Combinatorial Scientific Computing and Petascale Simulations (CSCAPES)

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CSCAPES Mission and Recent Activities

• Research and Development
  • Provide load balancing and parallelization toolkits for petascale computation.
  • Develop advanced automatic differentiation capabilities for complex applications.
  • Advance the state-of-the-art in large-scale graph and sparse matrix computations.
  • Develop data and iteration reordering algorithms for improving single processor performance.

• Training and Outreach
  • In collaboration with SciDAC CETs and SAPs, support scientific applications with underlying graph and hypergraph algorithms.
  • Develop data and iteration reordering algorithms based on approximation techniques.
  • Train researchers in CSC skills. Currently, 2 post-docs, 5 graduate and 1 undergraduate students are being trained.

Performance Improvement

Modern microprocessors are highly sensitive to spatial and temporal locality of data. In a mesh smoothing application, for example, reordering the vertices and elements of a mesh can lead to a significant improvement in single processor performance. CSCAPES is developing several data and iteration reordering algorithms based on hypergraph models.

Graph Coloring

Graph coloring problems are powerful abstractions for minimizing the execution time, memory, and storage space needed in computing sparse derivative matrices using automatic differentiation. Graph coloring is also useful in discovering concurrency in parallel computation. CSCAPES researchers are developing novel sequential and parallel algorithms for various coloring problems. Implementations of the parallel algorithms are being made available via Zoltan.

Structuredly orthogonal column partition and its representation as a distance-2 coloring in the adjacency graph of a Hessian (left) or bipartite graph of a Jacobian.

Performance of a recently developed parallel distance-2 coloring algorithm on select applications.

Further Information

www.cscapes.org

Automatic Differentiation (AD)

AD is a technology for computing analytic derivatives of functions specified by computer programs. Efficient derivative accumulation can be posed as a transformation (vertex or edge elimination) problem on a computational graph. Sparsity exploitation in large-scale derivative matrix computation gives rise to a variety of graph coloring problems. Checkpointing in irregular computation is another source of combinatorial problems in AD. CSCAPES is developing efficient algorithms for these problems. It is also extending the capabilities of the Argonne-housed AD tools ADIC and ADIFOR within the OpenAD framework, and plans to provide users with integrated load balancing and coloring capabilities.

Load Balancing

In parallel computation, data and tasks need to be mapped to processors such that workload is balanced and communication cost is low. In dynamic or adaptive applications, these goals must be met as computation and communication change over time. Zoltan is a software toolkit for parallelization and load balancing.

A hypergraph-based dynamic repartitioning method with superior performance compared to earlier methods has recently been added to Zoltan. This work earned the Best Algorithms Paper Award at IPDPS07. The capabilities of Zoltan are being extended in several other ways to support petascale applications.

Performance comparison of hypergraph repartitioning (PGO-report) and several graph- and code-based methods in an adaptive mesh refinement problem from Sandra’s ALEGRA physics code. The top row shows finite element meshes at time-steps 0, 54, and 108. The bottom row shows the reduced total communication volume obtained with hypergraph repartitioning, as well as repartitioning times.

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