CS 5220 – Project 3: Shortest Paths

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1 Introduction

In this assignment we develop a set of optimized and parallelized programs that compute the shortest path between all pars of vertices in a directed graph. In Section 2, we profile the release implementation which uses a repeated squares $O(N^3 \log N)$ algorithm. In Section 3, we describe the repeated squares algorithm in depth, and present two additional algorithms that we implemented: a blocked repeated squares algorithm and the Floyd−Warshall algorithm. In Section 4, we describe the three parallelization mechanisms we used: OpenMP, MPI, and a hybrid of the two. Finally in Section 5 and Section 6, we evaluate the performance of our implementations and conclude.

2 Profiling

The release implementation of all-pairs shortest paths is a naive implementation of repeated squares algorithm that uses OpenMP for parallelization. We profiled the release code using VTune Amplifier and the vectorization reports produced by `icc`.

2.1 VTune Amplifier

The profiling results produced by VTune Amplifier are shown in Figure 1 and Figure 2, which show that the release implementation spends most of its time inside the `square` function. The majority of the time in `square` is spent accessing the `l` array. Although in contrast to many applications that spend most of their time on computation, this is unsurprising as the only computation done in the release implementation is a single addition and comparison.

These results suggest that we optimize our implementations to have good memory access patterns to take full advantage of the cache as much as possible. This optimization will be discussed in detail in Section 3.

Function	Module	CPU Time
square	omp.x	41.807s
__kmp_barrier	libiomp5.so	13.993s
__kmpc_reduce_nowait	libiomp5.so	6.397s
__kmp_fork_barrier	libiomp5.so	2.962s
__intel_ssse3_rep_memcpy	omp.x	0.040s
fletcher16	omp.x	0.030s
gen_graph	omp.x	0.020s
__kmp_join_call	libiomp5.so	0.010s
genrand	omp.x	0.010s

Figure 1: A snippet of the vectorization report produced by VTune Amplifier that shows the longest running functions.

```
Source Line  Source                                                              CPU Time
-----------  ------------------------------------------------------------------  --------
41           int square(int n,               // Number of nodes
42                      int* restrict l,     // Partial distance at step s
43                      int* restrict lnew)  // Partial distance at step s+1
44           {
45               int done = 1;
46               #pragma omp parallel for shared(l, lnew) reduction(&& : done)
47               for (int j = 0; j < n; ++j) {
48                   for (int i = 0; i < n; ++i) {                                0.020s
49                       int lij = lnew[j*n+i];                                   0.030s
50                       for (int k = 0; k < n; ++k) {                            8.072s
51                           int lik = l[k*n+i];                                 25.646s
52                           int lkj = l[j*n+k];
53                           if (lik + lkj < lij) {                               3.644s
54                               lij = lik+lkj;
55                               done = 0;                                        4.395s
56                           }
57                       }
58                       lnew[j*n+i] = lij;
59                   }
60               }
61               return done;
62           }
```

Figure 2: A snippet of the vectorization report produced by VTune Amplifier that shows the longest running sections of the `square` function.

2.2 Vectorization Reports

A snippet of the `icc` vectorization report is shown in Figure 3, which shows that most loops in the release implementation are vectorized. However, the vectorized loops have unaligned memory accesses because `l` and `lnew` are not allocated into aligned memory. This suggested that we optimized our code to allocate memory at aligned addresses.

```
LOOP BEGIN at path.c(108,5) inlined into path.c(258,5)
   remark #15388: vectorization support: reference l has aligned access   [ path.c(110,13) ]
   remark #15388: vectorization support: reference l has aligned access   [ path.c(110,13) ]
   remark #15300: LOOP WAS VECTORIZED
   remark #15448: unmasked aligned unit stride loads: 2
   remark #15449: unmasked aligned unit stride stores: 1
   remark #15475: --- begin vector loop cost summary ---
   remark #15476: scalar loop cost: 14
   remark #15477: vector loop cost: 1.250
   remark #15478: estimated potential speedup: 9.830
   remark #15479: lightweight vector operations: 10
   remark #15488: --- end vector loop cost summary ---
LOOP END
```

Figure 3: `icc` vectorization report.

3 Algorithms

In this section, we describe the three algorithms we have implemented to compute all-pairs shortest paths.

3.1 Repeated Squares

The release implementation uses a simple repeated squares (RS) dynamic programming algorithm. Let l_{ij}^s represent the length of the shortest path from vertex i to vertex j of at most length 2^s. RS relies on the following recurrence:

$$l_{ij}^{s+1} = \min_k \left(l_{ik}^s + l_{kj}^s \right)$$

The base case l_{ij}^0 is the weight of the edge from vertex i to vertex j or ∞ if no such edge exists. This recurrence is nearly identical to the formula used to compute the square of a matrix A:

$$a_{ij}^2 = \sum_k a_{ik} a_{kj}$$

The algorithm initializes a distance matrix L^0 and iteratively computes L^{s+1} by squaring L^s. The algorithm terminates once squaring L reaches a fixpoint; that is, once $L^2 = L$. Each squaring requires $O(N^3)$ operations where N is the number of vertices in the graph and the side-length of L. A shortest path can be of at most length N, so the algorithm terminates after at most $\log N$ iterations. Thus, the worst-case running time of RS is $O(N^3 \log N)$.

3.2 Blocked Repeated Squares

The release implementation of RS uses a naive matrix multiplication kernel to square L. We developed an optimized matrix multiplication kernel that implements a variety of optimizations. We use this kernel in an optimized repeated squares implementation that we call BLOCK. In this subsection, we describe the optimizations implemented by BLOCK.

Blocking A naive matrix multiplication kernel has very poor cache locality. BLOCK implements a blocked matrix multiplication to greatly improve cache locality. The optimal block size of 128 was found empirically.

Copy Optimization When BLOCK multiplies two sub-blocks, it first copies them into a smaller, aligned buffer, which allows the compiler to more aggressively vectorize loops over the sub-blocks and it makes memory accesses to the sub-blocks much more regular.

Compile-Time Loop Bounds If the size of a matrix is not divisible by the size of a block, then not all sub-blocks have the same size, and the size of a sub-blocks is only known at runtime. When BLOCK multiplies two sub-blocks, it first checks to see if they are full-sized blocks, and if they are, it multiplies them using a kernel whose loop bounds are known at compile-time. By knowing loop-bounds at compile time, the compiler more aggressively optimizes this code path. If the sub-blocks are not full-sized blocks, then it multiplies them using loops with bounds known at runtime. Since most blocks are full-sized blocks, BLOCK often performs block multiplication with the fully optimized kernel.

Vectorization BLOCK organizes all loops and array accesses to be fully vectorized.

3.3 Floyd-Warshall

The Floyd-Warshall algorithm (FW) is a dynamic programming algorithm developed by Robert Floyd and Stephen Warshall in the 1960's. Consider a directed graph with N nodes

ordered $1, \ldots, N$. Let $l_{i,j}^k$ be the length of the shortest path from vertex i to vertex j using only intermediate nodes from $\{1, \ldots, k\}$ or ∞ if no such path exists. FW relies on the following recurrence:

$$l_{i,j}^{k+1} = \min\left(l_{i,j}^k, l_{i,k+1}^k + l_{k+1,j}^k\right)$$

The base case $l_{i,j}^0$ is the weight of the edge from vertex i to vertex j or ∞ if no such edge exists. FW initializes L^0 and iteratively computes L^{k+1} from L^k using the above recurrence. L^{k+1} can be computed in $O(N^2)$ time and the algorithm terminates when it computes L^N. Thus, the algorithm runs in $O(N^3)$ time.

4 Parallelization

We parallelized the RS, BLOCK, and FW algorithm using three parallelization mechanisms: OpenMP, MPI, and a hybrid of the two. In this section, we describe how each mechanism was used for parallelization in detail.

4.1 OpenMP

Parallelizing each algorithm using OpenMP is simply a matter of annotating the outer loop of respective `square` functions with `#pragma omp parallel for`. The implementations of RS, BLOCK, and FW using OpenMP are in `rs-omp.c`, `block-omp.c`, and `fw-omp.c`.

4.2 MPI

Parallelizing the algorithms using MPI requires decomposing the problem into sub parts, which is similar to the idea of domain decomposition from the last project. We drew inspiration from previous work about distance-vector routing using the Bellman−Ford algorithm in determining shortest distances between routers. In that algorithm, each router sends its distances to all other routers (each time there is a change) to its neighbors which then use that information to update their own distances. This continues until no routers have changed distances.

In our case, we probably do not have a single thread per node, as there may not be enough hardware threads available. Instead, each "router" is an MPI rank and is responsible for a set of nodes rather than a single node. Each MPI rank calculates the minimum distance to each of its nodes from all other nodes going through each node between 1 and N.

For RS and BLOCK, each rank also determines if any distances in its range have changed. All MPI ranks then synchronize to gather distances from others and determine if any distances have changed. If none have changed, then the algorithm terminates and the "master" rank (rank 0) outputs checksum and timing information. To synchronize the distances across all ranks, we use `mpi_allgather` which sends each rank's distances to all other ranks and collects them from every rank including itself into a single buffer. To determine if any distances have changed, we use `mpi_allreduce` on each rank's "done" variable. The implementation of FW must synchronize for every iteration of k, and does not need to check if its finished as the algorithm will always finish in the same number of loops (N).

The implementations of RS, BLOCK, and FW using MPI are in `rs-mpi.c`, `block-mpi.c`, and `fw-mpi.c`.

4.3 Hybrid

MPI and OpenMP interact seamlessly when put together, making it easy to combine our MPI implementation with the release OpenMP implementation. Given a fixed number of MPI ranks r, and p available threads, then each MPI rank will have access to $\frac{p}{r}$ threads which can be used in OpenMP parallel sections of code. This means we do not take full advantage of all threads available to us if p is not divisible by r. We implemented a hybrid version of each algorithm (by combining our MPI implementation with the OpenMP portitons of the original implementation) in `rs-hybrid.c`, `block-hybrid.c`, and `fw-hybrid.c`.

5 Evaluation

We evaluated our MPI and hybrid implementations of RS, BLOCK, and FW with strong scaling studies across a range of problem sizes. For RS and BLOCK, we used a baseline of RS-OMP, which has access to 24 threads. For FW, we used a baseline of FW-OMP, which has access to 24 threads. For RS and BLOCK, we also performed a weak scaling study with a constant amount of work per thread corresponding to a graph of size $N = 500$.

5.1 RS

5.1.1 MPI

In strong scaling (Figure 4a), we can see that increasing the number of MPI ranks does increase speedup as a general trend, but for any problem size larger than 960 the speedup does not get above 1. Further there is a drop when ranks goes beyond 12, due to the increased MPI overhead across 2.

In weak scaling (Figure 4b), we can see that the performance per thread drops as speedup falls, due to the increased overhead of synchronizing with 1 more thread as we add 1 more thread.

5.1.2 Hybrid

In strong scaling (Figure 4c), we can see that increasing the number of MPI ranks (which in turn decreases the number of OMP threads per rank) has mixed speedup for most n. When the number of MPI ranks is less than 10 we sometimes have speedup larger than 1, but as we go beyond 10 and 12 speedup drops off. This is because of increased MPI overhead across 2 chips and the hybrid codes inability to take advantage of all possible threads when there are more than 12 MPI ranks.

The hybrid implementation drops speedup more rapidly than the MPI implementation for weak scaling (Figure 4d). This is probably because inability to take advantage of the full 24 hardware threads when the number of ranks does not divide 24 perfectly.

5.2 Block

5.2.1 MPI

Our block implementation with MPI has much higher speedups than our repeated squares with MPI. It crosses 5x speedup for almost all problem sizes at some point (Figure 4e). In

particular we see that smaller problems (960 being a notable outlier) with larger speedup. Speedup increases until 12 and then drops (due to multiple chips) and then increases again.

In weak scaling (Figure 4f), we can see that the speedup is around 1 when the number of threads is up to 6, and then is between 0.75 and 0.9 when the number of threads is more than 6 after a sudden drop at 7, which might be explained by the increased overhead of synchronizing with more threads as well.

5.2.2 Hybrid

Our block implementation with hybrid has much higher speedups than our repeated squares with hybrid (Figure 5a), however the speedups are smaller than for MPI. Speedup varies between sizes, particular with fewer than 12 ranks due to not always taking advantage of all 24 hardware threads. Similarly, problem size 960 has much more speedup than other sizes.

In weak scaling (Figure 5b), we can see that the speedup is decreasing as a general trend although it goes up and down alternatively, which might be explained by the increased overhead of synchronizing with more threads again.

5.3 FW

5.3.1 MPI

The performance of FW with MPI is typically poor (Figure 5c), which makes sense because of the increased workload of synchronizations ($O(N)$) in FW compared to $O(\log(N))$ in RS. The speedup slowly increases for all sizes, but never surpasses one in all sizes except for the smallest one (480); in fact, all but 480 and 960 never cross 0.5x speedup.

5.3.2 Hybrid

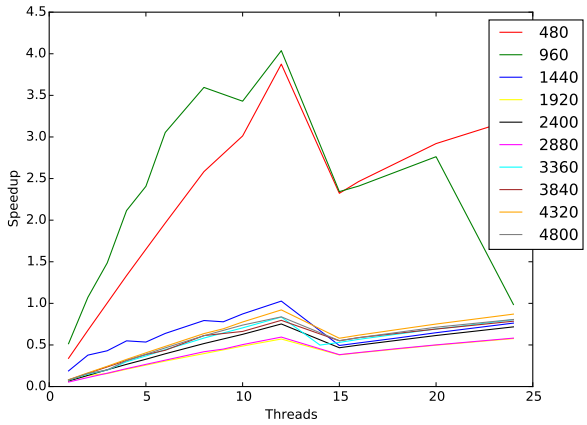
The performance of FW with hybrid actually tends to decrease as ranks increase (Figure 5d), which makes sense because of the increased workload of synchronizations again along with inability to use all 24 hardware threads.

At last, we compare the performance of all algorithms excluding fw-mpi and fw-hybrid in Figure 6 below, in order to have a big picture of what did work and what did not work.

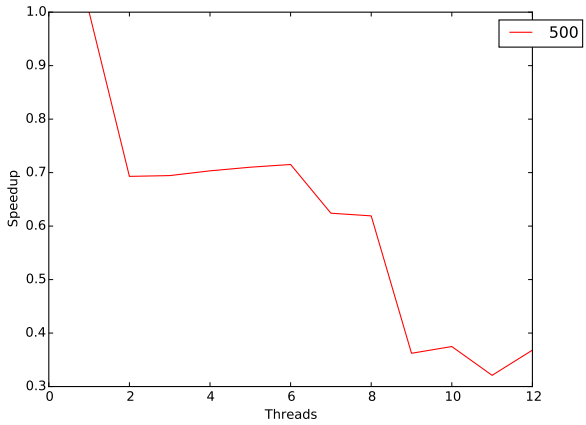
6 Conclusion

In conclusion, we have implemented an optimized and parallelized implementation of RS, BLOCK, and FW using OpenMP, MPI, and a hybrid of the two. The optimization of the implementations was guided by profiles generated by VTune Amplifier and `icc`. Ultimately, our BLOCK implementations are roughly an order of magnitude faster than the release implementation and our other implementations for large graphs.

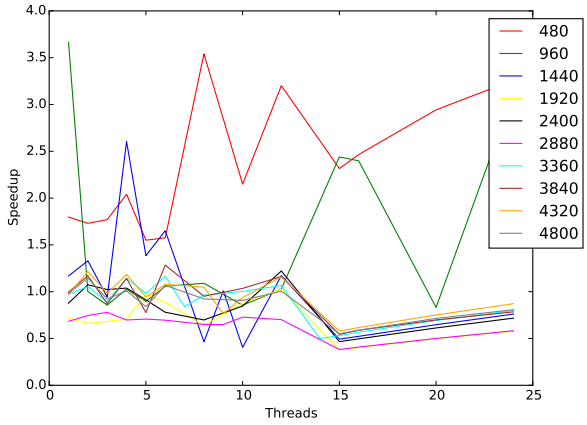
Perhaps the most important thing we learn from this project is that we should be aware of the synchronization cost when we work on a parallel problem. The Floyd-Warshall (FW) which has $O(N^3)$ in computation and $O(N)$ in synchronization, is beaten by the repeated squares (RS) which has $O(N^3 \log N)$ in computation and $O(\log N)$ in synchronization. It is always a good manner to trade-off the computation and synchronization when we evaluate an algorithm in the parallel world.



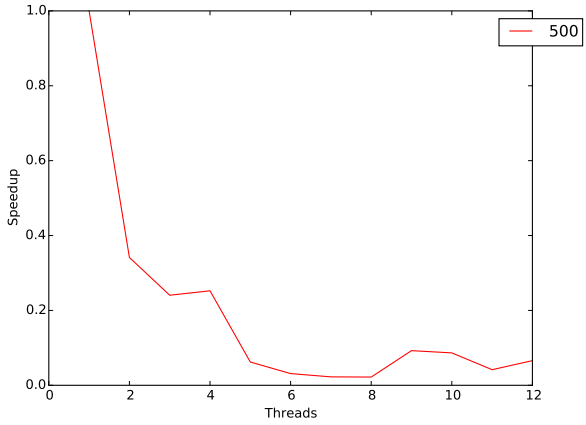
(a) RS-MPI strong scaling (RS-OMP baseline)



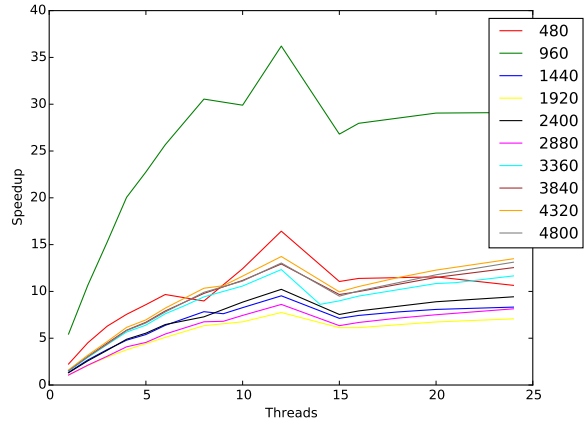
(b) RS-MPI weak scaling



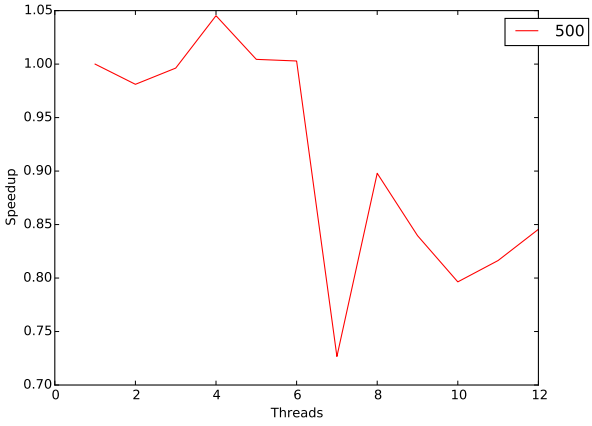
(c) RS-HYBRID strong scaling (RS-OMP baseline)



(d) RS-HYBRID weak scaling

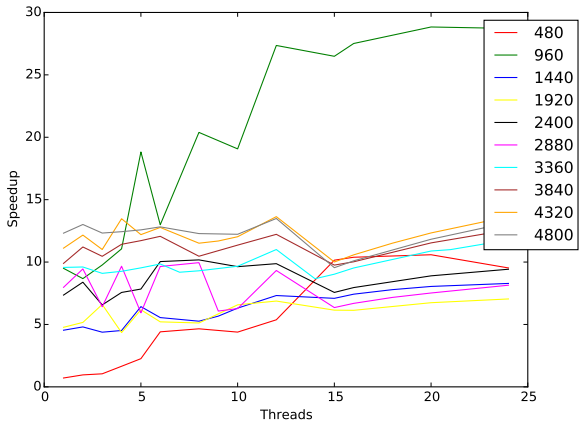


(e) BLOCK-MPI strong scaling (RS-OMP baseline)

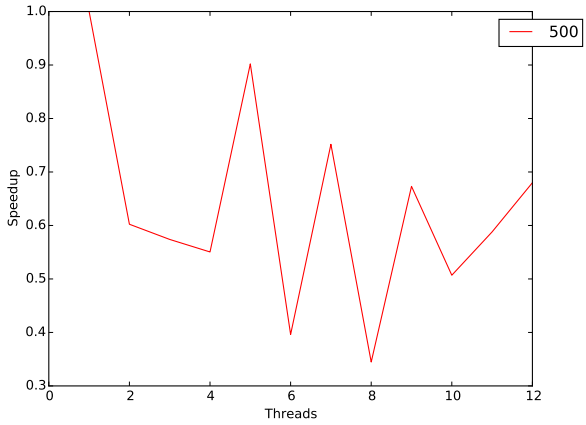


(f) BLOCK-MPI weak scaling

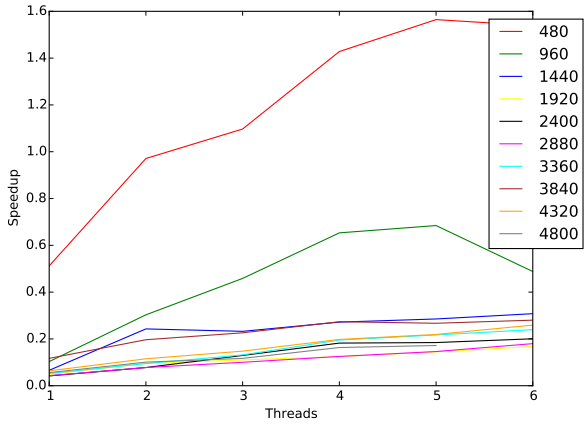
Figure 4: RS-MPI, RS-HYBRID, and BLOCK-MPI



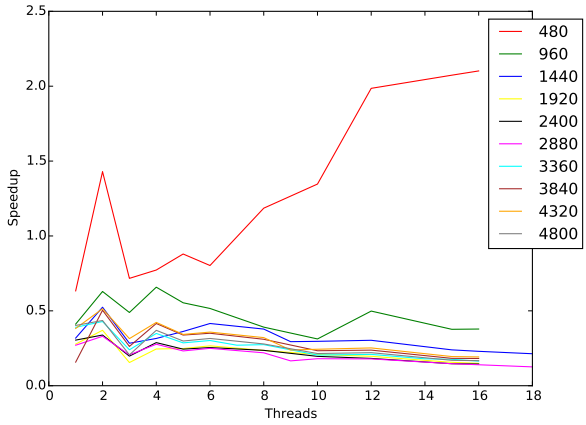
(a) BLOCK-HYBRID strong scaling (RS-OMP baseline)



(b) BLOCK-HYBRID weak scaling



(c) FW-MPI strong scaling (FW-OMP baseline)



(d) FW-HYBRID strong scaling (FW-OMP baseline)

Figure 5: BLOCK-HYBRID, FW-MPI, and FW-HYBRID

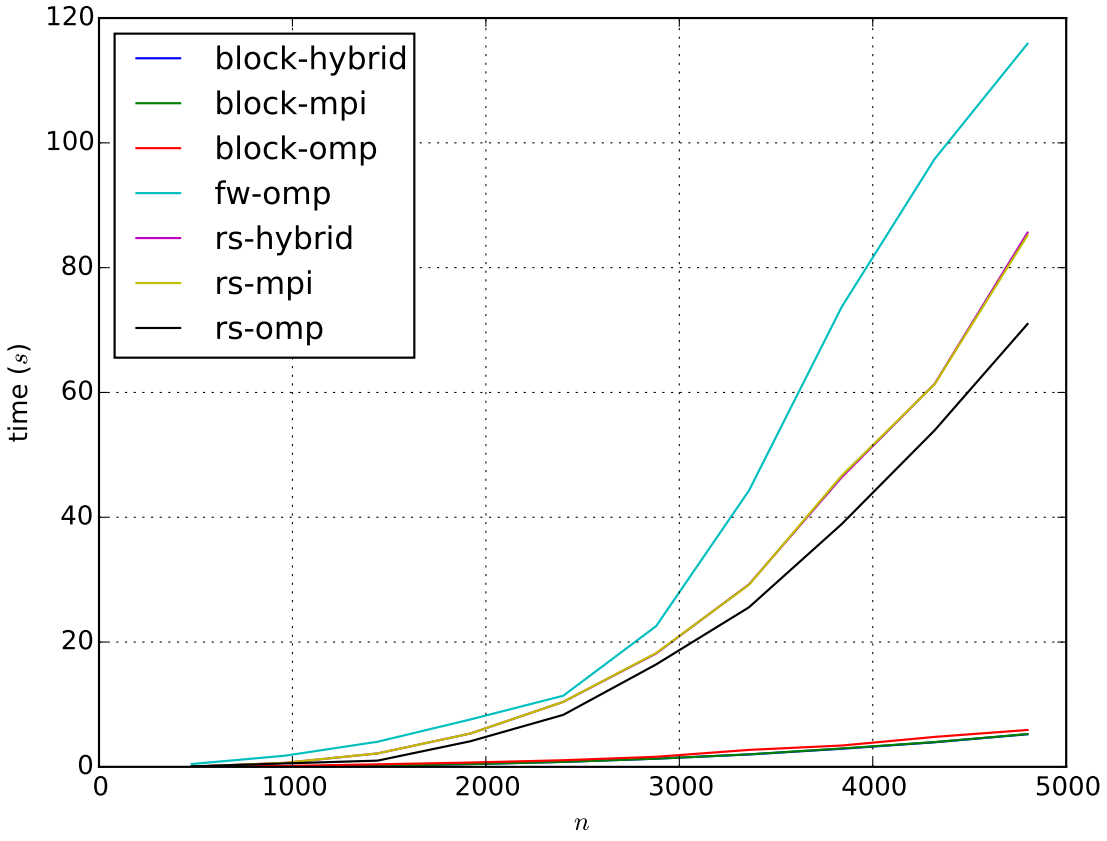


Figure 6: Performance comparison of all algorithms excluding FW-MPI and FW-HYBRID.