PT-Scotch in Solstice and beyond: where to go now

17/06/2010

INSTITUT NATIONAL
DE RECHERCHE
EN INFORMATIQUE
ET EN AUTOMATIQUE

INRIA

centre de recherche
BORDEAUX - SUD-OUEST

François Pellegrini

Sparse Day'10

Summary of the talk

- The Scotch project
- The multi-level framework and its parallelization
- Parallel static mapping
- Conclusion

The Scotch project

INSTITUT NATIONAL
DE RECHERCHE
EN INFORMATIQUE
ET EN AUTOMATIQUE

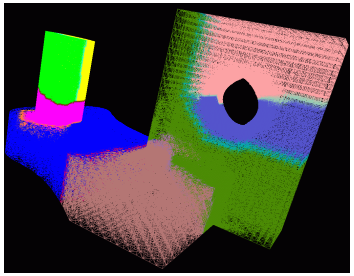
INRIA

centre de recherche
BORDEAUX - SUD-OUEST

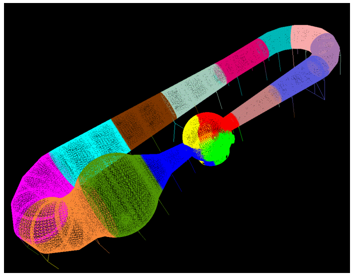
Graph partitioning (1)

- Graph partitioning is an ubiquitous technique which has proven useful in a wide number of application fields
  - Used to model domain-dependent optimization problems
  - “Good solutions” take the form of partitions which minimize vertex or edge cuts, while balancing the weight of graph parts
- NP-complete problem in the general case
- Many algorithms have been proposed in the literature :
  - Graph algorithms, evolutionary algorithms, spectral methods, linear optimization methods, …

Graph partitioning (2)



- Two main problems for our team :
  - Sparse matrix ordering for direct methods
  - Domain decomposition for iterative methods



- These problems can be modeled as graph partitioning problems on the adjacency graph of symmetric positive-definite matrices
  - Edge separator problem for domain decomposition
  - Vertex separator problem for sparse matrix ordering by nested dissection

The Scotch roadmap

- Devise robust parallel graph partitioning methods
  - Should handle graphs of more than a billion vertices distributed across one thousand processors
- Improve sequential graph partitioning methods if possible
  - Multi-level FM-like algorithms are both fast and efficient on a very large class of graphs but FM algorithms are intrinsically sequential
- Investigate alternate graph models (meshes/hypergraphs)
- Provide a software toolbox for scientific applications
  - Scotch sequential software tools
  - PT-Scotch parallel software tools

Design constraints

- Parallel algorithms have to be carefully designed
  - Algorithms for distributed memory machines
  - Preserve independence between the number of parts k and the number of processing elements P on which algorithms are to be executed
  - Algorithms must be “quasi-linear” in |V| and / or |E|
  - Constants should be kept small !
    - Theory is not likely to help much...
- Data structures must be scalable :
  - In |V| and/or |E| : graph data must not be duplicated
  - In P and k : arrays in k|V| , k^2, kP, P|V| or P^2 are forbidden

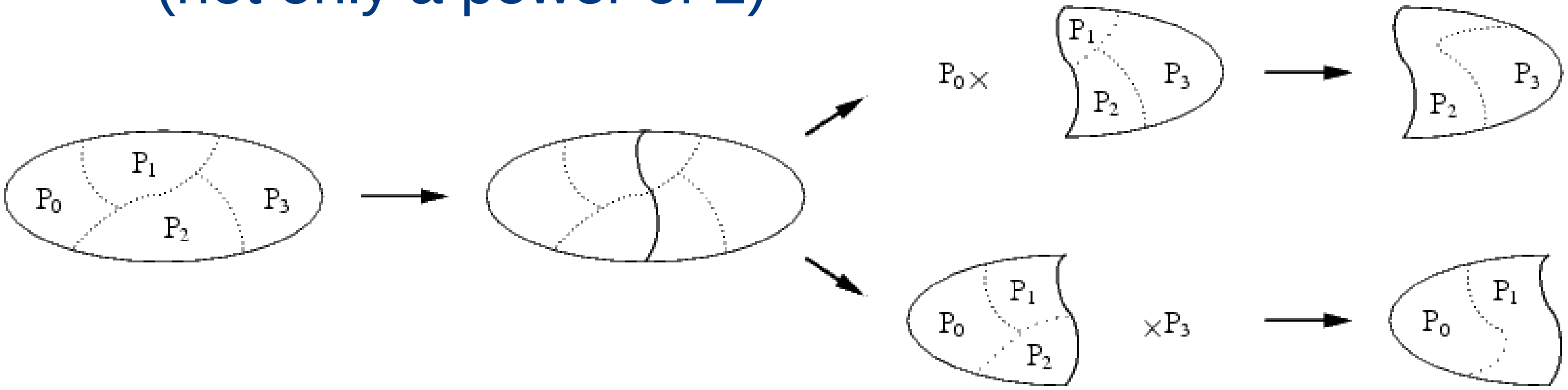
The multi-level framework and its parallelization

From k-partitioning to recursive bipartitioning

- *K*-way graph partitioning can be approximated by a sequence of recursive bipartitionings
  - Bipartitioning is easier to implement than *k*-way partitioning
    - No need to choose the destination part of vertices
- It is only an approximation, but a rather good one [Simon & Teng, 1993]

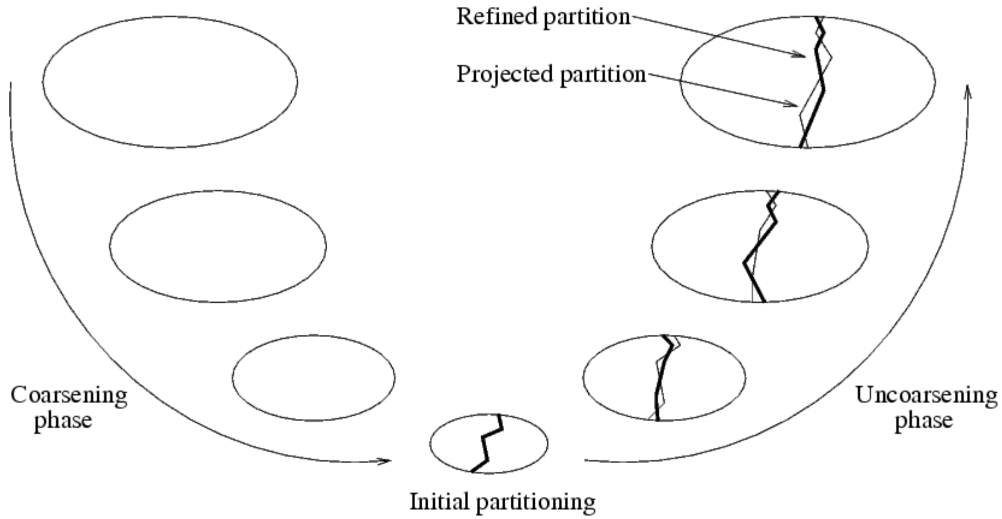
Recursive bipartitioning in parallel

- After a separator has been computed, the two separated subgraphs are folded and redistributed each on a half of the available processors
  - All subgraphs at a same level are processed concurrently on separate subsets of processors
  - Ability to fold a graph on any number of processors (not only a power of 2)



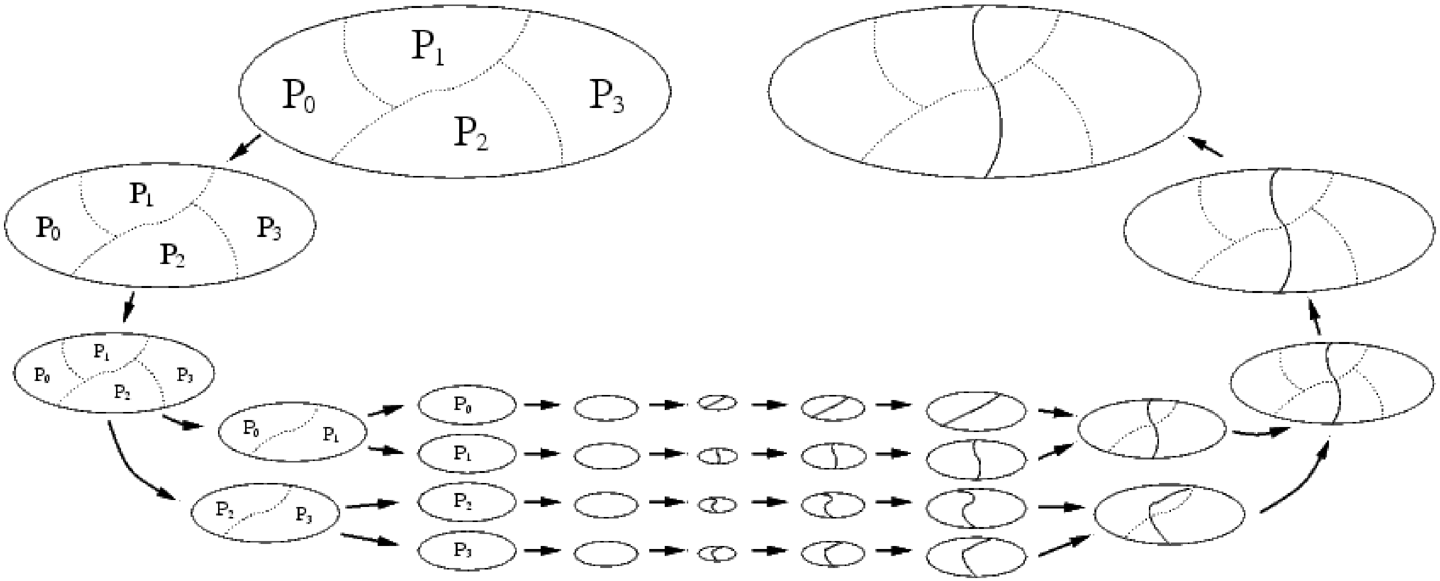
Multi-level framework

- Principle [Hendrickson & Leland, 1994]
  - Create a family of topologically equivalent coarser graphs by clustering groups of vertices
  - Compute an initial partition of the smallest graph
  - Propagate back the result, with local refinement



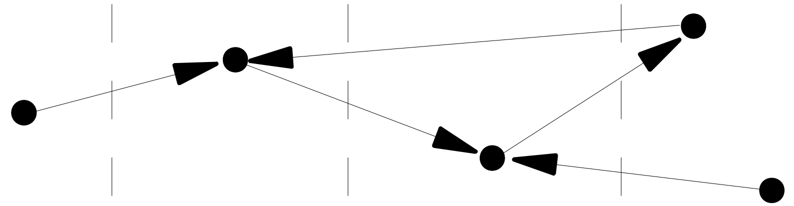
Coarsening in parallel

- The coarsened graph can either be:
  - Kept on the same number of processors: decreases memory and processing cost
  - Folded and duplicated on two subsets of processors: increases quality but also cost



Parallel matching

- Parallel coarsening bases on parallel matching
  - These matchings do not need to be maximal
- Synchronization between non-local neighbors is critical
  - Dependency chains or loops between mating requests can stall the whole algorithm because of sequential constraints



- Some distributed tie-breaking is required
- Too many requests decrease matching probability

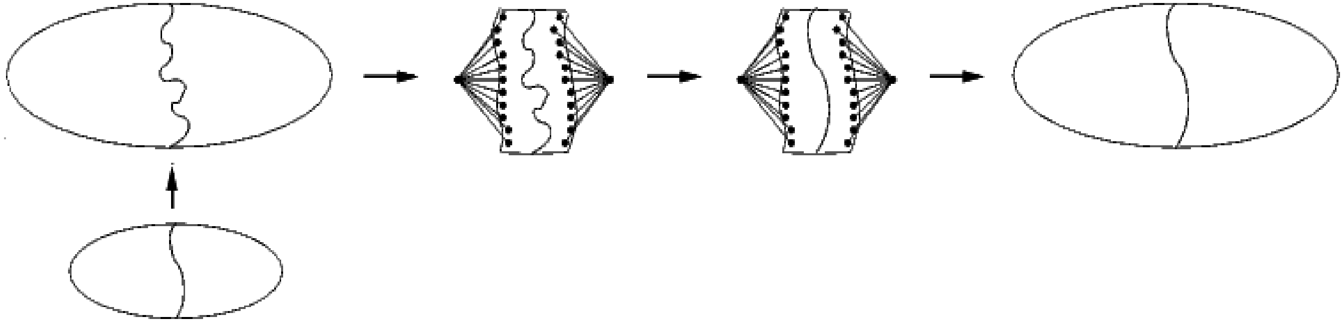
Parallel probabilistic matching

- Principle [Chevalier, 2007]
  - Do not discriminate between local and non-local neighbors when selecting a neighbor for mating
  - Vertices request for matings with their neighbors (whether local or remote) with a prescribed probability
- Reduces topological biases and converges quickly
  - 5 collective passes are enough to match 80 % of the vertices on average

Pass	Matching		Coarsening	
	Avg.	M.a.d.	Avg.	M.a.d.
C1	53.3	12.3	50.4	0.7
C2	68.7	13.6	51.6	2.2
C3	76.2	12.2	52.5	3.3
C4	81.0	10.6	53.2	4.0
C5	84.5	9.1	53.7	4.5
LF	100.0	0.0	59.4	6.8

Band graphs

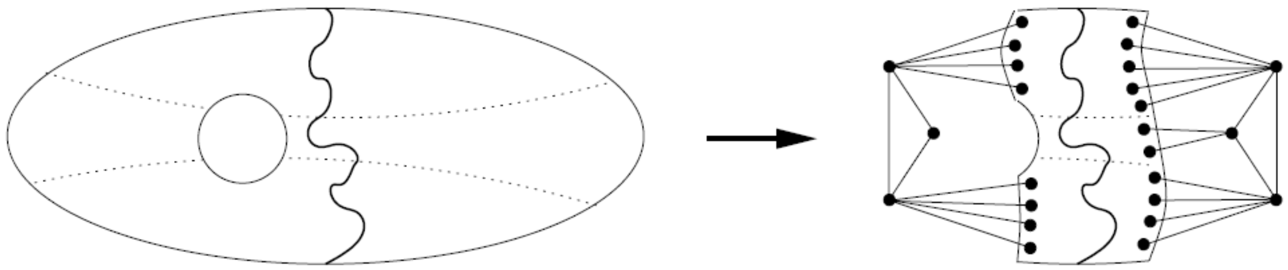
- Principle [Chevalier & Pellegrini, 2006]
  - Only local improvements along the projected cut are necessary, so work only on a small band around the cut



- Reduce problem space dramatically
  - Allow one to use expensive algorithms, such as genetic algorithms

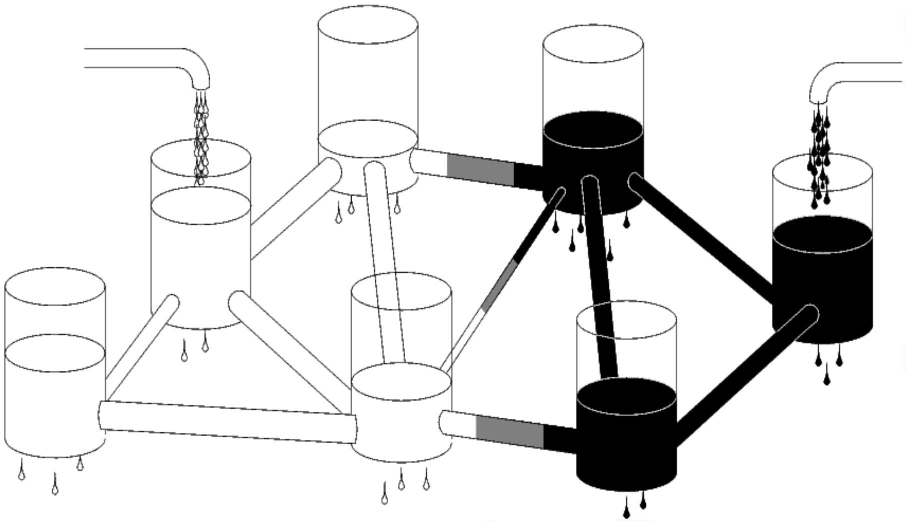
Band graphs in parallel

- Anchor vertices may have very high degrees compared to sequential band graphs
  - Two anchor vertices per process
  - Remote anchor vertices for each part form a clique
    - Will soon be a hypercube to accommodate for large numbers of processes



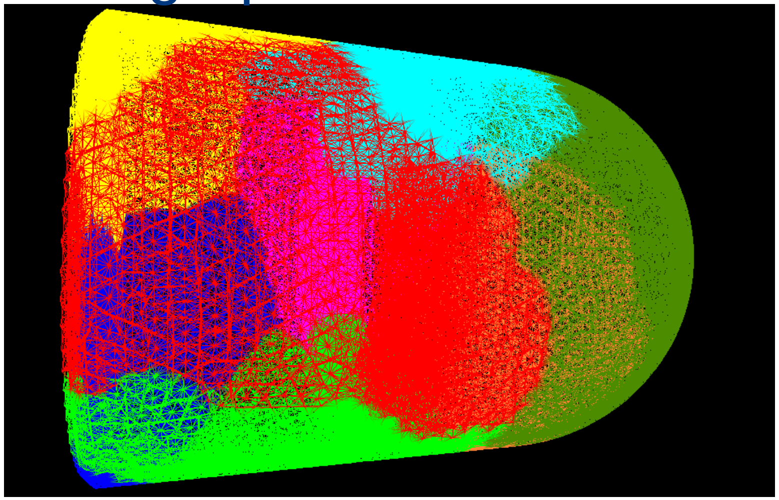
Jug of the Danaides (1)

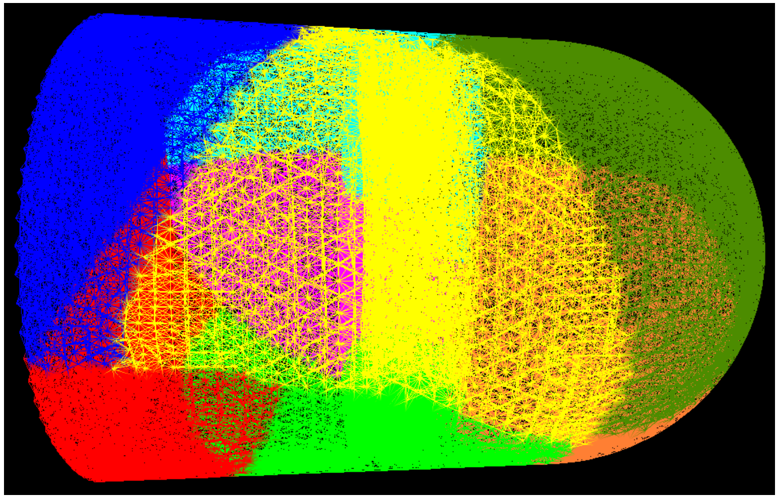
- Principle [Pellegrini, 2007]
  - Analogous to “bubble growing” algorithms but natively integrates the load balancing constraint
  - The graph is modeled as a set of leaking barrels and pipes
  - Two antagonistic liquids flow from two source vertices
  - Liquids vanish when they meet



Jug of the Danaides (2)

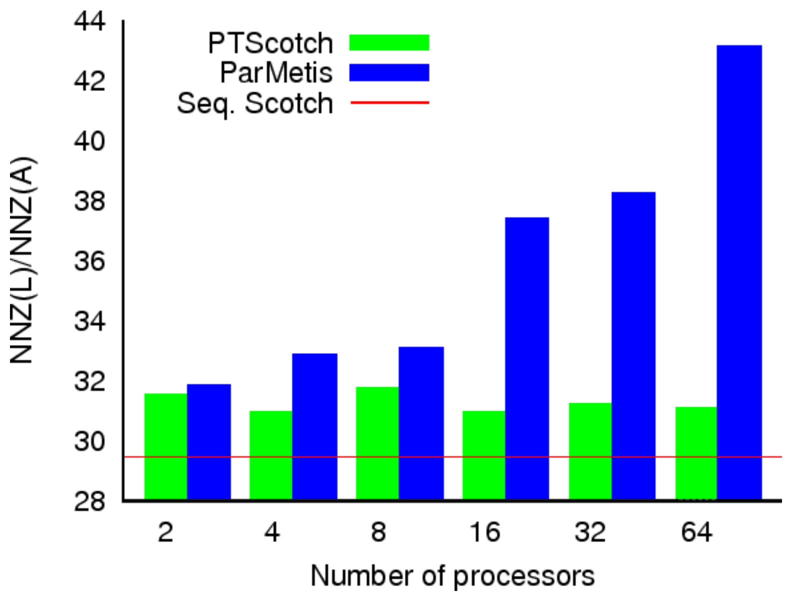
- Using JotD as the refinement algorithm in the multi-level process :
  - Yields mooth interfaces
  - Is slower than sequential FM (20 times for 500 iterations, but only 3 times for 40 iterations)
- Band graph anchor vertices used as source vertices

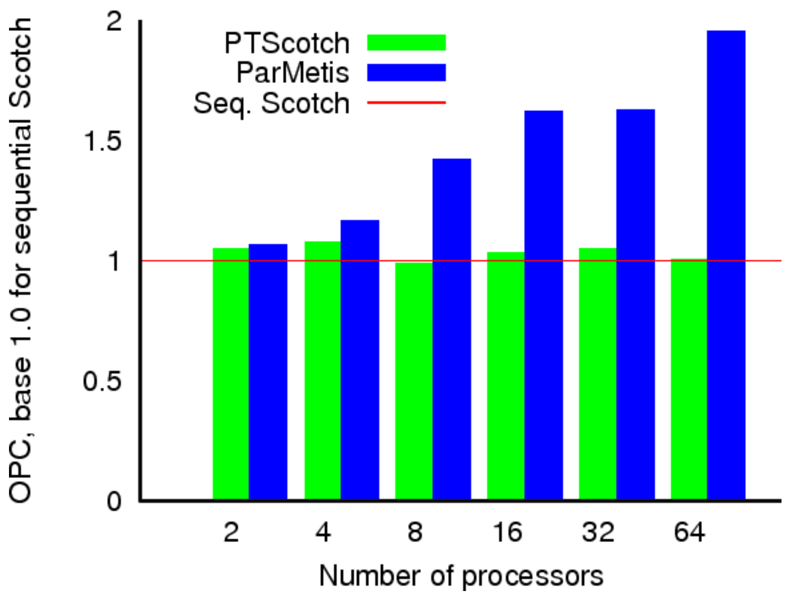




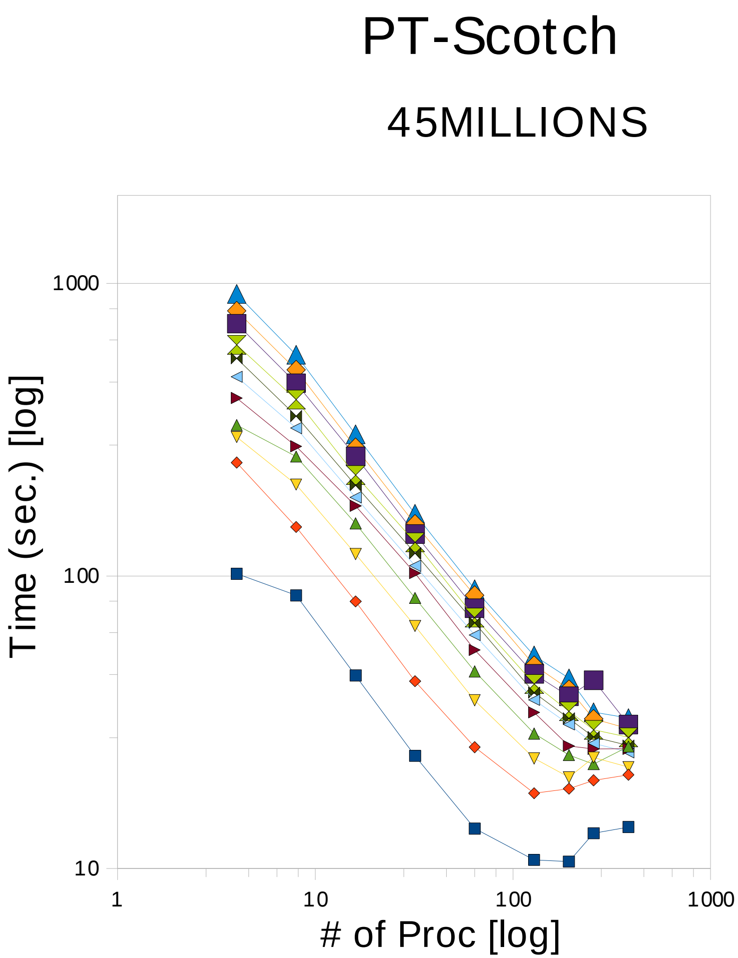
Runtime and sparse matrix ordering quality

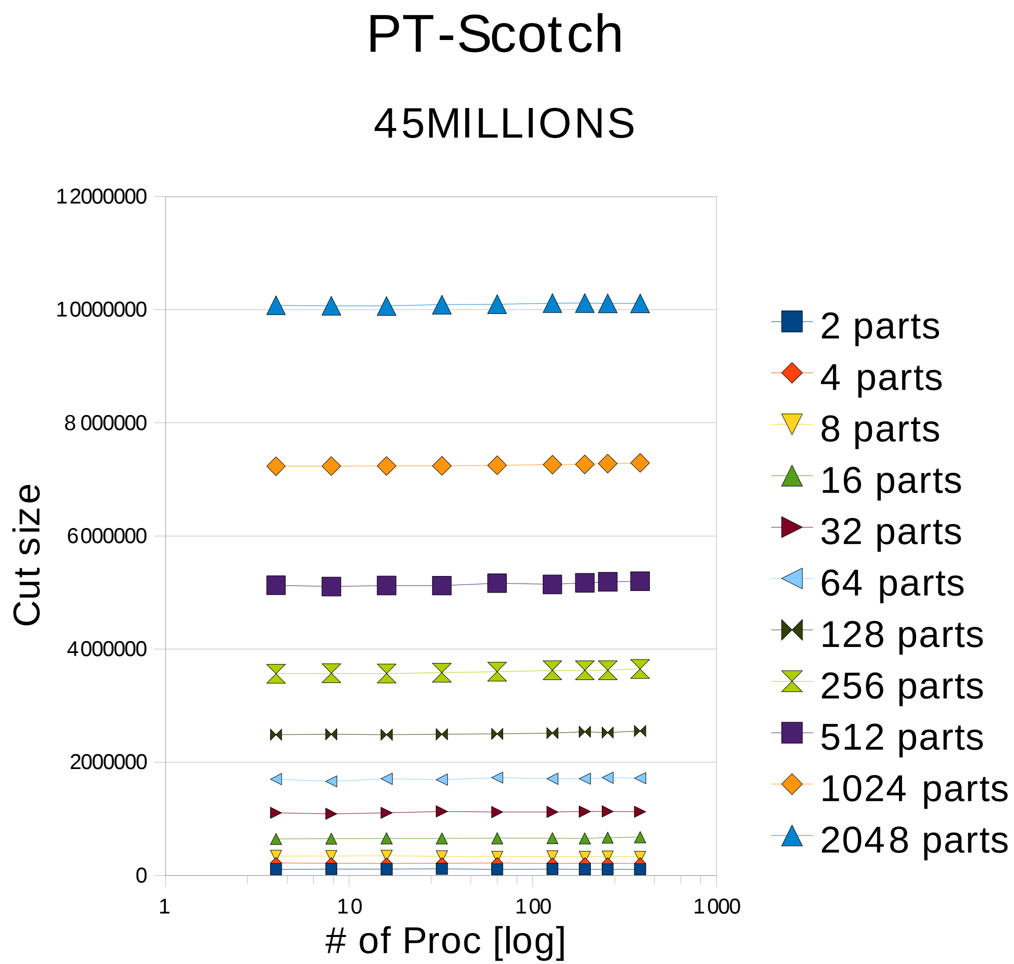
Test case	Number of processes					
	2	4	8	16	32	64
audikw1						
O_{PTS}	**5.73E+12**	**5.65E+12**	**5.54E+12**	**5.45E+12**	**5.45E+12**	**5.45E+12**
O_{PM}	5.82E+12	6.37E+12	7.78E+12	8.88E+12	8.91E+12	1.07E+13
t_{PTS}	64.14	43.72	31.25	20.66	13.86	9.83
t_{PM}	32.69	23.09	17.15	9.80	5.65	3.82





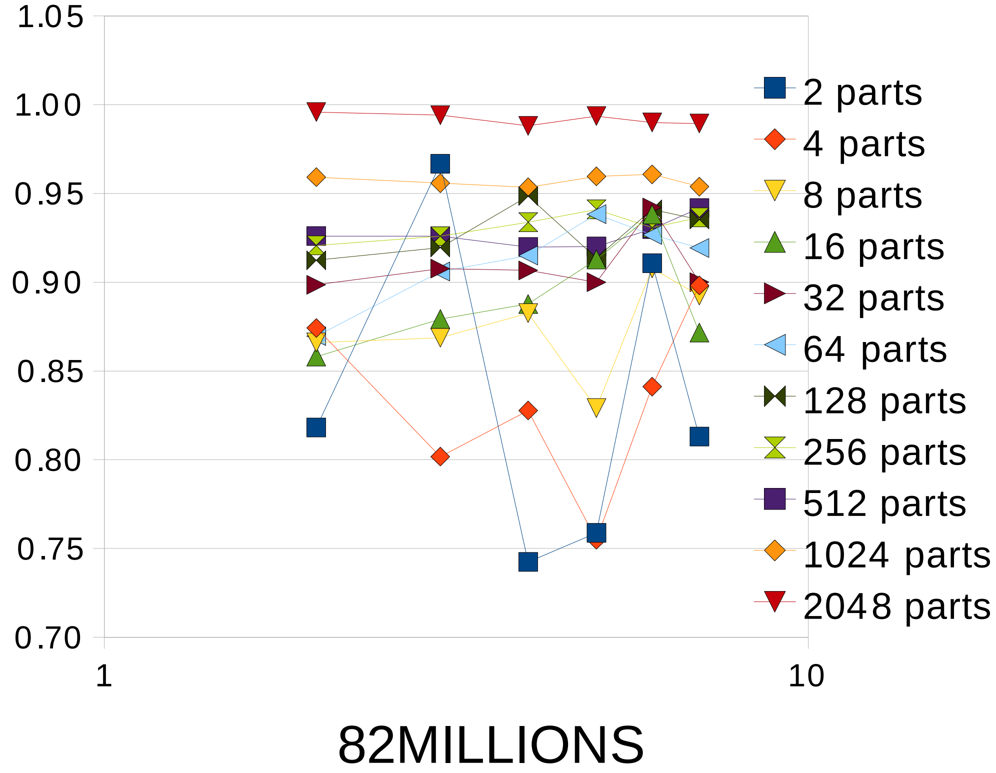
Runtime and partition quality (1)





Runtime and partition quality (2)

- Cut size ratio is most often in favor of PT-Scotch vs. ParMeTiS up to 2048 parts
  - Partition quality of ParMeTiS is irregular for small numbers of parts
  - Gets worse when number of parts increases as recursive bipartitioning prevents performing global optimization

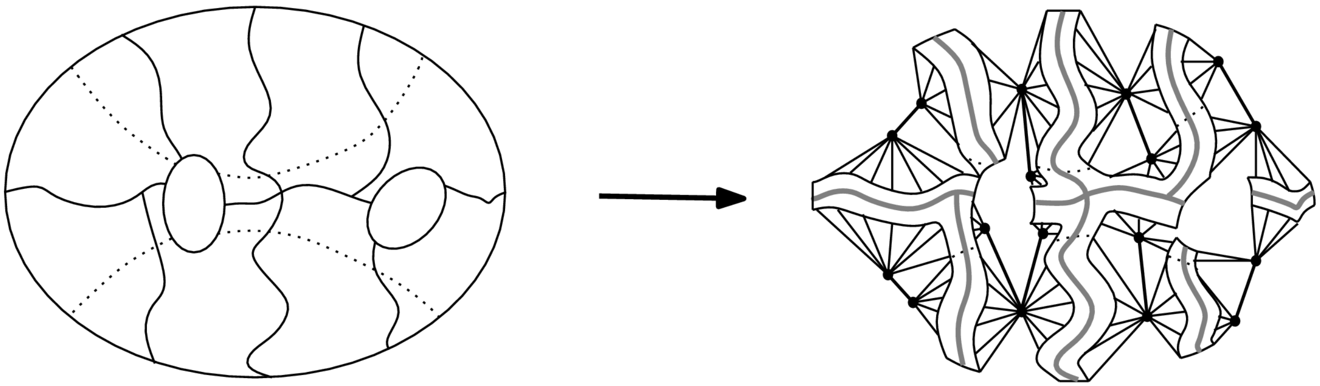


Runtime and partition quality (3)

- For most of the cases, PTS shows better partition quality
  - About 20% better in the bipartitioning cases for graph 82MILLIONS
- For the highest numbers of partitions, ParMeTiS shows slight better quality for AUDIKW1, THREAD, and BRGM
  - The graphs have high average degree
  - Greedy nature of recursive bipartitioning scheme emphasized for these graphs

Parallel direct k-way graph partitioning

- Extension to k parts of the multilevel framework used for recursive bipartitioning
  - Straightforward for the multi-level framework itself
  - Relies on distributed k-way band graphs



- Stability problems with our diffusion-based algorithms
  - Artifacts when there are too few vertices per part

Parallel static mapping

Architectural considerations matter

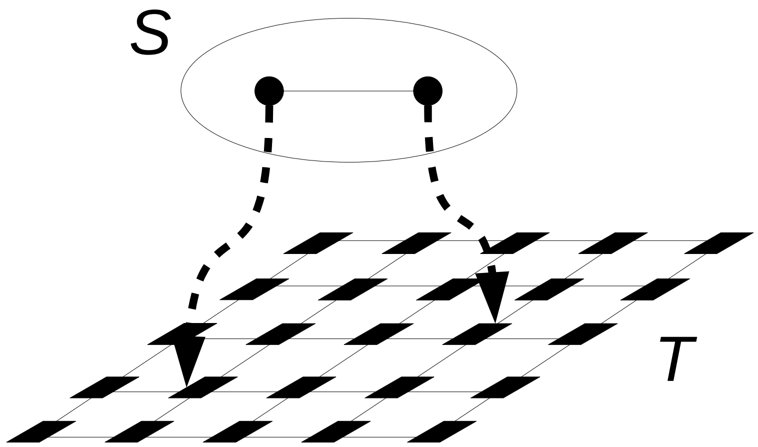
- Upcoming machines will comprise very large numbers of processing units, and will possess NUMA / heterogeneous architectures
  - More than a million processing elements on the *Blue Waters* machine to be built at UIUC (joint lab with INRIA)
- Impacts on our research :
  - Topology of target architecture has to be taken into account
    - Static mapping and not only graph partitioning
  - Dynamic repartitioning capabilities are mandatory

Parallel static mapping (1)

- Compute a mapping of *V*(*S*) and *E*(*S*) of source graph S to *V*(*T*) and *E*(*T*) of target architecture graph T, respectively
- Communication cost function accounts for distance

$$f_C(\tau_{S,T}, \rho_{S,T}) \stackrel{\text{def}}{=} \sum_{e_S \in E(S)} w(e_S)\, |\rho_{S,T}(e_S)|$$

- Static mapping features are already present in the sequential Scotch library
  - We have to go parallel

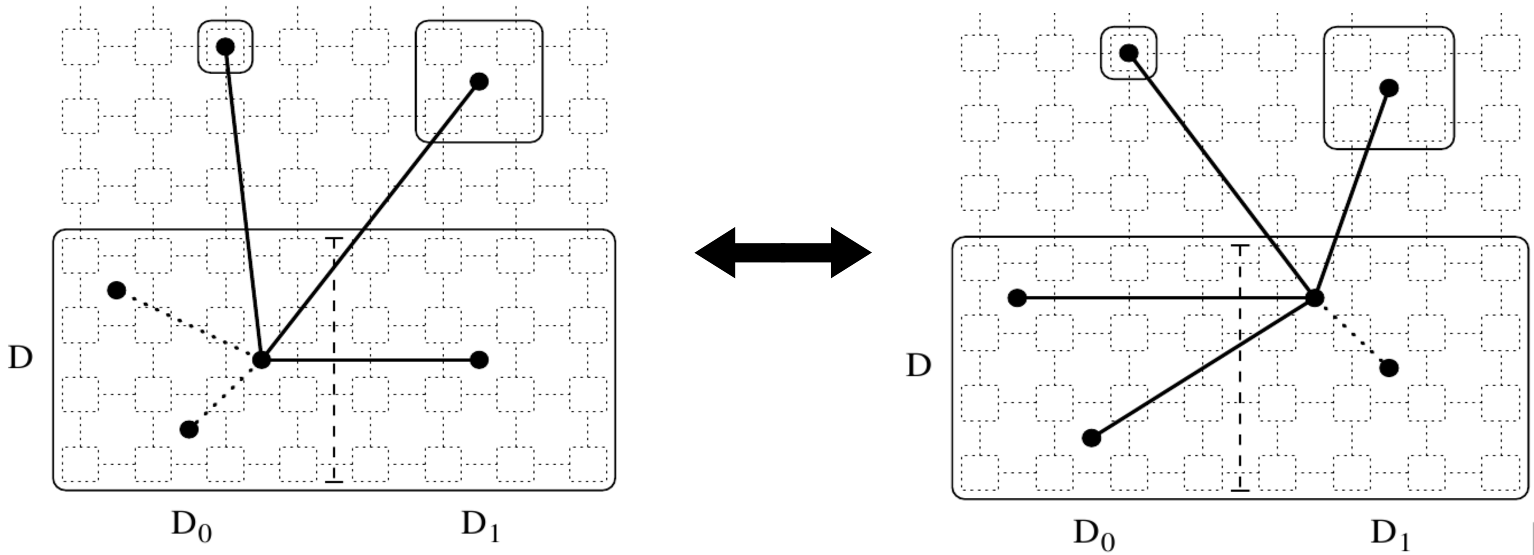


Parallel static mapping (2)

- Partial cost function in the context of recursive bipartitioning

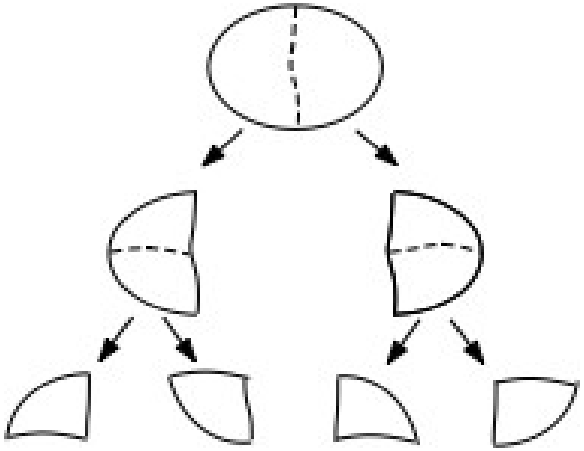
$$f'_C(\tau_{S,T}, \rho_{S,T}) \stackrel{\text{def}}{=} \sum_{\substack{v \in V(S') \\ \{v,v'\} \in E(S)}} w(\{v,v'\}) \, |\rho_{S,T}(\{v,v'\})|$$

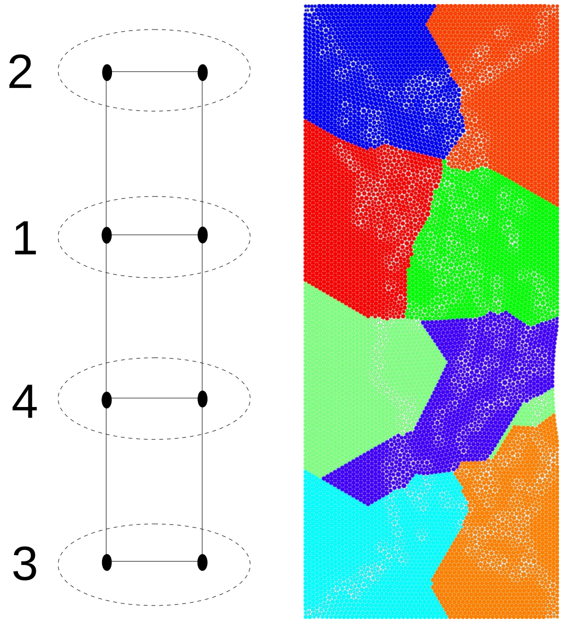
- Decision making depends on available mapping information



Parallel static mapping (3)

- Recursive bi-mapping cannot be transposed in parallel
  - All subgraphs at some level are supposed to be processed simultaneously for parallel efficiency
  - Yet, ignoring decisions in neighboring subgraphs can lead to "twists"

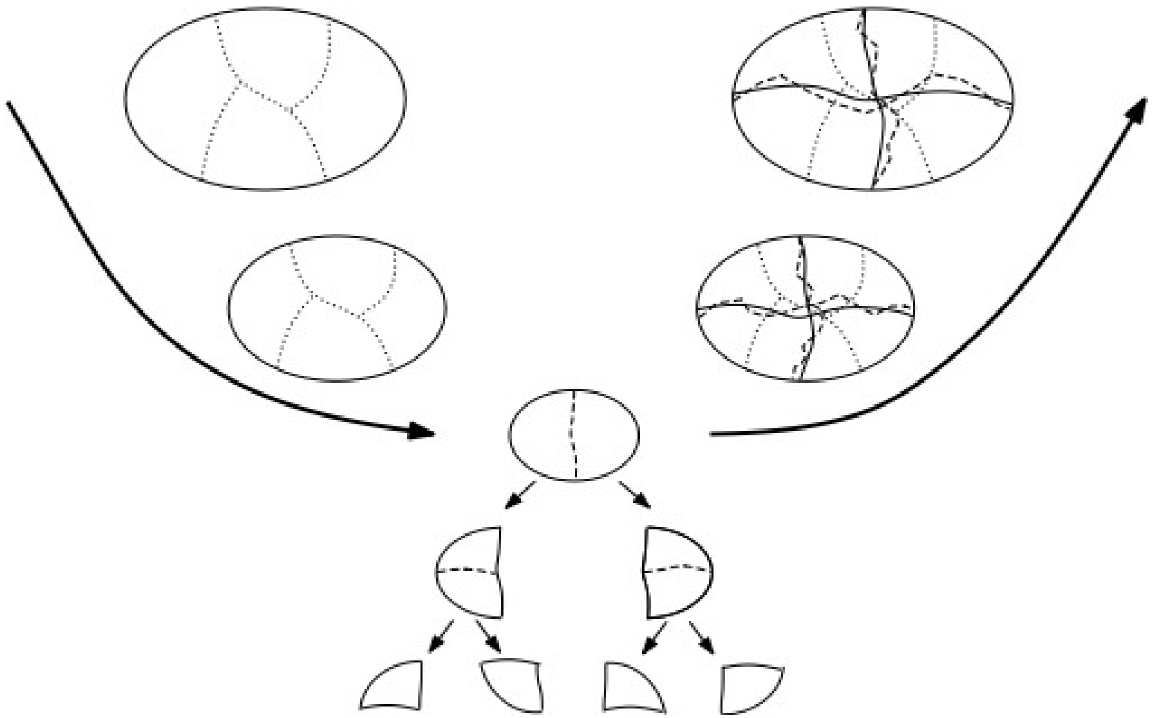




- Only sequential processing works!

Parallel static mapping (4)

- Parallel multilevel framework for static mapping
  - Parallel coarsening and k-way mapping refinement
  - Initial mapping by sequential recursive bi-mapping



Parallel static mapping (5)

- If the number of parts gets bigger than the size of the biggest graph to be stored on a single node, the sequential initial mapping phase cannot take place
  - Above 1 million parts (that is, cores)
- New roadmap : be able to map graphs of about a trillion vertices spread across a million processing elements
  - Focus on scalability problems related to the number of processors

Conclusion

Solstice goals achieved !

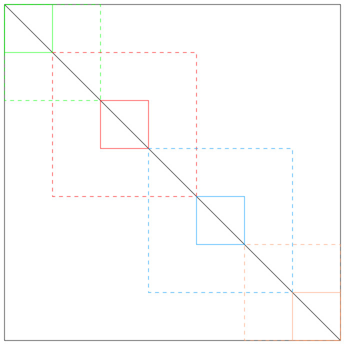
- Some users have experimented with Scotch up to the symbolic frontiers that we had defined
  - Katie Lewis at LLNL : graphs up to 800 Mvertices and 2 Gedges partitioned on 4096 procs
  - Scalability in terms of memory and runtime
  - Load imbalance increases along with the number of processes
- We are stuck by MPI interface limitations
  - All displacement and count values are expressed as ints (32 bits)
  - We must have full 64-bit MPI implementations

The Scotch software package

- All of the algorithms are available to the community
  - Scientific reproducibility
  - Freely available from the INRIA Gforge
  - Modular and documented code (≈100k lines of C)
- Upgrades on a regular basis
  - Version 4.0 : February 2004 : 2500+ direct downloads
  - About one major release per year (5.2 almost ready)
- Usage by third-party software
  - Emilio (CEA/CESTA), Code_Aster (EDF), Dolfin/Fenics (Simula), MUMPS (ENSEEITH, LIP & LaBRI), PaStiX (LaBRI), SuperLU (U. C. Berkeley), Zoltan (Sandia), ...

K-way vertex partitioning with overlap (1)

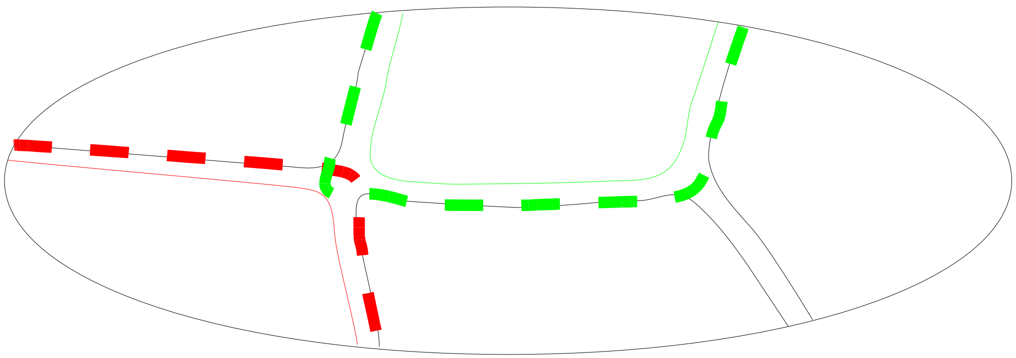
- Parallel matrix computations
  - Block decomposition with overlap

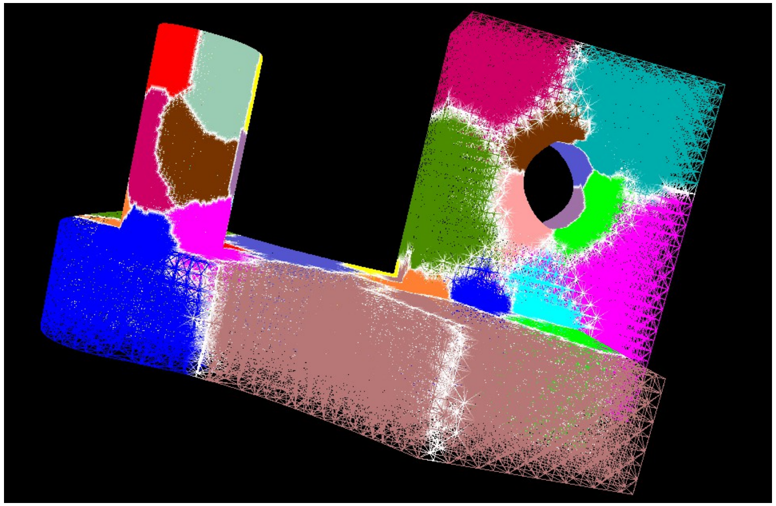


- Several application domains
  - Quantum chemistry
  - Schur complement techniques for linear system solving

K-way vertex partitioning with overlap (2)

- Compute k vertex-separated parts
- Balance part loads according to inner vertices as well as neighboring separator vertices
  - Separator vertices may contribute to several parts





Dynamic remeshing and repartitioning

- Move upwards from the production of general-purpose tools to more specific application domains
  - Motivation for joining the Bacchus team
- Parallel adaptive remeshing
  - Take into account the numerical stability of the problem being studied
  - Take advantage of the work done in PT-Scotch on distributed graphs
- Dynamically repartition the remeshed graphs

Thanks !

- To all the past and present “Scotch-men” :
  - Cédric Chevalier
  - Charles-Edmond Bichot
  - Jun-Ho Her
  - Sébastien Fourestier
  - Cédric Lachat
- The journey is going on...