OpenMP and pthreads Assignment

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1) Lower-Upper Decomposition

LU Decomposition is a technique to factorise a matrix A into the product of one upper (U) and one lower (L) triangular matrix. The pseudocode provided in the assignment is for LU decomposition with partial pivoting (it uses Gaussian Elimination)which only allows us to permute the rows. A permutation vector P is updated after the rows are interchanged. At the end the following condition should be satisfied:

$$PA = LU$$

Pseudocode 1 inputs: a(n,n) 2 outputs: $\pi(n)$, l(n,n), and u(n,n)Initialization 4 initialize π as a vector of length n 5 initialize u as an n x n matrix with 0s below the diagonal 6 initialize l as an n x n matrix with 1s on the diagonal and 0s above the diagonal 7 for i = 1 to n $\pi[i] = i$ 10 for k = 1 to n 11 max = 0for i = k to n12 13 if max < |a(i,k)|**Find Max** max = |a(i,k)|14 15 k' = iif max == 0 16 17 error (singular matrix) 18 19 swap $\pi[k]$ and $\pi[k']$ **Row Pivoting** 20 swap a(k,:) and a(k',:)swap l(k,1:k-1) and l(k',1:k-1)21 u(k,k) = a(k,k)22 23 for i = k+1 to n 24 25 l(i,k) = a(i,k)/u(k,k)Update L and Uu(k,i) = a(k,i)26 27 for i = k+1 to n 28 29 for j = k+1 to n Update A a(i,j) = a(i,j) - l(i,k)*u(k,j)30 31 32 Here, the vector π is a compact representation of a permutation matrix p(n,n), 33 which is very sparse. For the ith row of p, $\pi(i)$ stores the column index of 34 the sole position that contains a 1.

All the major steps have been labelled in figure above.

Initialization

Matrix A is initialised with random double values and the 0s were positioned above and below the diagonals for L and U. This can be achieved with two nested for-loops (complexity = $O(n^2)$). π (compact representation of P) is initialised with the index values (possible in one for loop) (complexity = O(n)).

Find Max

We iterate over all the columns and find the max absolute value in k^{th} column below the diagonal. The value is stored in **max** and the row (ith) in which it was found is stored in **k**'. One for loop is required for each column (two-nested loops). (complexity = $O(n^2)$)

Row Pivoting

When the absolute max value has been identified in the kth column, we swap the rows k and k' (where it was found). Depending on the implementation the complexity would vary. If we store A, L, U as 2-D matrices or use an array to store column pointers then this would require one for-loop. But if we use a pointer for each row then pointers for both the rows can be swapped in a single command.

Update L and U

The values below the diagonal in L need to be scaled. This is possible with one for-loop (complexity = O(n)).

Update A

This is the most important stage in the algorithm where Gaussian Elimination takes place and requires maximum time (>95%). There are three-nested for loops (complexity = $O(n^3)$) and during parallelization it would become important to determine the optimal order to reduce the runtime. This depends on concepts like cache hit/miss and shared memory. If we are storing the data as an array of n column pointers then the second loop (in i) should come before the jth loop as all the elements in a row can be loaded together. But if we are using column pointers then jth loop should come before ith loop. A significant reduction in runtime was observed after arranging the loops in the correct order.

Verification

L and U matrices obtained can be verified by finding the $L_{2,1}$ norm of |PA - LU| =Residual matrix. This value should be close to zero. This is not a part of the implementation and doesn't need to be parallelized.

2) Sequential Results

Time taken by different steps in the sequential implementation was measured for (n=4000).

	Time (seconds)	Percentage of total time (%)
Initialization	0.4	0.25
Find Max	0.15	0.10
Row Pivoting	3.9	2.48
Update \boldsymbol{L} and \boldsymbol{U}	0.92	0.58
Update A	152.03	96.59
Total	157.4	100

3) Implementation Details

Optimizations

The following optimizations were performed to increase the performance:

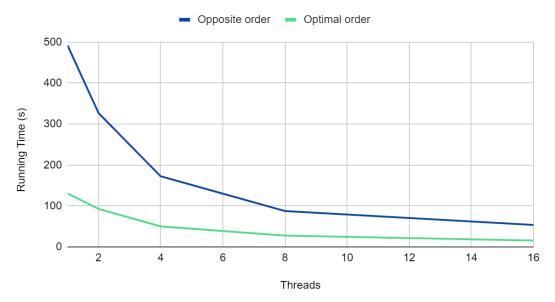
a) Choosing an appropriate data structure:

We had the option of choosing between 2-D arrays and n pointers to n-element data vectors. Representing them as n pointers is more efficient because it allows continuous memory access and negligible cache misses (because large chunks of continuous values can be accessed together). Now we have to make another decision about whether we want to store n-row pointers or n-columns pointers. Based on the pseudocode, column pointers are better. In *L* and *U Update* and *Find Max* sections of the code, loops iterate over elements of a column. If we store column pointers, then we will be able to access all the elements in a column at once (without cache miss).

As discussed above, in *Update A* step, the order of the loops is very important. In my case, since I had stored n-column pointers to n-element vectors, I ensured that the outer loop iterates on the columns and the inner loop iterates on the rows. I have compared the performance increase observed by changing the order in the following graph.

n = 4000	1	2	4	8	16
Opposite order	492.125	326.641	172.375	87.589	53.763
Optimal order	130.326	92.772	50.059	27.56	15.488

Difference in time because of cache hits and misses



- b) <u>Initialization</u>: drand48_r() was used to randomly initialise *A* of size (n x n) with doubles in the range (0,1). This required two nested loops, and the outer one was parallelized. *L*, *U*, and *P* can be initialised in the same loop.
- c) Find Max: The inner loop which iterates on the rows ($k \le i < n$) of the k^{th} column is parallelized.
- d) <u>Update L and U</u>: This is a single for loop that iterates on the columns and can be easily parallelized.
- e) <u>Update A</u>: Since there are no loop dependencies, there are two nested for loops inside the main loop which can be parallelized. This optimization has the maximum impact on the total runtime. (I have discussed the order above)

Performance Metrics

Total Runtime, speedup and efficiency were used to analyse the performance of our parallel programs.

$$S_t = \frac{T_1}{T_t}$$

$$\mathbf{eff}_t = \frac{T_1}{t * T_t}$$

CPU Information (HPC IITD)

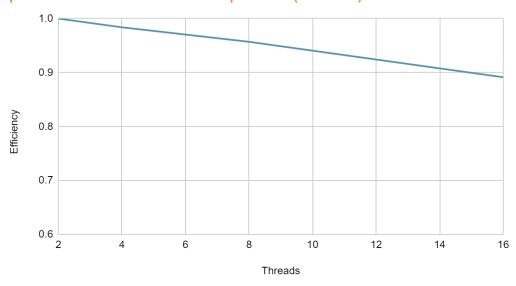
All the experiments were run on Intel Xeon Gold-6148 @ 2.40GHz.

4) pthreads Results

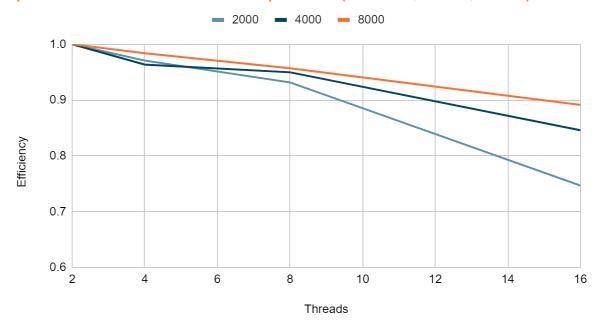
n threads	1 (Sequential)	2	4	8	16
4	0.000385	0.000486	0.000705	1	1
10	0.000784	0.000914	0.001355	0.002292	1
100	0.01006	0.010878	0.012822	0.021336	0.037941
2000	19.13316	9.853762	5.134571	3.202602	3.392026
4000	144.1306	74.7928	37.93881	21.2989	20.34223
8000	1133.601	576.0936	296.1369	158.9794	132.1915

Efficiency vs Number of Threads

pthreads: Performance Comparison (n=8000)

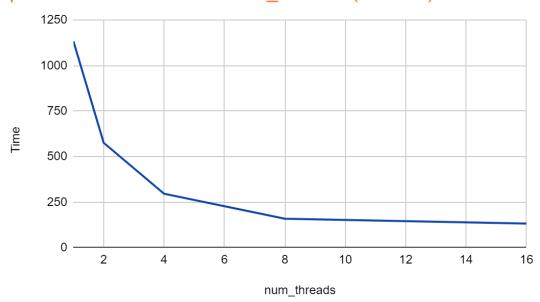


pthreads: Performance Comparison (n=2000, 4000, 8000)



Running time vs Number of Threads

pthreads: Variation with num_threads (n=8000)

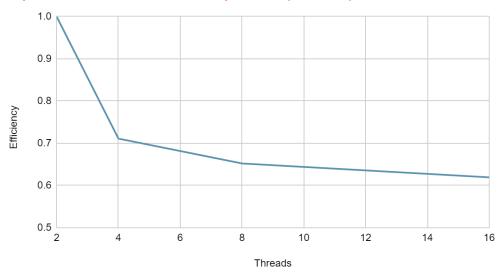


5) OpenMP Results

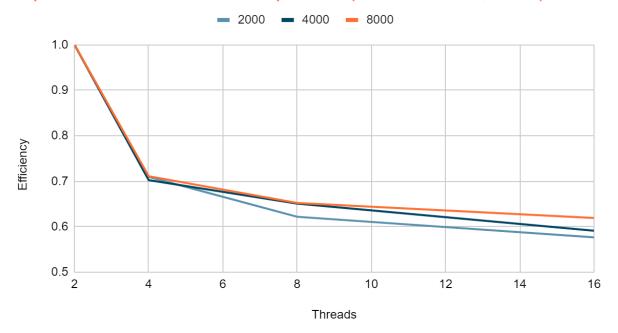
n threads	1 (Sequential)	2	4	8	16
4	0.000127	0.000200	0.000315	1	1
10	0.000163	0.000254	0.000266	0.000439	-
100	0.002691	0.003199	0.003072	0.003443	1.047959
2000	16.44022	11.58318	6.609498	3.563321	2.128477
4000	130.3256	92.77135	50.05883	27.56014	15.48819
8000	1028.224	722.9866	394.1345	207.5554	113.441

Efficiency vs Number of Threads

OpenMP: Performance Comparison (n=8000)

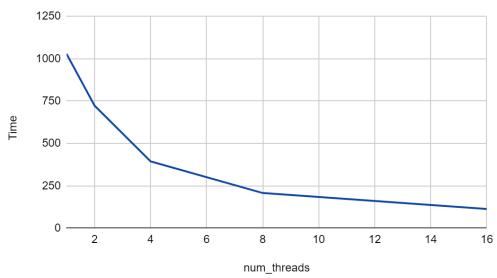


OpenMP: Performance Comparison (n=2000, 4000, 8000)



Running time vs Number of Threads

OpenMP: Variation with num_threads (n=8000)



OpenMP: Performance Comparison (n=2000, 4000, 8000)

