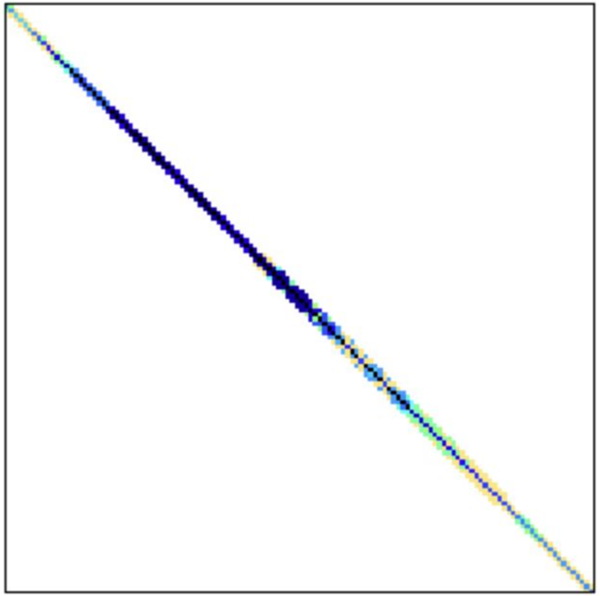
symPACK: A GPU-Capable Fan-Out Sparse Cholesky Solver

Julian Bellavita[1], Mathias Jacquelin[2], Esmond G. Ng[1], Dan Bonachea[1], Johnny Corbino[1], and Paul H. Hargrove[1]

[1]Lawrence Berkeley National Laboratory
[2]Cerebas Systems

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



Introduction

symPACK is a parallel sparse Cholesky solver that effectively utilizes heterogeneous processing units and employs a novel one-sided communication algorithm

https://github.com/symPACK/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

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

  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
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

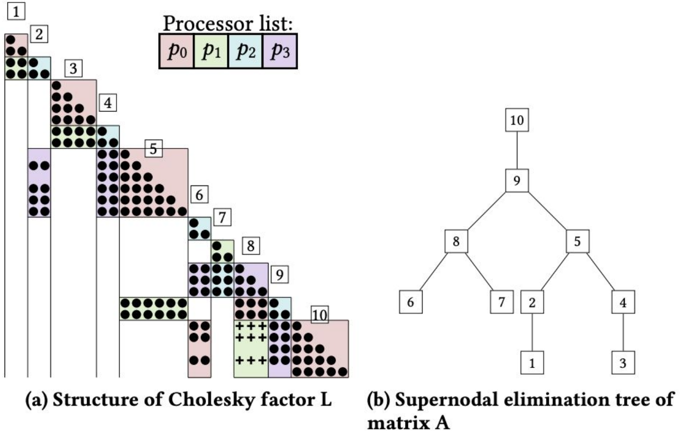


Figure 1: Sparse matrix A partitioned into supernodes and dense blocks. $\boxed{i}$ denotes the i-th supernode, • represents original nonzero elements in A, while + denotes fill-in entries. Colors correspond to the four distributed-memory nodes onto which blocks are mapped in a 2D block-cyclic way.

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 $F_{i,j}$: Factorize block i in supernode j
    - Update $U_{i,j,k}$: 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

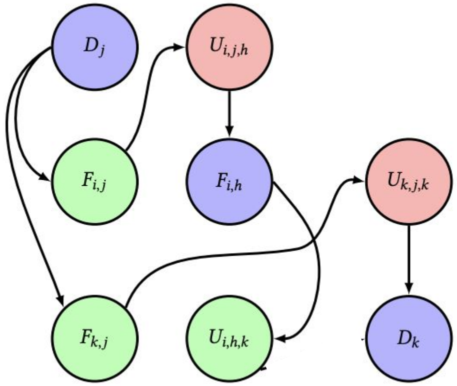


Figure 2: ***fan-out*** **task dependencies for four columns** j, i, k, **and** h

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
- Psource owns T_1, Ptarget owns T_2

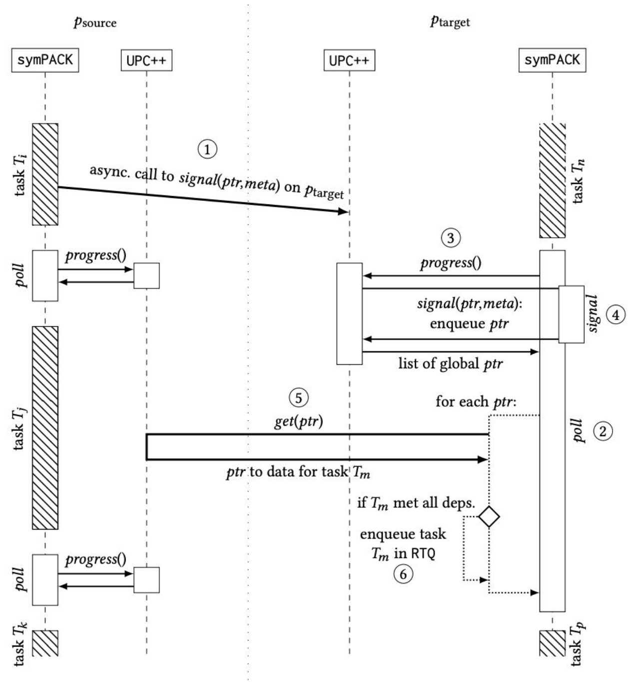


Figure 4: Data exchange protocol in symPACK. Notifications are performed using UPC++ asynchronous RPC, and the actual data is fetched using non-blocking one-sided RMA get.

Communication Paradigm

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

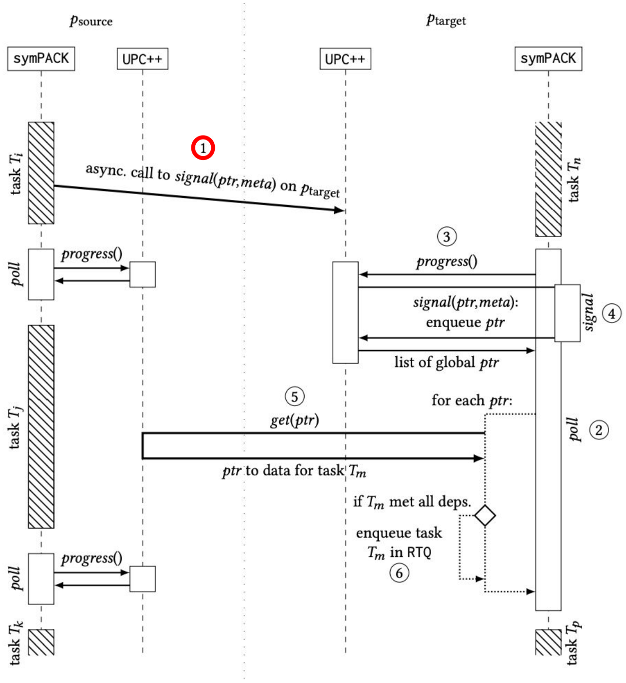
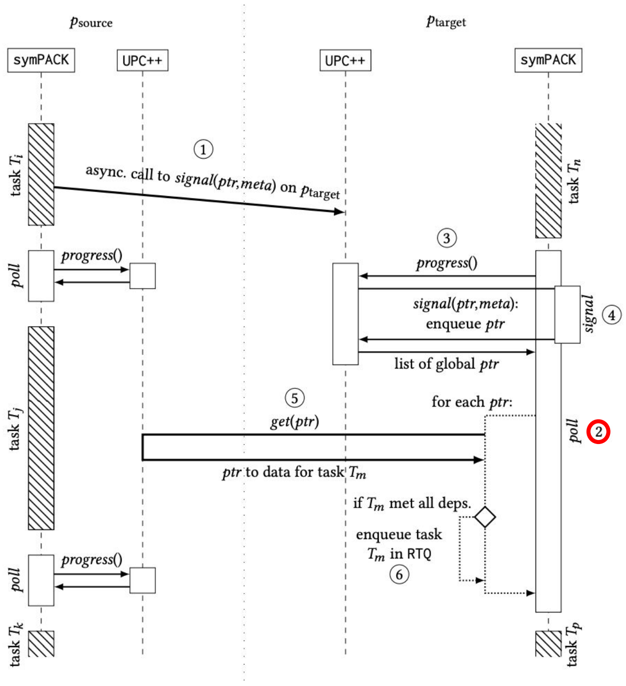


Figure 4: Data exchange protocol in symPACK. Notifications are performed using UPC++ asynchronous RPC, and the actual data is fetched using non-blocking one-sided RMA get.

Communication Paradigm

- Step 2: call `poll()` function on Ptarget, which dispatches a call to `upcxx::progress()`



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Communication Paradigm

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

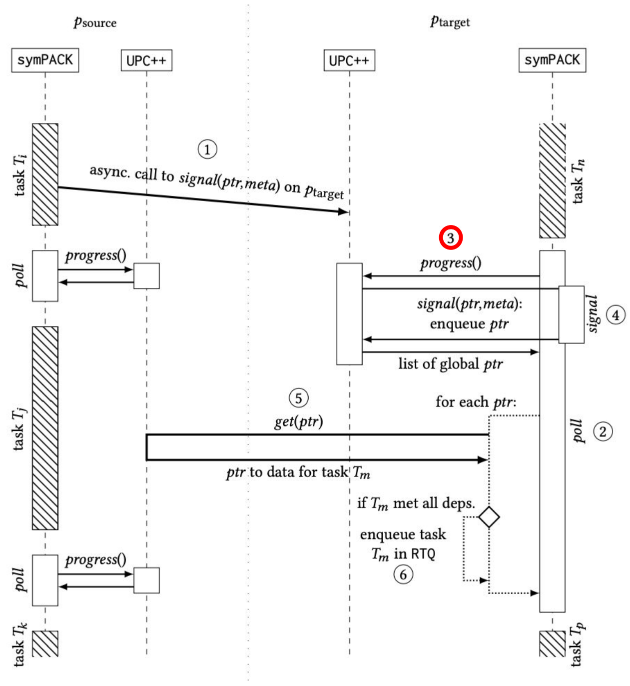


Figure 4: Data exchange protocol in symPACK. Notifications are performed using UPC++ asynchronous RPC, and the actual data is fetched using non-blocking one-sided RMA get.

Communication Paradigm

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

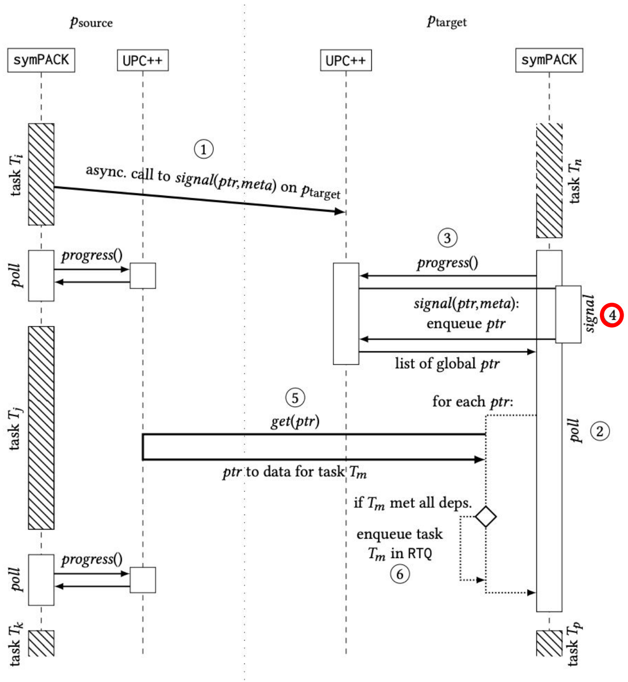
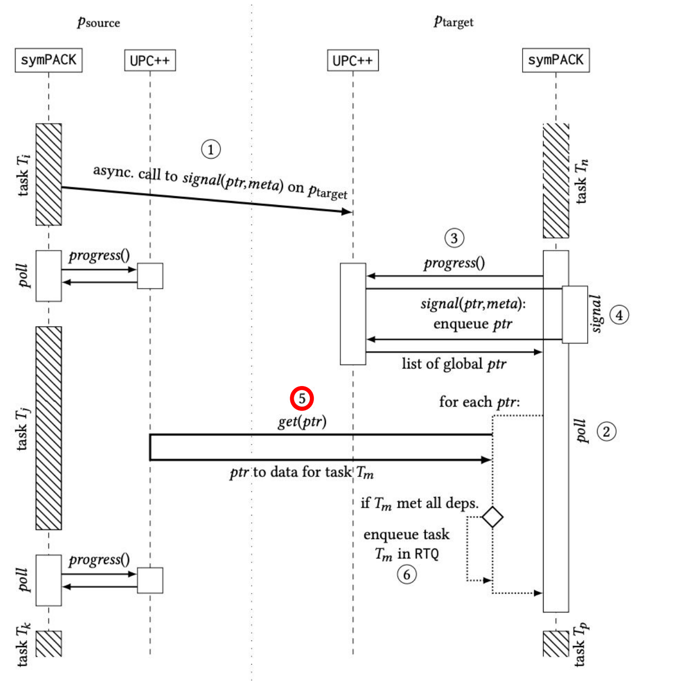


Figure 4: Data exchange protocol in symPACK. Notifications are performed using UPC++ asynchronous RPC, and the actual data is fetched using non-blocking one-sided RMA get.

Communication Paradigm

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



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Communication Paradigm

- Step 6: Decrement T_2 dependency counter, push on RTQ if all dependencies are satisfied

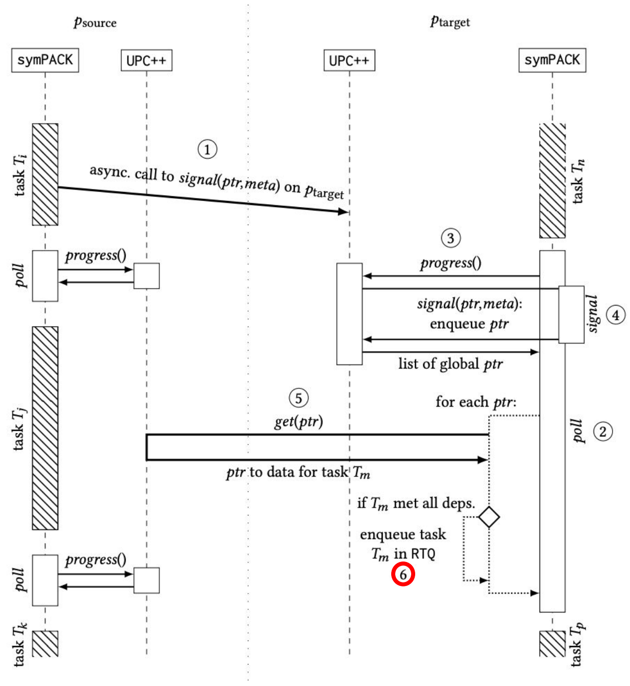


Figure 4: Data exchange protocol in symPACK. Notifications are performed using UPC++ asynchronous RPC, and the actual data is fetched using non-blocking one-sided RMA get.

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

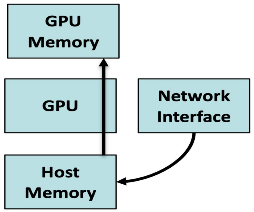
GPU Functionality

- 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

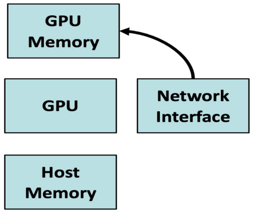
- For each BLAS/LAPACK operation, define a <u>size threshold</u> that determines whether we map the an instance of each operation to the GPU or the CPU
  - If an operation involves a block > size threshold, do it on the GPU, otherwise do it on the CPU
  - cuBLAS/cuSolver handles local computation

Optimizing GPU Communication with Memory Kinds

- 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)



Data movement without acceleration



Data movement with acceleration

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

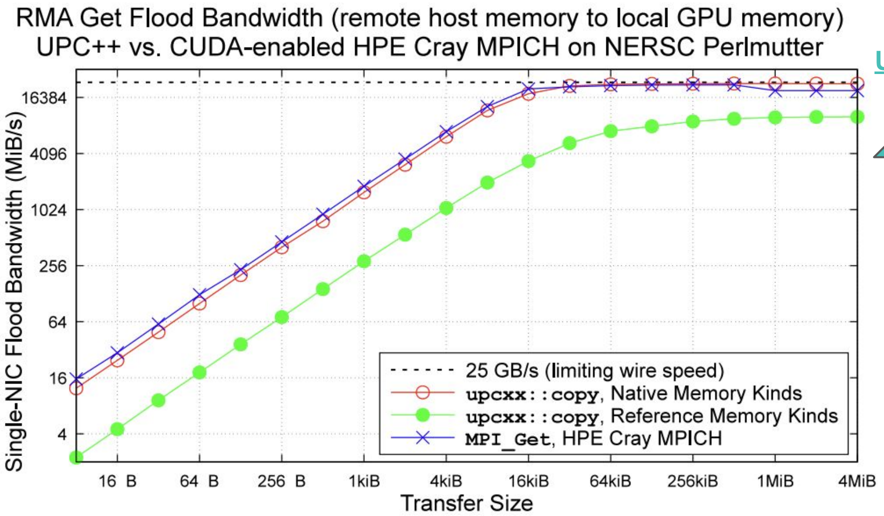
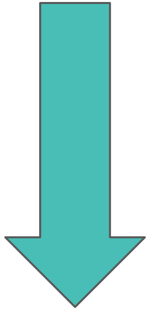


Figure 5: Microbenchmark comparison of one-way point-to-point communication bandwidth for non-blocking RMA gets involving GPU-resident buffers using GPUDirect RDMA technology versus the same transfer staged through an intermediate buffer in host memory.

Up is good

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

Performance Evaluation



Down is good

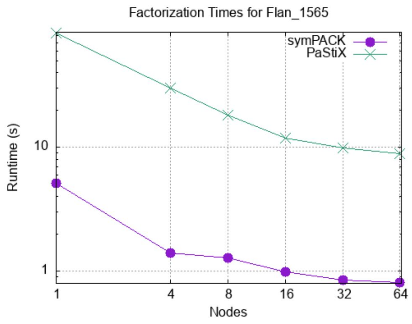


Figure 7: Strong scaling of symPACK's Cholesky factorization on Flan_1565

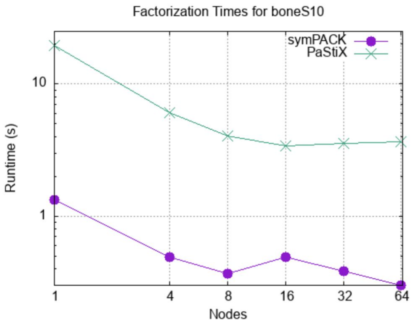


Figure 9: Strong scaling of symPACK's Cholesky factorization on boneS10

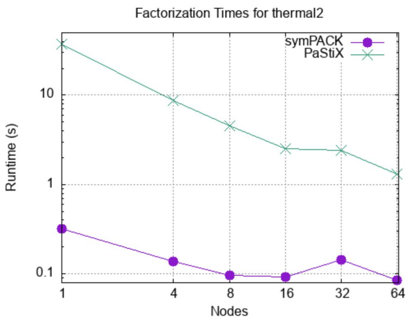


Figure 11: Strong scaling of symPACK's Cholesky factorization on thermal2

Matrices from SuiteSparse matrix collection			
Name	Description	*n*	*nnz*
Flan_1565	3D model of a steel flange	1,564,794	114,165,372
boneS10	3D trabecular bone	914,898	40,878,708
thermal2	steady state thermal	1,228,045	8,580,313

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

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