Fast and Parallel Direct Linear Solvers

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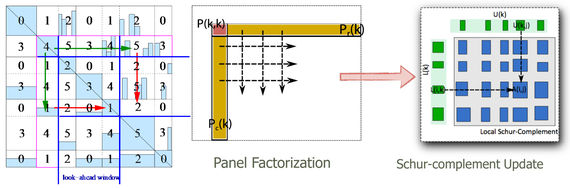
Scalable direct solvers for large-scale sparse and dense linear systems arising from scientific and engineering applications

SuperLU: Unsymmetric Sparse Direct Solver

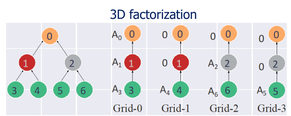
Overview

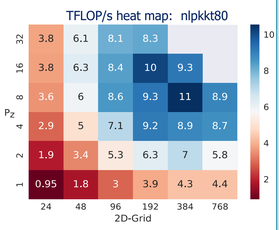
- Direct solver for general unsymmetric sparse linear systems: LU factorization, triangular solution, ILUTP preconditioner (serial).
- $O(N^2)$ flops, $O(N^{4/3})$ memory for typical 3D PDEs.



Communication-avoiding 3D sparse LU factorization on CPU + GPU.

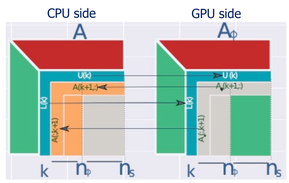
- Trade off memory for reduced communication, more parallelism. Up to **27.4x** speedup for 2D problems, up to **3.3x** speedup for 3D problems.





Improving Triangular Solve

- Improve strong scaling: customized binary broadcast & reduction trees. Up to **7x** speedup.



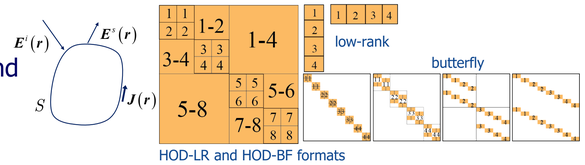
	CPU	+ GPU
2D Algo	1x	0.9 – 3x
3D Algo	0.6 – 27x	2.5 – 27x

P. Sao, X. Li, R. Vuduc, IPDPS 2015, IPDPS 2018.
Y. Liu, M. Jacquelin, P. Ghysels, X.S. Li, SIAM CSC18

ButterflyPACK: Dense Direct Solver for Wave Equations

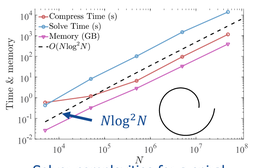
Overview

- Direct solver for rank-structured dense matrices.
- Support distributed-memory HOD-LR (low-rank) and HOD-BF (butterfly) formats.
- Targeted at electromagnetic, acoustic and elastic applications.

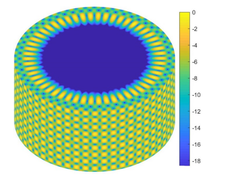


Parallel matrix construction and factorization

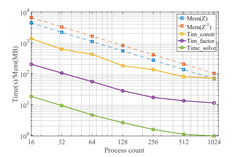
- Hierarchical blocked ACA, ID-based butterfly. compression with neighboring information, cost $O(N\log^2 N)$.
- Randomized algebras for factorization, cost at most $O(N^{1.5}\log N)$. Preconditioner, cost $O(N\log^2 N)$.
- Distributed-memory butterfly and low-rank up to 4000 MPI ranks.



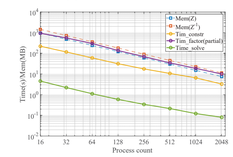
Solver complexities for a spiral



$TM_{10,8,2}$ mode of a RF cavity



Strong Scaling for HOD-LR



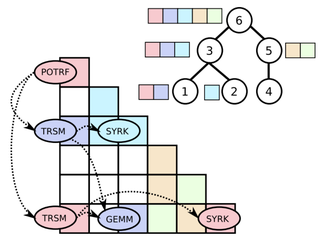
Strong Scaling for HOD-BF

Y. Liu, W. Sid-Lakhdar, E. Rebrova, P. Ghysels, and X. Sherry Li, Linear Algebra Appl. 2019.
Y. Liu, and H. Yang, J. Comp. Phys., 2019

symPACK: Symmetric Sparse Direct Solver

Overview

- Direct linear solver for sparse symmetric matrices: fewer storage and computations are required.
- Factorization is a crucial preprocessing step to PEXSI (www.pexsi.org), a library used in electronic structure computations.
- A new highly scalable 2D data distribution leading to much improved strong scalability and significant speedups over the previous 1D data distribution.



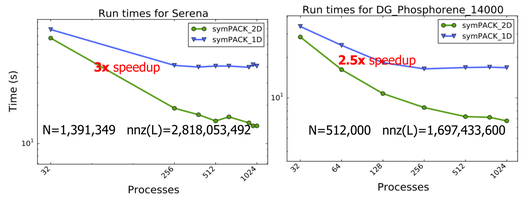
(1) Proportional mapping assign groups of processes to subtrees

(2) Nonzero blocks corresponding to a supernode are distributed across processes within each sub-groups

(3) Corresponding task graph has finer granularity than 1D counterpart

Research details

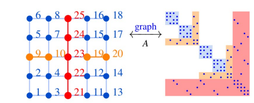
- New task-based 2D data distribution.
- Proportional mapping + explicit load balancing.
- Balances flops, memory.
- New distribution and task based computations lead to higher strong scalability for both numerical factorization and solution phases.

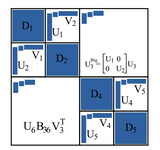


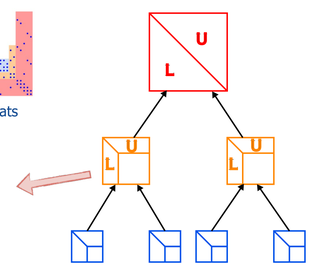
STRUMPACK: Rank-structured Dense and Sparse Direct Solver

Overview

- Direct solver for dense and sparse systems using rank-structured matrix approximations.
- Dense matrix: HSS, BLR, HOD-LR and HOD-BF formats. Applicable to Toeplitz, Cauchy, BEM, QuantumChem, machine learning, covariance…
- Sparse matrix: Multifrontal LU Factorization with rank-structured sub-matrices. Aimed at PDE applications.

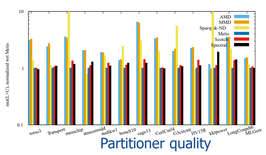


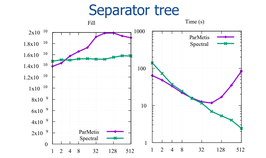




Spectral nested-dissection code

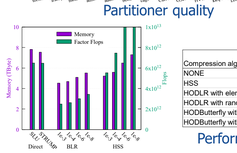
- Partition based on Fiedler vector from graph Laplacian. Reuse existing scalable eigensolvers.





More rank-structured formats for indefinite Maxwell

- BLR, HOD-LR, HOD-BF with sampling and extraction
- Significantly better compression with HOD-BF



Compression algorithm	Factor flops	Factor memory on Top Fronts	Compression Rank	Maximum Rank	GMRES Iterations	Total time (sec)
NONE	4.38E+14	128 GB	100 %		1	1215.2
HSS	3.25E+14	96 GB	11.9 %	2003	6	965.7
HODLR with element extraction	2.58E+14	96 GB	13.1 %	2112	4	1097.7
HODLR with random sampling	7.82E+14	96 GB	17.7 %	2923	55	2735.1
HODButterfly with element extraction	2.59E+14	92 GB	4.9 %	303	18	1145.9
HODButterfly with random sampling	1.24E+15	94 GB	9.2 %	451	16	3965.8

Performance of different rank-structured formats

More Information: http://www.fastmath-scidac.org or contact Xiaoye Sherry Li, LBNL, xsli@lbl.gov