, migrate data here.
*/
if (!rc){
  exPrintGlobalResult("Recursive Coordinate Bisection",
                      nprocs, me,
                      MyNumPts, numImport, numExport, changes);
}
else{
  free(Pts);
  free(Gids);
  Zoltan_Destroy(&zz);
  MPI_Finalize();
  exit(0);
}
```

Example zoltanSimple.c: Cleanup

Sandia National Laboratories

```
/* Free Zoltan memory allocated by Zoltan_LB_Partition. */
Zoltan_LB_Free_Part(&importGlobalGids, &importLocalGids,
                    &importProcs, &importToPart);
Zoltan_LB_Free_Part(&exportGlobalGids, &exportLocalGids,
                    &exportProcs, &exportToPart);

/* Free Zoltan memory allocated by Zoltan_Create. */
Zoltan_Destroy(&zz);

/* Free Application memory */
free(Pts); free(Gids);

/************************
** all done ************
************************/

MPI_Finalize();
```

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Performance Results

- Experiments on Sandia's Thunderbird cluster.
  - Dual 3.6 GHz Intel EM64T processors with 6 GB RAM.
  - Infiniband network.
- Compare RCB, HSFC, graph and hypergraph methods.
- Measure …
  - Amount of communication induced by the partition.
  - Partitioning time.

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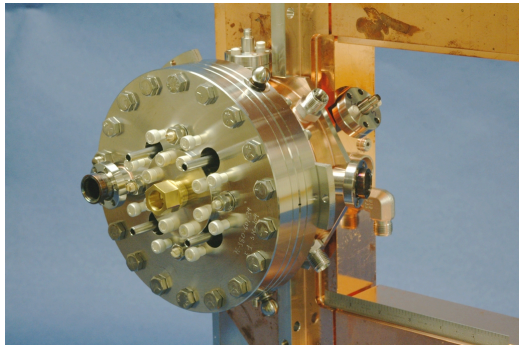
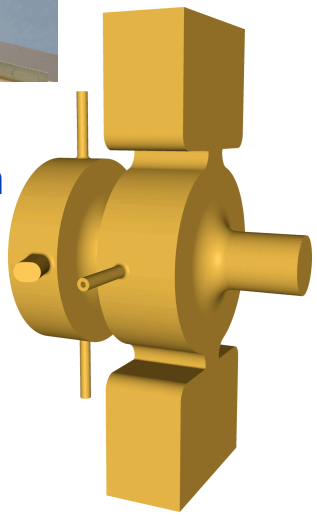
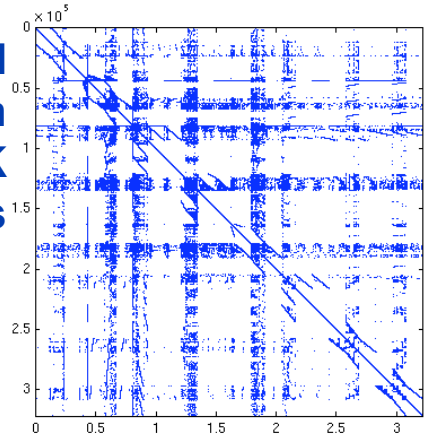
Test Data



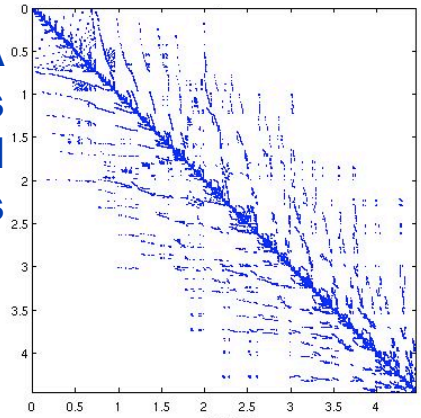
SLAC *LCLS
Radio Frequency Gun
6.0M x 6.0M
23.4M nonzeros



Xyce 680K ASIC Stripped
Circuit Simulation
680K x 680K
2.3M nonzeros



Cage15 DNA
Electrophoresis
5.1M x 5.1M
99M nonzeros



SLAC Linear Accelerator
2.9M x 2.9M
11.4M nonzeros

Communication Volume: Lower is Better

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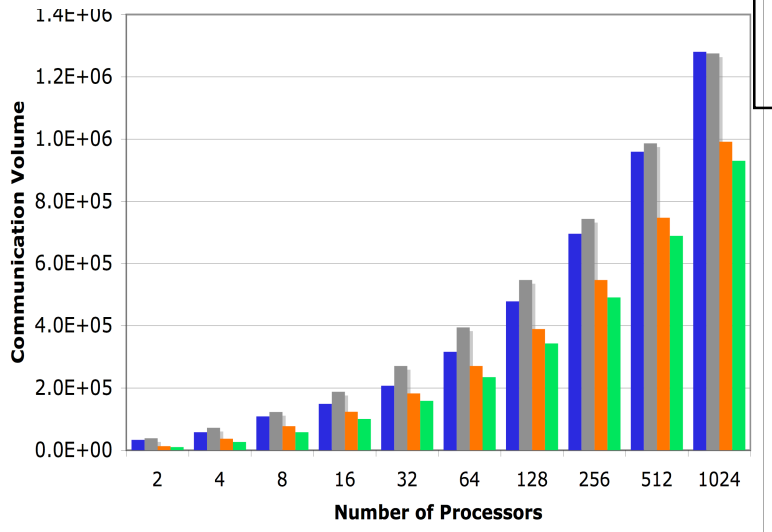
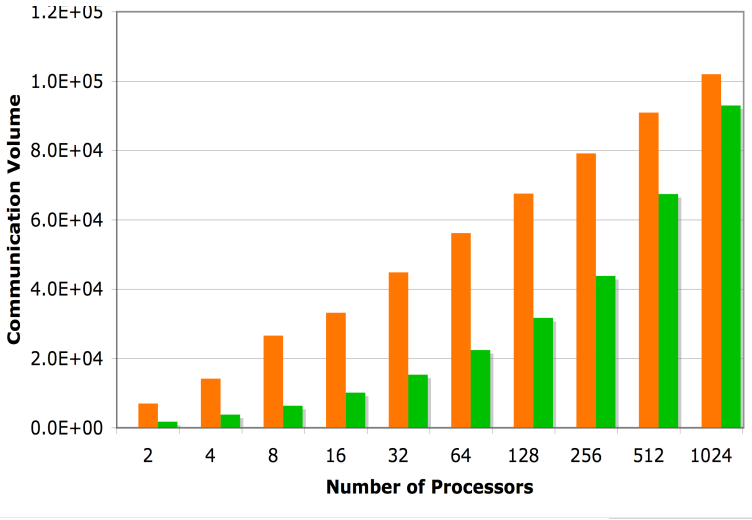
Number of parts = number of processors.

SLAC 6.0M LCLS

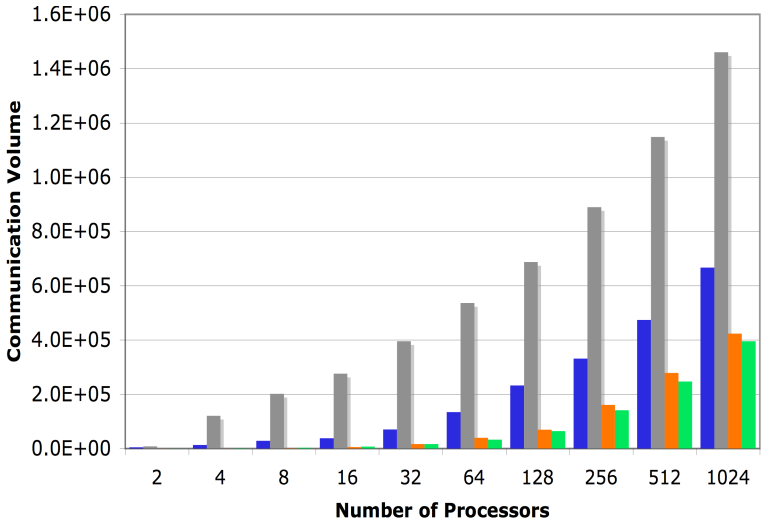


Xyce 680K circuit

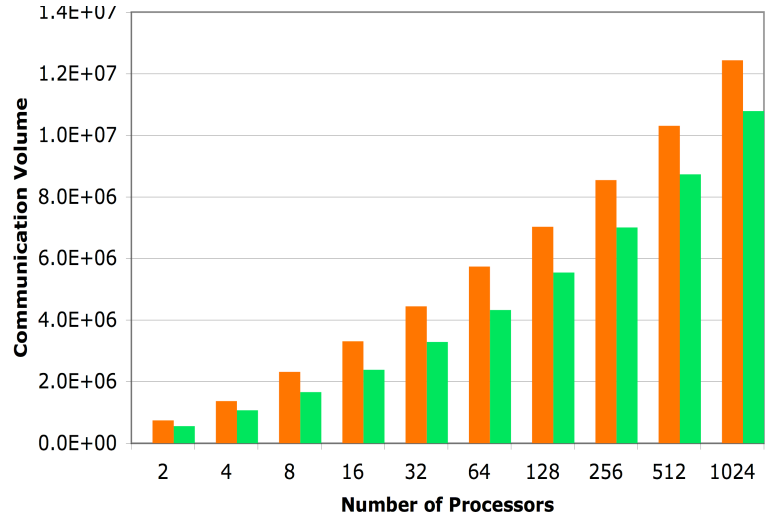


RCB
HSFC
Graph
Hypergraph

SLAC 2.9M Linear Accelerator



Cage15 5.1M electrophoresis



Partitioning Time: Lower is better

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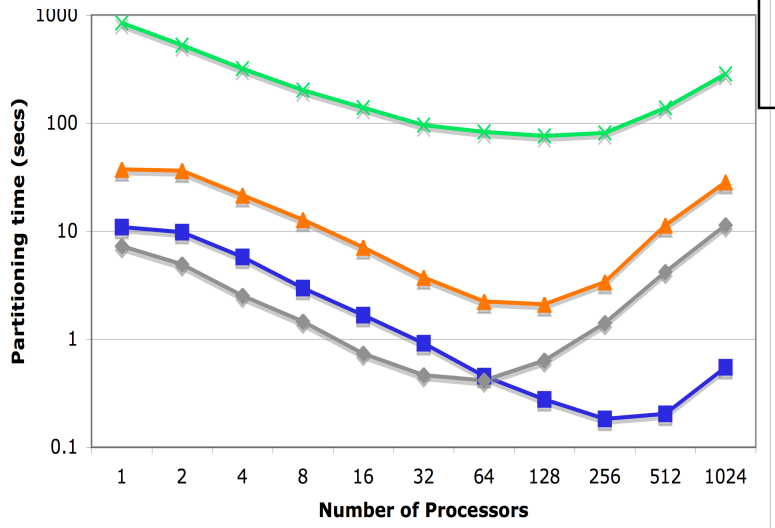
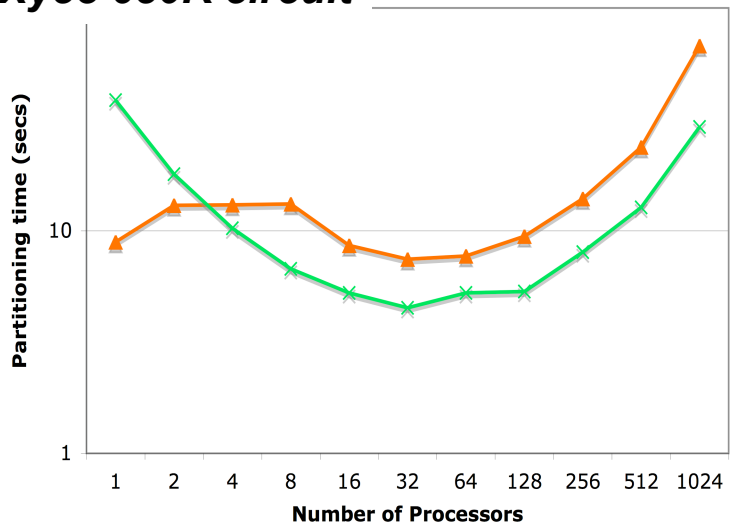
1024 parts. Varying number of processors.

RCB
HSFC
Graph
Hypergraph

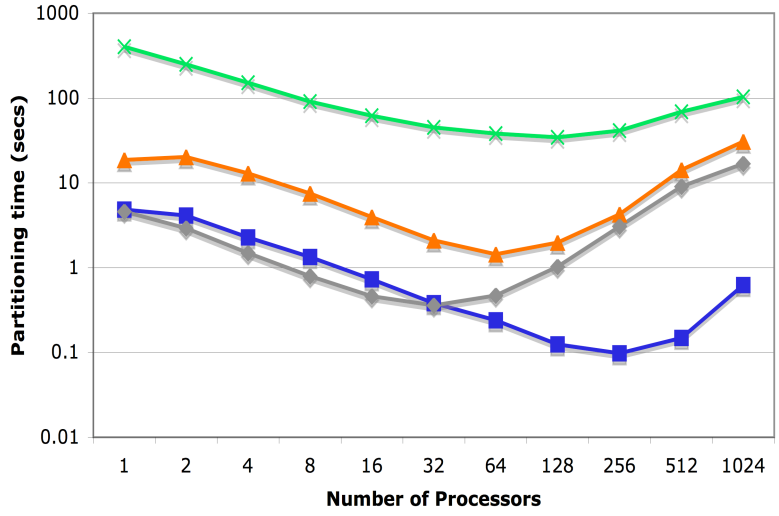
SLAC 6.0M LCLS



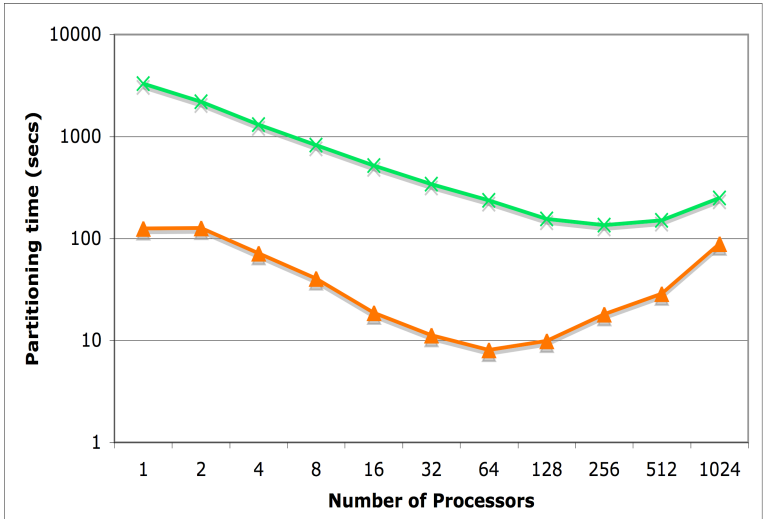
Xyce 680K circuit



SLAC 2.9M Linear Accelerator



Cage15 5.1M electrophoresis



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Repartitioning Experiments

- Experiments with 64 parts on 64 processors.
- Dynamically adjust weights in data to simulate, say, adaptive mesh refinement.
- Repartition.
- Measure repartitioning time and total communication volume:

  Data redistribution volume

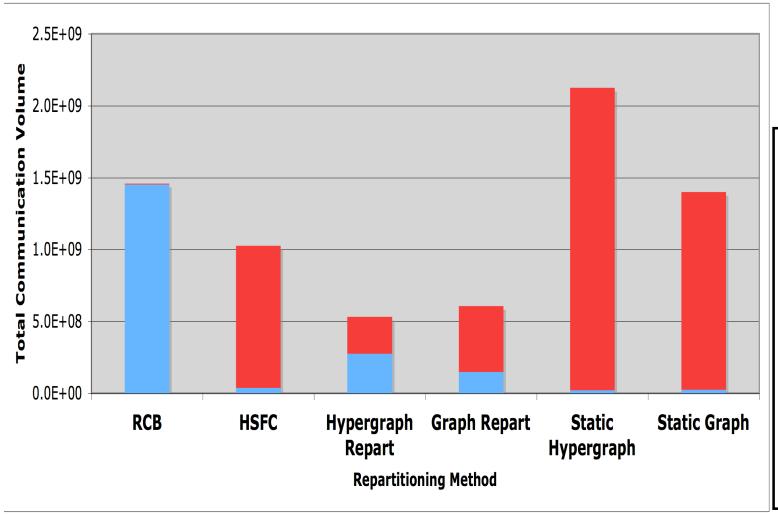
  \+ Application communication volume

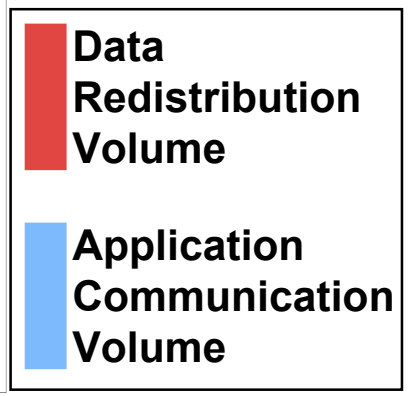
  Total communication volume

Repartitioning Results: Lower is Better

Sandia National Laboratories

SLAC 6.0M LCLS





Xyce 680K circuit