Cholesky Factorization on Tile Low-Rank Matrices for Distributed-Memory Systems

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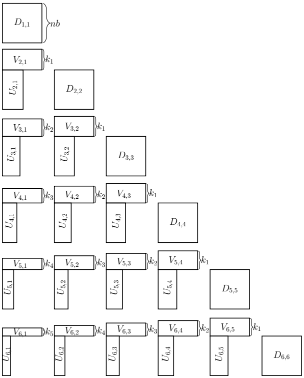

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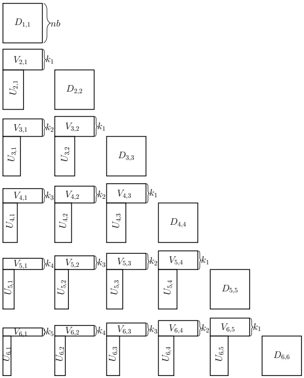

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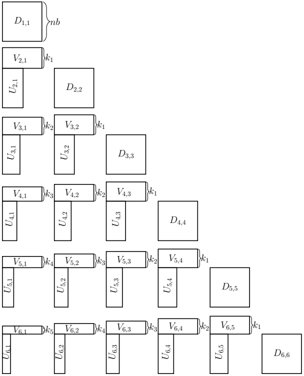

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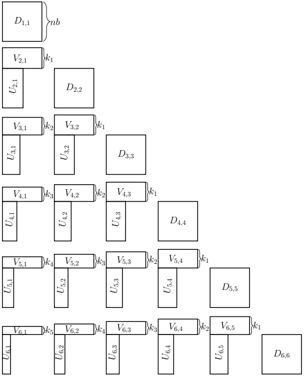

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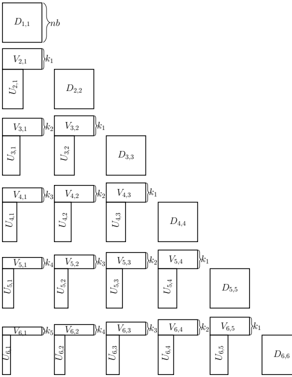

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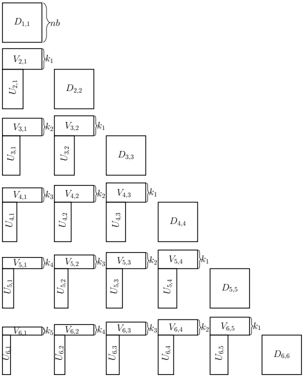

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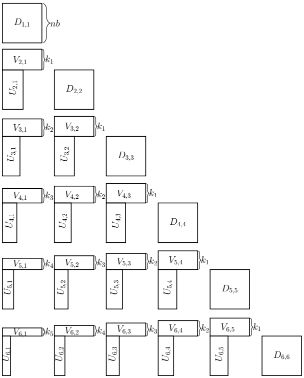
    - `pdpotrf` $\rightarrow$ `pdpotrf_tlr`?

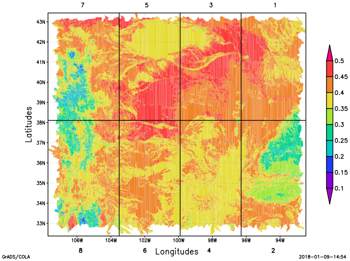


Climate/Weather Forecasting

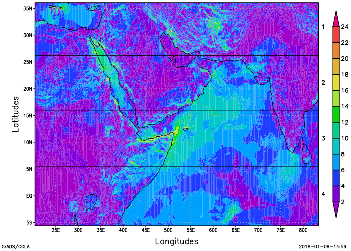
- Computational statistics: multivariate large spatial data sets in climate/weather modeling:

$$\ell(\boldsymbol{\theta}) = -\frac{1}{2}\mathbf{Z}^T\Sigma^{-1}(\boldsymbol{\theta})\mathbf{Z} - \frac{1}{2}\log|\Sigma(\boldsymbol{\theta})|$$

(a) Problem Definition.



(b) Soil moisture.



(c) Wind speed.

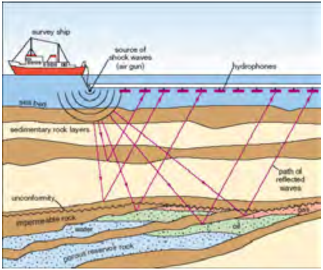
w/ Y. Sun and M. Genton

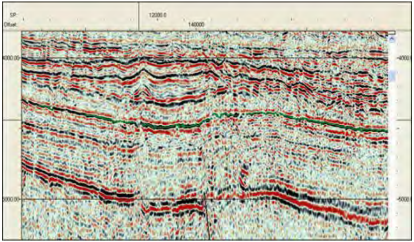
Earth Science

- Seismic imaging: Imaging the subsurface by solving the Helmholtz equation (acoustic wave equation):

$$(-\triangle - k^2)u(x, w) = s(x, w)$$

$k = \frac{w}{v(x)}$, w is the angular frequency, v(x) is the seismic velocity field, and u(x, w) is the time-harmonic wavefield solution to the forcing term s(x, w).





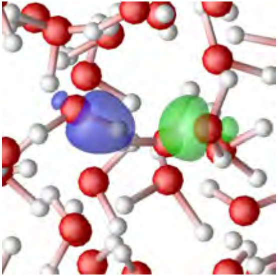
w/ S. Zampini

Materials Science

- Structural and vibrational analysis to problems in computational physics and chemistry like electronic and band structure calculations

$$(A - \lambda B)\, x = 0$$

(a) Problem Definition.



(b) Electronic structure.

Figure: Design of new materials.

w/ U. Schwingenschlogl

Common Properties

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- (Apparently) dense matrices
- Often data-sparse
    - Decay of parameter correlations with distance

Common Kernel: Cholesky Factorization (`potrf`)

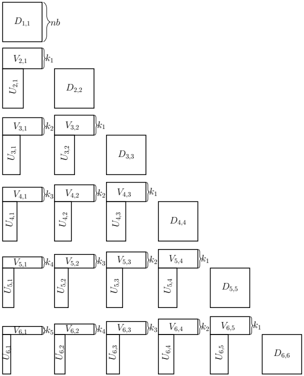
The Cholesky factorization of an $N \times N$ real symmetric, positive-definite matrix A has the form

$$A = LL^T,$$

where L is an $N \times N$ real lower triangular matrix with positive diagonal elements.

Ranks after Compression into Tile Low Rank (TLR) Format

- TLR format with varying ranks



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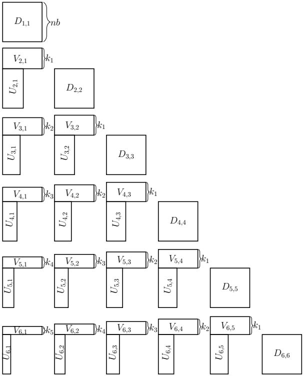
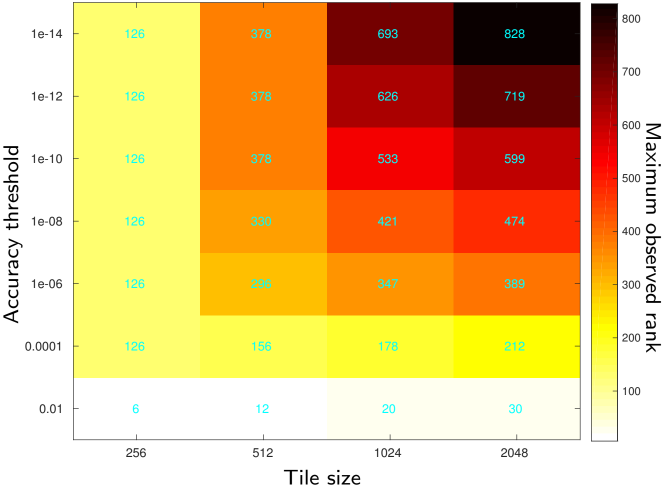


- Geospatial statistics, matrix size: 20000, block size: 500, accuracy threshold: 10^{-9}, 2D problem

	0					5					10					15				
0	500	133	47	35	154	83	44	33	59	49	38	30	40	37	33	29	33	32	30	27
	133	500	139	48	86	163	86	44	50	59	50	38	37	41	37	33	32	33	32	30
	47	139	500	137	44	86	153	83	38	49	59	49	33	37	41	37	30	32	33	32
	35	48	137	500	33	44	83	164	30	38	49	59	29	33	37	41	27	30	32	33
	154	86	44	33	500	134	48	34	165	84	44	33	59	50	38	30	41	37	33	30
5	83	163	86	44	134	500	139	48	86	163	85	44	49	59	50	38	37	40	37	33
	44	86	153	83	48	139	500	137	44	86	172	86	38	50	59	49	33	37	40	37
	33	44	83	164	34	48	137	500	33	44	86	166	30	39	50	59	29	33	37	41
	59	50	38	30	165	86	44	33	500	143	48	35	164	85	44	33	59	49	38	31
	49	59	49	38	84	163	86	44	143	500	143	48	84	159	87	44	49	59	49	38
10	38	50	59	49	44	85	172	86	48	143	500	134	44	86	156	81	38	49	58	49
	30	38	49	59	33	44	86	166	35	48	134	500	33	45	86	157	30	39	49	59
	40	37	33	29	59	49	38	30	164	84	44	33	500	138	48	35	162	86	44	33
	37	41	37	33	50	59	50	39	85	159	86	45	138	500	142	48	85	165	85	45
	33	37	41	37	38	50	59	50	44	87	156	86	48	142	500	133	44	84	159	85
15	29	33	37	41	30	38	49	59	33	44	81	157	35	48	133	500	33	44	81	157
	33	32	30	27	41	37	33	29	59	49	38	30	162	85	44	33	500	142	47	34
	32	33	32	30	37	40	37	33	49	59	49	39	86	165	84	44	142	500	136	48
	30	32	33	32	33	37	40	37	38	49	58	49	44	85	159	81	47	136	500	130
	27	30	32	33	30	33	37	41	31	38	49	59	33	45	85	157	34	48	130	500

Maximum Ranks after Compression into Tile Low Rank (TLR) Format

- Seismic imaging: 3D Helmholtz with $N = 128$ and $k = N \times 0.625$ (10 grid points / wavelength) on $\Omega = [0, 1]^3$
- Heat map



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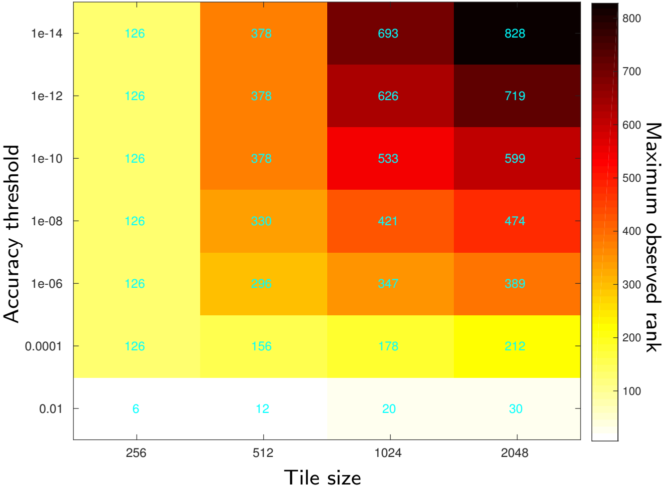

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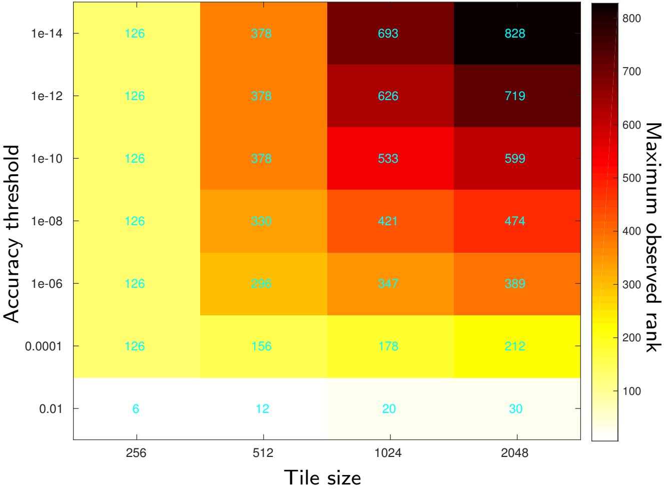

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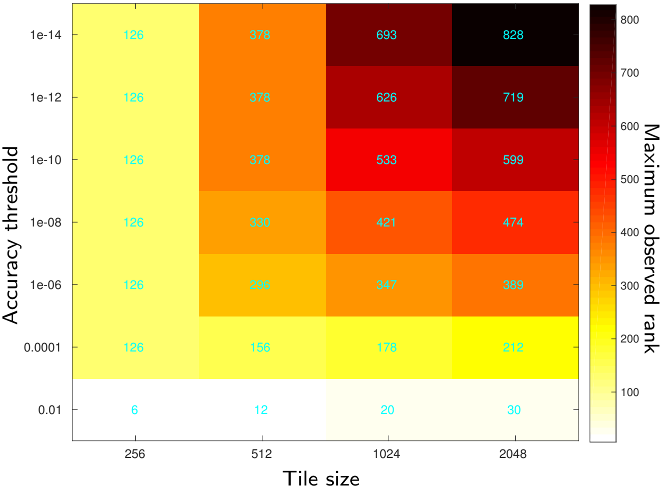
- value/color: maximum rank in TLR matrix for a specific tile size and accuracy



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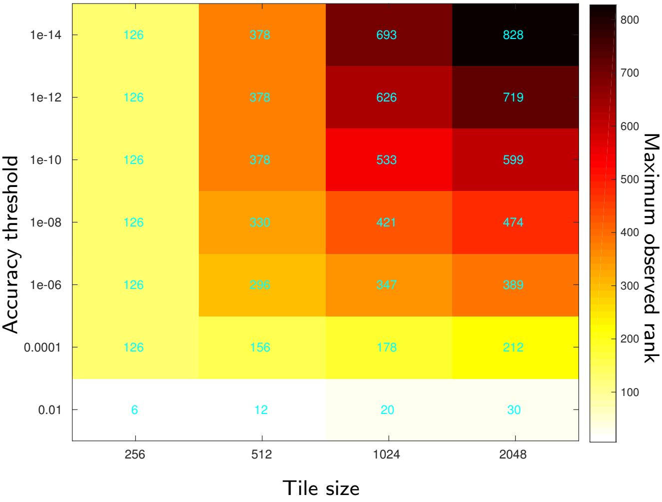
- lighter color: smaller maxrank



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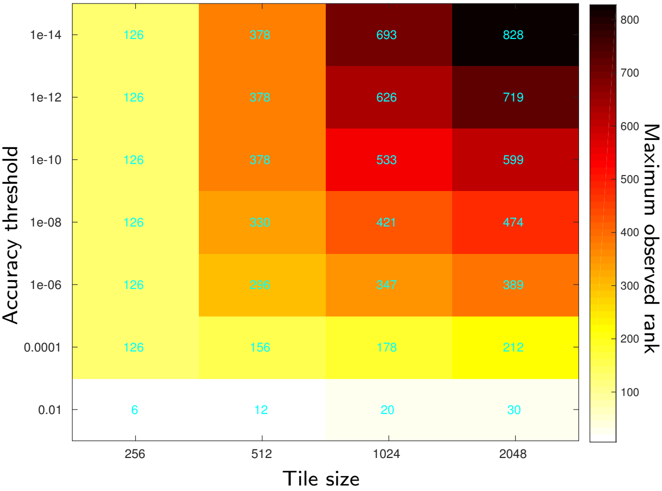
- Even for accuracy of 1e-14, ranks are smaller than half of tile size.



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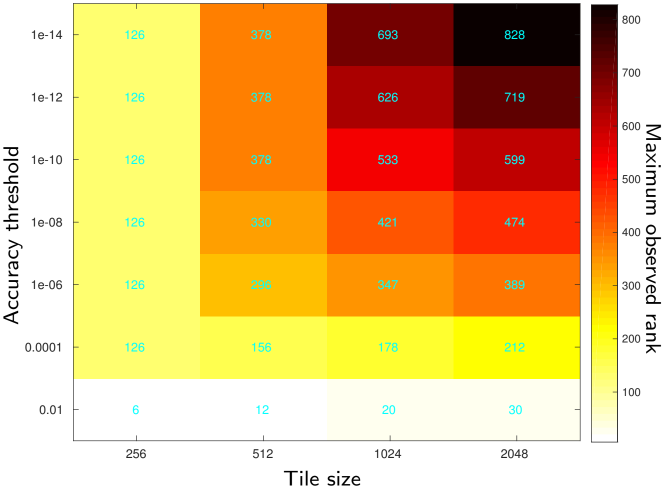
- Even for tiles of size 2048, rank is smaller than 2048/2=1024.



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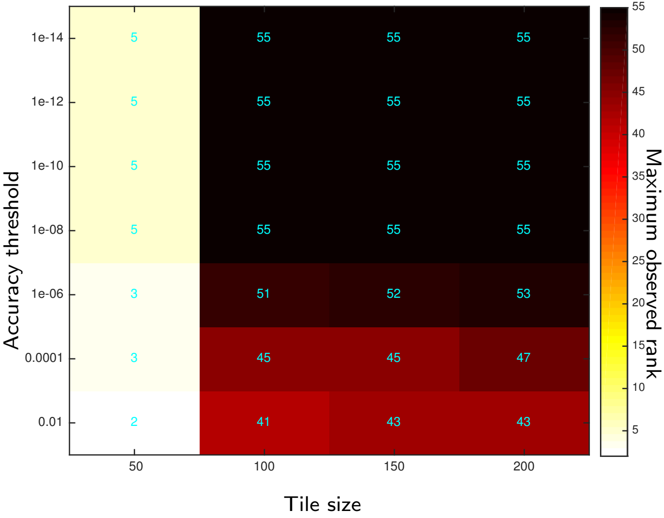

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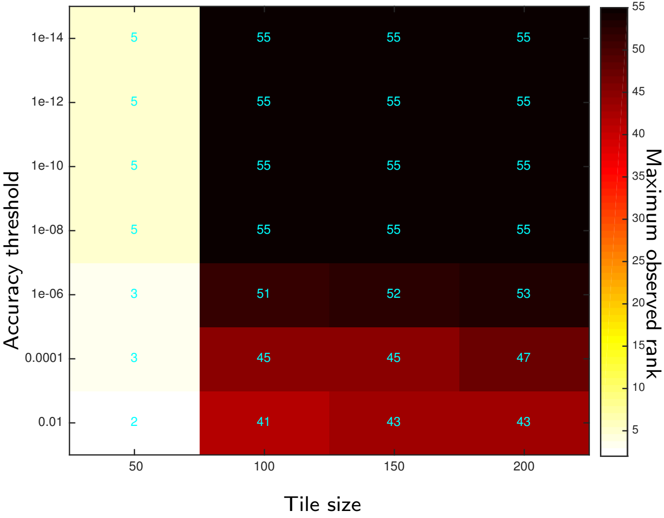
- x axis: different tile sizes



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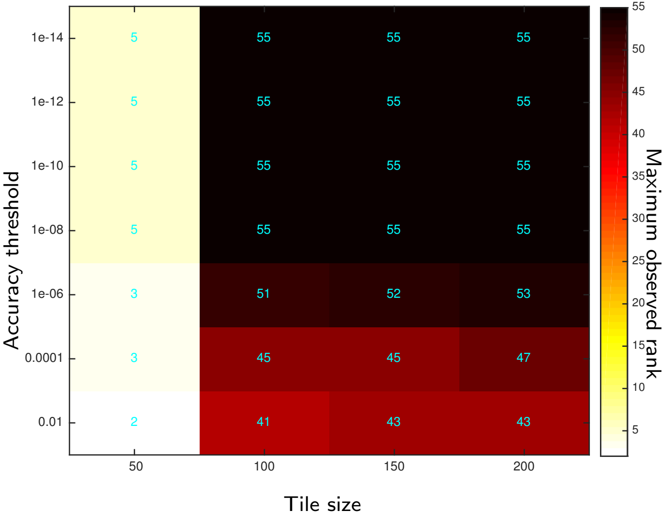

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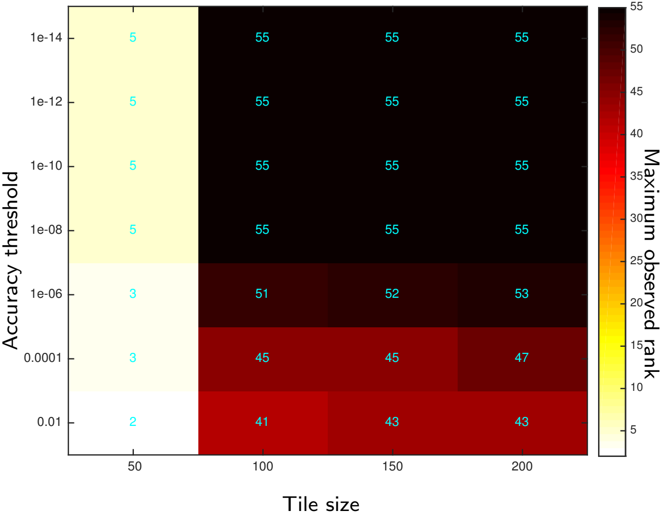

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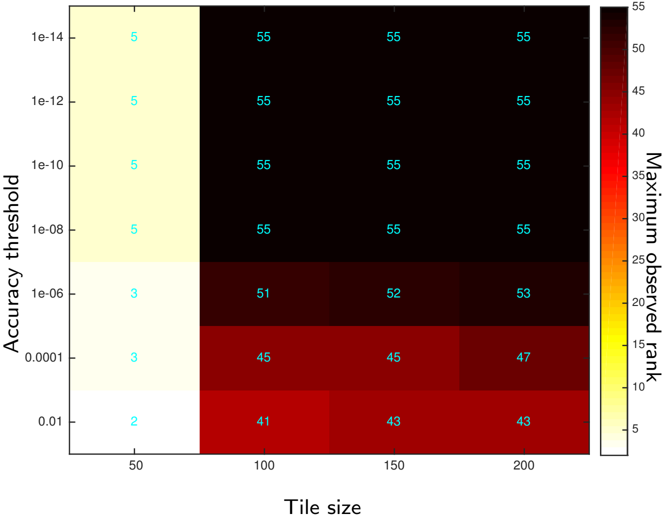

Maximum Ranks after Compression into Tile Low Rank (TLR) Format

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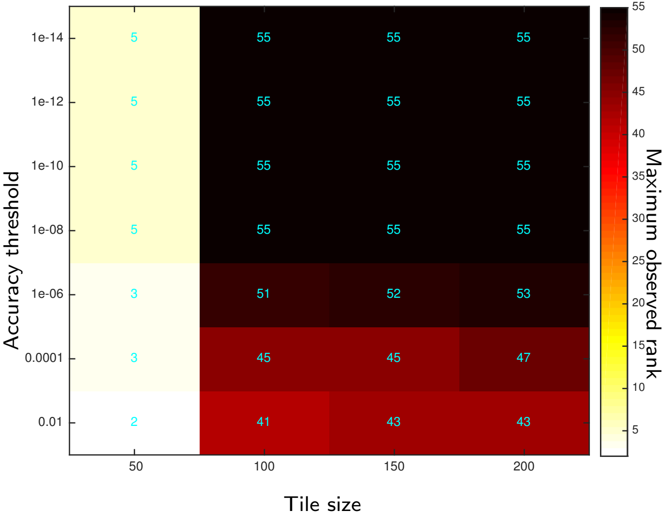
- Even for accuracy of 1e-14, maximum rank is 55 which is considerably smaller than tile size.



Maximum Ranks after Compression into Tile Low Rank (TLR) Format

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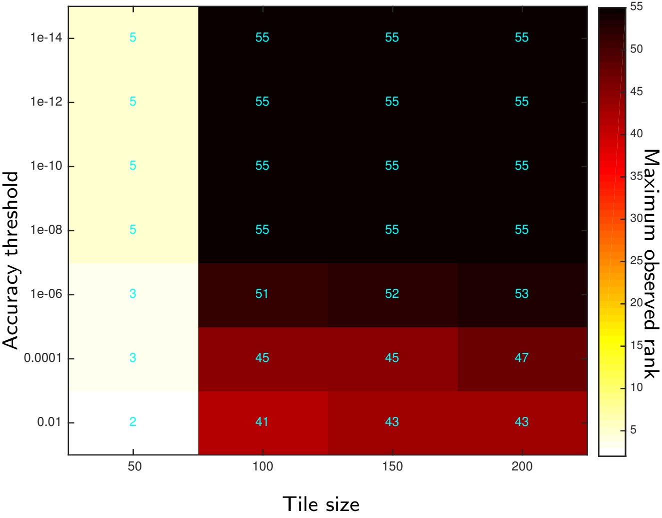
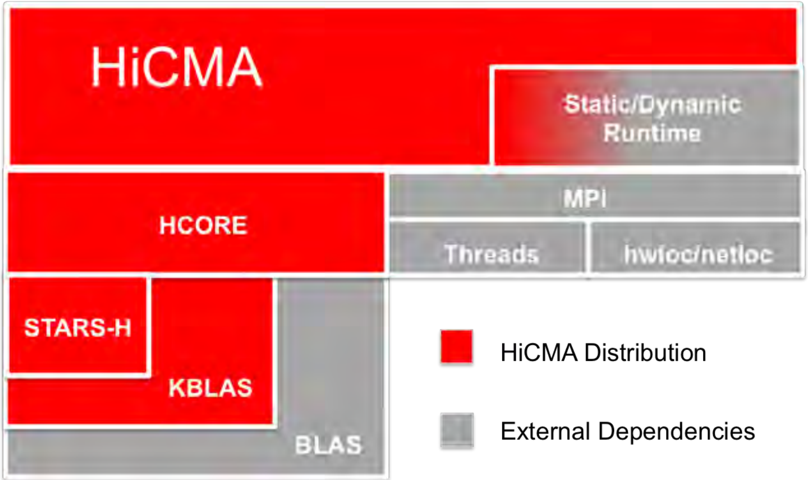
- Even for larger tiles, maximum rank is 55.

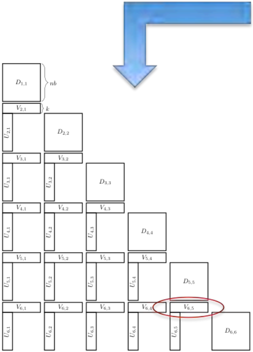


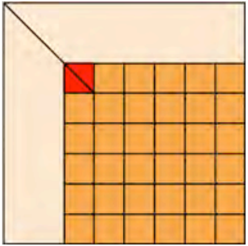
The HiCMA Library: Hierarchical Computations on Manycore Architectures



Available at http://github.com/ecrc/hicma

Dense Linear Algebra Renaissance

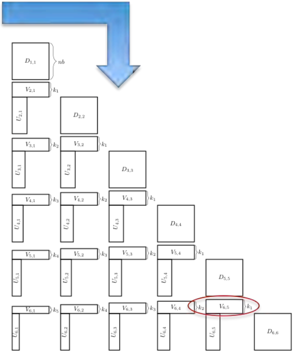




dense tiles
Cholesky: O(n³)

↓

tile low rank
Cholesky: O(kn²)



Fixed ranks
Preconditioners
Performance oriented

Fixed accuracy
Variable ranks
Dense/Sparse Direct Solvers

HiCMA dpotrf

The tile low-rank (TLR) Cholesky algorithm can be expressed with the following four computational kernels:

hcore_dpotrf: The kernel performs the Cholesky factorization of a diagonal (lower triangular) tile. It is similar to DPOTRF since the diagonal tiles are dense.

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`hcore_dtrsm`: The operation applies an update to an off-diagonal low-rank tile of the input matrix, resulting from factorization of the diagonal tile above it and overrides it with the final elements of the output matrix: $V_{(i,k)} = V_{(i,k)} \times D^{-1}_{(k,k)}$. The operation is a triangular solve.

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- `hcore_dsyrk`: The kernel applies updates to a diagonal (lower triangular) tile of the input matrix, resulting from factorization of the low-rank tiles to the left of it: $D_{(j,j)} = D_{(j,j)} - (U_{(j,k)} \times V^T_{(j,k)}) \times (U_{(j,k)} \times V^T_{(j,k)})^T$. The operation is a symmetric rank-k update.

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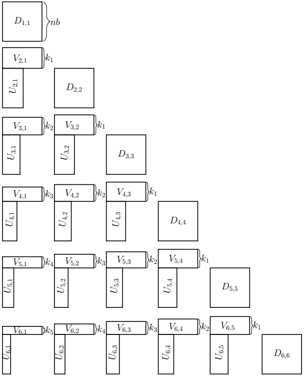
- **hcore_dgemm**: The operation applies updates to an off-diagonal low-rank tile of the input matrix, resulting from factorization of the low-rank tiles to the left of it. The operation involves two QR factorizations, one reduced SVD (depending on the rank and/or the accuracy parameter) and two matrix-matrix multiplications.

HiCMA dpotrf

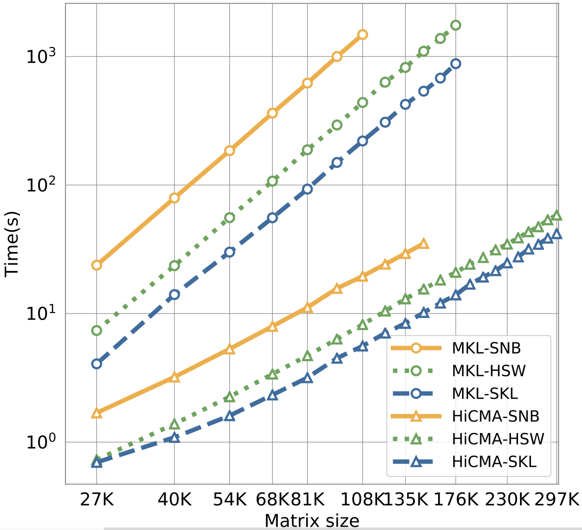
Algorithm 1 `hicma_dpotrf` (HicmaLower, D, U, V, N, nb, rank, acc)

```
p = N / nb
for k = 1 to p do
    #task access(read&write:D(k))
    hcore_dpotrf (HicmaLower, D(k))
    for i = k+1 to p do
        #task access(read:D(k), read&write:V(i,k))
        hcore_dtrsm (V(i,k), D(k,k))
    end for
    for j = k+1 to p do
        # task access(read:U(j,k), read:V(j,k), read&write:D(j))
        hcore_dsyrk (D(j), U(j,k), V(j,k))
        for i = j+1 to p do
            #task access(read:U(i,k),
                read:V(i,k)), read:U(j,k), read:V(j,k),
                read&write:U(i,j), read&write:V(i,j))
            hcore_dgemm (U(i,k), V(i,k), U(j,k), V(j,k), U(i,j), V(i,j), rank, acc)
        end for
    end for
end for
```



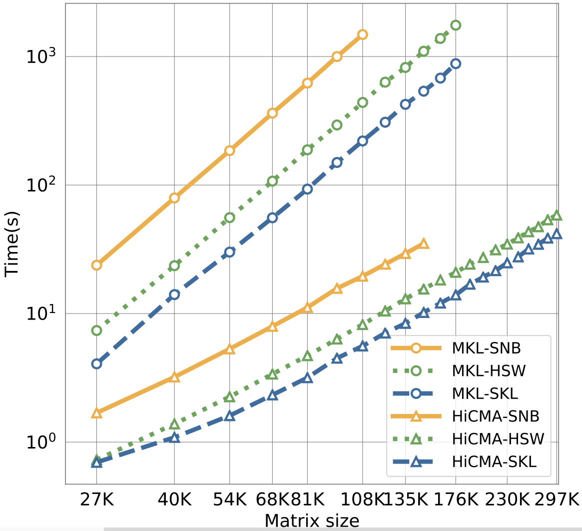
Dense vs TLR Cholesky on a Single Node

- Execution times for MKL dpotrf (dense) vs HiCMA dpotrf (TLR).
  Smaller the better.



Dense vs TLR Cholesky on a Single Node

- Execution times for MKL dpotrf (dense) vs HiCMA dpotrf (TLR). Smaller the better.
- Application: Geospatial statistic, square exp. kernel



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- Execution times for MKL dpotrf (dense) vs HiCMA dpotrf (TLR).
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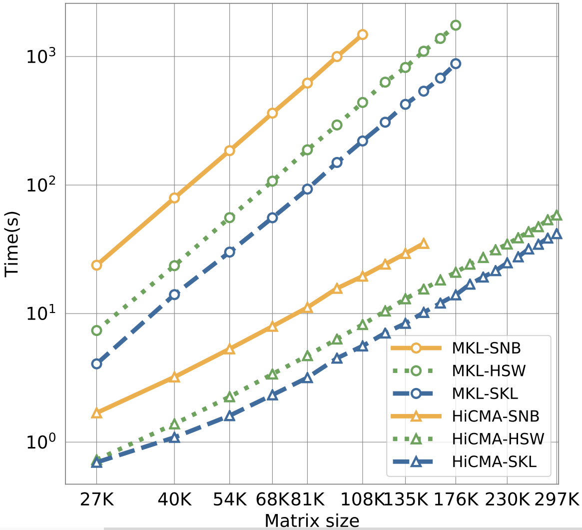
- Accuracy threshold: 10^{-9}. This accuracy level is enough for a large amount of cases encountered in the geospatial statistics application.



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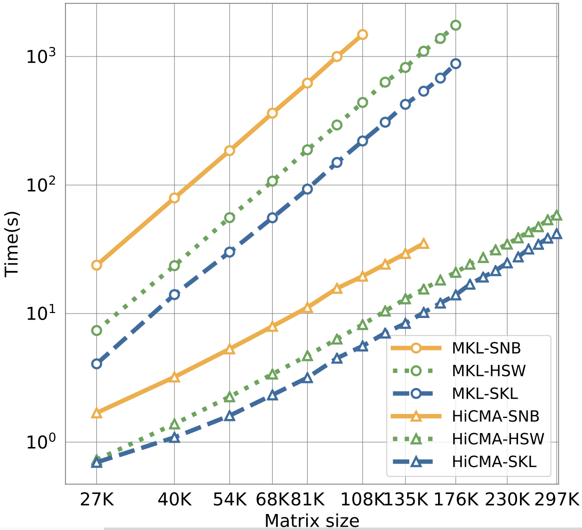
- StarPU (task-based runtime)



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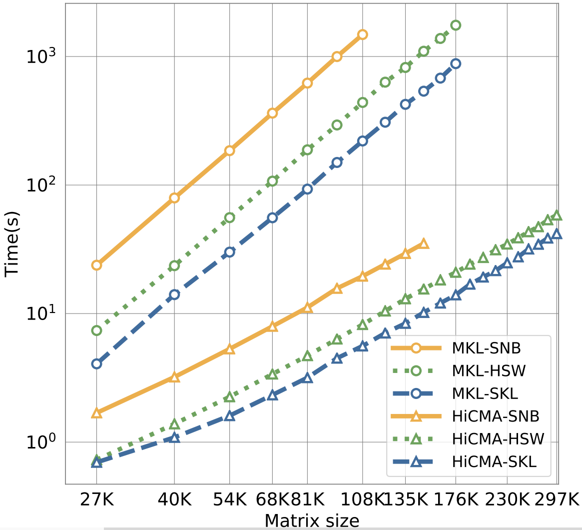
- Accuracy threshold: 10^{-9}. This accuracy level is enough for a large amount of cases encountered in the geospatial statistics application.
- StarPU (task-based runtime)
- Three architectures:
    - Sandy Bridge (SNB): AVX, 2.0GHz 2 sockets x 8 cores
    - Haswell (HSW): AVX2, 2.4GHz 2 sockets x 18 cores
    - Skylake (SKL): AVX512, 2.1GHz 2 sockets x 28 cores



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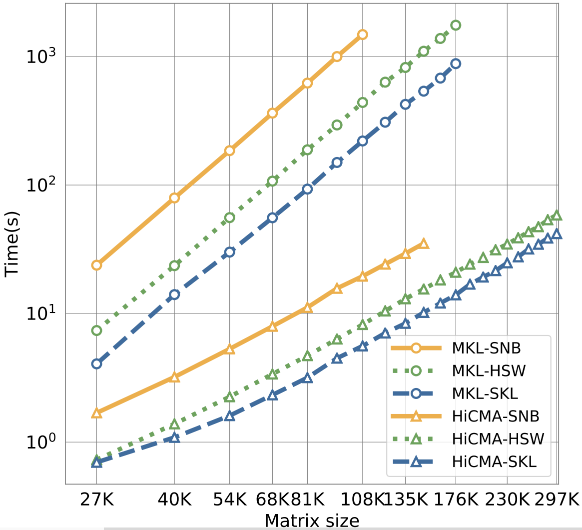
  Smaller the better.
- *x* axis (*log*-scale): different matrix sizes



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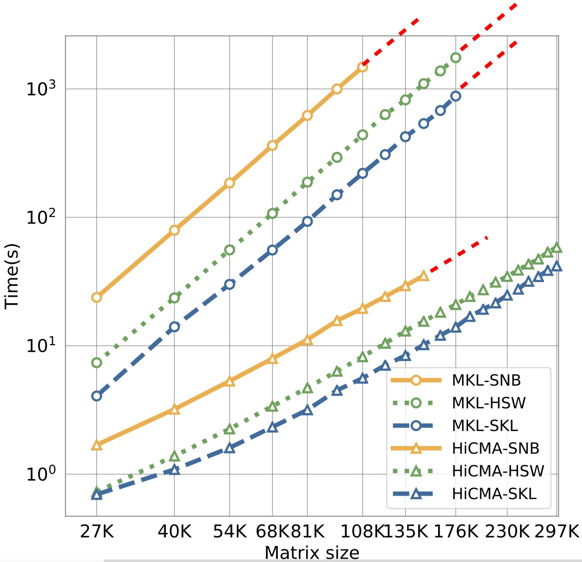
  Smaller the better.
- *x* axis (*log*-scale): different matrix sizes
  - Missing points due to not enough memory for larger matrices



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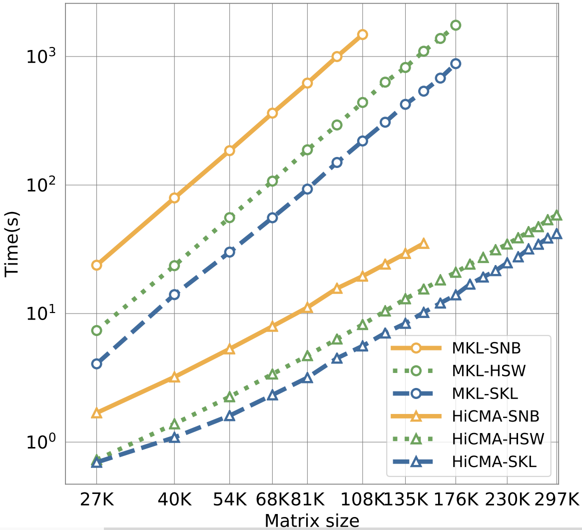
- *y* axis (*log*-scale): time of `dpotrf` in seconds



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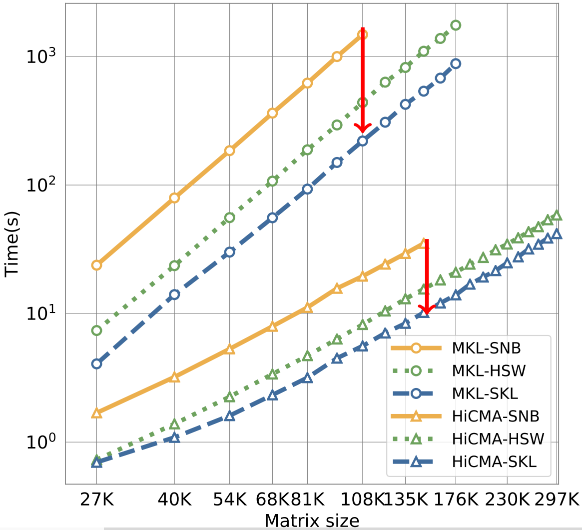
- *y* axis (*log*-scale): time of `dpotrf` in seconds
- Smaller time as chips get better



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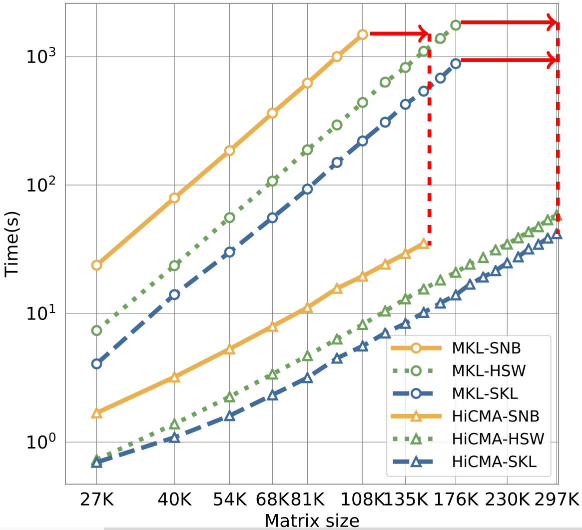
- Smaller time as chips get better
- Solve larger problems



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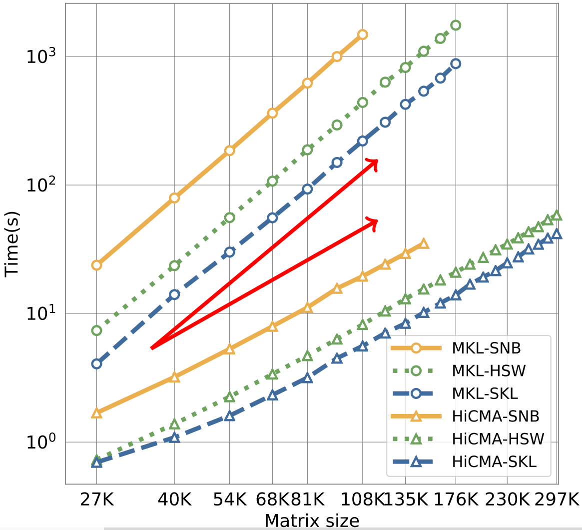
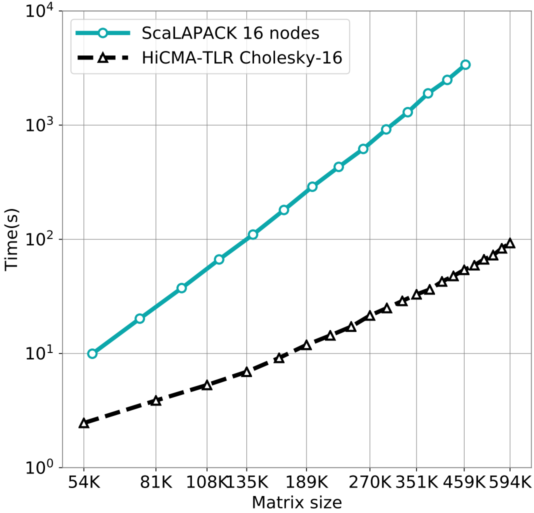
- Smaller time as chips get better
- Solve larger problems
- Smaller slope: $O(n^3) \rightarrow O(kn^2)$



ScaLAPACK vs TLR Cholesky (*Shaheen-2*, HSW, acc$=10^{-9}$)

- Execution times for ScaLAPACK dpotrf (dense) vs HiCMA dpotrf (TLR). Smaller the better.



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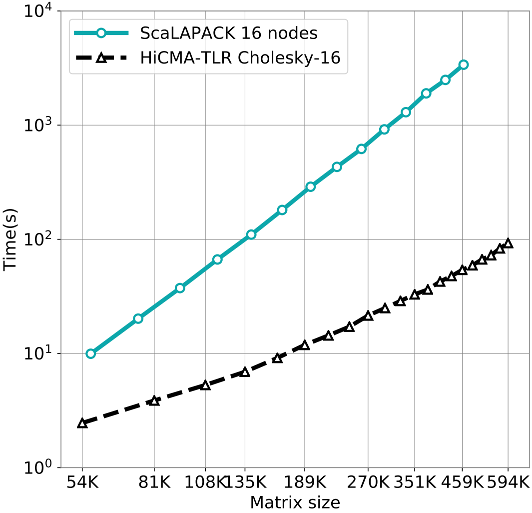

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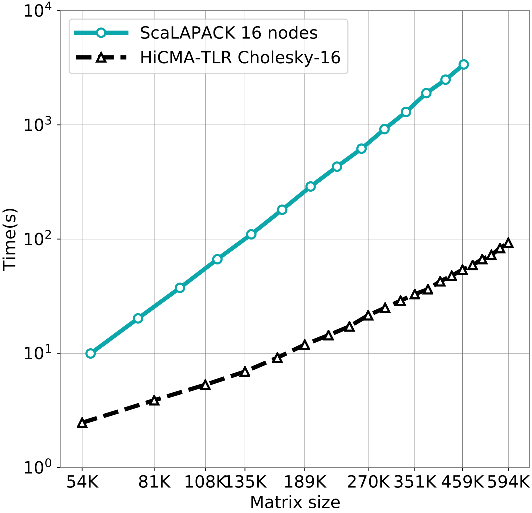

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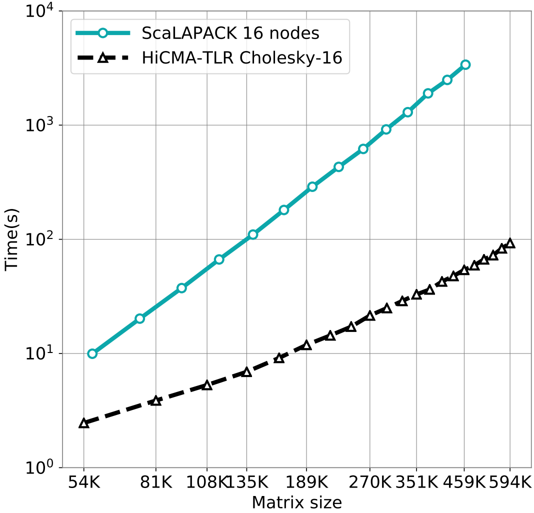
- StarPU (task-based runtime)



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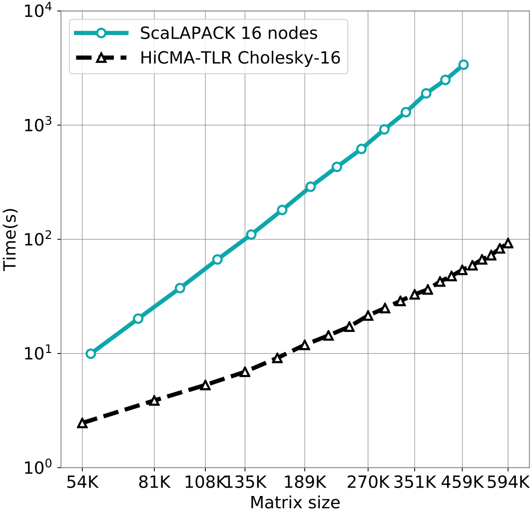

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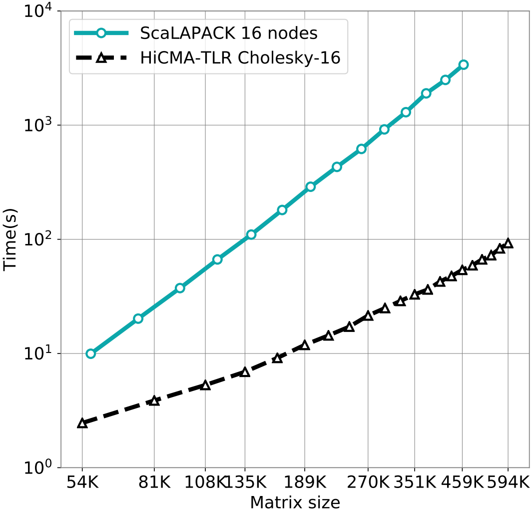

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- x axis (*log*-scale): different matrix sizes
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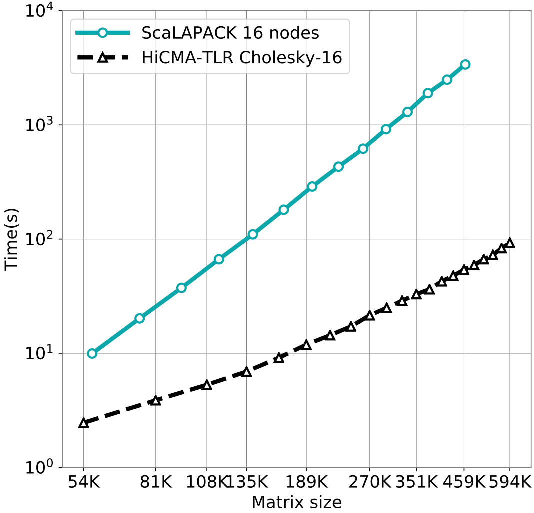
- 85x speedup



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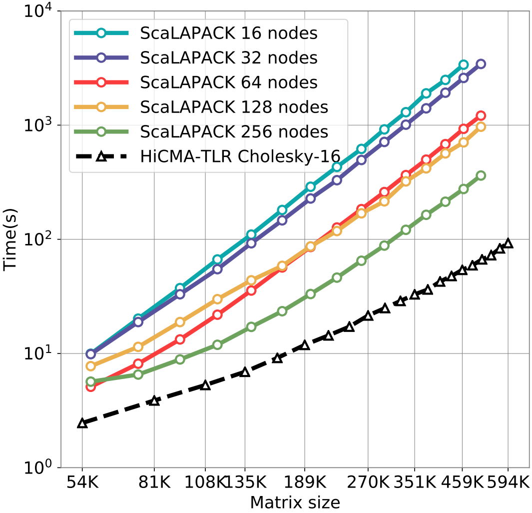

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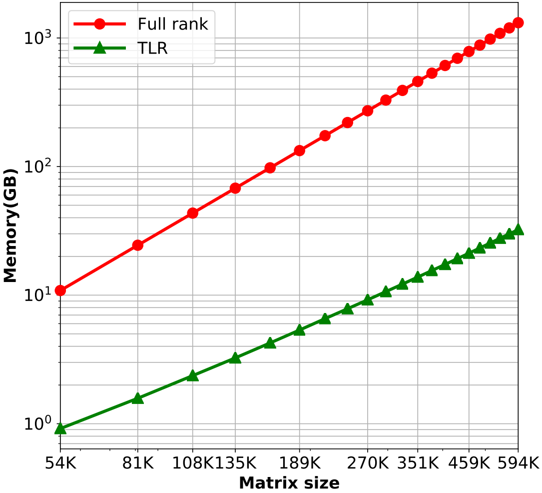
TLR Cholesky: Memory Footprint (acc$=10^{-9}$)

- Memory footprint for dense vs TLR matrices.
  Smaller the better.



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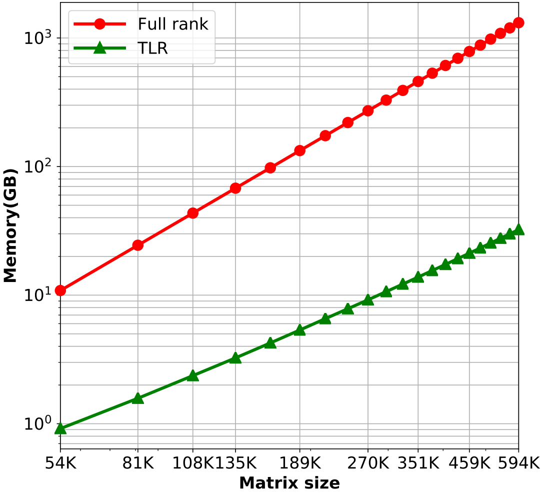

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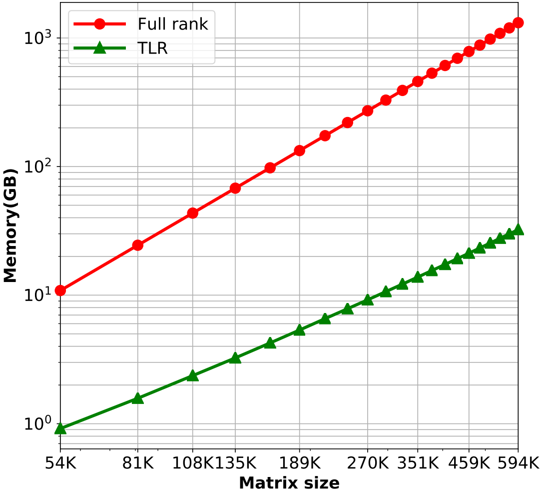

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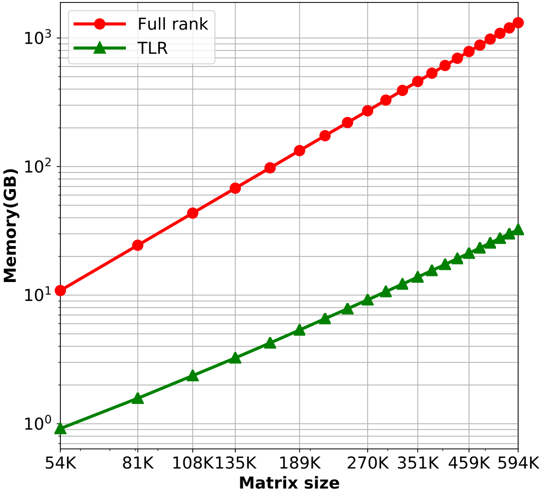
- x axis (*log*-scale): different matrix sizes (N)



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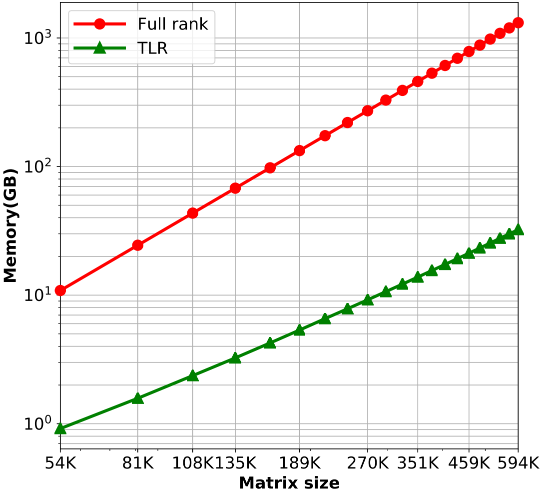

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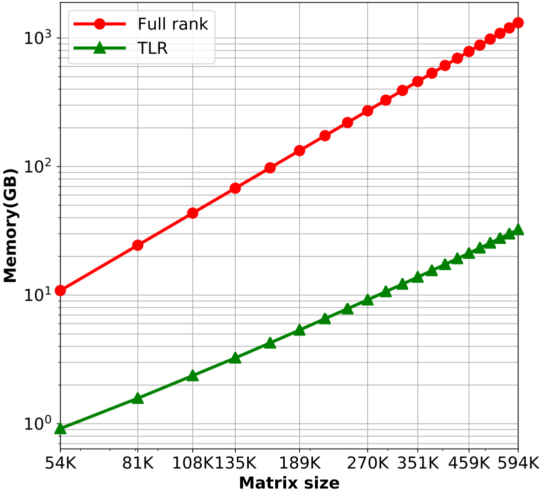
- Full rank: N^2



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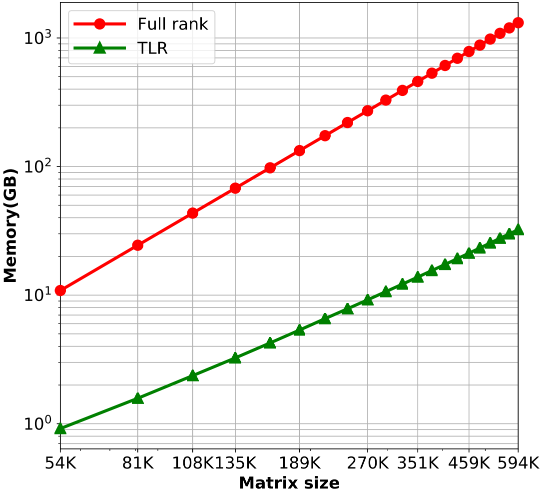
- y axis (*log*-scale): memory required for storing matrix in terms of giga bytes
- Full rank: N^2
- TLR: $\frac{N^2 k}{nb}$



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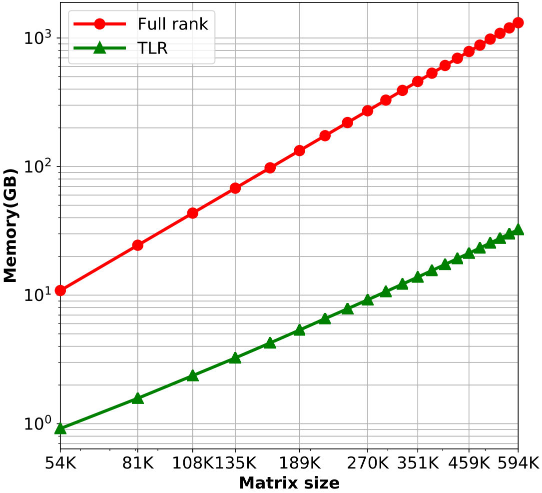
- Full rank: N^2
- TLR: $\frac{N^2 k}{nb}$
    - k: average rank



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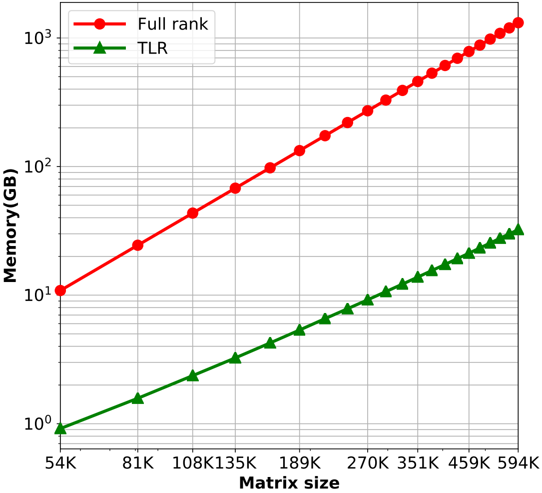
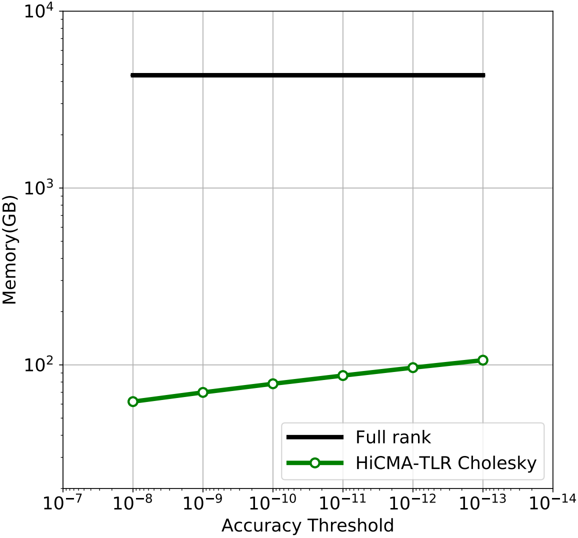
  - k: average rank
  - nb: tile size



Impact of Accuracy Thresholds, **1M** Matrix Size, nb=2700

- Memory footprint for dense vs TLR matrices. Smaller the better.



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Impact of Accuracy Thresholds, **1M** Matrix Size, nb=2700

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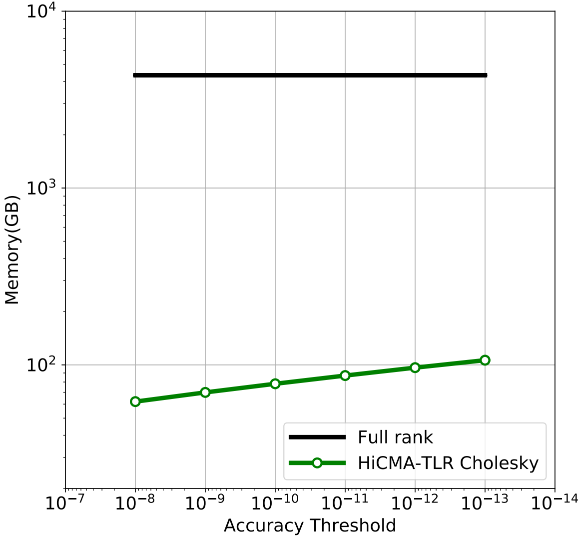

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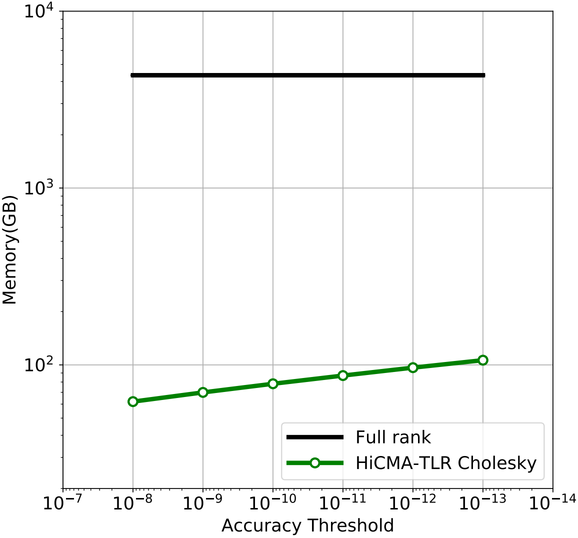
- *x* axis (*log*-scale): different accuracy thresholds



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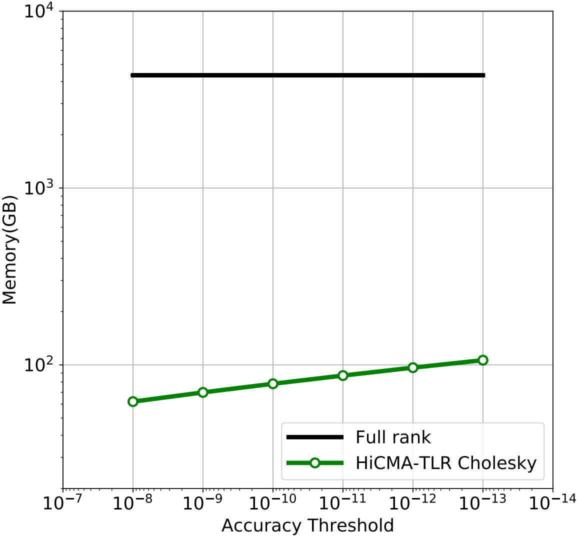

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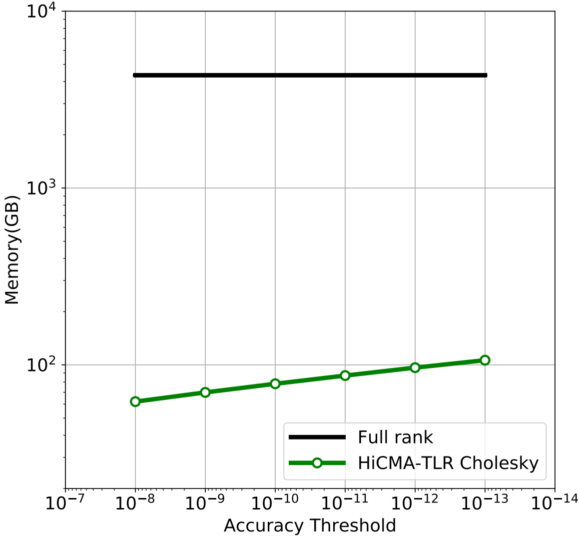
- *x* axis (*log*-scale): different accuracy thresholds
- *y* axis (*log*-scale): memory required for storing matrix in terms of giga bytes
- Being more accurate requires higher ranks so larger memory is used.



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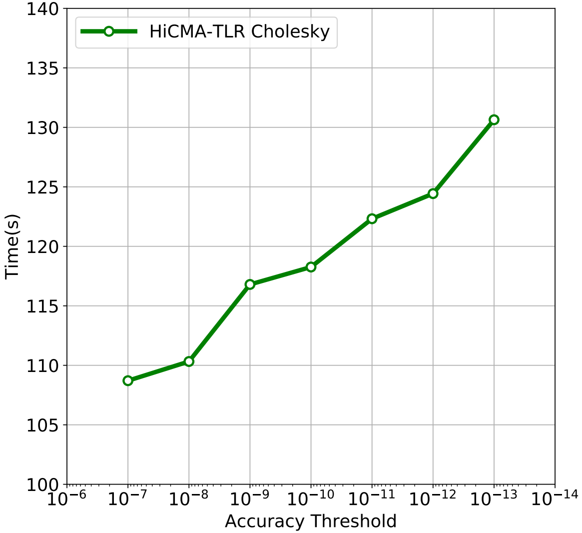
Impact of Accuracy Thresholds, **1M** Matrix Size, nb=2700, 64 nodes, *Shaheen-2*

- Execution times for HiCMA dpotrf (TLR)



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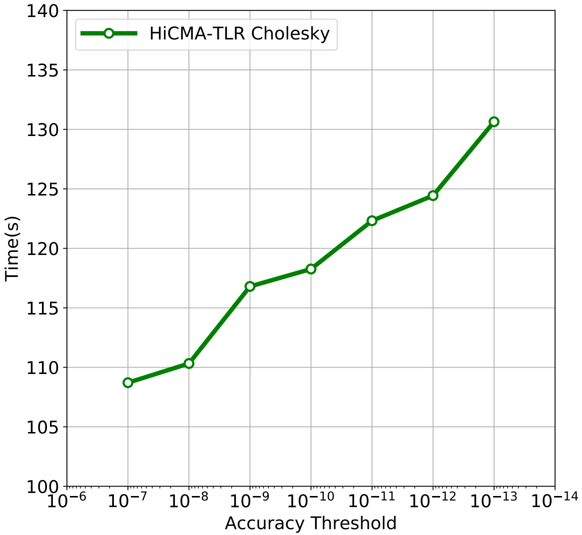

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Impact of Accuracy Thresholds, **1M** Matrix Size, nb=2700, 64 nodes, *Shaheen-2*

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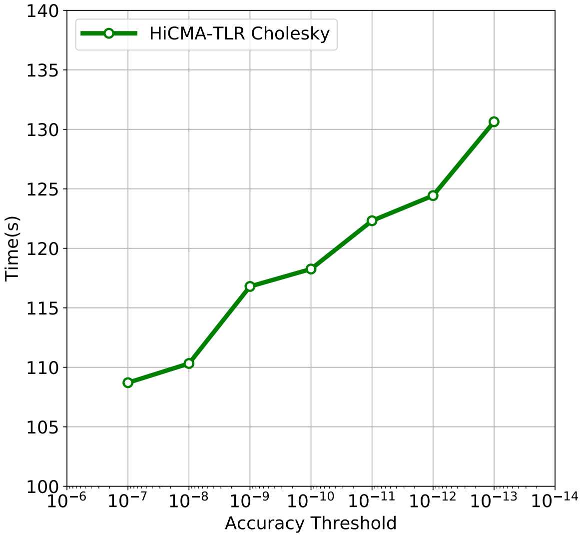

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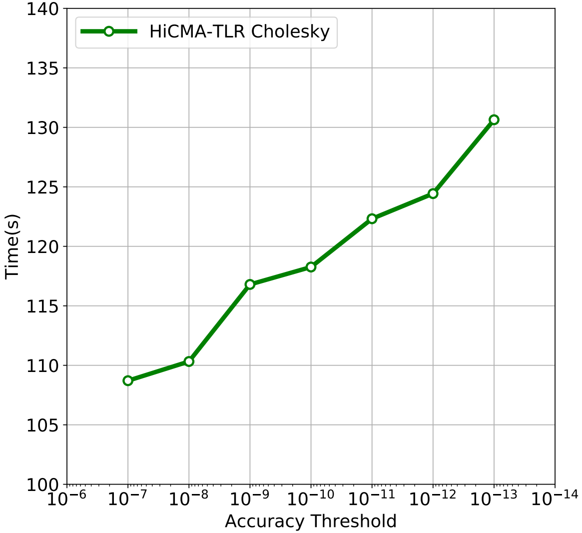
- x axis (*log*-scale): different accuracy thresholds
- y axis (*log*-scale): time of `dpotrf` in seconds



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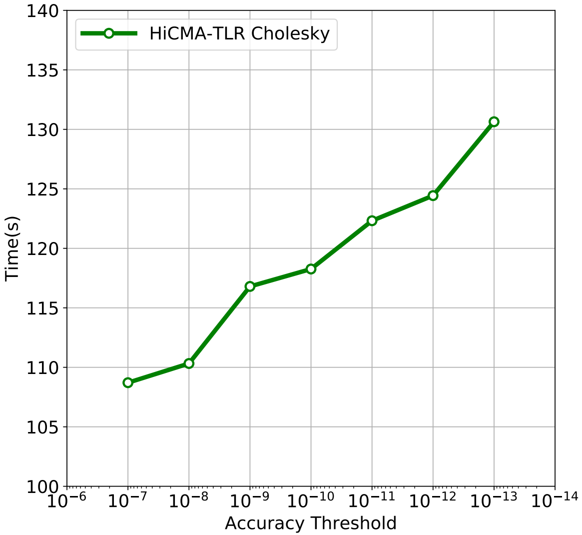
Impact of Accuracy Thresholds, **1M** Matrix Size, nb=2700, 64 nodes, *Shaheen-2*

- Execution times for HiCMA dpotrf (TLR)
- Application: Geospatial statistic, square exp. kernel
- x axis (*log*-scale): different accuracy thresholds
- y axis (*log*-scale): time of `dpotrf` in seconds
- Being more accurate requires higher ranks so more flops are done.



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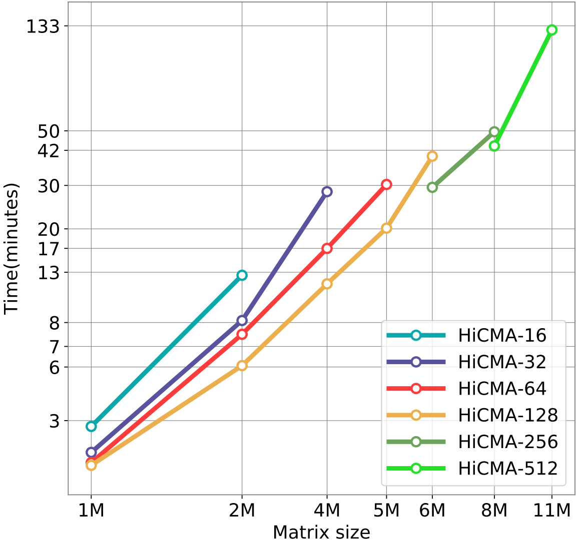
TLR Cholesky up to 11M (*Shaheen-2*, HSW, Statistics - SqExp kernel, acc=10^{-9})

- Execution times for HiCMA dpotrf (TLR) for different number of nodes



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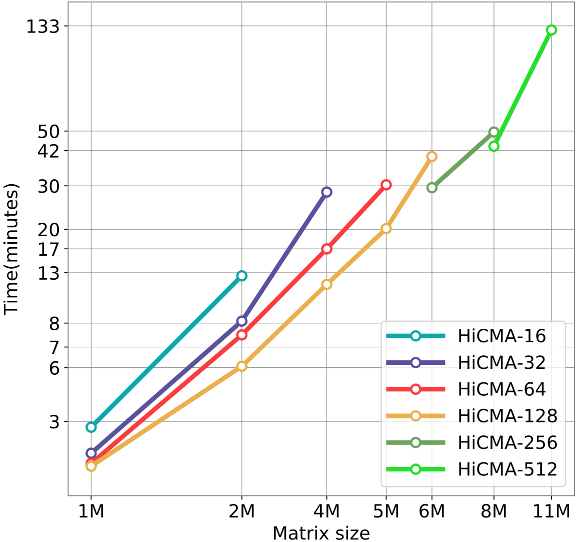

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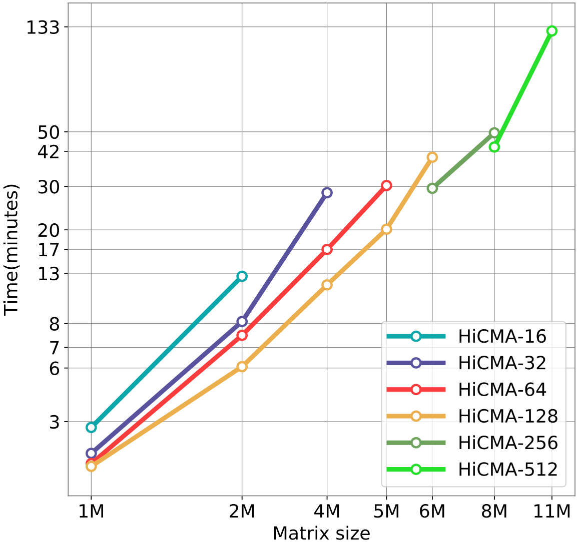
- Application: Geospatial statistic, square exp. kernel
- *x* axis (*log*-scale): different matrix sizes



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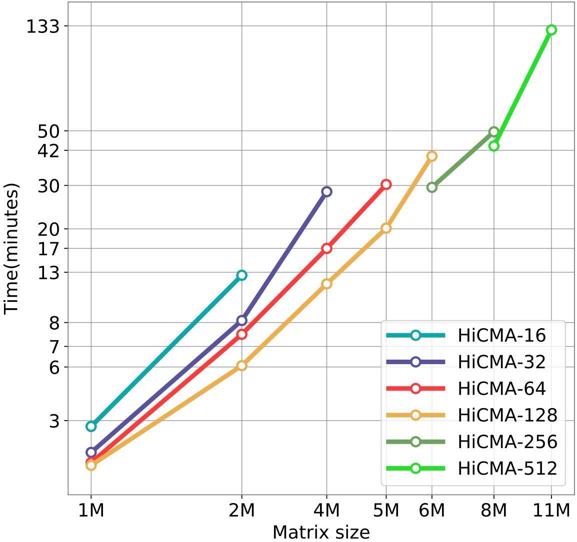

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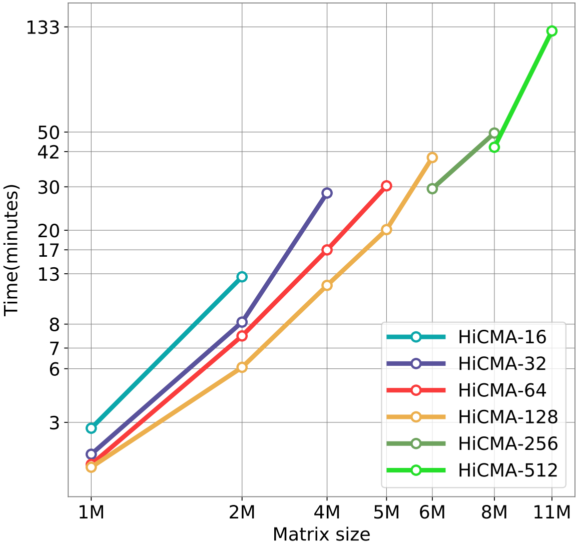
- Running ScaLAPACK for larger cases is not feasible because of time and memory.



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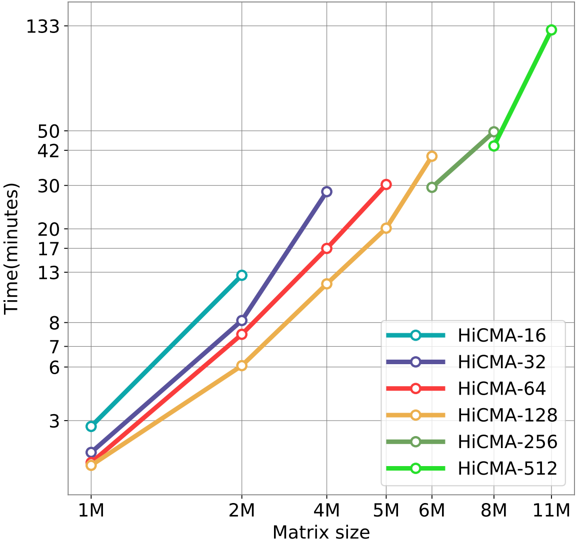
- Missing points for larger matrices: not enough memory



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- Application: Geospatial statistic, square exp. kernel
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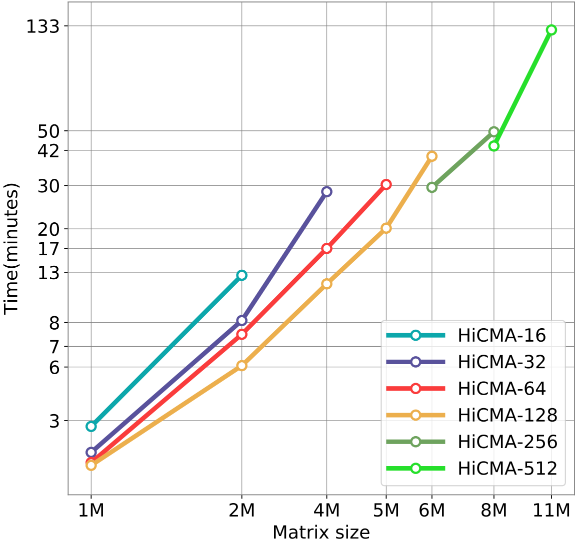
- Running ScaLAPACK for larger cases is not feasible because of time and memory.
- Missing points for larger matrices: not enough memory
- Missing points for smaller matrices: not enough work



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TLR Cholesky up to 8M (SKL Cluster, Turbo On, Statistics - SqExp, acc=10^{-9})

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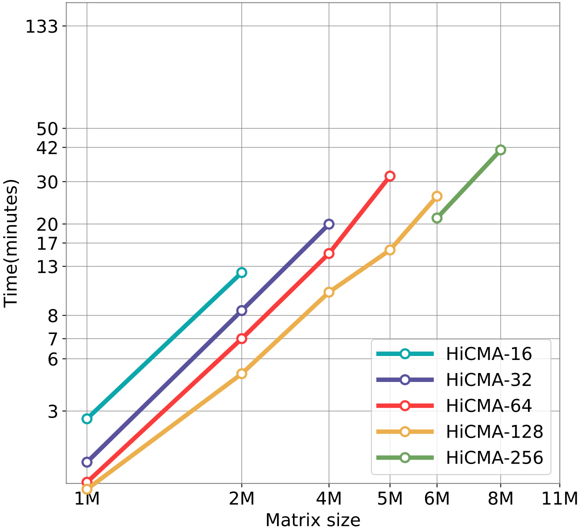

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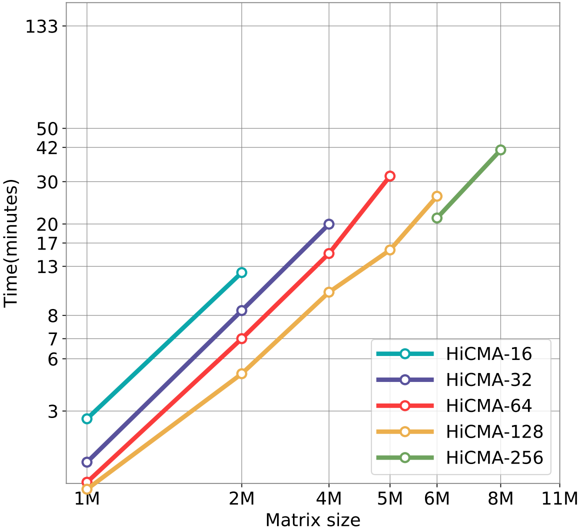

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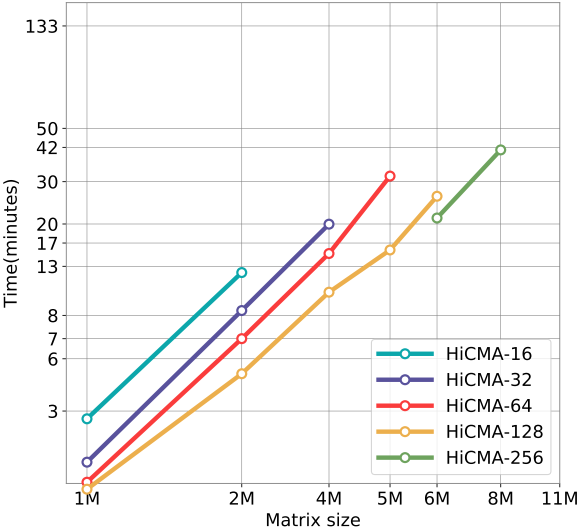

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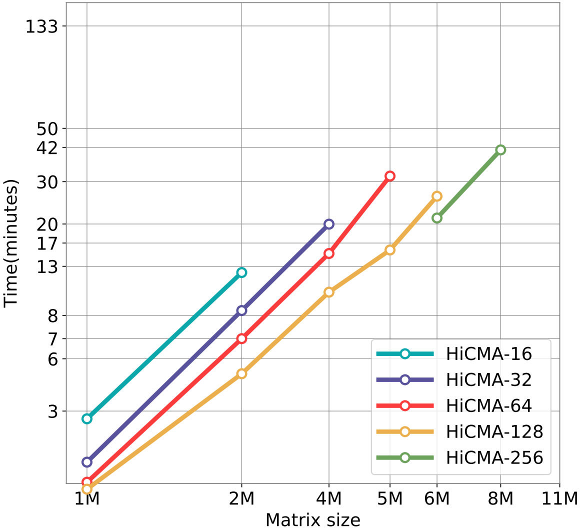

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- Application: Geospatial statistic, square exp. kernel
- *x* axis (*log*-scale): different matrix sizes
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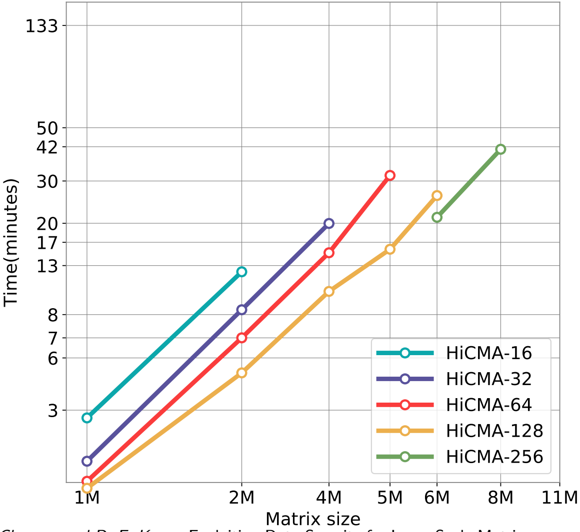
- We ran HiCMA on the latest Intel deployment.



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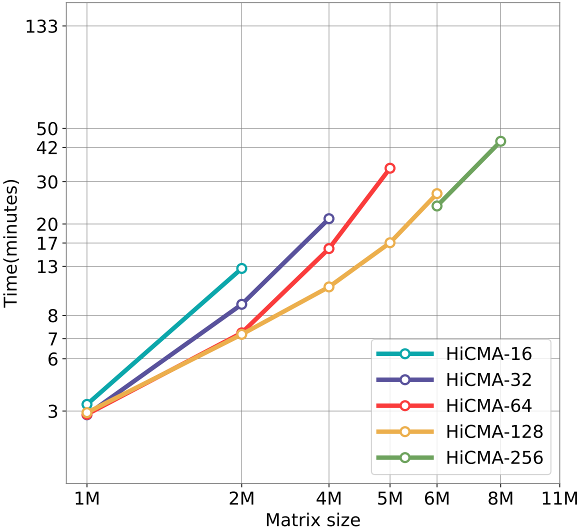

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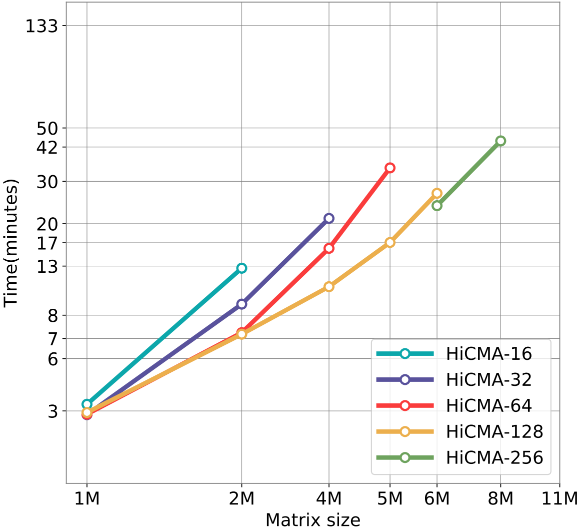

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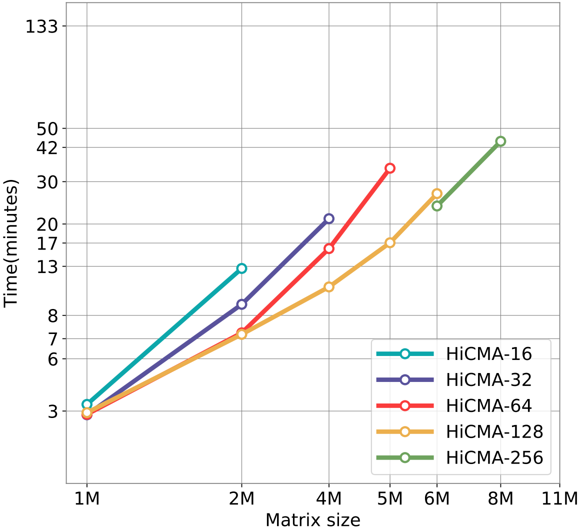

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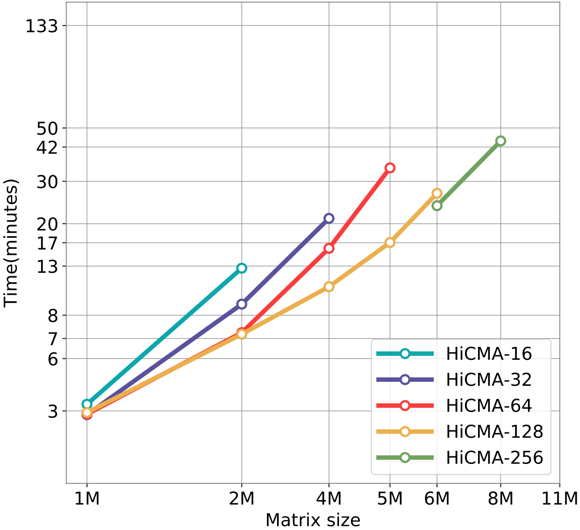

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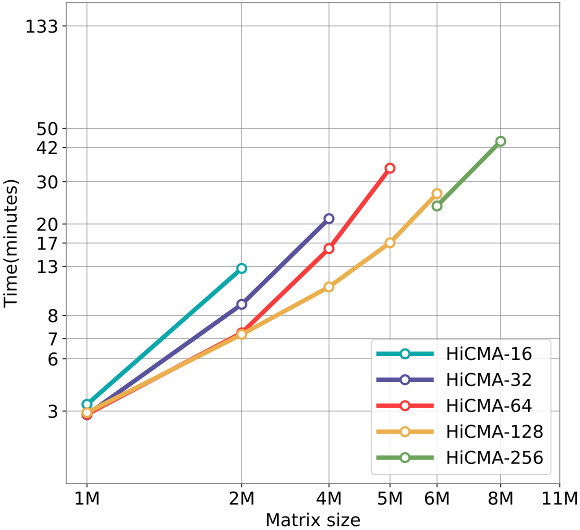
- Execution times for HiCMA dpotrf (TLR) for different number of nodes
- Application: Geospatial statistic, square exp. kernel
- *x* axis (*log*-scale): different matrix sizes
- *y* axis (*log*-scale): time of `dpotrf` in minutes
- Not big difference between turbo on and off due low arithmetic intensity



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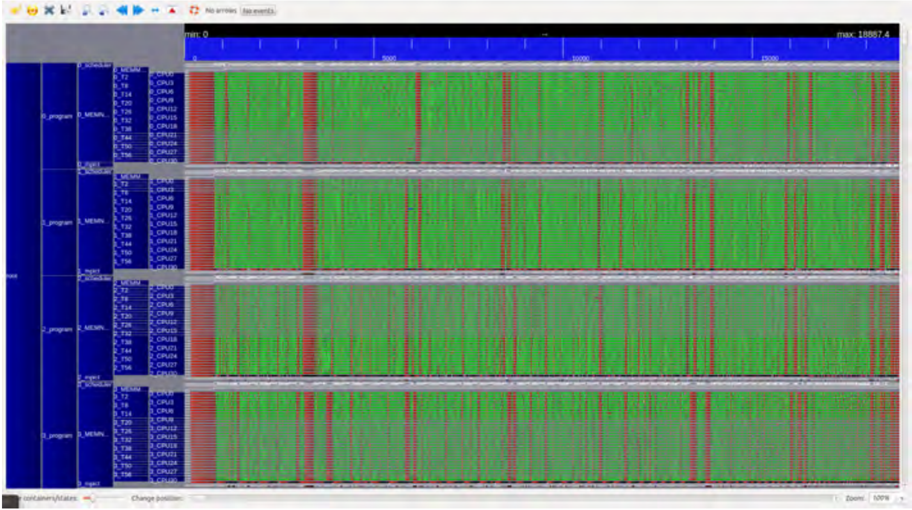
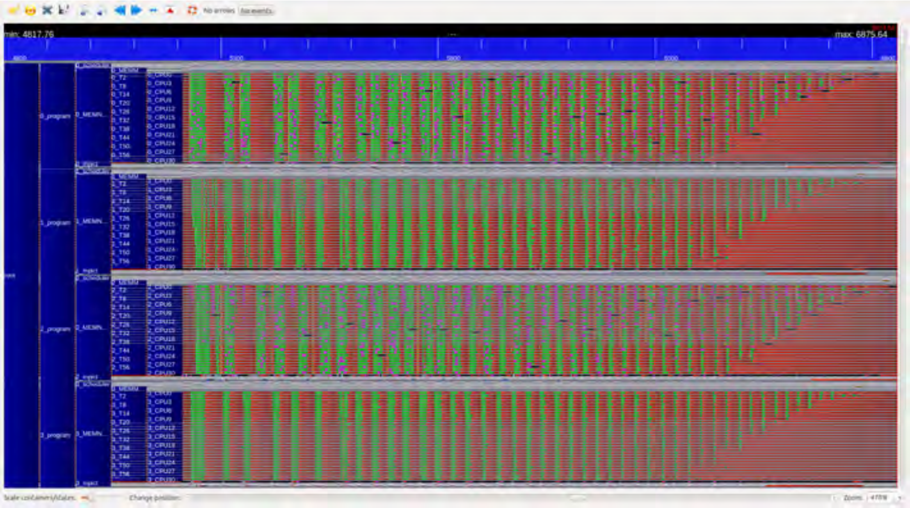
Traces Chameleon: Dense dpotrf time=18.1s on 4 nodes of *Shaheen-2* with a matrix size of 54K



Traces HiCMA: Data-sparse `dpotrf` time=1.8s on 4 nodes of *Shaheen-2* with a matrix size of 54K

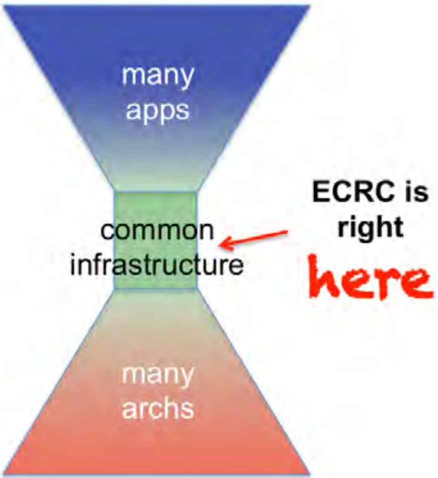


Conclusion & Future Work

- We cut down flops through compression.
- We use less memory.
- Accuracy requirement is satisfied.
- HiCMA is for both shared and distributed memory systems.

- HODLR/H (non-nested bases) data compression format.
- More matrix computation algorithms (LU/QR, eigenvalue solvers/SVD, matrix inversion, etc.)
- Support for more large-scale scientific applications.

The Hourglass Revisited



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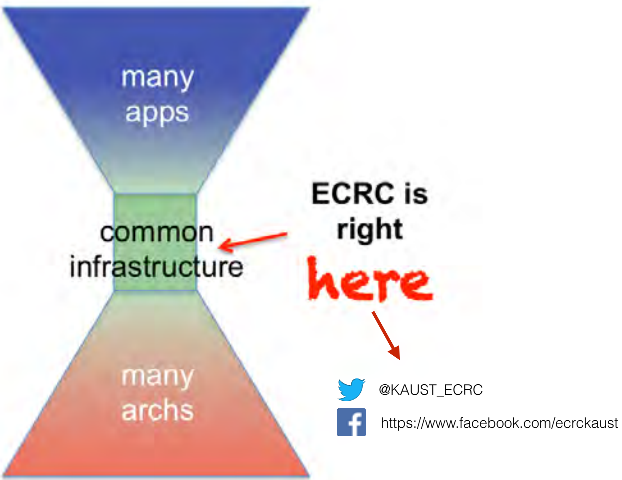

Students/Collaborators/Vendors

- Extreme Computing Research Center @ KAUST: **R. Abdelkhalek, S. Abdullah, K. Akbudak, R. AlOmairy, A. Alonazy, T. Alturkestani, W. Boukaram, A. Charara, N. Doucet, M. Genton, E. A. Gonzalez Fisher, D. Keyes, H. Ltaief, A. Mikhalev, D. Sukkari and Y. Sun**
- Tokyo Institute of Technology, Japan: **R. Yokota**
- Innovative Computing Laboratory @ UTK, USA: **PLASMA/MAGMA/PaRSEC Teams**
- INRIA/INP/LaBRI Bordeaux, France: **Runtime/HiePACS Teams**
- Max-Planck Institute@Leipzig, Germany: **R. Kriemann**
- American University of Beirut, Lebanon: **G. Turkiyyah**
- KAUST Supercomputing Lab
- Intel Parallel Computing Center
- Cray Center of Excellence

Thank You!

Questions?