The Zoltan Toolkit – Partitioning, Ordering, and Coloring

Erik Boman, Cedric Chevalier, Karen Devine
Sandia National Laboratories, NM

Ümit Çatalyürek
Ohio State University

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Outline

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

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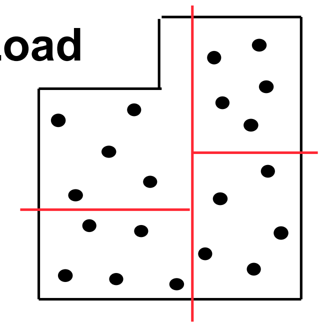
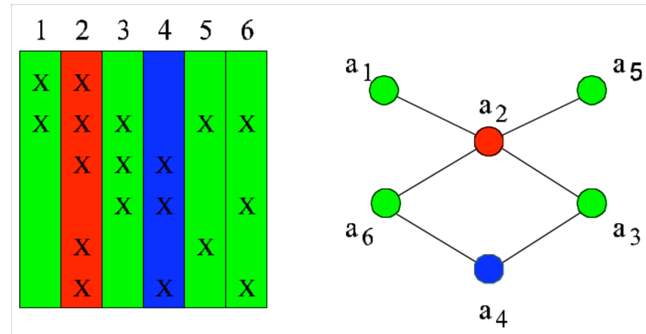
The Zoltan Toolkit

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

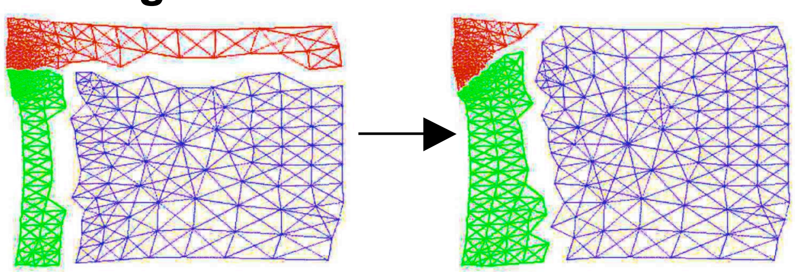
Dynamic Load Balancing



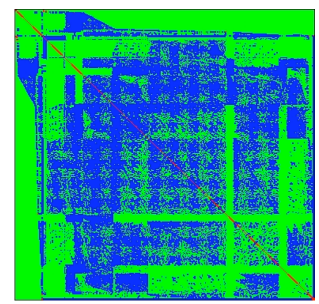
Graph Coloring



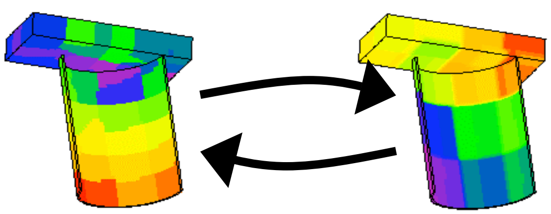
Data Migration



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

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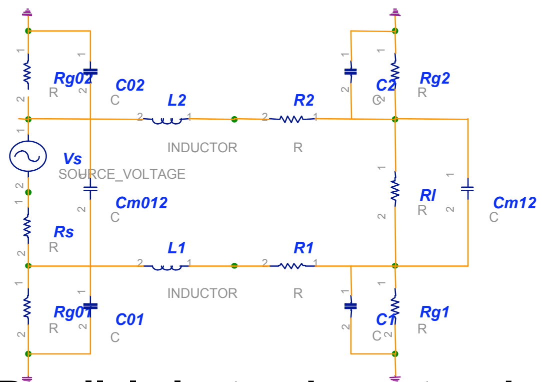
Zoltan System Assumptions

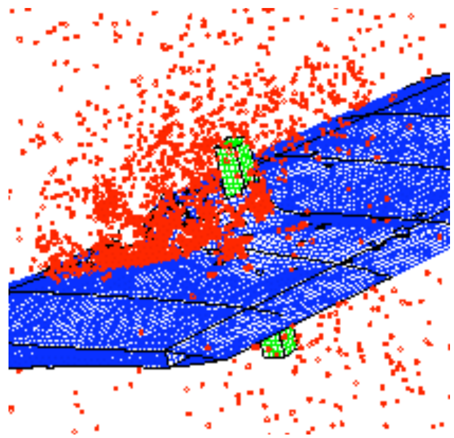
- **Assume distributed memory model.**
- **Data decomposition + “Owner computes”:**
  - **The data is distributed among the processors.**
  - **The owner performs all computation on its data.**
  - **Data distribution defines work assignment.**
  - **Data dependencies among data items owned by different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

Zoltan Supports Many Applications

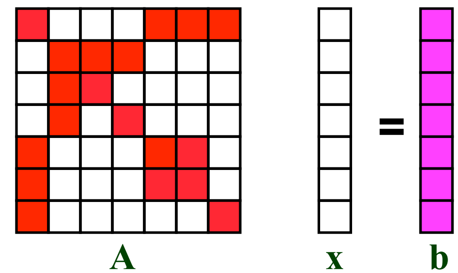
- **Different applications, requirements, data structures.**



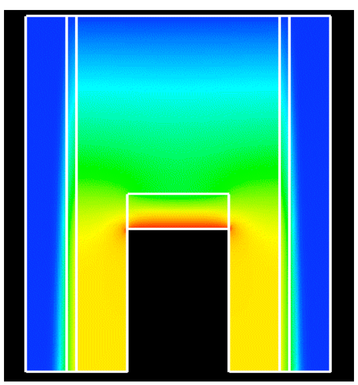
Parallel electronics networks



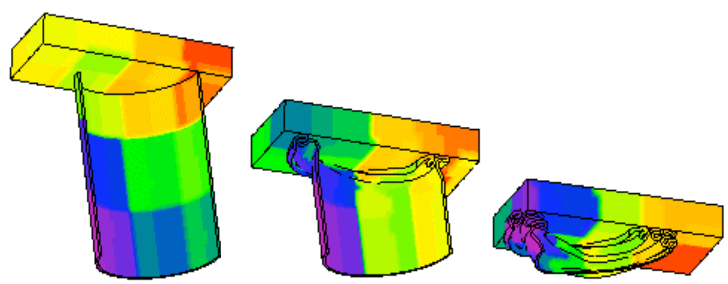
Particle methods



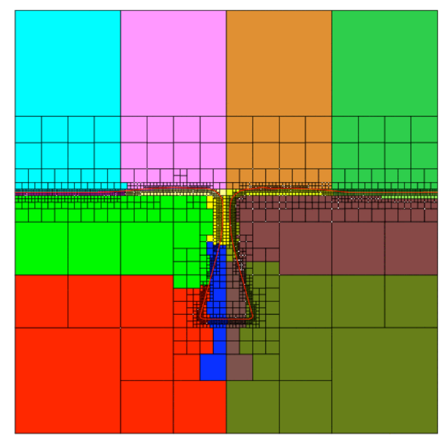
Linear solvers & preconditioners



Multiphysics simulations



Crash simulations



Adaptive mesh refinement

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Zoltan Interface Design

- 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

- Fairly 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)

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Zoltan Application Interface

- 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.

Zoltan Application Interface

APPLICATION

Initialize Zoltan
(Zoltan_Initialize, Zoltan_Create)

Select Method and Parameters
(Zoltan_Set_Params)

Register query functions
(Zoltan_Set_Fn)

(Re)partition
(Zoltan_LB_Partition)

Move data
(Zoltan_Migrate)

COMPUTE

Clean up
(Zoltan_Destroy)

ZOLTAN

Zoltan_LB_Partition:
- **Call query functions.**
- **Build data structures.**
- **Compute new decomposition.**
- **Return import/export lists.**

Zoltan_Migrate:
- **Call packing query functions for exports.**
- **Send exports.**
- **Receive imports.**
- **Call unpacking query functions for imports.**

Zoltan Query Functions

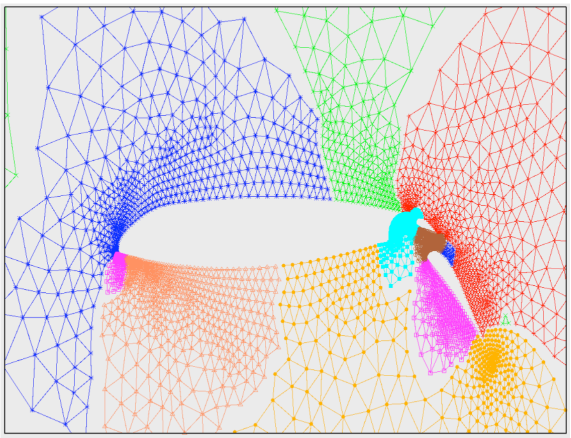
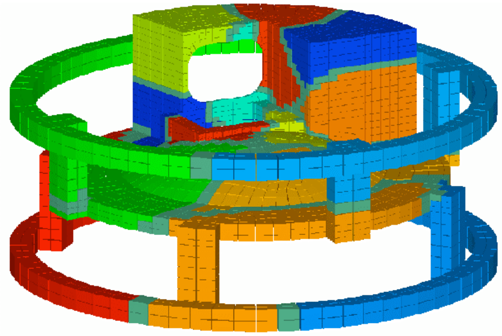
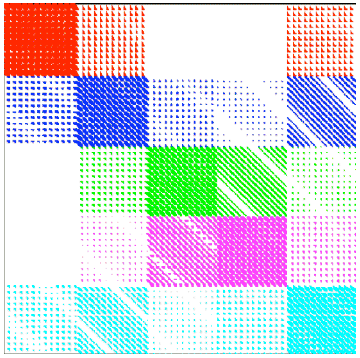
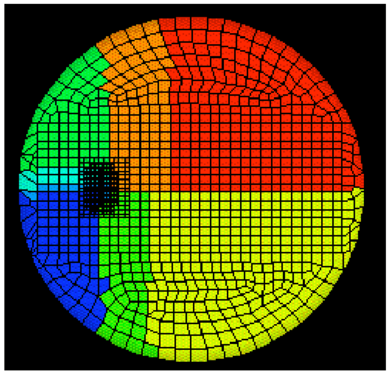
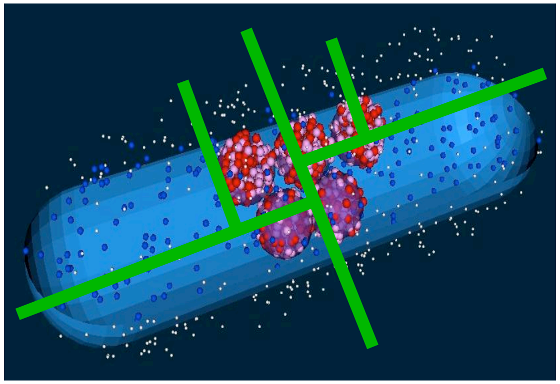
General Query Functions	
`ZOLTAN_NUM_OBJ_FN`	Number of items on processor
`ZOLTAN_OBJ_LIST_FN`	List of item IDs and weights.
Geometric Query Functions	
`ZOLTAN_NUM_GEOM_FN`	Dimensionality of domain.
`ZOLTAN_GEOM_FN`	Coordinates of items.
Hypergraph Query Functions	
`ZOLTAN_HG_SIZE_CS_FN`	Number of hyperedge 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.

Using Zoltan in Your Application

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

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)

Note that parts may differ from processors.

```
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);
```

Static Partitioning

Initialize Application → Partition Data → Distribute Data → Compute Solutions → Output & End

- Static partitioning in an application:
  - Data partition is computed.
  - Data are distributed according to partition map.
  - Application computes.

- Ideal partition:
  - Largest processor time is minimized.
  - Inter-processor communication costs are kept low.

- Zoltan_Set_Param(zz, “LB_APPROACH”, “PARTITION”);

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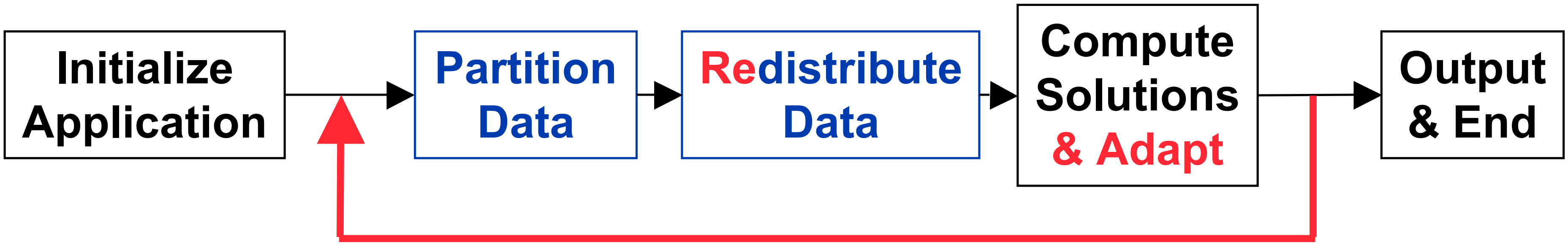
Dynamic Repartitioning (a.k.a. Dynamic Load Balancing)



- **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:**
  - **Largest processor time is minimized.**
  - **Inter-processor communication costs are kept low.**
  - **Cost to redistribute data is also kept low.**

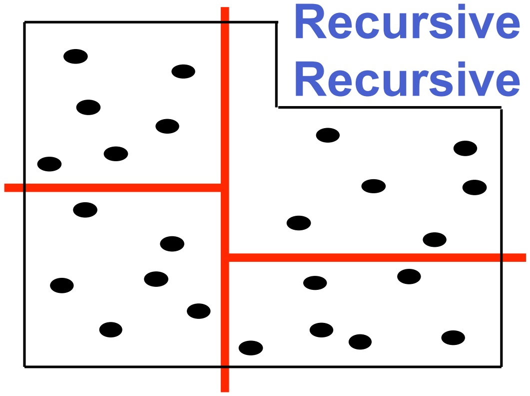
- **Zoltan_Set_Param(zz, “LB_APPROACH”, “REPARTITION”);**

Zoltan Toolkit: Suite of Partitioners

- 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.

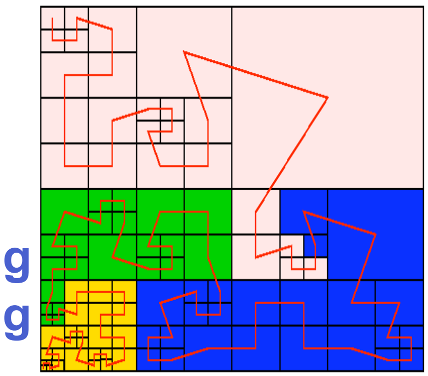
Partitioning Algorithms in the Zoltan Toolkit

Geometric (coordinate-based) methods

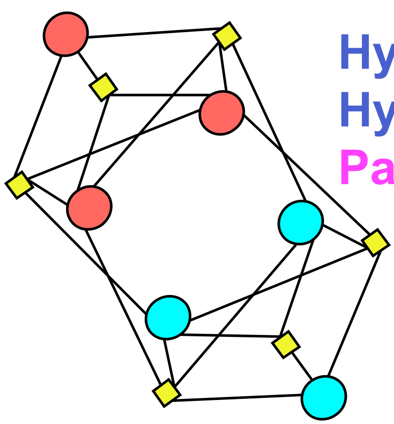


Recursive Coordinate Bisection
Recursive Inertial Bisection

Space Filling Curve Partitioning
Refinement-tree Partitioning

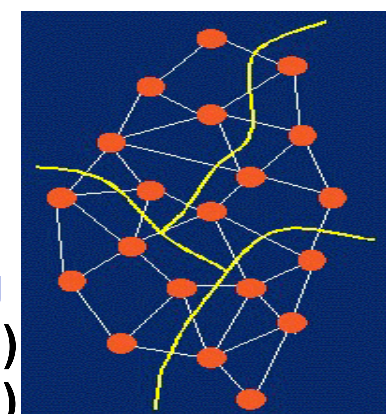


Combinatorial (topology-based) methods



Hypergraph Partitioning
Hypergraph Repartitioning
PaToH (Catalyurek & Aykanat)

Graph Partitioning
ParMETIS (Karypis et al.)
PT-Scotch (Pellegrini et al.)



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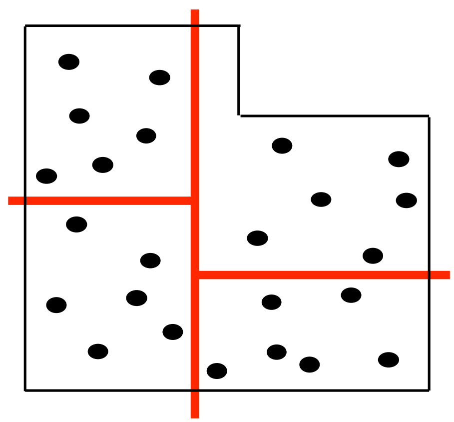
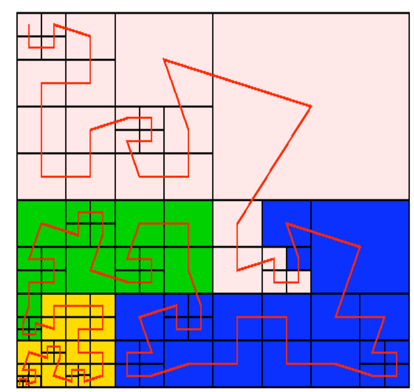
Geometric Partitioning

- Partition based on geometric locality of objects.
  - Assign physically close objects to the same processor.
- Communication costs are controlled only implicitly.
  - Assumption: objects that depend on each other are physically near each other.
  - Reasonable assumption for particle simulations, contact detection and some meshes.



Recursive Coordinate Bisection (RCB)
Berger & Bokhari, 1987

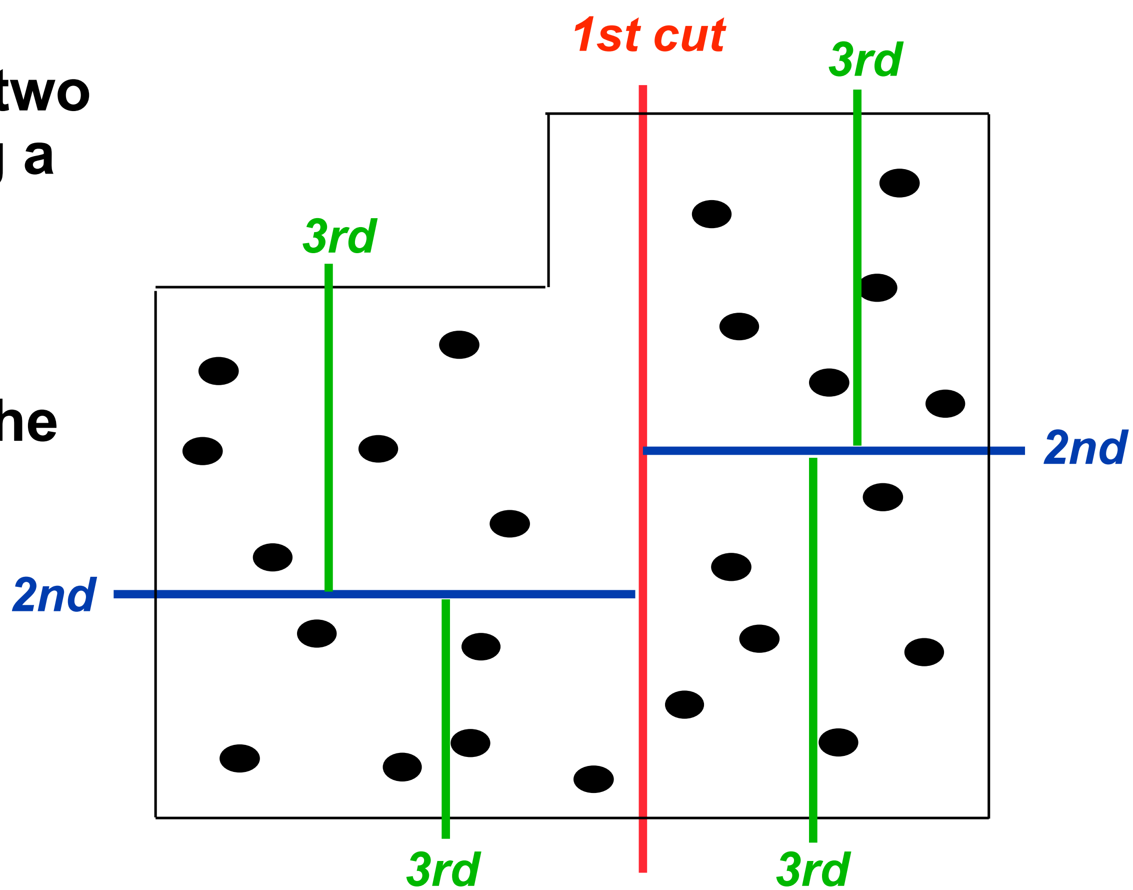
Recursive Inertial Bisection (RIB)
Simon, 1991; Taylor & Nour Omid, 1994



Space Filling Curve Partitioning (HSFC)
Warren & Salmon, 1993;
Pilkington & Baden, 1994; Patra & Oden, 1995

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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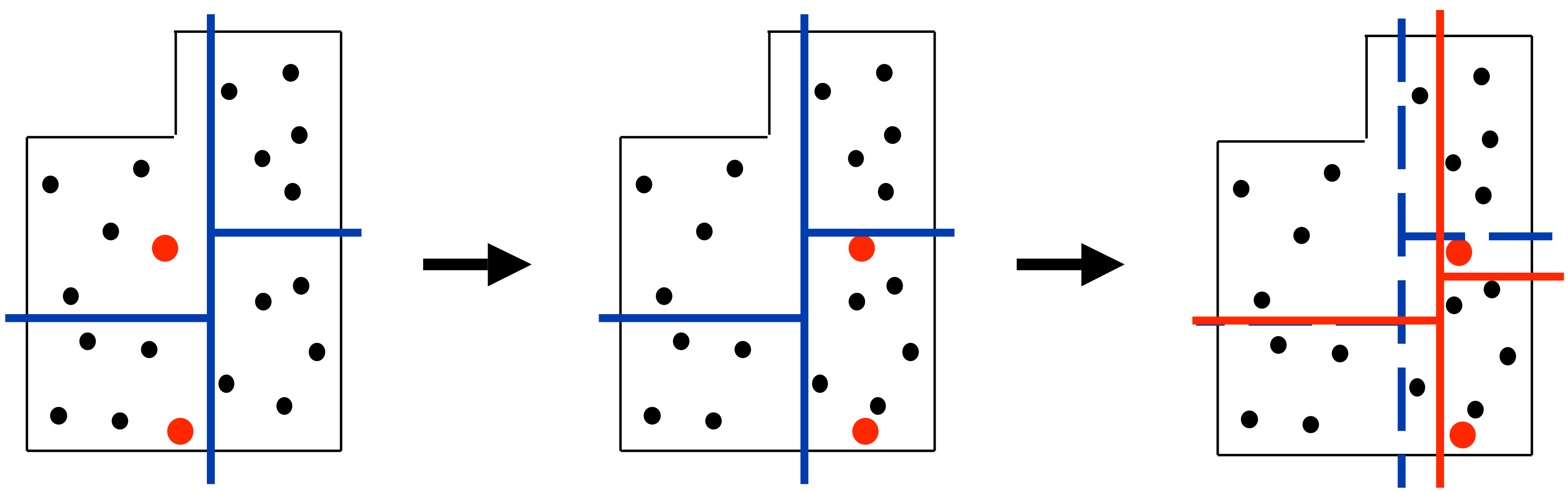
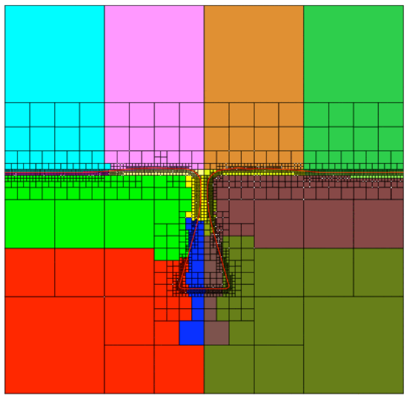
Geometric Repartitioning

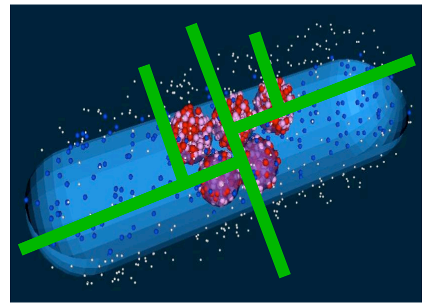
- Implicitly achieves low data redistribution costs.
- For small changes in data, cuts move only slightly, resulting in little data redistribution.

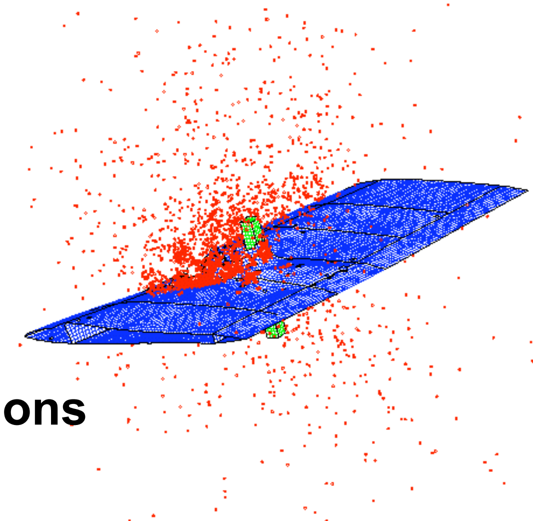


Applications of Geometric Methods

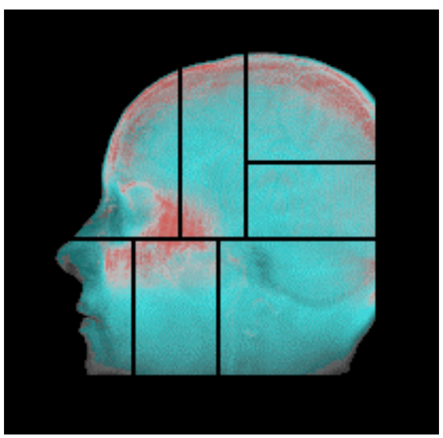


Adaptive Mesh Refinement

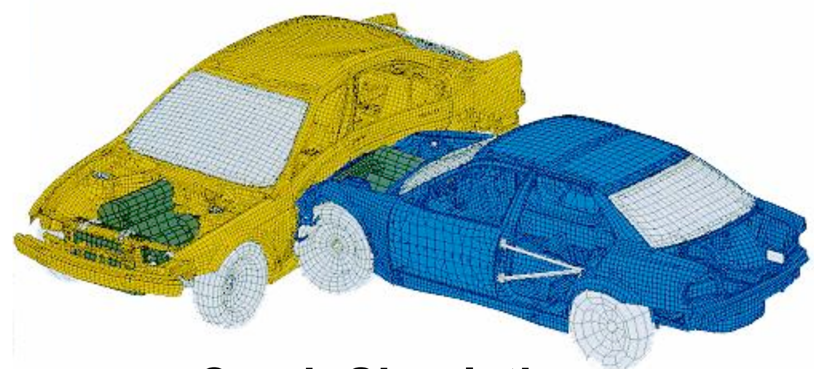




Particle Simulations



Parallel Volume Rendering



Crash Simulations
and Contact Detection

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Geometric Methods: 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.

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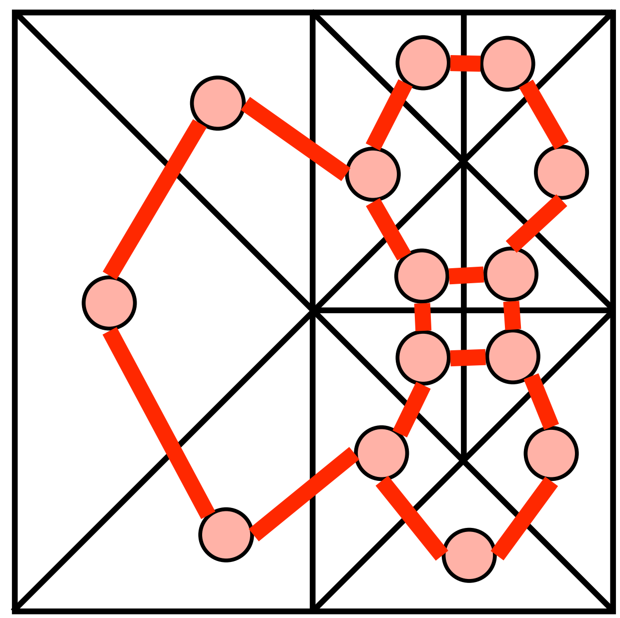
Graph Partitioning

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

- Kernighan, Lin, 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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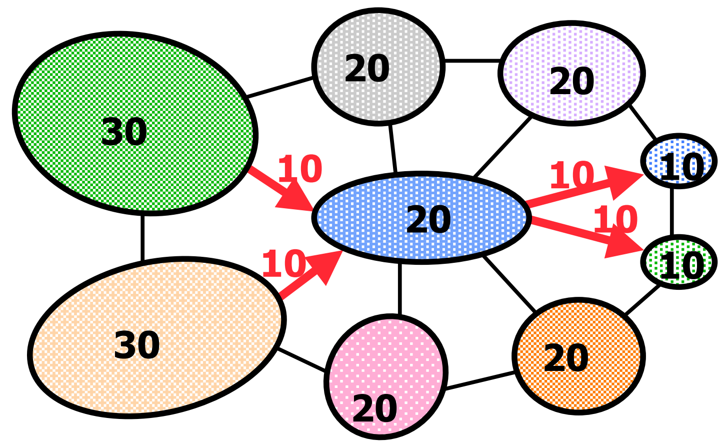
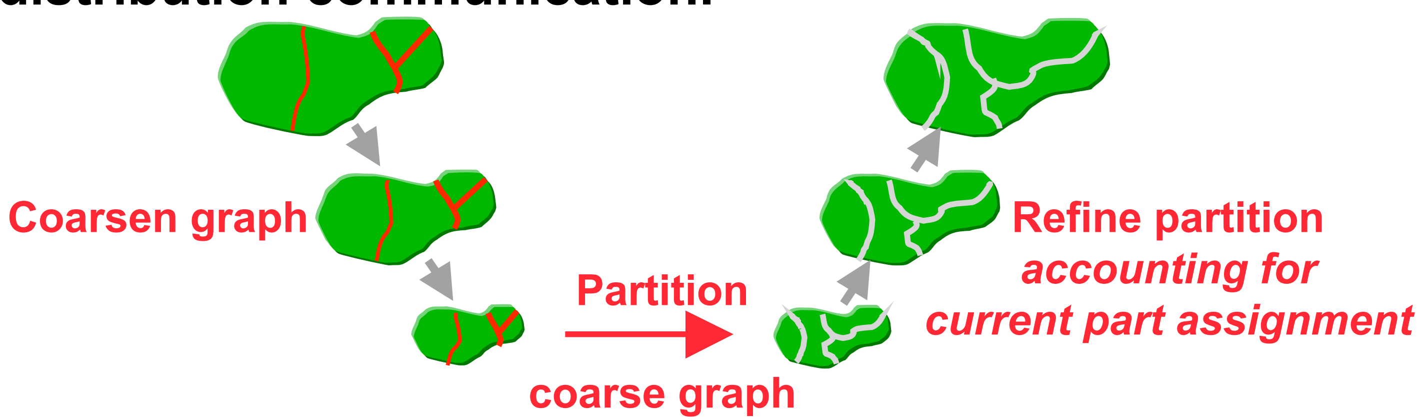
Graph Repartitioning

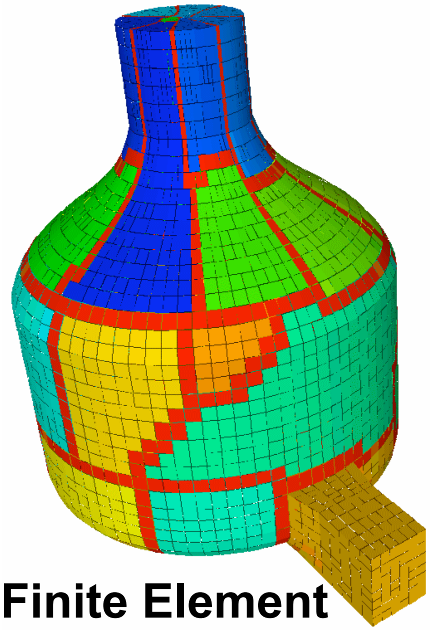
- **Diffusive strategies (Cybenko, Hu, Blake, Walshaw, Schloegel, et al.)**
  - **Shift work from highly loaded processors to less loaded neighbors.**
  - **Local communication keeps data redistribution costs low.**



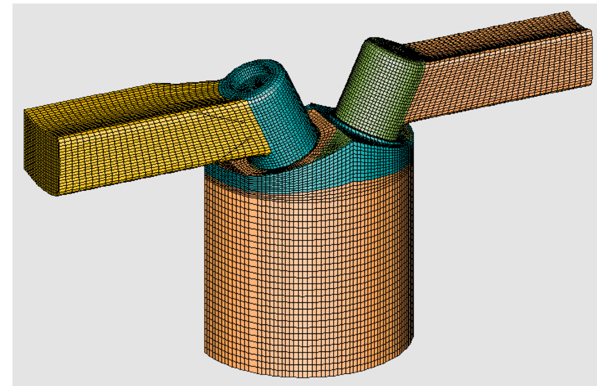
- **Multilevel partitioners that account for data redistribution costs in refining partitions (Schloegel, Karypis)**
  - **Parameter weights application communication vs. redistribution communication.**



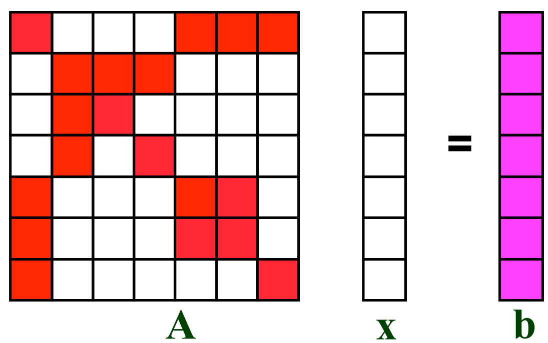
Applications using Graph Partitioning



Finite Element Analysis



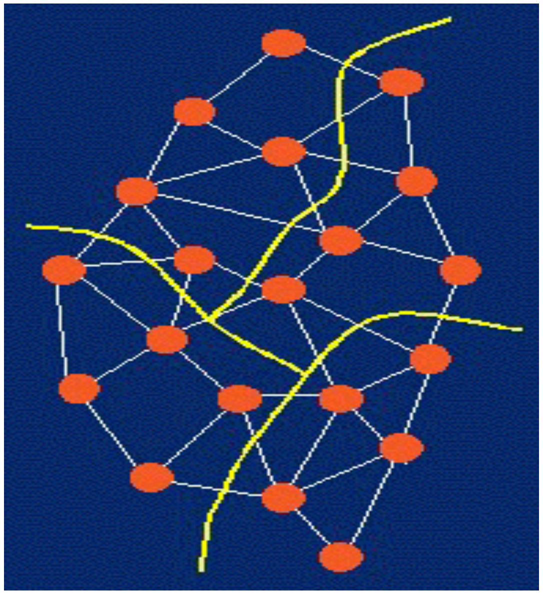
Multiphysics and multiphase simulations



Linear solvers & preconditioners
(square, structurally symmetric systems)

Graph Partitioning: Advantages and Disadvantages

- **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.)
      Scotch (U. Bordeaux)
    - Parallel: Zoltan (SNL)
      ParMETIS (U. Minn.)
      PJostle (U. Greenwich)
      PT-Scotch (LaBRI/INRIA)

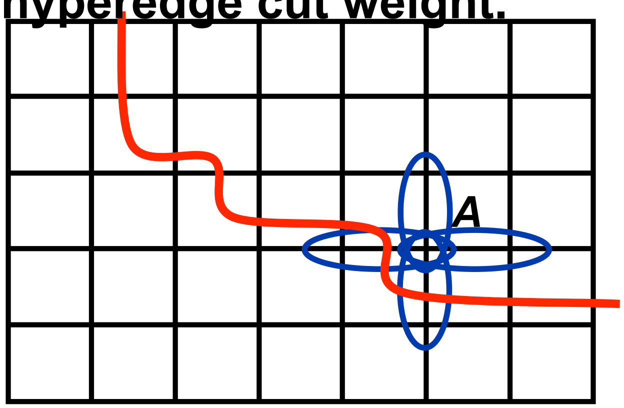


- **Disadvantages:**
  - More expensive than geometric methods.
  - Edge-cut model only approximates communication volume.

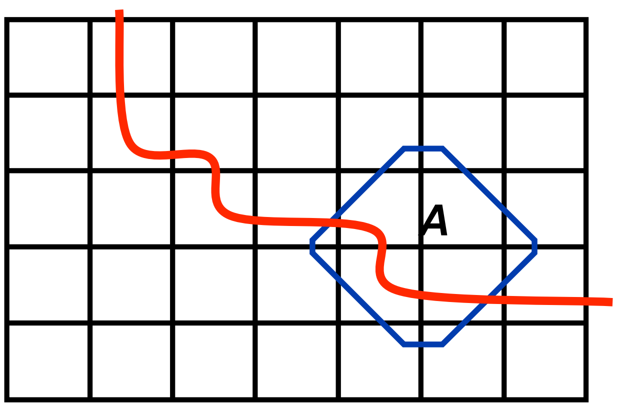
Hypergraph Partitioning

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

- Schweikert, Kernighan, Fiduccia, Mattheyes, Sanchis, 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

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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:**

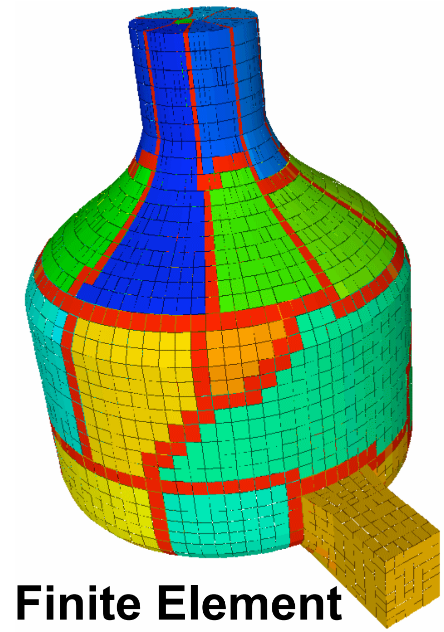
  Data redistribution volume

  + Application communication volume

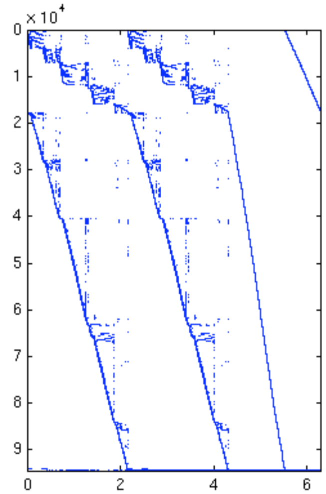
  Total communication volume
- **Data redistribution volume: callback returns data sizes.**
  - **Zoltan_Set_Fn(zz, ZOLTAN_OBJ_SIZE_MULTI_FN_TYPE, myObjSizeFn, 0);**
- **Application communication volume = Hyperedge cuts * Number of times the communication is done between repartitionings.**
  - **Zoltan_Set_Param(zz,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

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

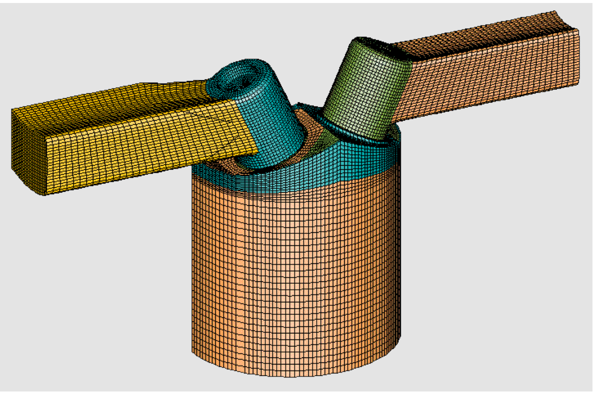
Hypergraph Applications



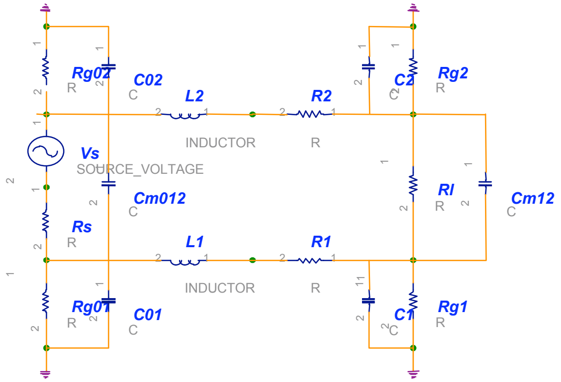
Finite Element Analysis



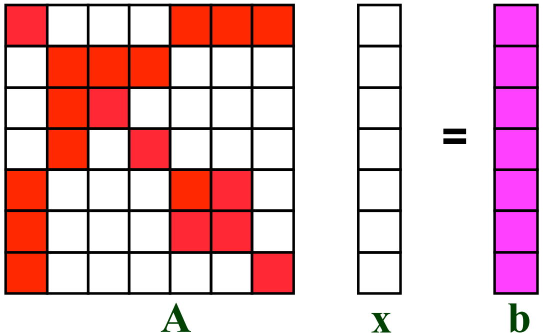
Linear programming for sensor placement



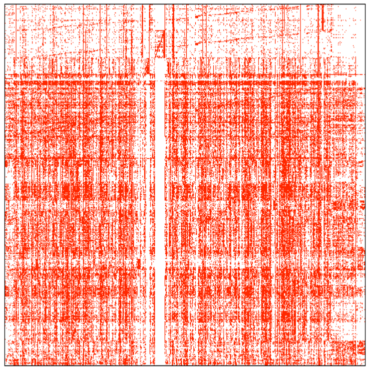
Multiphysics and multiphase simulations



Circuit Simulations



Linear solvers & preconditioners
(no restrictions on matrix structure)



Data Mining

Hypergraph Partitioning: Advantages and Disadvantages

- **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:**
  - Usually more expensive than graph partitioning.

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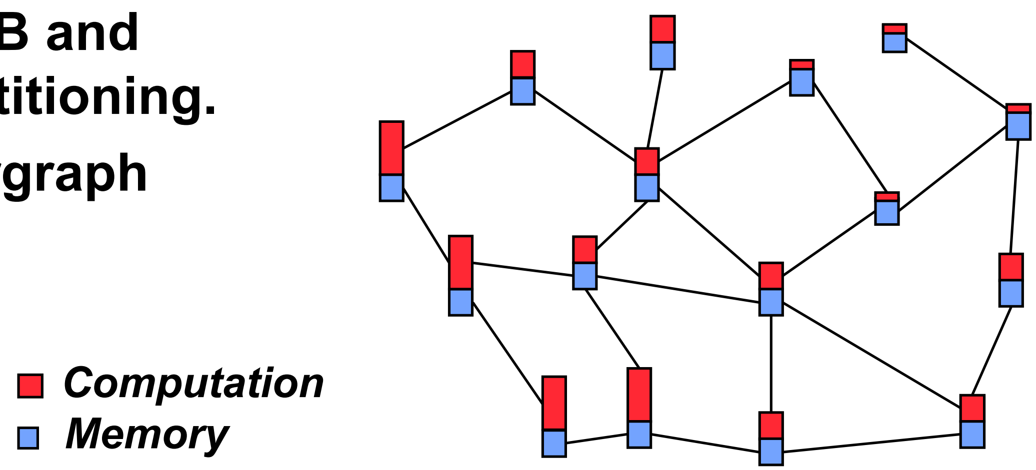
Multi-criteria Load-balancing

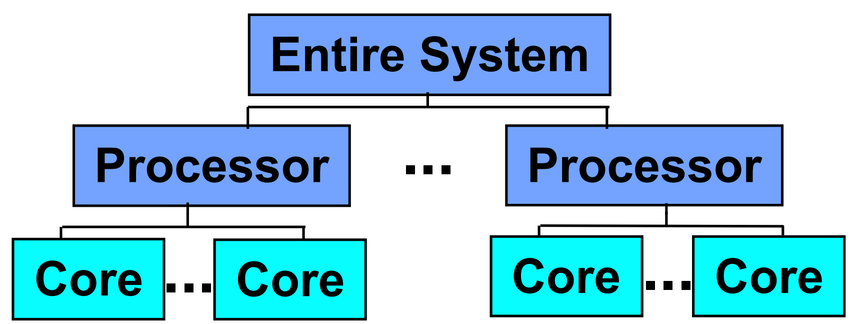
- Multiple constraints or objectives
  - Compute a single partition that is good with respect to multiple factors.
    - Balance both computation and memory.
    - Balance meshes in loosely coupled physics.
    - Balance multi-phase simulations.
  - Extend algorithms to multiple weights
    - Difficult. No guarantee good solution exists.
- Zoltan_Set_Param(zz, “OBJ_WEIGHT_DIM”, “2”);
  - Available in RCB, RIB and ParMETIS graph partitioning.
  - In progress in Hypergraph 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(…);**
    - **Note: Can use this function to specify part sizes for any purpose.**
- **Balance with respect to processor capacity.**

- **Hierarchical partitioning: Allows different partitioners at different architecture levels.**
  - **Zoltan_Set_Param(zz, "LB_METHOD", "HIER");**
  - **Requires three additional callbacks to describe architecture hierarchy.**
    - **ZOLTAN_HIER_NUM_LEVELS_FN**
    - **ZOLTAN_HIER_PARTITION_FN**
    - **ZOLTAN_HIER_METHOD_FN**



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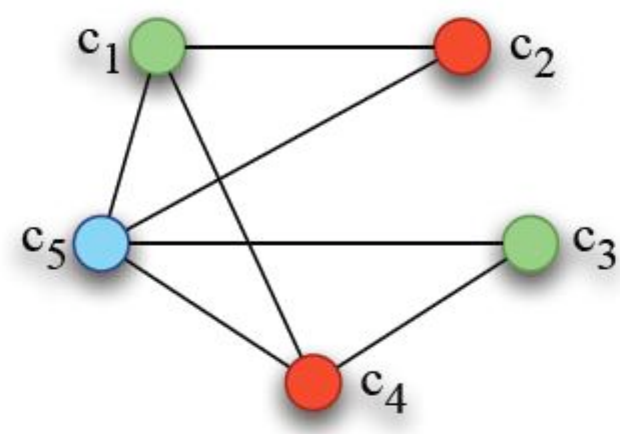
Graph Coloring

- **Problem:** Color the vertices of a graph with as few colors as possible such that no two adjacent vertices have the same color.
  - Distance-2: No vertices connected by a length-2 path have the same color
- **Applications**
  - Iterative sparse solvers
  - Preconditioners
  - Automatic differentiation
  - Sparse tiling



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'09* (in submission).**

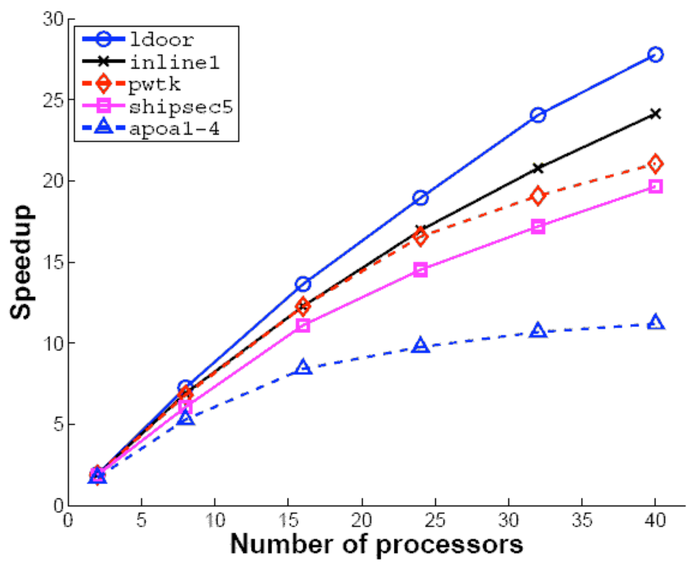
Coloring Interface in Zoltan

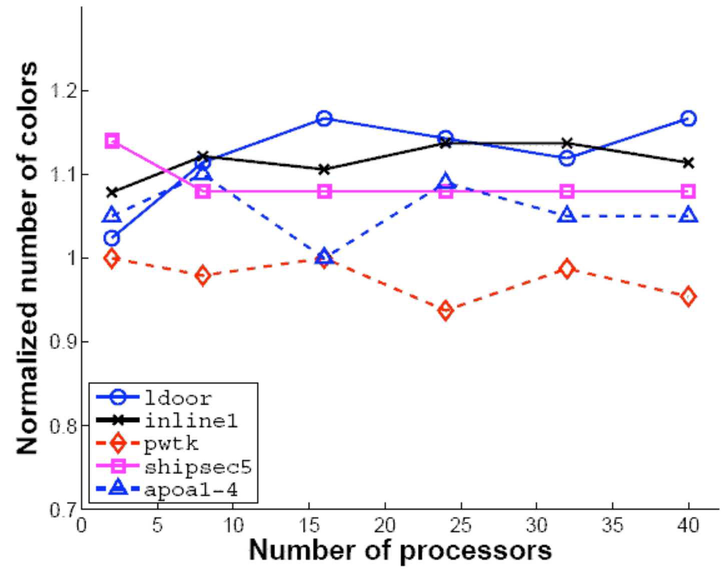
- Both distance-1 and distance-2 coloring routines are invoked by the Zoltan_Color function.
- Graph query functions required.
- The colors assigned to the objects are returned in an array of integers.

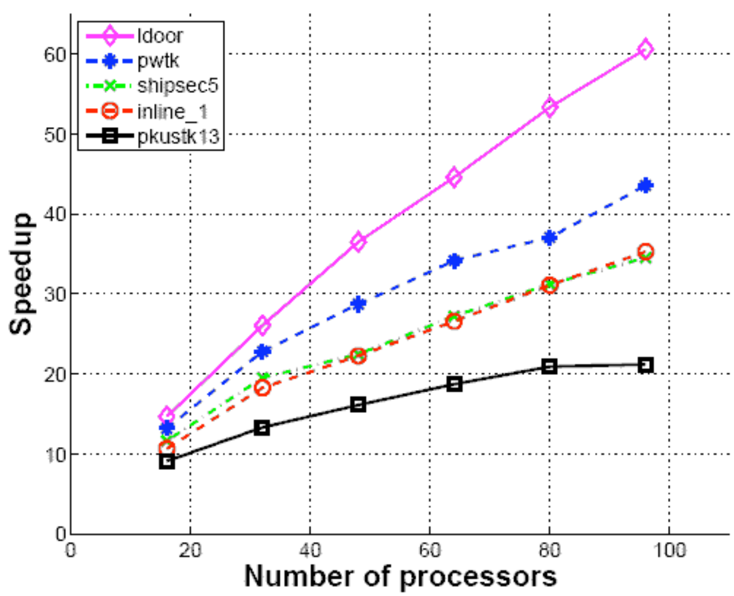
A Parallel Coloring Framework

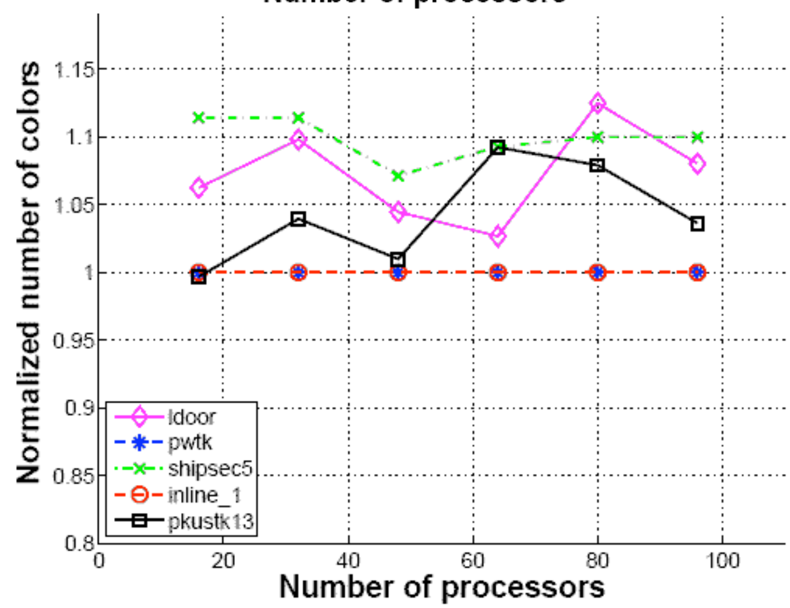
- Color vertices iteratively in rounds using a first fit strategy.
- Each round is broken into supersteps:
  - Color a certain number of vertices.
  - Exchange recent color information.
- Detect conflicts at the end of each round.
- Repeat until all vertices receive consistent colors.

Experimental Results



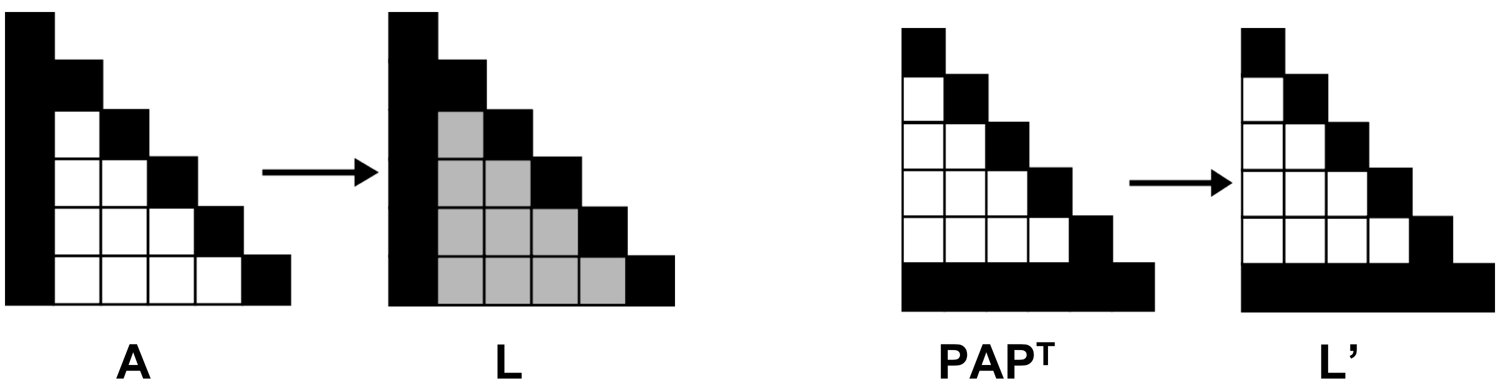






Sparse Matrix Ordering Problem

- Work and fill in sparse direct solvers (Cholesky, LU) depend on the matrix ordering.
  - Optimal ordering is NP-hard.
  - Many heuristics: Nested dissection, minimum degree, etc.
  - Nested dissection is preferred for parallel processing.



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Matrix ordering within Zoltan

- Computed by third party libraries:
  - ParMETIS
  - Scotch (actually PT-Scotch, the parallel part)
  - Easy to add another one.
- The calls to the external ordering library are transparent for the user. Thus Zoltan’s API can be a standard way to compute ordering.
- Native ordering in Zoltan planned.

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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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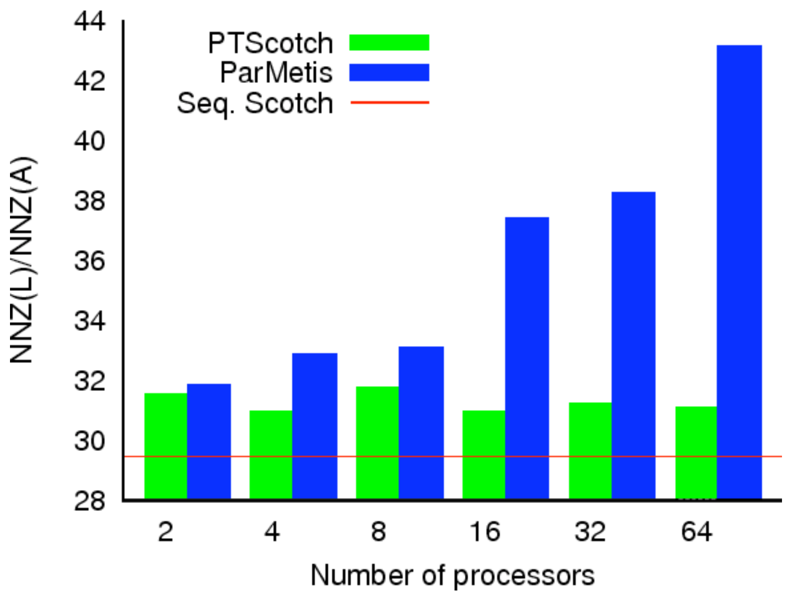
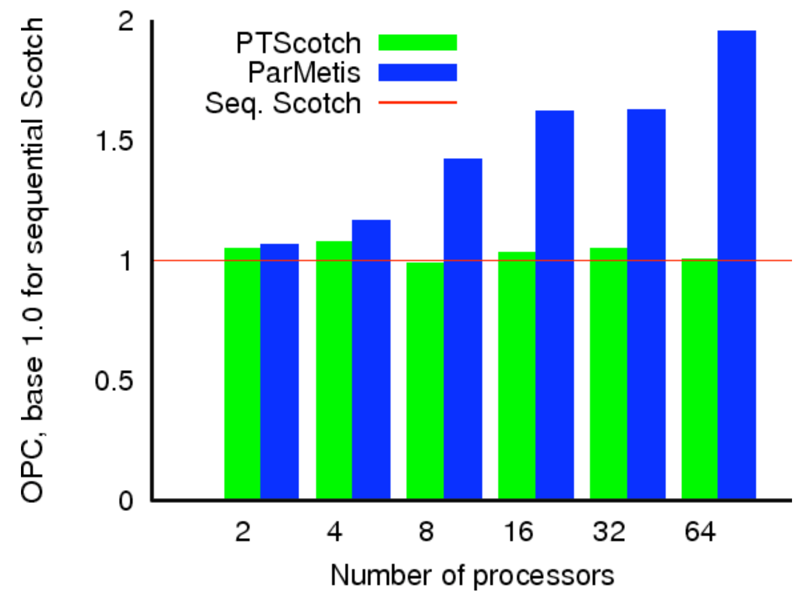
Comparison PT-Scotch vs ParMetis

Test case	Number of processes					
	2	4	8	16	32	64
audikw1						
O_{PTS}	**5.73E+12**	**5.65E+12**	**5.54E+12**	**5.45E+12**	**5.45E+12**	**5.45E+12**
O_{PM}	5.82E+12	6.37E+12	7.78E+12	8.88E+12	8.91E+12	1.07E+13
t_{PTS}	73.11	53.19	45.19	33.83	24.74	18.16
t_{PM}	32.69	23.09	17.15	9.80	5.65	3.82





Summary of Matrix Ordering

- Zoltan provides access to efficient parallel ordering for sparse matrices.
  - PT-Scotch gives best quality (but longer time).
- Zoltan provides a standard way to call parallel ordering.
- Zoltan will provide also its own ordering tool in the future, for non-symmetric problems.
  - HUND algorithm (talk by S. Donfack)

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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**

Alternate Interfaces to Zoltan

- C++ and F90 interfaces in Zoltan.
- Isorropia package in Trilinos solver toolkit.
  - Epetra Matrix interface to Zoltan partitioning.
    - B = Isorropia::Epetra::create_balanced_copy(A, params);
  - Trilinos v9 includes ordering and coloring interfaces in Isorropia (in addition to partitioning).
- ITAPS iMesh interface to Zoltan.
  - New iMeshP parallel mesh interface in progress.

Zoltan for CSC Developers

- Zoltan is an open-source project.
  - We welcome contributions from the CSC community!
  - Data-neutral interface makes it easy to integrate new packages as third-party libraries.
- Requirements for 3rd party software:
  - Open source
  - Written in C or C++
  - Library interface
- Talk to us if you may be interested!

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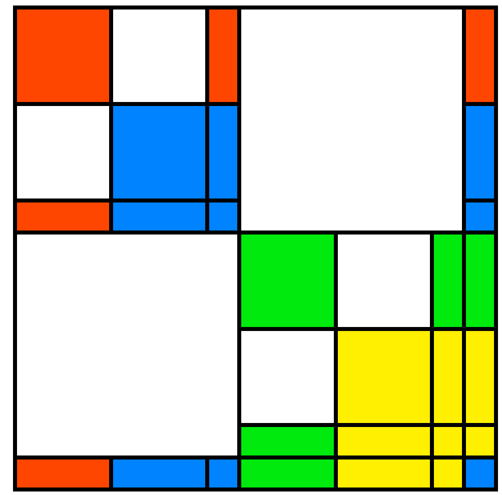
Current Work

- Two-dimensional matrix partitioning
  - Fine-grain hypergraph method
    - Catalyurek & Aykanat (2000)
  - Nested dissection matrix partitioning
    - Boman & Wolf (2008)
  - Will require Isorropia (Trilinos).
- Multi-criteria hypergraph partitioning
  - May be used for "checkerboard" matrix partitioning.
- Non-symmetric matrix ordering (HUND).
  - For sparse LU factorization.



Future Zoltan extensions

- May add support for:
  - Matching
    - MatchBox (Dobrian)
    - MatchBoxP (Halappanavar)
  - More coloring
    - ColPack (Gebremedhin)

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DEMO and HANDS ON!

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Demo: Mesh partitioning

- For a demo, we'll use the Zoltan test driver (zdrive).
- Zdrive reads data from a file and outputs a static partition.
  - Visualize the result with gnuplot.
- Designed for testing, not for users!
  - Code is ugly; do NOT use as example.
- Show mesh with different partitioning algorithms.
  - BLOCK, RCB, GRAPH, HYPERGRAPH

How to get Zoltan?

- A) Stand-alone:
  - Download tarball from Zoltan home page.
    - http://www.cs.sandia.gov/Zoltan
- B) As part of Trilinos:
  - Download from Trilinos web site (~35 packages).
    - http://trilinos.sandia.gov
  - Best if you want to use other Trilinos packages.
- You should already have Zoltan!
  - Just ‘cd zoltan’.

Configuring and Building Zoltan

- Create and enter the Zoltan directory.
  - tar xfz zoltan_distrib_v3.1.tar.gz
  - cd Zoltan
- Configure and make Zoltan library.
  - Currently two build systems:
    - Autotools (preferred)
    - Manual (fallback option if above fails…)
  - Create a build directory: mkdir BUILD
    - Zoltan allows multiple builds from same source.
  - cd BUILD; ../configure <options>
  - Then just type ‘make’!
    - make install

Example of configure script

```
../configure \
--prefix=/home/urmel/zoltan/BUILD \
--enable-mpi --with-mpi-compilers \
--with-parmetis \
--with-parmetis-incdir="/home/urmel/ParMETIS3_1" \
--with-parmetis-libdir="/home/urmel/ParMETIS3_1"
```

Tips:

- Remember to configure in your BUILD directory.
- Use --enable-mpi to build for parallel execution.
- Keep configure command in a script.
- See sample scripts in zoltan/SampleConfigureScripts.

How to run Zoltan?

- Recall Zoltan is “just” a library!
  - Run your app and call Zoltan.
- There is no “Hello World” for Zoltan. ☹
- Fairly simple examples in zoltan/example.
  - cd zoltan/example/C

SimpleRCB and SimpleGRAPH

- simpleRCB.c
  - Example of RCB on 5x5 regular mesh.
  - Objects to be partitioned are mesh nodes.
- simpleGRAPH.c
  - Same example, but use graph model.
- Each program has 5 phases:
  - Initialize.
  - Set parameters and callbacks.
  - Partition (call Zoltan).
  - Use the partition (e.g. move data).
  - Clean up.

simpleRCB.c: Initialization

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

/*
** Initialize application data.  In this example,
** we split a 5*5 mesh among processors, see simpleGraph.h
*/

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

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

Example zoltanRCB.c: Set Parameters and Callbacks

```
/* 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
   (defined in simpleQueries.h). */
Zoltan_Set_Num_Obj_Fn(zz, get_number_of_objects, NULL);
Zoltan_Set_Obj_List_Fn(zz, get_object_list, NULL);
Zoltan_Set_Num_Geom_Fn(zz, get_num_geometry, NULL);
Zoltan_Set_Geom_Multi_Fn(zz, get_geometry_list, NULL);
```

Example simpleRCB.c: Partitioning

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 simpleRCB.c: Use the Partition


```
  /* Process partitioning results;
  ** in this case, just print information;
  ** in a "real" application, migrate data here.
  */
  draw_partitions("initial distribution", ngids, gid_list, 1,
wgt_list, 0);
   ...
  /* update gid_flags from import/export  lists. */
   ...
  draw_partitions("new partitioning", nextIdx, gid_flags, 1,
wgt_list, 0);
```

Example simpleRCB.c: Cleanup


```
/* 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);

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

MPI_Finalize();
```

Compile and Run it!

- We could use autotooled makefiles.
- But let's do it "from scratch."
  - `mpicc simpleRCB.c –o simpleRCB -I/home/urmel/zoltan/BUILD/include/ -L/home/urmel/zoltan/BUILD/lib –lzoltan -L/home/urmel/ParMETIS3_1 -lparmetis -lmetis`
  - `mpirun –np 2 simpleRCB`

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

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 simpleRCB.c: ZOLTAN_NUM_OBJ_FN

```
/*****************************************************
 * Prototype: ZOLTAN_NUM_OBJ_FN
 * Return the number of objects I own.
 *****************************************************
 * Zoltan partitions a collection of objects distributed
 * across processes. In this example objects are vertices.
 * They are dealt out like cards based on process rank.
 */
static int get_number_of_objects(void *data, int *ierr)
{
int i, numobj=0;

  for (i=0; i<simpleNumVertices; i++){
    if (i % numProcs == myRank) numobj++;
  }

  *ierr = ZOLTAN_OK;

  return numobj;
}
```

Example simpleRCB.c: ZOLTAN_OBJ_LIST_FN

```
void get_object_list(void *userData,
                     int sizeGID, int sizeLID,
                     ZOLTAN_ID_PTR globalID,
                     ZOLTAN_ID_PTR localID,
                     int wgt_dim, float *obj_wgts,
                     int *err)
{
int i, next;
 if (sizeGID != 1){  /* My global IDs are 1 integer */
    *ierr = ZOLTAN_FATAL;
    return;
  }
  for (i=0, next=0; i<simpleNumVertices; i++){
    if (i % numProcs == myRank){
      globalID[next] = i+1;   /* application wide global ID */
      localID[next] = next;   /* process specific local ID  */
      obj_wgts[next] = (float)simpleNumEdges[i];  /* weight */
      next++;
    }
  }
  *ierr = ZOLTAN_OK;
  return;
}
```

Example simpleRCB.c: ZOLTAN_GEOM_MULTI_FN

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```
void get_geometry_list(void *data, int sizeGID, int sizeLID,
                      int num_obj,
             ZOLTAN_ID_PTR globalID, ZOLTAN_ID_PTR localID,
             int num_dim, double *geom_vec, int *ierr)
{
int i;
int row, col;

  for (i=0;  i < num_obj ; i++){
    row = (globalID[i] - 1) / 5;
    col = (globalID[i] - 1) % 5;

    geom_vec[2*i] = (double)col;
    geom_vec[2*i+1] = (double)row;
  }

  *ierr = ZOLTAN_OK;
  return;
}
```

Example: simpleGRAPH.c

- Same example, but now use graph partitioning.
- Changes needed:
  - Zoltan_Set_Param(zz, “LB_METHOD”, “GRAPH”);
  - Set method-specific parameters (optional).
  - Register graph call-back query functions.
  - Everything else stays the same!

For graph partitioning, coloring & ordering, use …

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.

Changing Partitioner of Same Type

- By default, “GRAPH” uses Zoltan’s native graph/hypergraph partitioner.
- To use ParMetis or Scotch:
  - Zoltan_Set_Param(zz, “GRAPH_PACKAGE", "PARMETIS");
  - Zoltan_Set_Param(zz, “GRAPH_PACKAGE", “SCOTCH");
  - Define third-party libraries at configure time.
- Single parameter to switch partitioner.
  - Try it!

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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:
  - zoltan-users@software.sandia.gov
  - {kddevin,ccheval,egboman}@sandia.gov
  - umit@bmi.osu.edu

The End

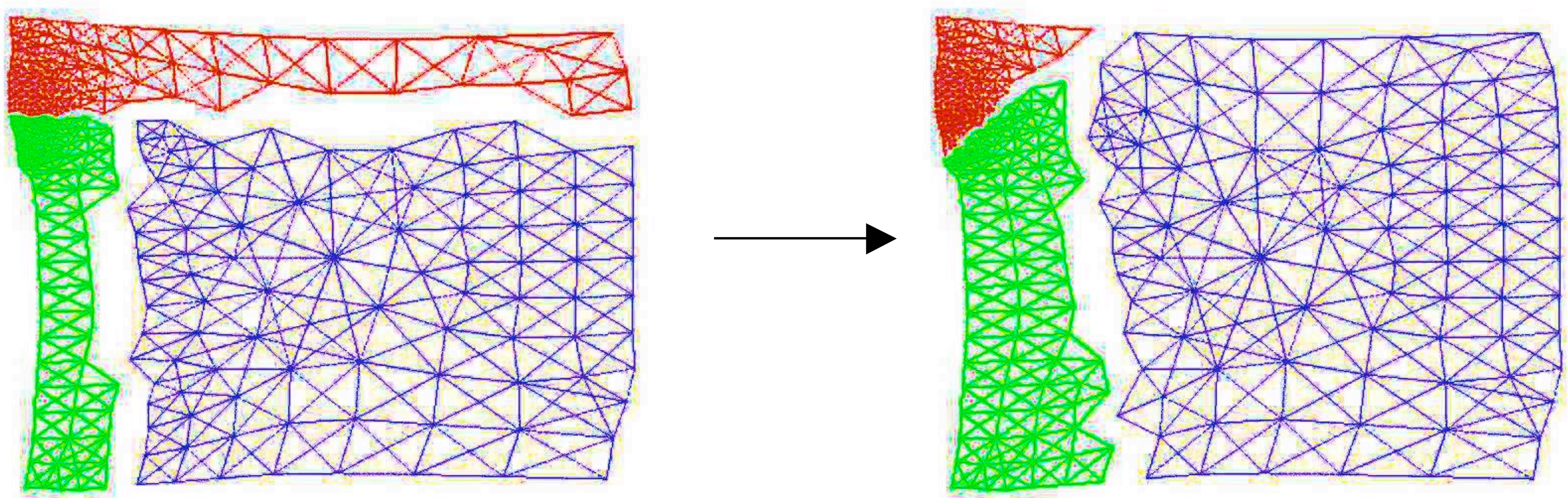
More Details on Query Functions

- 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)
```

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);
```

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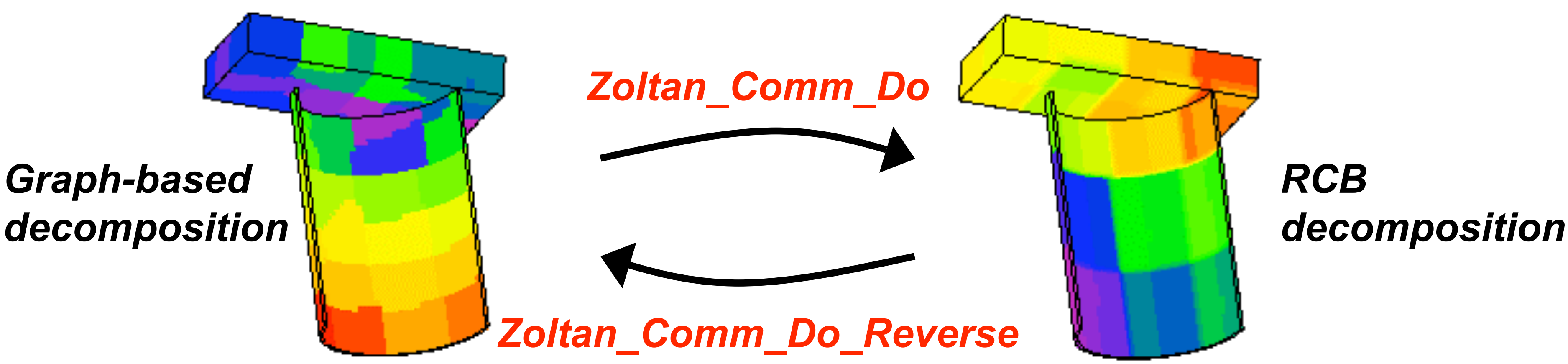
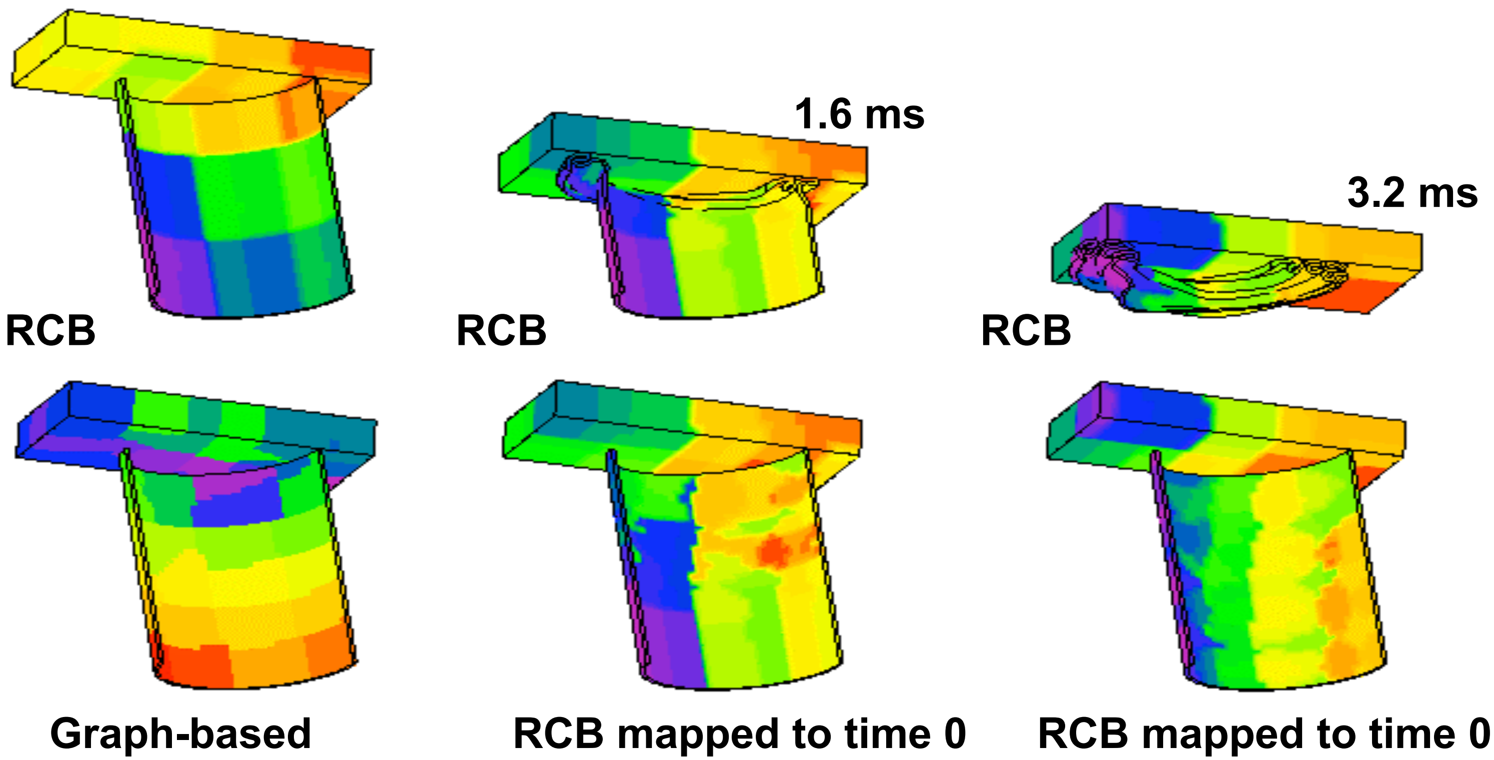
Zoltan Unstructured Communication Package

- 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.
  - Similar to BSP model.



Example Application: Crash Simulations

- **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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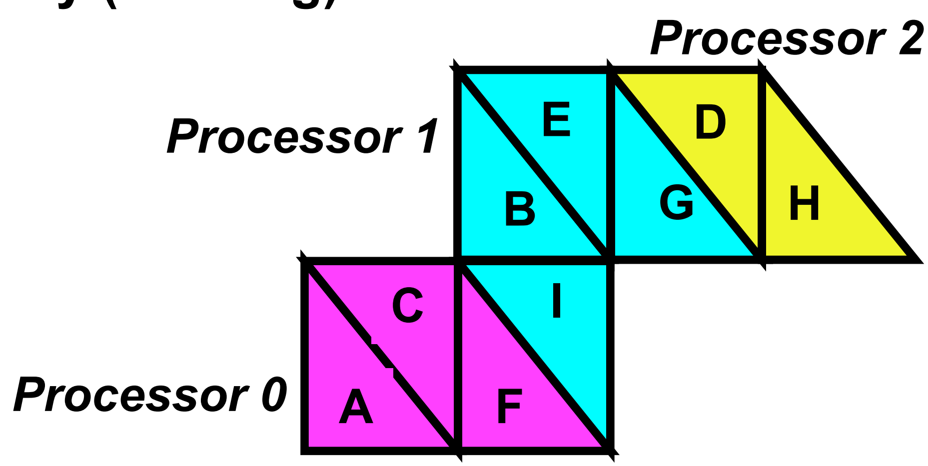
- Helps applications locate off-processor data.
  - Zoltan does not keep track of user data.
- Rendezvous algorithm (Pinar, 2001).
  - Directory distributed in known way (hashing) across processors.
  - Requests for object location sent to processor storing the object's directory entry.



Directory Index →
Location →

Directory Index	A	B	C
Location	0	1	0

Processor 0

Directory Index	D	E	F
Location	2	1	0

Processor 1

Directory Index	G	H	I
Location	1	2	1

Processor 2

For hypergraph partitioning and repartitioning, use …

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.

Or can use graph queries to build hypergraph.

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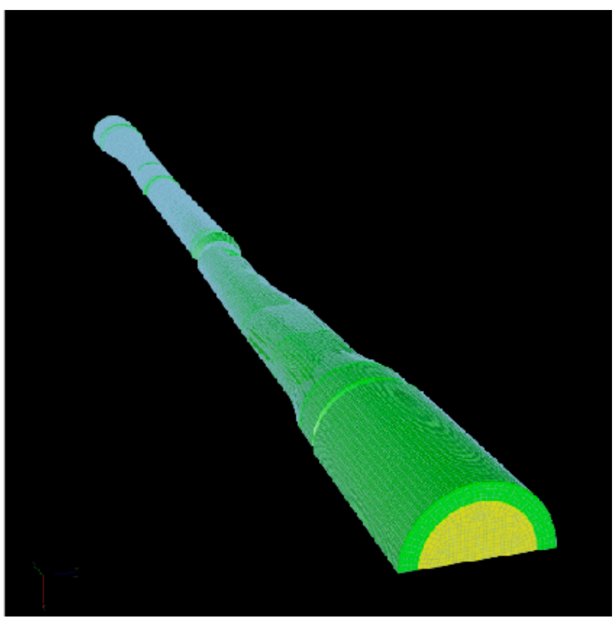
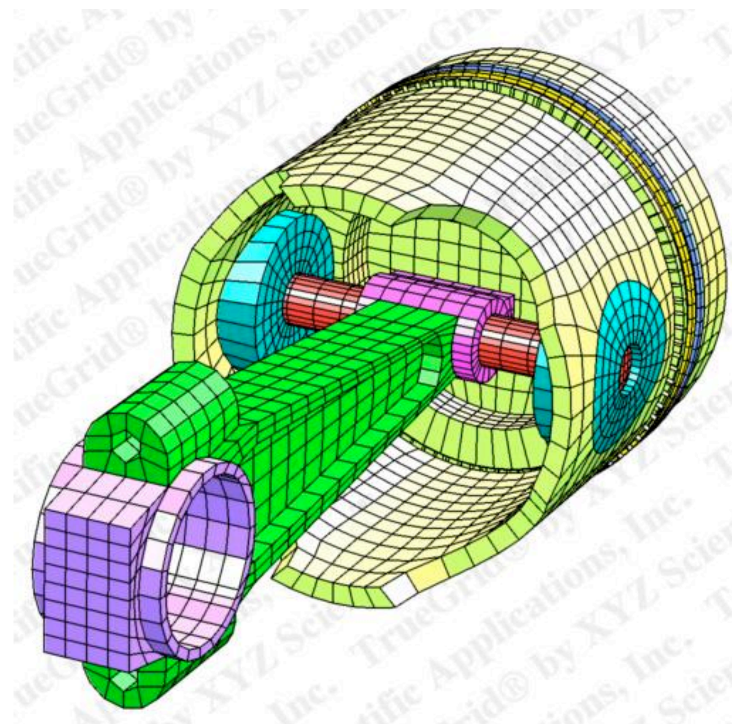
General Query Functions	
ZOLTAN_NUM_OBJ_FN	Number of items on processor
ZOLTAN_OBJ_LIST_FN	List of item IDs and weights.
Geometric Query Functions	
ZOLTAN_NUM_GEOM_FN	Dimensionality of domain.
ZOLTAN_GEOM_FN	Coordinates of items.
Hypergraph Query Functions	
ZOLTAN_HG_SIZE_CS_FN	Number of hyperedge pins.
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.

Variations on RCB : Recursive Inertial Bisection

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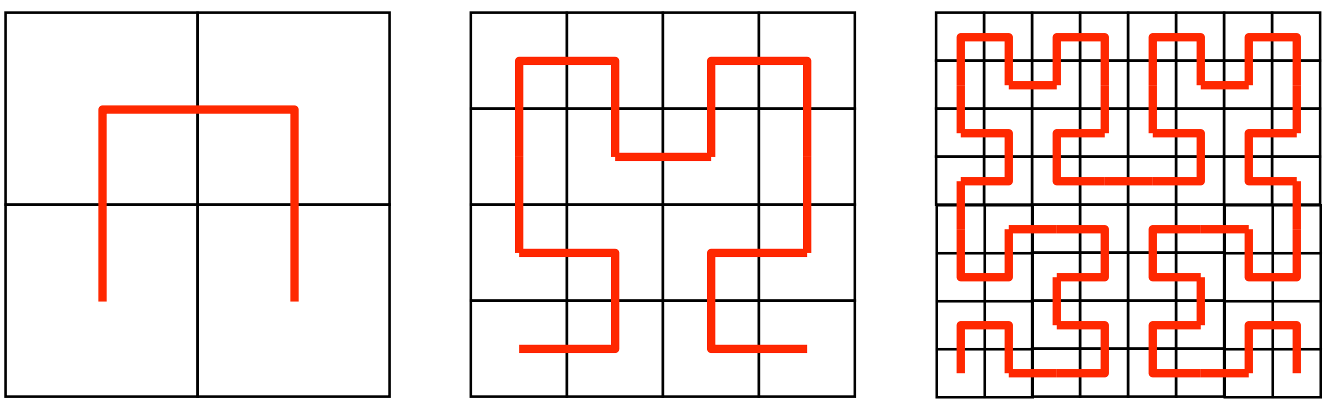
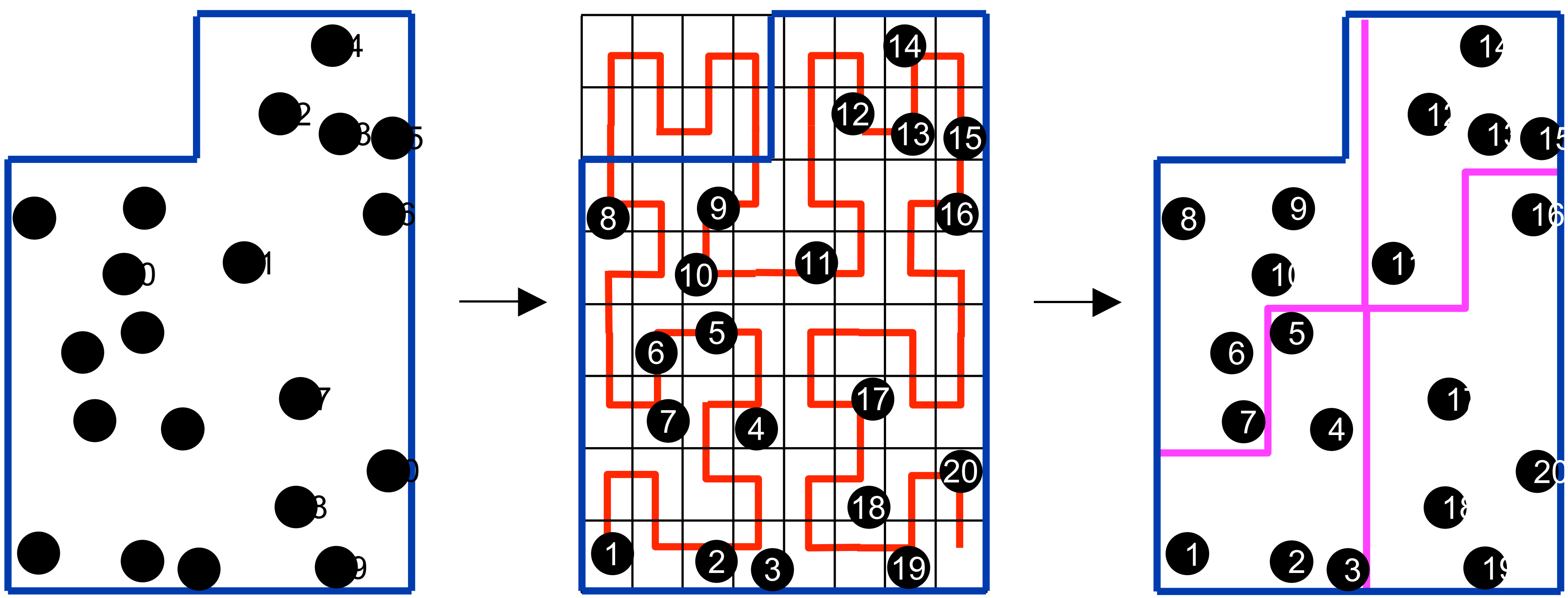
- Zoltan_Set_Param(zz, “LB_METHOD”, “HSFC”);
- Space-Filling Curve (Peano, 1890):
  - Mapping between R^3 to R^1 that completely fills a domain.
  - Applied recursively to obtain desired granularity.
- Used for partitioning by …
  - Warren and Salmon, 1993, gravitational simulations.
  - Pilkington and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



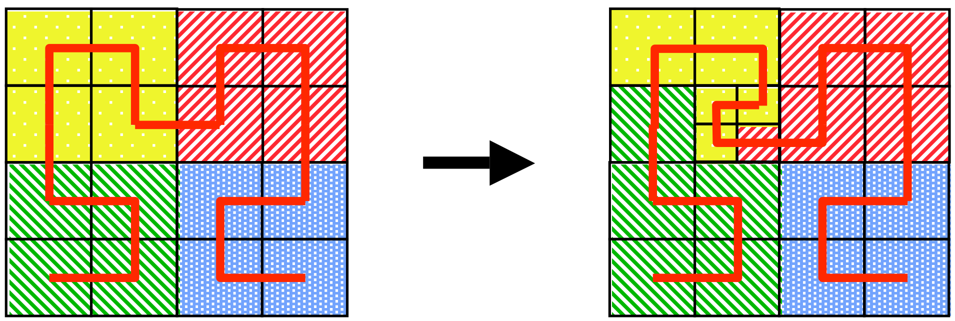
SFC Algorithm

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



SFC Advantages and Disadvantages

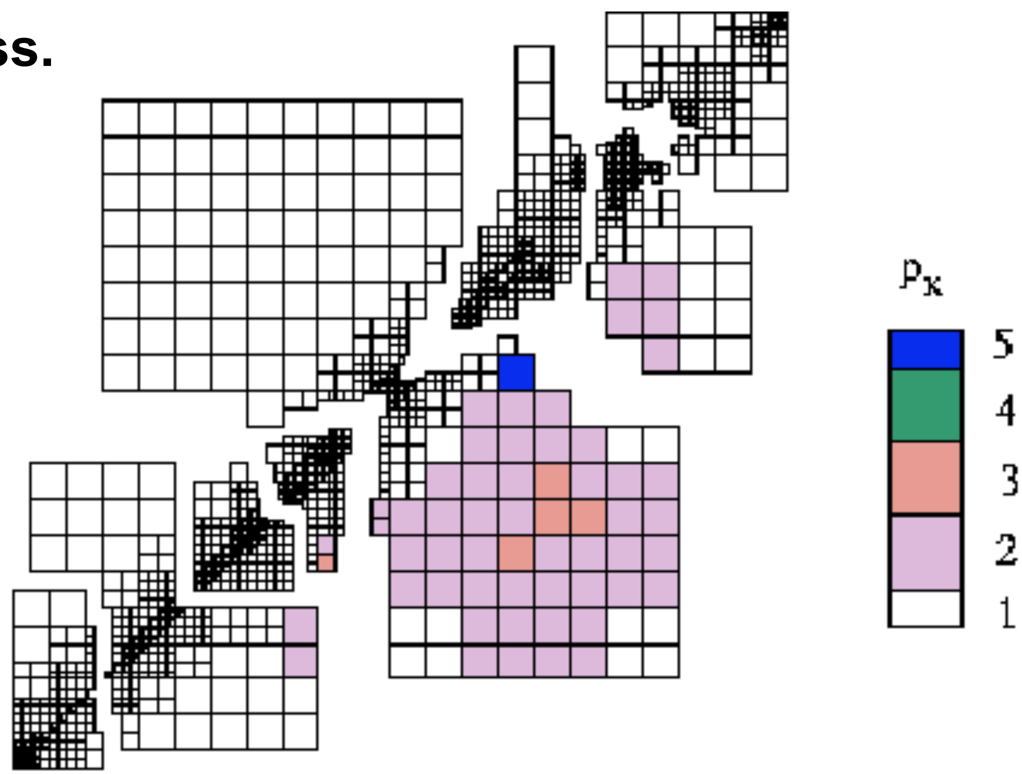
- **Advantages:**
  - Simple, fast, inexpensive.
  - Maintains geometric locality of objects in processors.
  - All processors can inexpensively know entire partition (e.g., for global search in contact detection).
  - Implicitly incremental for repartitioning.



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

Applications using SFC

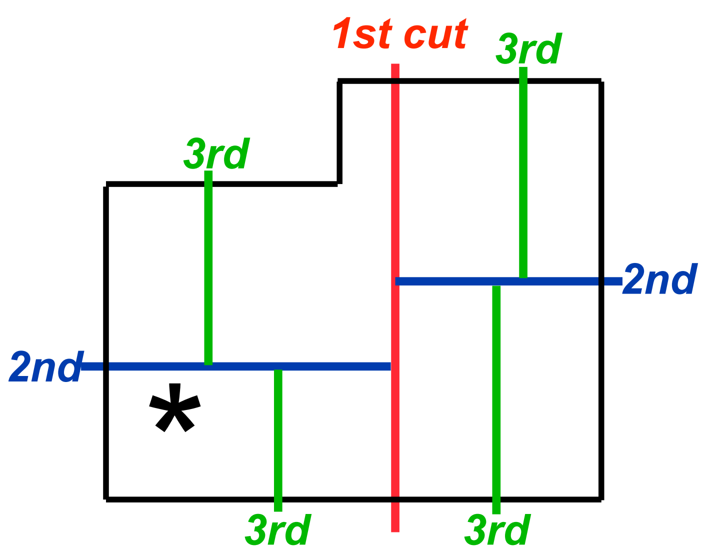
- **Adaptive hp-refinement finite element methods.**
  - **Assigns physically close elements to same processor.**
  - **Inexpensive; incremental; fast.**
  - **Linear ordering can be used to order elements for efficient memory access.**



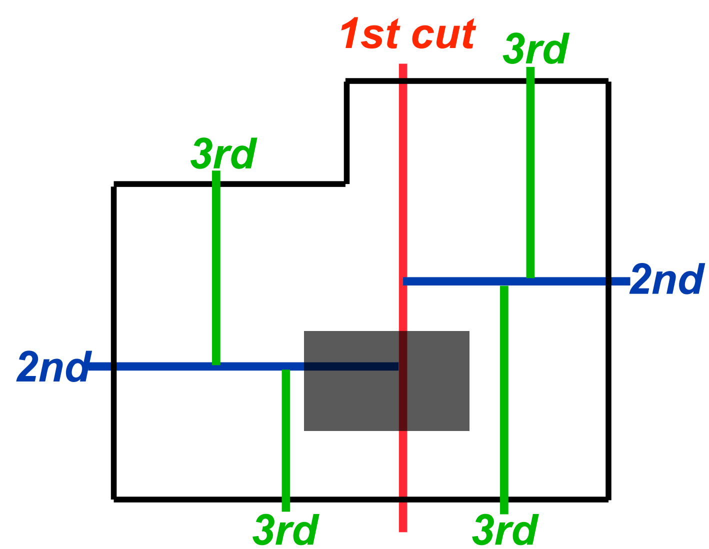
hp-refinement mesh; 8 processors. Patra, et al. (SUNY-Buffalo)

Auxiliary Capabilities for Geometric Methods

- Zoltan can store cuts from RCB, RIB, and HSFC inexpensively in each processor.
  - Zoltan_Set_Param(zz, “KEEP_CUTS”, “1”);
- Enables parallel geometric search without communication.
  - Useful for contact detection, particle methods, rendering.



Determine the part/processor owning region with a given point.
Zoltan_LB_Point_PP_Assign

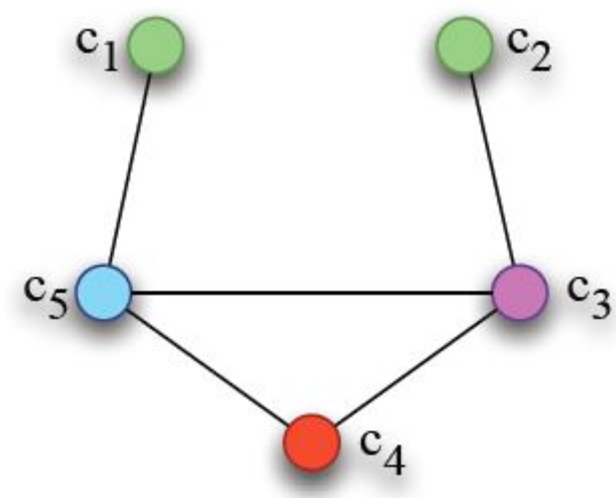


Determine all parts/processors overlapping a given region.
Zoltan_LB_Box_PP_Assign

Distance-2 Graph Coloring

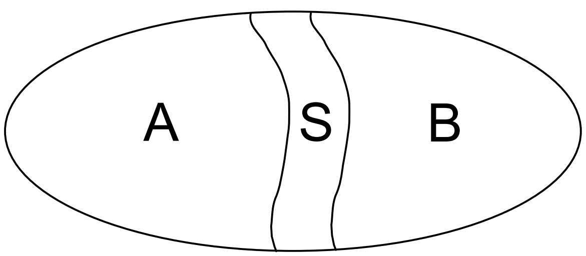
- **Problem (NP-hard)**
  Color the vertices of a graph with as few colors as possible such that a pair of vertices connected by a path on two or less edges receives different colors.

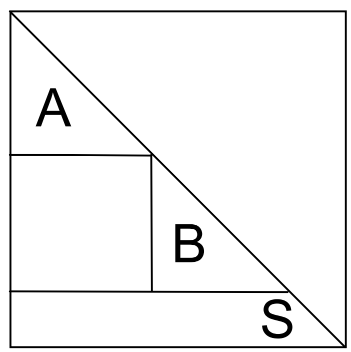
- **Applications**
  - **Derivative matrix computation in numerical optimization**
  - **Channel assignment**
  - **Facility location**
- **Related problems**
  - **Partial distance-2 coloring**
  - **Star coloring**

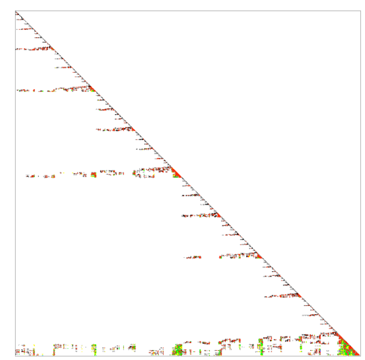


Nested dissection (1)

- 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.*



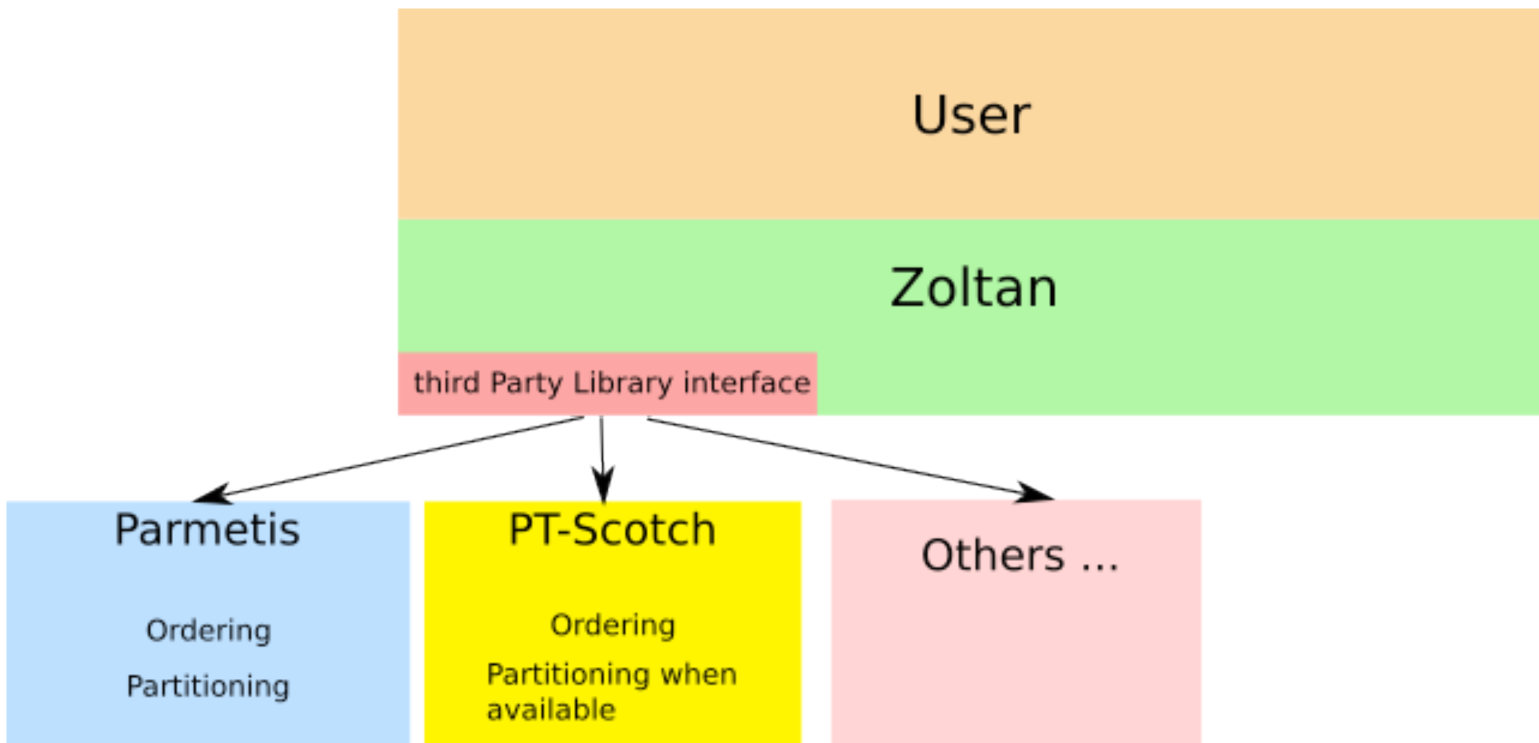




Nested dissection (2)

- **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.**
      - **The ordering itself can be computed in parallel.**

Zoltan ordering architecture



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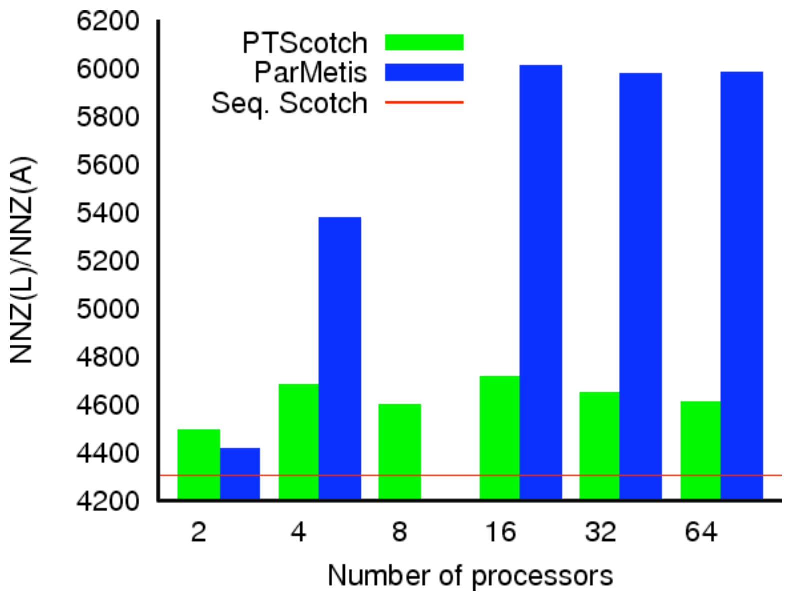
Experimental results (1)

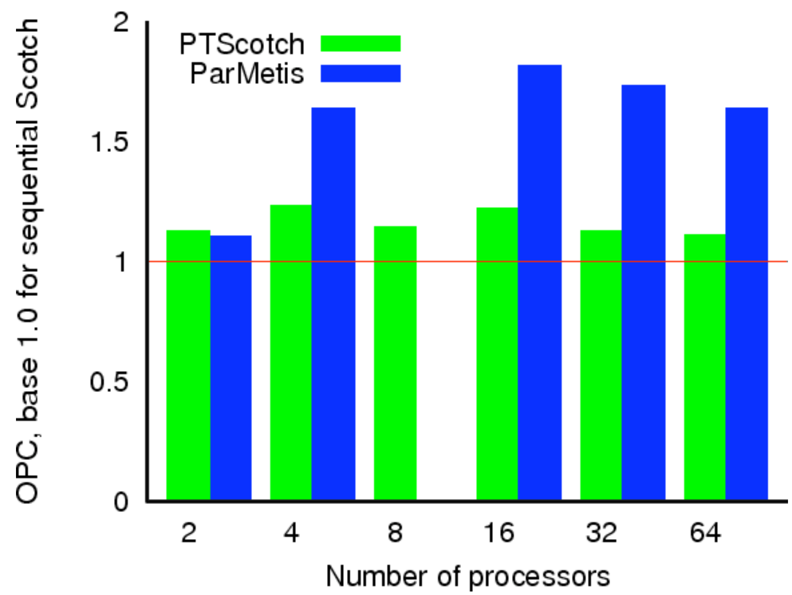
- Metric is OPC, the operation count of Cholesky factorization.
- Largest matrix ordered by PT-Scotch: 83 millions of unknowns on 256 processors (CEA/CESTA).
- Some of our largest test graphs.

Graph	Size (x1000)		Average degree	O_{SS}	Description
	|V|	|E|			
audikw1	944	38354	81.28	5.48E+12	3D mechanics mesh, Parasol
cage15	5154	47022	18.24	4.06E+16	DNA electrophoresis, UF
quimonda07	8613	29143	6.76	8.92E+10	Circuit simulation, Quimonda
23millions	23114	175686	7.6	1.29E+14	CEA/CESTA

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+16**
O_{PM}	**4.47E+16**	6.64E+16	†	7.36E+16	7.03E+16	6.64E+16
t_{PTS}	540.46	427.38	371.70	340.78	351.38	380.69
t_{PM}	195.93	117.77	†	40.30	22.56	17.83





Experimental results (4)

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

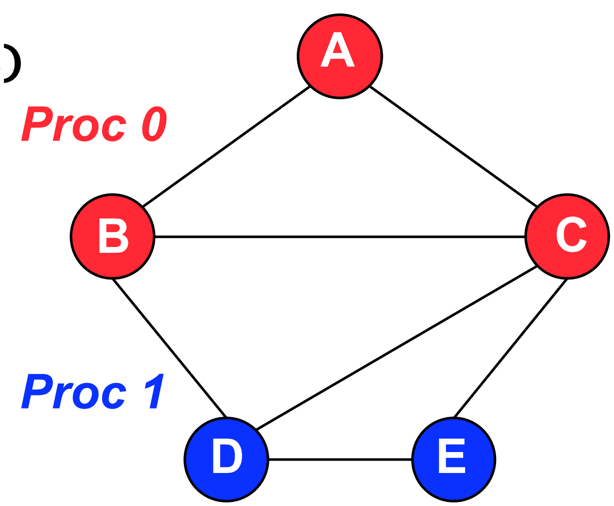
Test case	Number of processes					
	2	**4**	**8**	**16**	**32**	**64**
quimonda07						
O_{PTS}	-	-	**5.80E+10**	**6.38E+10**	**6.94E+10**	**7.70E+10**
t_{PTS}	-	-	34.68	22.23	17.30	16.62
23millions						
O_{PTS}	**1.45E+14**	**2.91E+14**	**3.99E+14**	**2.71E+14**	**1.94E+14**	**2.45E+14**
t_{PTS}	671.60	416.45	295.38	211.68	147.35	103.73

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
```

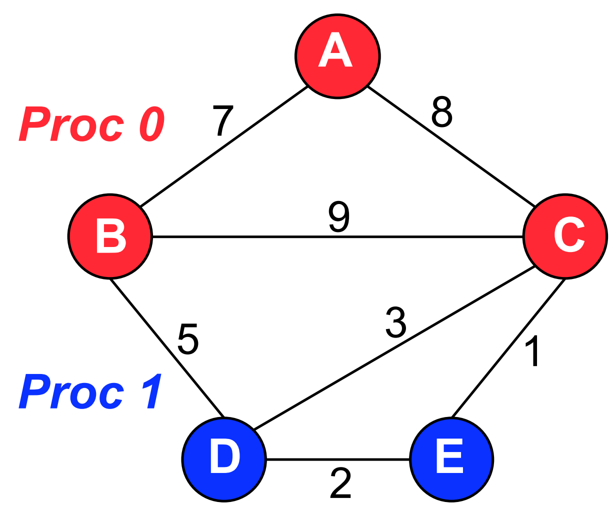


Example Graph Callbacks

```
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
```

Vertices

Hyperedges	Proc 0		Proc 1	
	A	B	C	D
a	X			X
b		X		X
c			X	X
d		X		X
e	X		X	X
f	X	X	X	X

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
```

	Vertices			
	Proc 0		Proc 1	
Hyperedges	A	B	C	D
a	X			X
b		X		X
c			X	X
d		X		X
e	X		X	X
f	X	X	X	X

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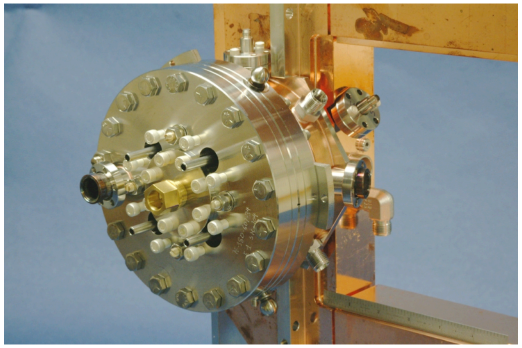
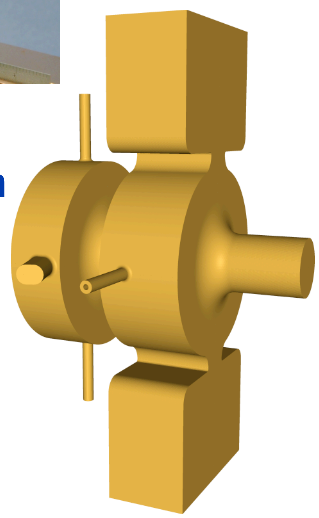
Performance Results

- 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.

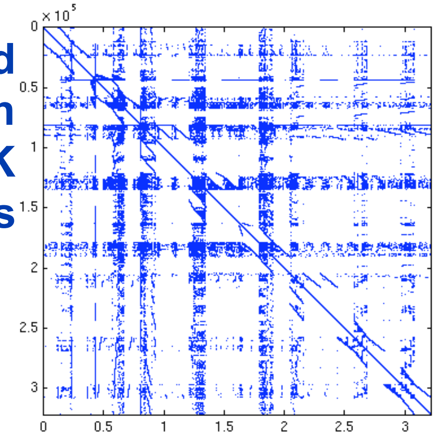
Test Data



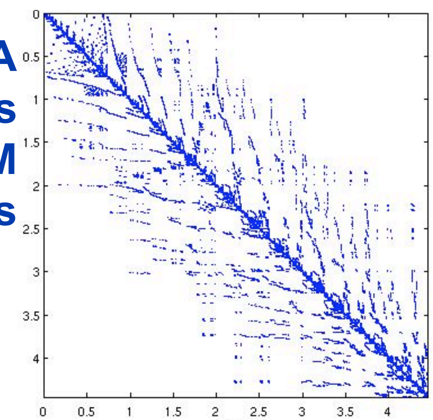


**SLAC *LCLS
Radio Frequency Gun
6.0M x 6.0M
23.4M nonzeros**

**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**

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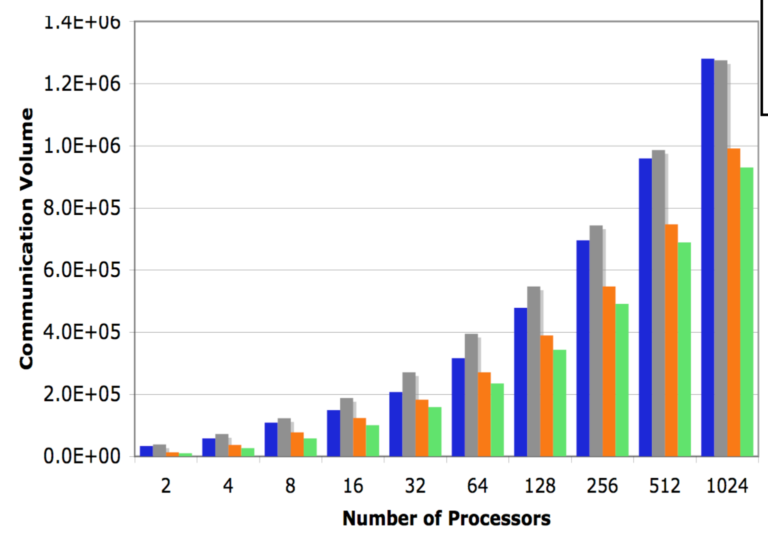
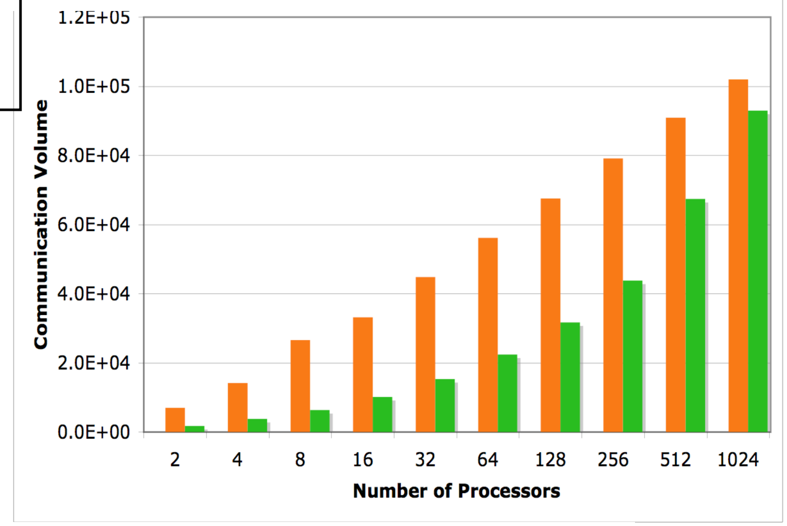
Communication Volume: Lower is Better

Number of parts = number of processors.

SLAC 6.0M LCLS

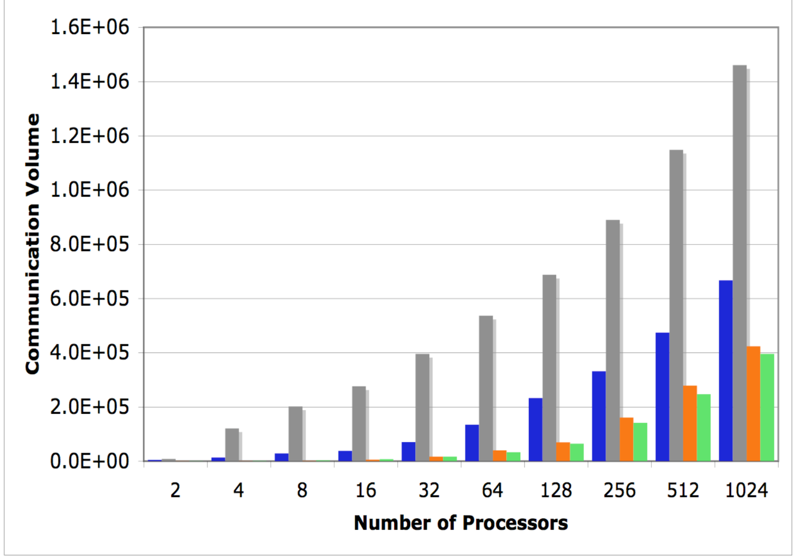


Xyce 680K circuit

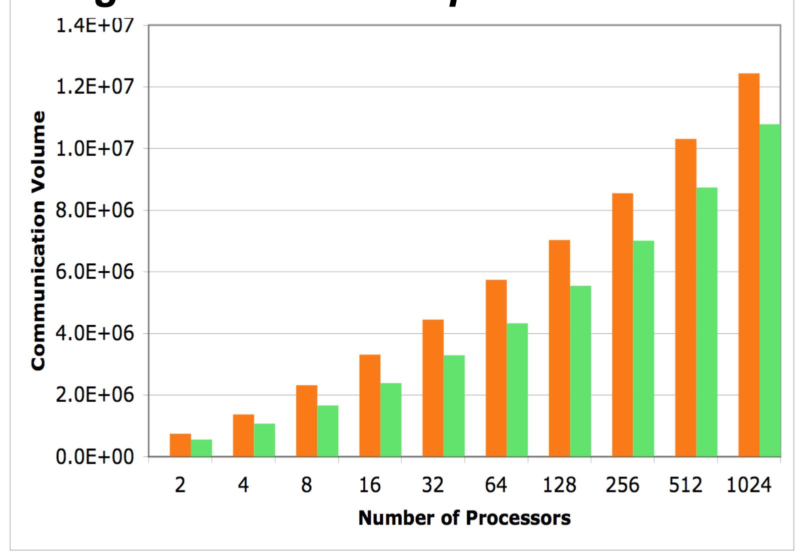


- RCB
- HSFC
- Graph
- Hypergraph

SLAC 2.9M Linear Accelerator

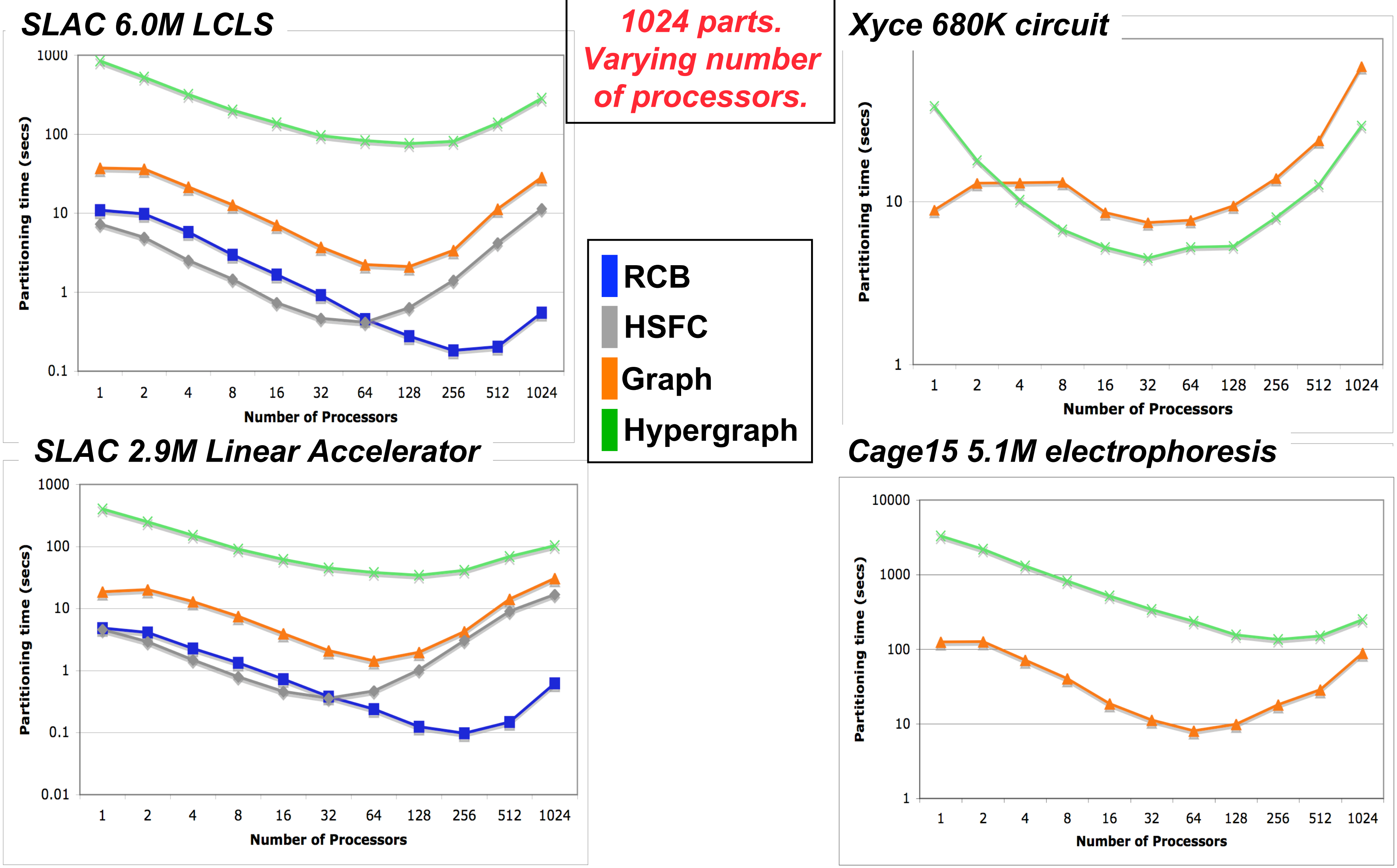


Cage15 5.1M electrophoresis



Partitioning Time: Lower is better

1024 parts. Varying number of processors.



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

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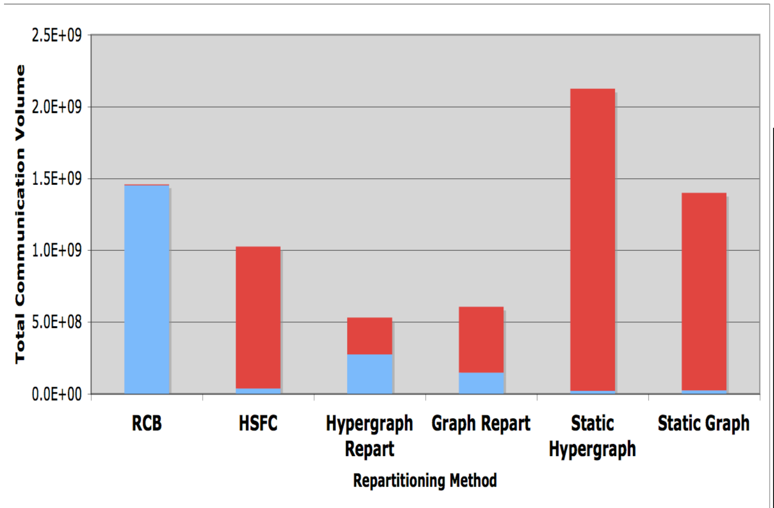
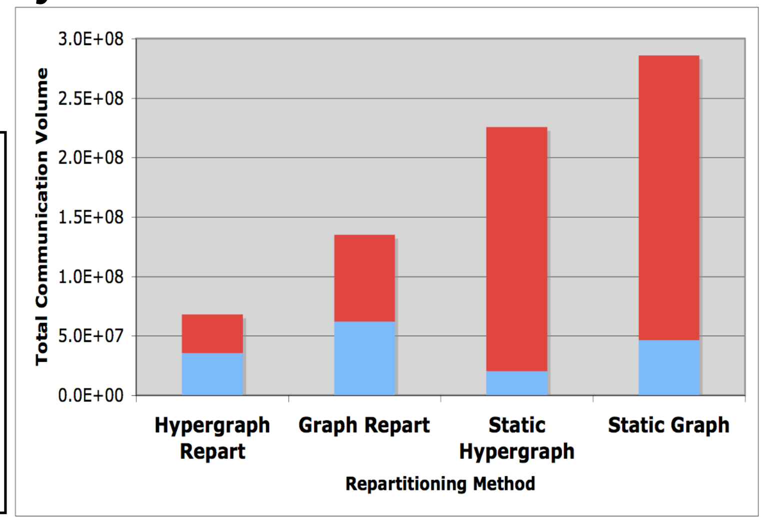
SLAC 6.0M LCLS

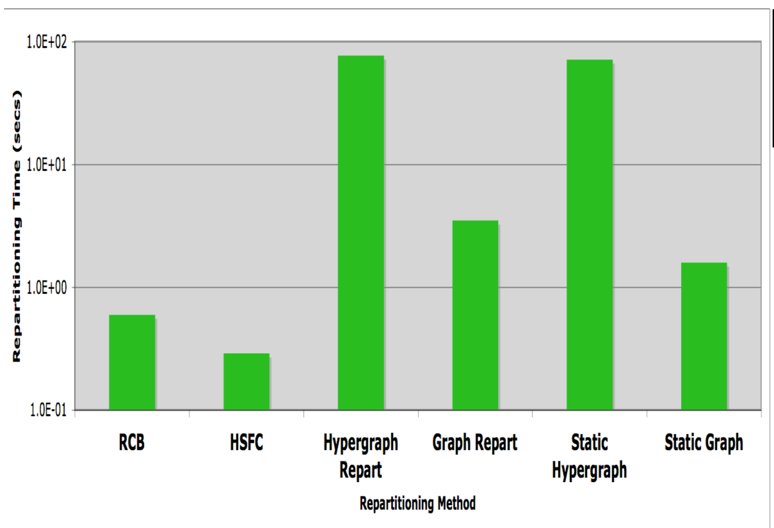


Data Redistribution Volume

Application Communication Volume

Xyce 680K circuit





Repartitioning Time (secs)