Basker: A Threaded Sparse LU factorization utilizing Hierarchical Parallelism and Data Layouts

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ShyLU and Subdomain Solvers: Overview

- **MPI+X based subdomain solvers**
  - Decouple the notion of one MPI rank as one subdomain: Subdomains can span multiple MPI ranks each with its own subdomain solver using X or MPI+X

- **Subpackages of ShyLU**: Multiple Kokkos-based options for on-node parallelism
  - **Basker**: LU or ILU (t) factorization
  - **Tacho**: Incomplete Cholesky - IC (k) (See K. Kim talk in HIPS workshop later today)
  - **Fast-ILU**: Fast-ILU factorization for GPUs
  - **KokkosKernels**: Coloring based Gauss-Seidel (see talk by M. Deveci Thursday), Triangular Solves

- Under active development. Jointly funded by ASC, ATDM, FASTMath, LDRD.
Themes for Architecture Aware Solvers and Kernels: Data layouts

- Specialized memory layouts
  - Architecture aware data layouts
    - Coalesced memory access
    - Padding
    - Array of Structures vs Structure of Arrays
    - Kokkos based abstractions (H. C. Edwards et al.)
- Two dimensional layouts for matrices
  - Allows using 2D algorithms for solvers and kernels
  - Bonus: Fewer synchronizations with 2D algorithms
  - Cons: Much more harder to design correctly
  - Better utilization of hierarchical memory like High Bandwidth Memory (HBM) in Intel Xeon Phi or NVRAM
- Hybrid layouts
  - Better for very heterogeneous problems
Synchronizations are expensive

- 1D algorithms for factorizations and solvers, such as ND based solvers have a huge synchronization bottleneck for the final separator
- Impossible to do efficiently in certain architectures designed for massive data parallelism (GPUs)
- This is true only for global synchronizations, fork/join style model.

Fine grained synchronizations

- Between handful of threads (teams of threads)
- Point to Point Synchronizations instead of global synchronizations
  - Park et al (ISC14) showed this for triangular solve
- Thread parallel reductions wherever possible
  - Atomics are cheap
    - Only when used judiciously
Themes for Architecture Aware Solvers and Kernels: Task Parallelism

- Statically Scheduled Tasks
  - Determine the static scheduling of tasks based on a task graph
  - Eliminate unnecessary synchronizations
    - Tasks scheduled in the same thread do not need to synchronize
    - Find transitive relationships to reduce synchronization even further
      - Jongsoo Park et al

- Dynamically scheduled tasks
  - Use a tasking model that allows fine grained synchronizations
    - Requires support for futures
    - Not the fork-join model where the parent forks a set of tasks and blocks till they finish
  - Kokkos Tasking API
    - Joint work with Carter Edwards, Stephen Olivier, Kyungjoo Kim, Jon Berry, George Stelle
  - See K. Kim’s talk in HIPS for a comparison with this style of codes
Themes for Architecture Aware Solvers and Kernels: Asynchronous Algorithms

- System Level Algorithms
  - Communication Avoiding Methods (s-step methods)
    - Not truly asynchronous but can be done asynchronously as well.
    - Multiple authors from early 1980s
  - Pipelined Krylov Methods
    - Recently Ghysels, W. Vanroose et al. and others
- Node Level Algorithms
  - Finegrained Asynchronous iterative ILU factorizations
  - An iterative algorithm to compute ILU factorization (Chow et al)
    - Asynchronous in the updates
  - Finegrained Asynchronous iterative Triangular solves
    - Jacobi iterations for the triangular solve.
Why Transistor-Level Circuit Simulation?

- Provides tradeoff between fidelity and speed/problem size
  - Xyce enables full system parallel simulation for large integrated circuits
- Essential simulation approach used to verify electrical designs
  - SPICE is the defacto industry standard (PSpice, HSPICE, etc.)
  - Xyce supports NW-specific device development
Simulation Challenges

Analog simulation models network(s) of devices coupled via Kirchoff’s current and voltage laws

- **Network Connectivity**
  - Hierarchical structure rather than spatial topology
  - Densely connected nodes: O(n)

- **Badly Scaled DAEs**
  - Compact models designed by engineers, not numerical analysts!
  - Steady-state (DCOP) matrices are often ill-conditioned

- **Non-Symmetric Matrices**

- **Load Balancing vs. Matrix Partitioning**
  - Balancing cost of loading Jacobian values unrelated to matrix partitioning for solves

- **Strong scaling and robustness is the key challenge!**

\[
f(x(t)) + \frac{dq(x(t))}{dt} = b(t)\]
ShyLU/Basker: LU factorization

- Basker: Sparse (I)LU factorization
  - Block Triangular form (BTF) based LU factorization, Nested-Dissection on large BTF components
  - 2D layout of coarse and fine grained blocks
    - Previous work: X. Li et al, Rothberg & Gupta
- Data-Parallel, Kokkos based implementation
- Fine-grained parallel algorithm with P2P synchronizations
- Parallel version of Gilbert-Peirels’ algorithm (or KLU)
- Left-looking 2D algorithm requires careful synchronization between the threads
  - All reduce operations between threads to avoid atomic updates
ShyLU/Basker: Steps in a Left looking factorization

- Different Colors show different threads
- Grey means not active at any particular step
- Every left looking factorization for the final separator shown here involves four independent triangular solve, a mat-vec and updates (P2P communication), two independent triangular solves, a mat-vec and updates, and triangular solve. (Walking up the nested-dissection tree)
ShyLU/Basker : Performance Results

- A set of problems selected from UF Sparse Matrix Collection and Sandia’s internal problem set
  - Representative problems with both high fill (fill-in density > 4.0) and low fill-in density
- OpenMP and Kokkos based implementation for CPU and Xeon Phi based architectures
- Testbed Cluster at Sandia
  - SandyBridge based two eight core Xeons (E5-2670), 24GB of DRAM
  - Intel Xeon Phi (KNC) co-processors with 61 cores with 16 GB main memory
- The number of non-zeros between the solvers are different due to the different ordering schemes used by the solvers
- Comparisons with KLU, SuperLU-MT and MKL-PARDISO
ShyLU/Basker : Performance Results

- Speedup 5.9x (CPU) and 7.4x (Xeon Phi) over KLU (Geom-Mean) and up to 53x (CPU) and 13x (Xeon Phi) over MKL
- Low-fill matrices Basker is consistently the better solver. High fill matrices MKL Pardiso is consistently the better solver
ShyLU/Basker: Performance Results

- Performance Profile for a matrix set with a high-fill and low-fill matrices shown (16 threads on CPUs /32 threads on Xeon Phi)
- Low-fill matrices Basker is consistently the better solver. High fill matrices MKL Pardiso is consistently the better solver
Conclusions

- Themes around Thread Scalable Subdomain solvers
  - Data Layouts
  - Fine-grained Synchronizations
  - Task Parallelism
  - Asynchronous Algorithms
- Basker LU factorization
  - Uses 2D layouts with hierarchy from block triangular form and nested dissection
  - Uses fine-grained synchronizations between teams of threads
  - Uses a static tasking mechanism with data-parallelism
Questions ?