**SciDAC Institute:
Combinatorial Scientific Computing and Petascale Simulations
(CSCAPES)
DOE Award #DE-FC02-06ER25775
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Final Report (#DOE-OSU-25775-Final)**

Research Accomplishments:

Throughout the project we focused on six research areas. In accordance with the specific goals, we developed novel models to solve some of these. Some of the problems required scalable distributed memory algorithms, where as some required sequential solutions. Although several graduate students and collaborators were actively involved in all of these activities, only one PhD student was directly supported by the grant. Below is a brief overview of the research carried out in each of these areas.

1. Static and Dynamic Load Balancing:

We developed a new hypergraph-based repartitioning model for load-balancing problems in dynamic applications. Our model minimizes total communication volume during the application execution as well as total cost of data migration, which is needed due to re-partitioning. This model represents the current state of the application with a hypergraph where some vertices are fixed to partitions. Existing parallel hypergraph partitioning tools could not handle fixed-vertices, hence we have developed multi-level parallel hypergraph partitioning with fixed-vertices using Zoltan framework [1, 2, 3].

In addition to optimizing the total communication volume metric, we investigated direct minimization of maximum total volume sent by a single processor. We also evaluated total number of messages and maximum number of messages sent by a single processor [4].

For applications where connectivity information was available, we also investigated at spatial partitioning problem. We developed the first-ever theoretical bounds for some of the existing spatial partitioning algorithms. We also developed dynamic-programming based exact polynomial algorithms for some classes of spatial partitioning problems and developed new heuristic methods such as the m-jagged algorithm that outperformed all existing rectangular partitioning based techniques [5, 6].

2. Parallel Graph Coloring:

We developed the first-ever scalable parallel distributed memory distance-1 graph coloring technique based on speculative coloring [7]. We provided efficient

implementation of our algorithm on shared memory architectures [8, 9]. We evaluated the performance of the shared-memory algorithm on novel Intel MIC architecture [10]. Later we improved the performance of the distributed-memory algorithm by vertex visit ordering and recoloring [11] and also developing a hybrid distributed memory and shared memory implementation using MPI + OpenMP [12].

We developed distributed distance-2 graph coloring techniques using the framework we developed for distance-1 coloring. In the distance-2 algorithm, “neighbor” processors proactively compute a forbidden color list that is used to detect which colors are not allowed to color a specific vertex, and sends this information to the owner of the vertex [13].

3. Matrix Partitioning:

We investigated the scalability (on the problem size) of the hypergraph models for partitioning sparse matrices [14]. We evaluated the hypergraph-based models against known optimal solutions for particular problem instances.

We developed a matrix-partitioning interface to PaToH in Matlab [15] for partitioning sparse matrices. This allows Matlab users to partition their sparse matrices using 1D and 2D partitioning techniques we developed [16]. We also carried out an extensive evaluation of our proposed 2D matrix partitioning techniques and provided a simple decision technique, in other words a recipe, for selecting the appropriate matrix partitioning technique based on the properties of the input matrix [16].

4. Matrix Ordering:

We developed the first hypergraph-based matrix ordering techniques. Our approach is based on the formulation of graph partitioning by vertex separator (GPVS) problem as a hypergraph partitioning problem. This new formulation is immune to the deficiency of GPVS in a multilevel framework and hence enables better orderings [17].

We developed a new technique for solving hypergraph partitioning problems by using GPVS [18]. GPVS formulation cannot preserve exact load-balancing information but allows us to trade-off partitioning quality for execution time. We developed vertex-weighting scheme to achieve good node balancing. We also introduced vertex removal and vertex splitting techniques in order to accurately model cut-net and connectivity metrics during recursive bisection.

In book chapters [19, 20, 21] we presented a high level overview of PaToH hypergraph partitioning software, as well as various hypergraph models we developed during the course of this proposal. An overview of the Zoltan and Zoltan2 frameworks, which included load balancing, coloring and matrix ordering work, is presented in another book chapter [22] and a journal article [23].

5. Scheduling:

We investigated task assignment for pipelined executions and file transfer scheduling problems, and developed algorithms for various instances. For the

application that presents the scheduling problem via dependency graph, also known as directed acyclic graph (DAG), we developed scheduling techniques that optimize latency while taking throughput as a constraint [24] and vice versa [25]. We also investigated duplication-based scheduling [26], and scheduling of mixed-parallel applications [27]. In addition, we developed an extensive survey of pipelined workflow scheduling [28].

For data-intensive applications, we investigated coordinated scheduling of file transfers [29, 30]. We also developed hypergraph-based techniques for integrated task assignment and data placement [31].

In addition, we investigated moldable job scheduling, and developed novel algorithms that minimizes the stretch, the total execution time of a task (including wait time) divided by size of the task, in order to develop a “fair” scheduling technique that does not penalize the small tasks [32, 33].

6. Clustering:

We developed a new divisive clustering technique for graph clustering problems. Our approach achieves final clustering by recursive application of graph/hypergraph bisection heuristics followed by a refinement scheme [34]. The technique was tested on 13 problem instances common in the literature and the algorithm improves the best-known modularity in 9 cases.

We investigated multithreaded clustering for multi-level hypergraph partitioning. We developed simple matching-based and agglomerative clustering techniques for shared memory architectures [35].

Outreach

The results and findings of our research have been extensively published in numerous high profile scientific venues, including the proceedings of various prestigious conferences and in peer-reviewed journals (see below the publication list that includes 35 publications).

We have organized mini-symposiums (at SIAM CSE'09, SIAM PP'10, SIAM PP'12) and workshops (ParGraph at HiPC'2011 and HiPC'2012) targeted to the research community on combinatorial and graph algorithms. We have also organized a two-week summer program for high school students.

Furthermore, the methods and algorithms developed in this project are implemented and made available to the scientific community via various software packages.

Zoltan, Parallel Partitioning, Load Balancing and Data-Management Software (<http://www.cs.sandia.gov/Zoltan/>) includes the implementations of our dynamic load balancing techniques and parallel graph coloring frameworks.

PaToH, Partitioning Tools for Hypergraph, (<http://bmi.osu.edu/~umit/software.html>) includes hypergraph-based, load balancing, ordering and matrix partitioning tools. A new MATLAB interface for PaToH was released under the GNU Lesser General Public License.

OSU Personnel

Umit V. Catalyurek (OSU-PI).

PhD Student Doruk Bozdag defended his PhD Dissertation titled "Graph Coloring and Clustering Algorithms for Science and Engineering Applications" at the Department of Electrical and Computer Engineering of The Ohio State University on December 8, 2008.

Impact:

The algorithms and tools developed in this project clearly enhance the state-of-the-art in many areas of combinatorial scientific computing including load balancing, graph coloring, and matrix partitioning and ordering. Hypergraph models that have been enhanced and developed in this project become de facto standards for modeling complex interactions in scientific computing.

Publications:

1. Ü.V. Çatalyürek, E.G. Boman, K.D. Devine, D. Bozdağ, R. Heaphy, and L.A. Riesen, "Hypergraph-based Dynamic Load Balancing for Adaptive Scientific Computations", Proceedings of 21st IEEE International Parallel & Distributed Processing Symposium (IPDPS'07), Apr 2007. **Best paper award in the Algorithms track.**
2. Ü.V. Çatalyürek, D. Bozdağ, E.G. Boman, K.D. Devine, R. Heaphy and L.A. Riesen, "Hypergraph-based Dynamic Partitioning and Load Balancing", Advanced Computational Infrastructures for Parallel/Distributed Adaptive Applications, Wiley Press, Editors M. Parashar, X. Li, S. Chandra, Dec 2009.
3. Ü.V. Çatalyürek, E.G. Boman, K.D. Devine, D. Bozdağ, R.T. Heaphy, and L.A. Riesen, "A Repartitioning Hypergraph Model for Dynamic Load Balancing", Journal of Parallel and Distributed Computing, Vol. 69, No. 8, pp. 711-724, Aug 2009.
4. Ü.V. Çatalyürek, M. Deveci, K. Kaya, and B. Uçar, "UMPa: A Multi-objective, multi-level partitioner for communication minimization", 10th DIMACS Implementation Challenge - Graph Partitioning and Graph Clustering, Atlanta, GA, February 13-14, 2012. Published in Contemporary Mathematics, Vol. 588, Editors D.A. Bader, H. Meyerhenke, P. Sanders, D. Wagner, 2013.

5. E. Saule, E.Ö. Baş and Ü.V. Çatalyürek, "Partitioning Spatially Located Computations using Rectangles", Proceedings of 25th IEEE International Parallel & Distributed Processing Symposium (IPDPS'11), May 2011. *Acceptance rate 19%*.
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10. E. Saule and Ü.V. Çatalyürek, "An Early Evaluation of the Scalability of Graph Algorithms on the Intel MIC Architecture", Proceedings of 26th International Symposium on Parallel and Distributed Processing, Workshops and PhD Forum (IPDPSW), Workshop on Multithreaded Architectures and Applications (MTAAP), May 2012.
11. A.E. Sarıyüce, E. Saule and Ü.V. Çatalyürek, "Improving Graph Coloring on Distributed Memory Parallel Computers", Proceedings of 18th Annual International Conference on High Performance Computing (HiPC 2011), Dec 2011. *Acceptance rate 19.4%*.
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