symPACK: A GPU-Capable Fan-Out Sparse Cholesky Solver

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Introduction

- Sparse symmetric positive-definite systems of equations are ubiquitous
- Sparse direct solvers use Cholesky Factorization to efficiently solve such systems
- Parallel sparse Cholesky codes are essential
- But, modern HPC is heterogeneous
  - Codes need to exploit CPUs and GPUs
symPACK is a parallel sparse Cholesky solver that effectively utilizes heterogeneous processing units and employs a novel one-sided communication algorithm

https://go.lbl.gov/sympack
Cholesky Basics

- **Goal:** Solve $Ax=b$, where $A$ is spd
- **Factorize step:** $A = LL^T$
  - Proceed one column at a time
  - Compute each column of $L$ using column of $A$
  - Update trailing lower triangular region of $A$
- **Solve step:** Solve $Ly=b$ for $y$, then solve $L^Tx=y$ for $x$
  - Forward/Backward substitution

```plaintext
for column $j = 1$ to $n$ do
  $\ell_{j,j} = \sqrt{a_{j,j}}$
  for row $i = j + 1$ to $n$ do
    $\ell_{i,j} = a_{i,j}/\ell_{j,j}$
  end
end
for column $k = j + 1$ to $n$ do
  for row $i = k$ to $n$ do
    $a_{i,k} = a_{i,k} - \ell_{i,j} \cdot \ell_{k,j}$
  end
end
```

*Algorithm 1: Basic Cholesky algorithm*
Sparse Cholesky

- Group contiguous columns of A into “supernodes”
  - Group rows into dense blocks
  - Lets you use dense matrix operations
- Derive an elimination tree from the supernodes
  - This gives you a de-facto task graph
- Factorize each supernode according to the elimination tree
- Fill-in: nonzeros in L that were zero in A
  - Reduce fill-in this by reordering A with permutation matrices P, P^T

Figure 1: Sparse matrix A partitioned into supernodes and dense blocks. $i$ denotes the $i$-th supernode, • represents original nonzero elements in A, while + denotes fill-in entries. Colors correspond to the four distributed-memory nodes onto which blocks are mapped in a 2D block-cyclic way.
Parallel Cholesky

- Assign supernodes in the elimination tree to processors
- Elimination tree exposes needed communication between supernodes
- Three families of algorithms
  - Fan-in: compute update to remote supernode locally, then send the update to the remote supernode
  - Fan-out: send local supernode to remote processor, and compute the update on the remote processor
  - Fan-both: use both strategies
- symPACK is fan-out
symPACK Implementation
symPACK Task Formulation

- Formulate Cholesky factorization as tasks that operate on dense blocks of A
  - Supernode partitioning, then block partitioning
  - Computation is done using BLAS 3/LAPACK operations to achieve superior performance

- Three kinds of tasks
  - Diagonal Factorize $D_j$: Factorize diagonal block in supernode j
  - Factorize $F_{ij}$: Factorize block i in supernode j
  - Update $U_{ij,k}$: Update block i in supernode k using the factorized block i in supernode j (j < k)
Task Dependencies

- A diagonal block must be factorized before other blocks in the supernode can be factorized

- A block must be factorized before it can be used to update other blocks

- All updates must be applied to a block before it can be factorized

Figure 2: fan-out task dependencies for four columns $j$, $i$, $k$, and $h$
Task Scheduling

- Each processor has two task queues
  - Local task queue (LTQ): All tasks mapped to this processor
  - Ready task queue (RTQ): Tasks mapped to this processor that can be scheduled
- Tasks can be executed if all of their dependencies have been satisfied

- Tasks have a dependency counter

- Tasks are popped from the RTQ and executed, then they produce data used to satisfy dependencies between tasks
  - Once a task’s dependency counter hits zero, it is moved from the LTQ to the RTQ
Parallel Algorithm

- Individual blocks are mapped to processors using a 2D block-cyclic mapping
- All tasks involving a block are mapped to the processor owning that block

- 2 kinds of messages
  - Diagonal factorized blocks need to be sent to remote processors for factorize tasks
  - Off-diagonal factorized blocks need to be sent to remote processors for update tasks

- Communication is handled with one-sided RMA operations and remote procedure calls provided by UPC++
Communication Paradigm

- Four UPC++ constructs are important here
  - global address space: region of memory that each processor owns a region of
    - Processors can access regions of the global address space owned by other processors
  - rget: reads data located in a remote processor’s global address space using a global pointer
  - Remote procedure call: local processor enqueues a procedure on a remote processor
  - progress: advances internal UPC++ state, executes enqueued RPCs

- Example: Task $T_1$ produced data task $T_2$ needs
- $P_{source}$ owns $T_1$, $P_{target}$ owns $T_2$

Figure 4: Data exchange protocol in symPACK. Notifications are performed using UPC++ asynchronous RPC, and the actual data is fetched using non-blocking one-sided RMA get.
Communication Paradigm

- Step 1: Enqueue RPC to `signal()` on Ptarget
- One argument to `signal()` is a global pointer to the data $T_2$ needs

Figure 4: Data exchange protocol in symPACK. Notifications are performed using UPC++ asynchronous RPC, and the actual data is fetched using non-blocking one-sided RMA get.
Communication Paradigm

- Step 2: call \texttt{poll()} function on \texttt{Ptargrt}, which dispatches a call to \texttt{upcxx::progress()}

Figure 4: Data exchange protocol in symPACK. Notifications are performed using UPC++ asynchronous RPC, and the actual data is fetched using non-blocking one-sided RMA get.
Communication Paradigm

- **Step 3:** `upcxx::progress()` executes the RPC on Ptarget

Figure 4: Data exchange protocol in symPACK. Notifications are performed using UPC++ asynchronous RPC, and the actual data is fetched using non-blocking one-sided RMA `get`.
Communication Paradigm

- Step 4: `signal()` enqueues global pointer in a list of global pointers local to processor owning $T_2$

Figure 4: Data exchange protocol in symPACK. Notifications are performed using UPC++ asynchronous RPC, and the actual data is fetched using non-blocking one-sided RMA get.
Communication Paradigm

- Step 5: Iterate through list of global pointers, call `upcxx::rget()` on each one
- This actually satisfies the data dependency

Figure 4: Data exchange protocol in symPACK. Notifications are performed using UPC++ asynchronous RPC, and the actual data is fetched using non-blocking one-sided RMA get.
Step 6: Decrement $T_2$ dependency counter, push on RTQ if all dependencies are satisfied.
symPACK GPU Functionality
GPU Functionality

- **symPACK’s GPU functionality is built with UPC++ memory kinds**
  - Extends the global address space to include device memory
  - Allocate memory on devices with `upcxx::device_allocator`
  - Returns a global pointer to device memory

- **`upcxx::copy()` moves data between any combination of hosts and devices**
  - Local host <!-- Remote device
  - Local device <!-- Remote host
  - Local device <!-- Remote device
  - Local Host <!-- Remote host
GPU Functionality

- It’s best to use the GPU only for tasks that have a high arithmetic intensity
  - This translates to tasks that operate on large blocks
  - Inevitable overheads mean computation has to be much faster to justify overhead

- For each BLAS/LAPACK operation, define a size threshold that determines whether we map the task to the GPU or the CPU
  - cuBLAS/cuSolver handles local computation
Observation: If a block is large enough, all tasks involving the block will happen on the GPU

Naive approach: fetch data from remote host onto local host, then copy it to local device

Superior approach: fetch data from remote host directly to local device
  
  Memory kinds enable the superior approach through GASNet-EX’s support for GPUDirect RDMA (GDR)
Performance Evaluation
Performance Evaluation

- All experiments were run on NERSC Perlmutter GPU nodes
  - 1 AMD EPYC 7763 “Milan” CPU with 64 cores
  - 4 NVIDIA A100 “Ampere” GPUs
  - 4 HPE Slingshot 11 “Cassini” 200Gbps network cards

- Benchmarked GPU mode of symPACK using GPU mode of PaStiX as a baseline
  - Matrices are from SuiteSparse matrix collection
  - symPACK and PaStiX both use the Scotch ordering library
Performance Evaluation

- Impact of memory kinds
- Bandwidth vs message size for MPI one sided get, native `upcxx::copy()`, and reference `upcxx::copy()`

Figure 5: Microbenchmark comparison of one-way point-to-point communication bandwidth for non-blocking RMA gets involving GPU-resident buffers using GPUDirect RDMA technology versus the same transfer staged through an intermediate buffer in host memory.
Performance Evaluation

![Diagram showing factorization times for Flan_1565, boneS10, and thermal2](image)

- **Figure 7:** Strong scaling of symPACK's Cholesky factorization on Flan_1565
- **Figure 9:** Strong scaling of symPACK's Cholesky factorization on boneS10
- **Figure 11:** Strong scaling of symPACK's Cholesky factorization on thermal2

### Matrices from SuiteSparse matrix collection

<table>
<thead>
<tr>
<th>Name</th>
<th>Description</th>
<th>$n$</th>
<th>$nnz$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flan_1565</td>
<td>3D model of a steel flange</td>
<td>1,564,794</td>
<td>114,165,372</td>
</tr>
<tr>
<td>boneS10</td>
<td>3D trabecular bone</td>
<td>914,898</td>
<td>40,878,708</td>
</tr>
<tr>
<td>thermal2</td>
<td>steady state thermal</td>
<td>1,228,045</td>
<td>8,580,313</td>
</tr>
</tbody>
</table>

**Table 1:** Characteristics of symmetric matrices used in the experiments. $n$ denotes the number of rows/columns in the matrix, and $nnz$ denotes the number of nonzero elements in the matrix.
Future Work

● Develop a more sophisticated task scheduling policy

● Autotuning for GPU thresholds

● Supernode coalescing
Acknowledgements

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Thank you!

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