ARGONNE ATPESC 10 EXTREME-SCALE COMPUTING

Direct Sparse Linear Solvers, Preconditioners

SuperLU, STRUMPACK, with hands-on examples

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Agenda

- Setup for SuperLU hands-on (5 min)
- Overview of sparse direct solvers + SuperLU (30 min)

- Setup for STRUMPACK hands-on (5 min)
- STRUMPACK with compression techniques (30 min)

ThetaGPU setup

https://xsdk-project.github.io/MathPackagesTraining2022/setup_instructions/

- Copy all examples to your home:

cd ~

rsync -a /grand/ATPESC2022/EXAMPLES/track-5-numerical .

- Get a single GPU node

qsub -I -q single-gpu -n 1 -t 60 -A ATPESC2022

- Follow SuperLU lesson at:

https://xsdk-project.github.io/MathPackagesTraining2022/lessons/superlu_dist

Algorithm tour of sparse direct solvers

(illustration with SuperLU_DIST)

Gaussian Elimination (GE) to solve Ax=b

- First step of GE:

$$A = \begin{bmatrix} \alpha & w^T \\ v & B \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ v/\alpha & I \end{bmatrix} \cdot \begin{bmatrix} \alpha & w^T \\ 0 & C \end{bmatrix}$$

$$C = B - \frac{v \cdot w^T}{\alpha}$$

- Repeat GE on C
- Result in LU factorization (A = LU)
  - L lower triangular with unit diagonal, U upper triangular

- Then, x is obtained by solving two triangular systems with L and U, easier to solve

Strategies of solving sparse linear systems

- Iterative methods: (e.g., Krylov, multigrid, …)
  - **A is not changed (read-only)**
  - **Key kernel: sparse matrix-vector multiply**
    - **Easier to optimize and parallelize**
  - **Low algorithmic complexity, but may not converge**
- Direct methods:
  - **A is modified (factorized) : A = L*U**
    - **Harder to optimize and parallelize**
  - **Numerically robust, but higher algorithmic complexity**

- Often use direct method to precondition iterative method
  - **Solve an easier system: $M^{-1}Ax = M^{-1}b$**

Exploit sparsity

1) Structural sparsity
   - Defined by {0, 1} structure (Graphs)
   - LU factorization ~ $O(N^2)$ flops, for many 3D discretized PDEs

2) Data sparsity (usually with approximation)
   - On top of 1), can find data-sparse structure in dense (sub)matrices (often involve approximation)
   - LU factorization ~ O(N polylog(N))

SuperLU: only structural sparsity

STRUMPACK: both structural and data sparsity

PDE discretization leads to sparse matrices

- Poisson equation in 2D (continuum)

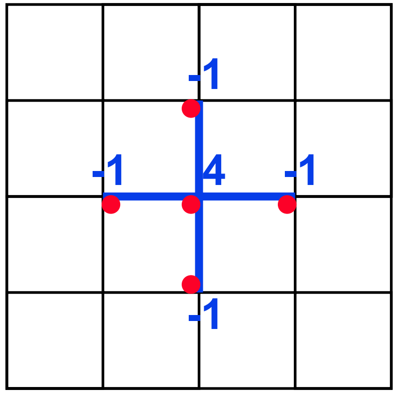
$$\frac{\partial^2 u}{\partial x^2}(x,y) + \frac{\partial^2 u}{\partial y^2}(x,y) = f(x,y), \quad (x,y) \in R$$

$$u(x,y) = g(x,y), \quad \text{(x,y) on the boundary}$$

- Stencil equation (discretized)

$$4 \cdot u(i,j) - u(i-1,j) - u(i+1,j) - u(i,j-1) - u(i,j+1) = f(i,j)$$

Graph and “stencil”



$$A = \left(\begin{array}{ccc:ccc:ccc}
4 & -1 & & -1 & & & & & \\
-1 & 4 & -1 & & -1 & & & & \\
& -1 & 4 & & & -1 & & & \\
\hdashline
-1 & & & 4 & -1 & & -1 & & \\
& -1 & & -1 & 4 & -1 & & -1 & \\
& & -1 & & -1 & 4 & & & -1 \\
\hdashline
& & & -1 & & & 4 & -1 & \\
& & & & -1 & & -1 & 4 & -1 \\
& & & & & -1 & & -1 & 4
\end{array}\right)$$

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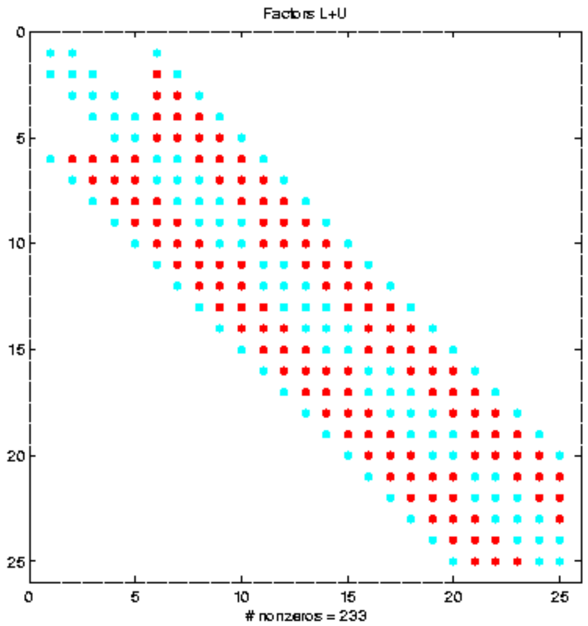
Fill-in in Sparse GE

Original zero entry A_{ij} becomes nonzero in L or U

– Red: fill-ins (Matlab: spy())

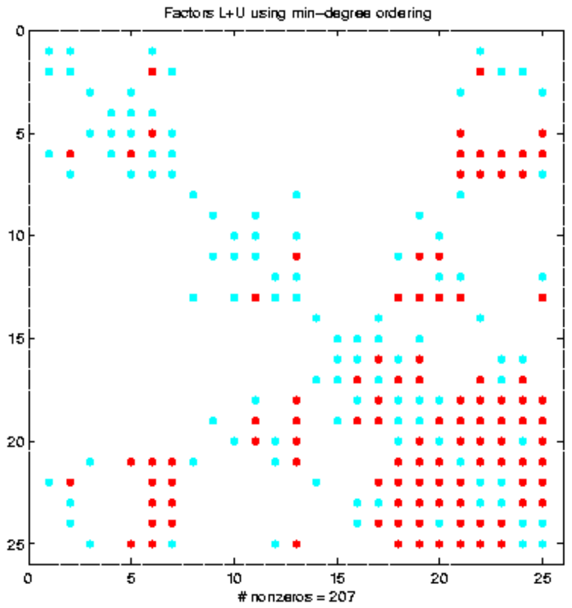
Natural order: NNZ = 233



Band solver

Fill-in: $O(N^{3/2})$
Flops: $O(N^2)$

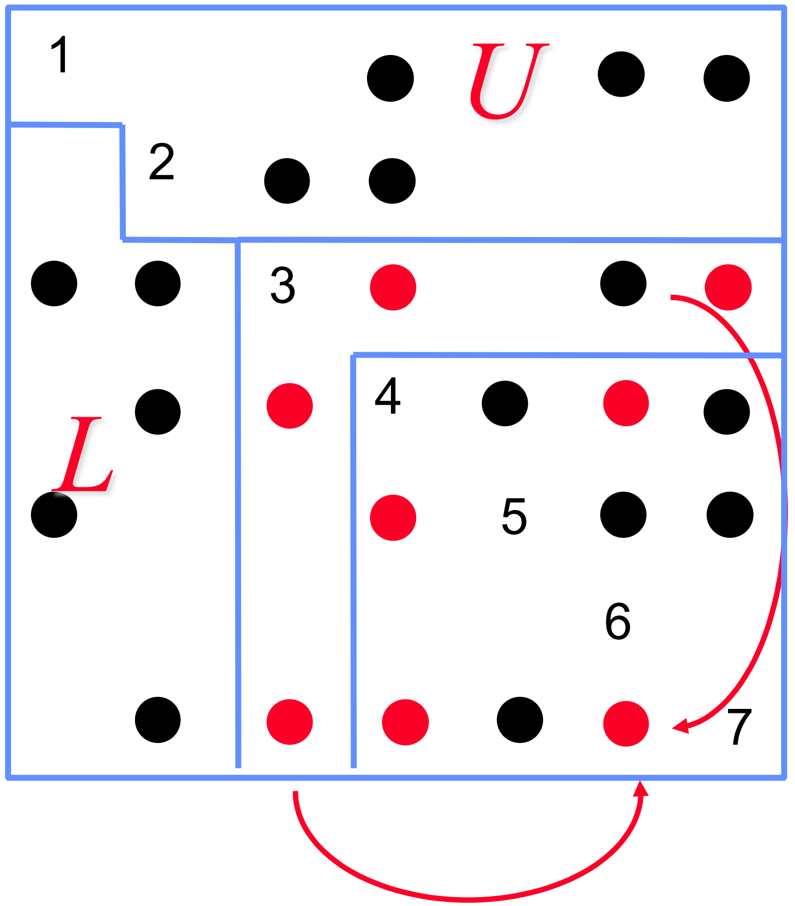
Minimum Degree order: NNZ = 207



General sparse solver

Fill-in: $O(N \log(N))$
Flops: $O(N^{3/2})$

Fill-in in sparse LU



Store general sparse matrix: Compressed Row Storage (CRS)

- **Store nonzeros row by row contiguously**
- **Example: N = 7, NNZ = 19**
- **3 arrays:**
  - **Storage: NNZ reals, NNZ+N+1 integers**

$$
\begin{pmatrix}
1 & & & a & & & \\
 & 2 & & & b & & \\
c & d & 3 & & & & \\
 & e & & 4 & f & & \\
 & & & & 5 & & g \\
 & & & h & i & 6 & j \\
 & & k & & l & & 7
\end{pmatrix}
$$

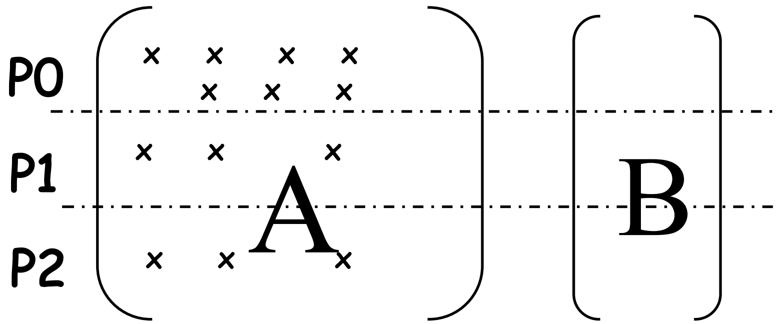
	1	3	5	8	11	13	17	20
nzval	1 a	2 b	c d 3	e 4 f	5 g	h i 6 j	k l 7	
colind	1 4	2 5	1 2 3	2 4 5	5 7	4 5 6 7	3 5 7	
rowptr	1 3 5 8 11 13 17 20							

Many other data structures: "Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods", R. Barrett et al.

Distributed input interface

- **Matrices involved:**
  - **A, B (turned into X) – input, users manipulate them**
  - **L, U – output, users do not need to see them**

- **A (sparse) and B (dense) are distributed by block rows**



Local A stored in *Compressed Row Format*

Distributed input interface

- **Each process has a structure to store local part of A**

Distributed Compressed Row Storage

```
typedef struct {
   int_t   nnz_loc;  // number of nonzeros in the local submatrix
   int_t   m_loc;    // number of rows local to this processor
   int_t   fst_row;  // global index of the first row
   void    *nzval;   // pointer to array of nonzero values, packed by row
   int_t   *colind;  // pointer to array of column indices of the nonzeros
   int_t   *rowptr;  // pointer to array of beginning of rows in nzval[]and colind[]
}  NRformat_loc;
```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Distributed Compressed Row Storage

SuperLU_DIST/FORTRAN/f_5x5.f90

A is distributed on 2 processors:

P0	s		u		u
	l	u			
P1		l	p		
				e	u
	l	l			r

- **Processor P0 data structure:**
  - **nnz_loc = 5**
  - **m_loc = 2**
  - **fst_row = 0 // 0-based indexing**
  - **nzval = { s, u, u, l, u }**
  - **colind = { 0, 2, 4, 0, 1 }**
  - **rowptr = { 0, 3, 5 }**

- **Processor P1 data structure:**
  - **nnz_loc = 7**
  - **m_loc = 3**
  - **fst_row = 2 // 0-based indexing**
  - **nzval = { l, p, e, u, l, l, r }**
  - **colind = { 1, 2, 3, 4, 0, 1, 4 }**
  - **rowptr = { 0, 2, 4, 7 }**

Direct solver solution phases

1. Preprocessing: Reorder equations to minimize fill, maximize parallelism (~10% time)
    - Sparsity structure of L & U depends on A, which can be changed by row/column permutations (vertex re-labeling of the underlying graph)
    - Ordering (combinatorial algorithms; “NP-complete” to find optimum [Yannakis ’83]; use heuristics)

2. Preprocessing: predict the fill-in positions in L & U (~10% time)
    - Symbolic factorization (combinatorial algorithms)

3. Preprocessing: Design efficient data structure for quick retrieval of the nonzeros
    - Compressed storage schemes

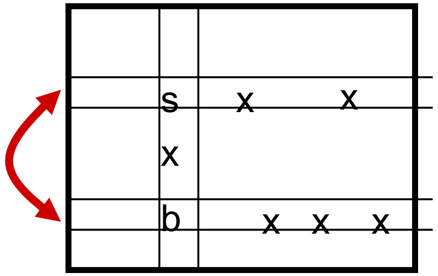
4. Perform factorization and triangular solutions (~80% time)
    - Numerical algorithms (F.P. operations only on nonzeros)
    - Usually dominate the total runtime

For sparse Cholesky and QR, the steps can be separate. For sparse LU with pivoting, steps 2 and 4 must be interleaved.

Numerical pivoting for stability

- Goal of pivoting is to control element growth in L & U for stability
  - For sparse factorizations, often relax the pivoting rule to trade with better sparsity and parallelism (e.g., threshold pivoting, static pivoting , . . .)

- **Partial pivoting** used in dense LU, sequential SuperLU and SuperLU_MT (GEPP)
  - Can force diagonal pivoting (controlled by diagonal threshold)
  - Hard to implement scalably for sparse factorization



Relaxed pivoting strategies:

- **Static pivoting** used in SuperLU_DIST (GESP)
  - Before factor, scale and permute A to maximize diagonal: $P_r D_r A D_c = A'$
  - During factor $A' = LU$, replace tiny pivots by $\sqrt{\varepsilon}\|A\|$, w/o changing data structures for L & U
  - If needed, use a few steps of iterative refinement after the first solution
  - quite stable in practice
- **Restricted pivoting**
- …

Can we reduce fill? -- various ordering algorithms

- Reordering (= permutation of equations and variables)

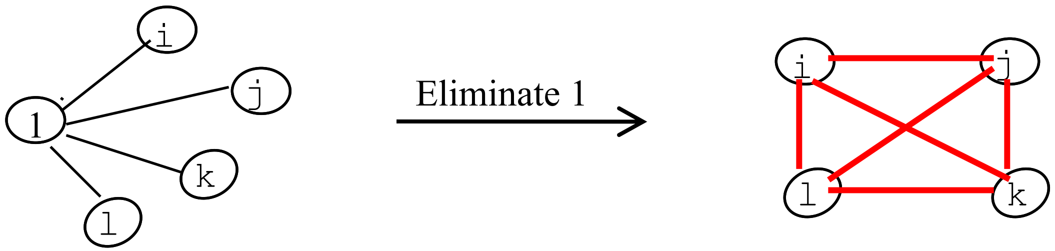
$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 2 & & & \\ 3 & & 3 & & \\ 4 & & & 4 & \\ 5 & & & & 5 \end{pmatrix} \text{(all filled after elimination)}$$

$$\Rightarrow \begin{pmatrix} & & & & 1 \\ & & & 1 & \\ & & 1 & & \\ & 1 & & & \\ 1 & & & & \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 2 & & & \\ 3 & & 3 & & \\ 4 & & & 4 & \\ 5 & & & & 5 \end{pmatrix} \begin{pmatrix} & & & & 1 \\ & & & 1 & \\ & & 1 & & \\ & 1 & & & \\ 1 & & & & \end{pmatrix} = \begin{pmatrix} 5 & & & & 5 \\ & 4 & & & 4 \\ & & 3 & & 3 \\ & & & 2 & 2 \\ 5 & 4 & 3 & 2 & 1 \end{pmatrix}$$

(no fill after elimination)

Ordering to preserve sparsity : Minimum Degree

$$
\begin{array}{c} \\ 1 \\ i \\ j \\ k \\ l \end{array}
\begin{array}{c}
\begin{array}{ccccc} & i & j & k & l \end{array} \\
\begin{bmatrix}
x & x & x & x & x \\
x & & & & \\
x & & & & \\
x & & & & \\
x & & & &
\end{bmatrix}
\end{array}
\xrightarrow{\text{Eliminate 1}}
\begin{array}{c} \\ 1 \\ i \\ j \\ k \\ l \end{array}
\begin{array}{c}
\begin{array}{ccccc} & i & j & k & l \end{array} \\
\left[\begin{array}{c|cccc}
x & x & x & x & x \\
\hline
x & \bullet & \bullet & \bullet & \bullet \\
x & \bullet & \bullet & \bullet & \bullet \\
x & \bullet & \bullet & \bullet & \bullet \\
x & \bullet & \bullet & \bullet & \bullet
\end{array}\right]
\end{array}
$$



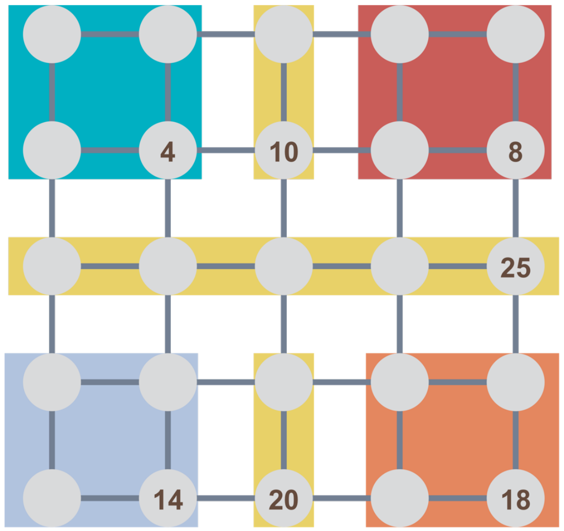
- Local greedy strategy: minimize upper bound on fill-in at each elimination step
- Algorithm: Repeat N steps:
  - Choose a vertex with minimum degree to eliminate
  - Update the remaining graph

Fast implementation: Quotient graph, approximate degree

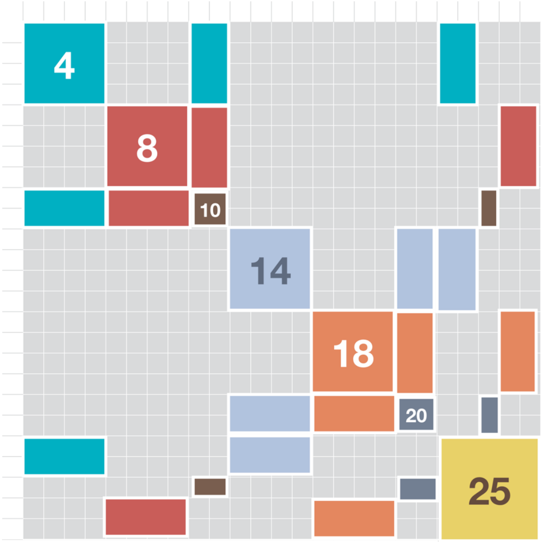
Ordering to preserve sparsity : Nested Dissection

- Model problem: discretized system Ax = b from certain PDEs, e.g., 5-point stencil on k x k grid, $N = k^2$
  - **Factorization flops: $O(k^3) = O(N^{3/2})$**
- Theorem: ND ordering gives optimal complexity in exact arithmetic [George '73, Hoffman/Martin/Rose]

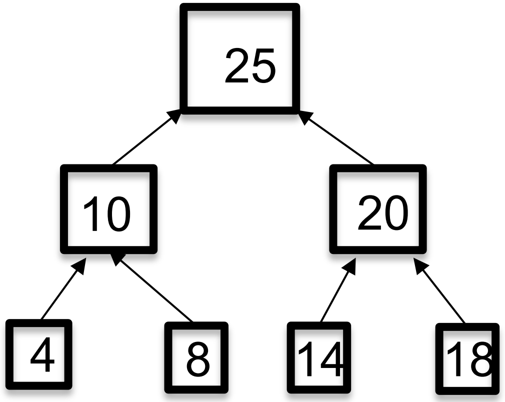
Geometry



Reordered Matrix



Separator Tree



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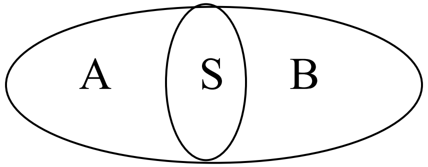
ND Ordering

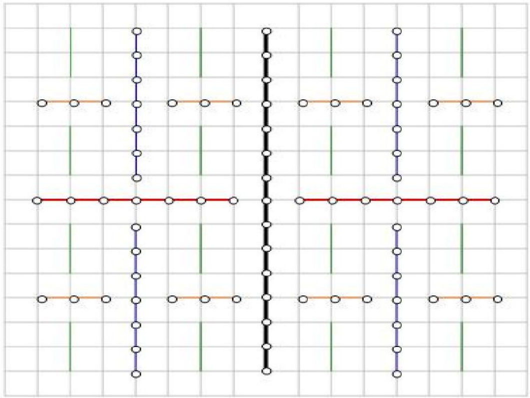
- Generalized nested dissection [Lipton/Rose/Tarjan ’79]
  - **Global graph partitioning: top-down, divide-and-conqure**
  - **Best for large problems**
  - **Parallel codes available: ParMetis, PT-Scotch**
    - First level



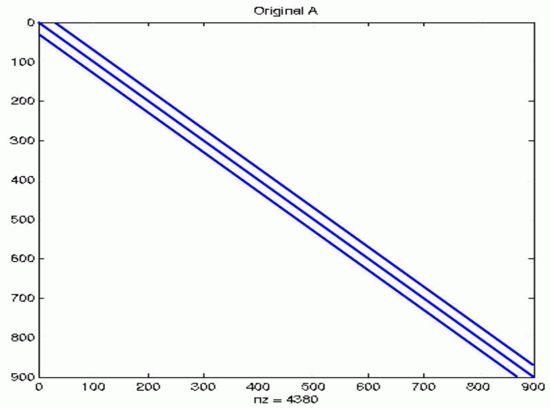
$$\longrightarrow \begin{bmatrix} A & 0 & x \\ 0 & B & x \\ x & x & S \end{bmatrix}$$

    - Recurse on A and B
- Goal: find the smallest possible separator S at each level
  - **Multilevel schemes:**
    - **Chaco [Hendrickson/Leland `94], Metis [Karypis/Kumar `95]**
  - **Spectral bisection [Simon et al. `90-`95, Ghysels et al. 2019-]**
  - **Geometric and spectral bisection [Chan/Gilbert/Teng `94]**

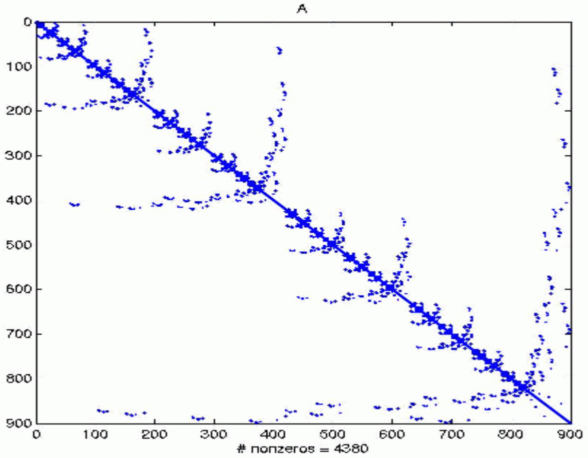
ND Ordering



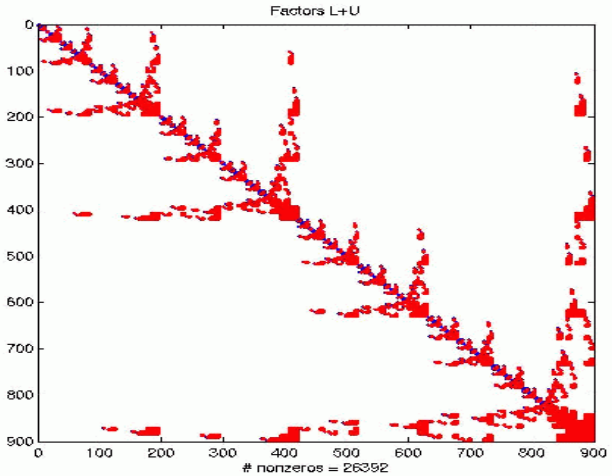
2D mesh



A, with row-wise ordering



A, with ND ordering



L &U factors

Ordering for LU with non-symmetric patterns

- Can use a symmetric ordering on a symmetrized matrix
- Case of partial pivoting (serial SuperLU, SuperLU_MT):
  - Use ordering based on A^T*A
- Case of static pivoting (SuperLU_DIST):
  - Use ordering based on A^T+A
- Can find better ordering based solely on A, without symmetrization
  - Diagonal Markowitz [Amestoy/Li/Ng `06]
    - Similar to minimum degree, but without symmetrization
  - Hypergraph partition [Boman, Grigori, et al. `08]
    - Similar to ND on A^TA, but no need to compute A^TA

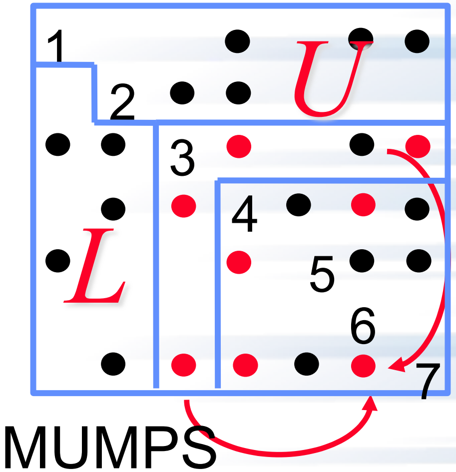
Algorithm variants, codes …. depending on matrix properties

Matrix properties	Supernodal (updates in-place)	Multifrontal (partial updates passing around)
Symmetric Pos. Def.: Cholesky LL' indefinite: LDL'	symPACK (DAG)	MUMPS (tree)
Symmetric pattern, non-symmetric value	PARDISO (DAG)	MUMPS (tree) STRUMPACK (binary tree)
Non-symmetric everything	SuperLU (DAG) PARDISO (DAG)	UMFPACK (DAG)

- Remarks:
  - SuperLU, MUMPS, UMFPACK can use any sparsity-reducing ordering
  - STRUMPACK can only use nested dissection (restricted to binary tree)

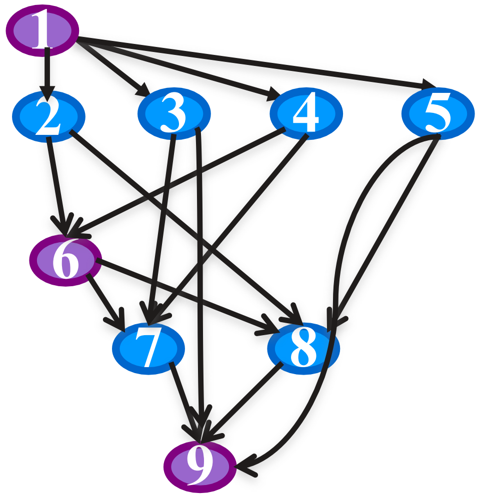
- Survey of sparse direct solvers (codes, algorithms, parallel capability):
  https://portal.nersc.gov/project/sparse/superlu/SparseDirectSurvey.pdf

Sparse LU: two algorithm variants



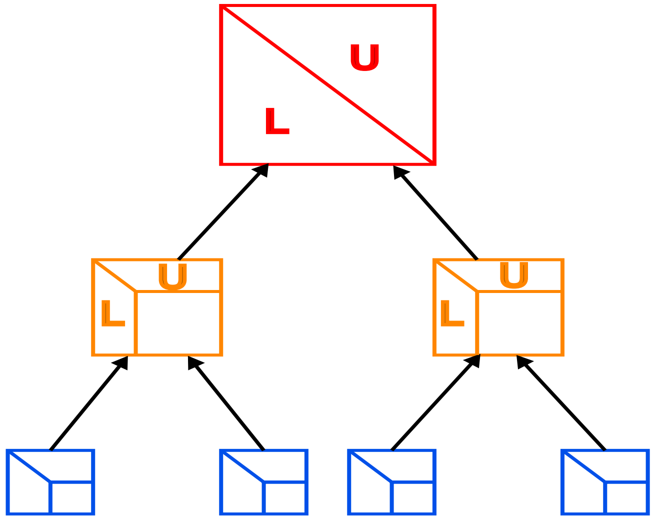
… depending on how updates are accumulated

DAG based
Supernodal: SuperLU



$S^{(j)} \leftarrow ((\ A^{(j)} - D^{(k1)}\ ) - D^{(k2)}\ ) - \ldots)$

Tree based
Multifrontal: STRUMPACK, MUMPS

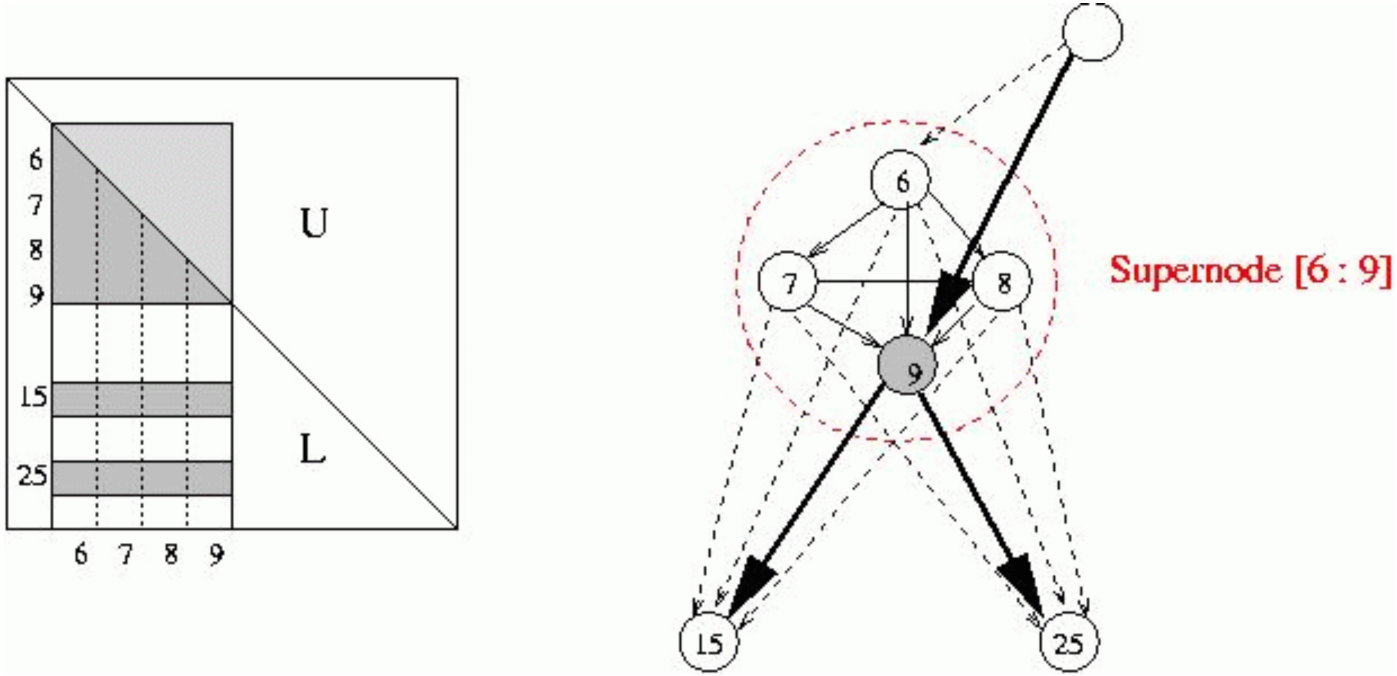


$S^{(j)} \leftarrow A^{(j)} - (..(D^{(k1)} + D^{(k2)}\ ) + \ldots)$

Supernode

Exploit dense submatrices in the factors

- Can use Level 3 BLAS
- Reduce inefficient indirect addressing (scatter/gather)
- Reduce graph traversal time using a coarser graph

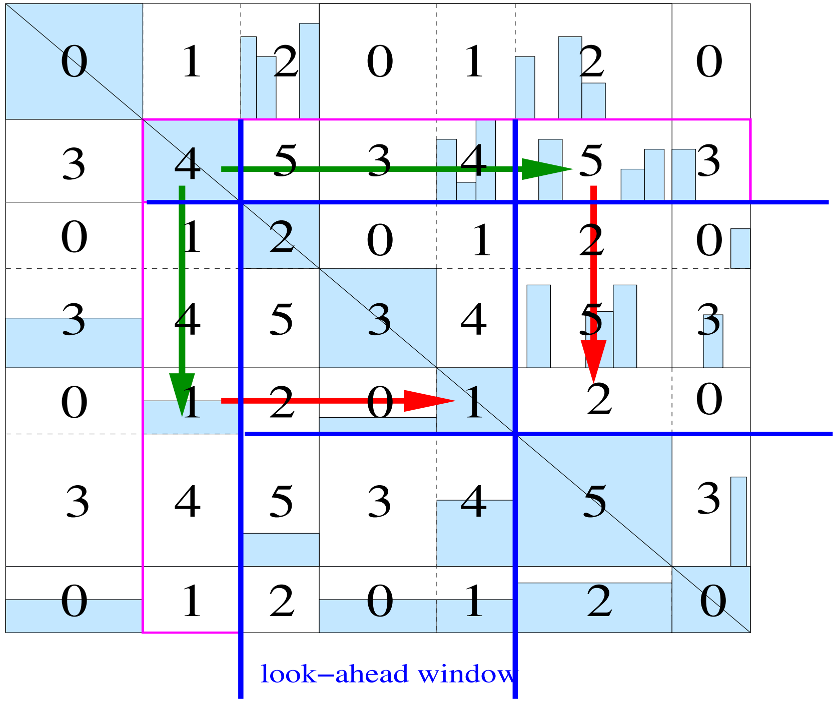


2D distributed L & U factored matrices (internal to SuperLU)

- 2D block cyclic layout – specified by user.
- Rule: process grid should be as square as possible.

  Or, set the row dimension (*nprow*) slightly smaller than the column dimension (*npcol*).

  - For example: 2x3, 2x4, 4x4, 4x8, etc.

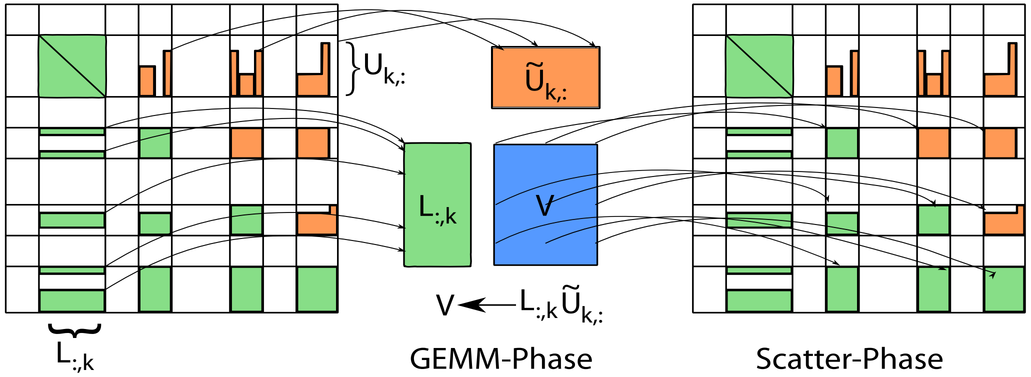


MPI Process Grid

0	1	2
3	4	5

Per-rank Schur complement update

Loop through N steps: (Gaussian Elimination)
FOR (k = 1, N) {
1) **Gather** sparse blocks A(:, k) and A(k,:) into dense work[]
2) Call dense **GEMM** on work[]
3) **Scatter** work[] into remaining sparse blocks
}



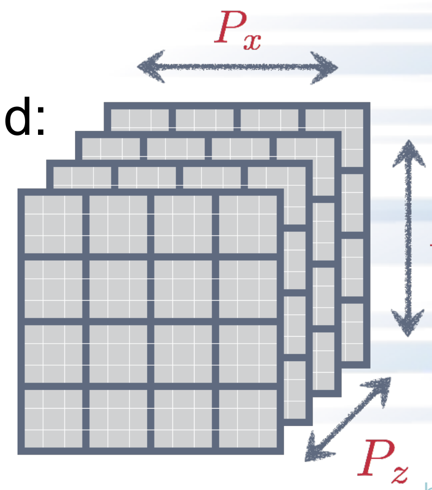
Communication-avoid 3D algorithm ('pddrive3d')

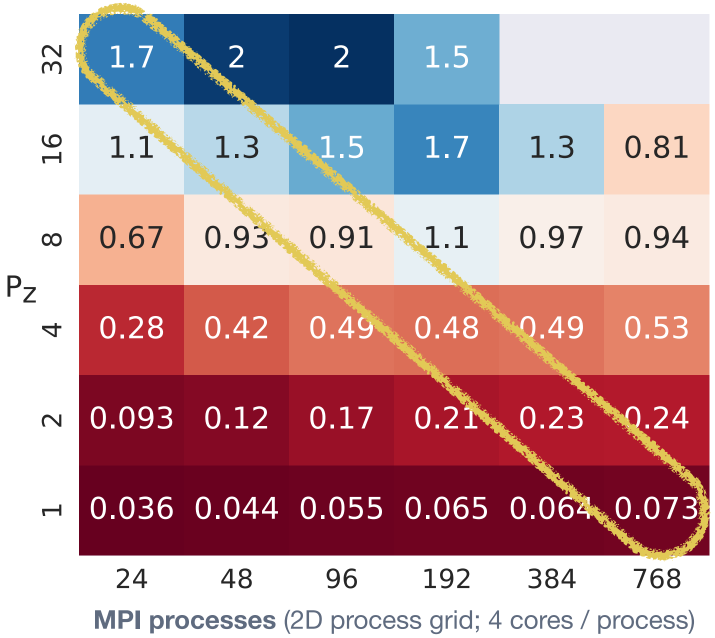
Sao, Li, Vuduc, JPDC 2019

- For matrices from planar graph, provably asymptotic lower communication complexity:
  - Comm. volume reduced by a factor of sqrt(log(n)).
  - Latency reduced by a factor of log(n).
- Strong scale to 24,000 cores.

  Compared to 2D algorithm:
  - Planar graph: up to 27x faster, 30% more memory @ $P_z = 16$
  - Non-planar graph: up to 3.3x faster, 2x more memory @ $P_z = 16$

3D process grid: $\{P_{XY}, P_Z\}$





2D to 3D:
→ **23x speedup**

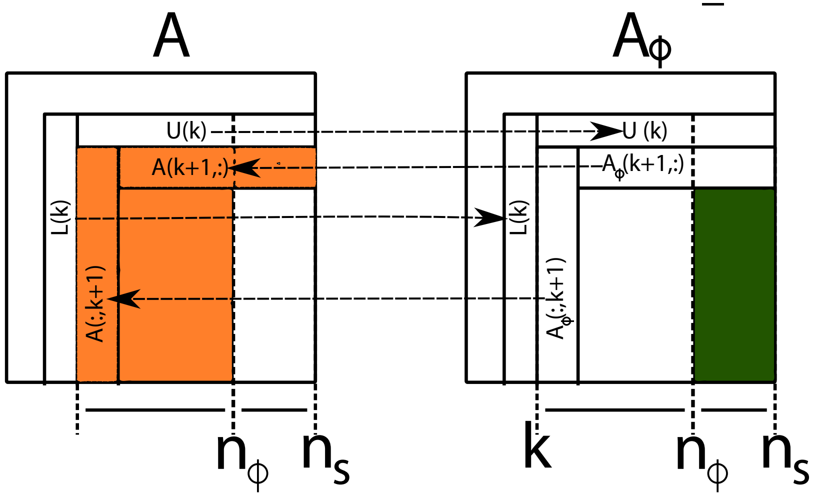
Teraflop/s
(32x procs → 2x speedup)

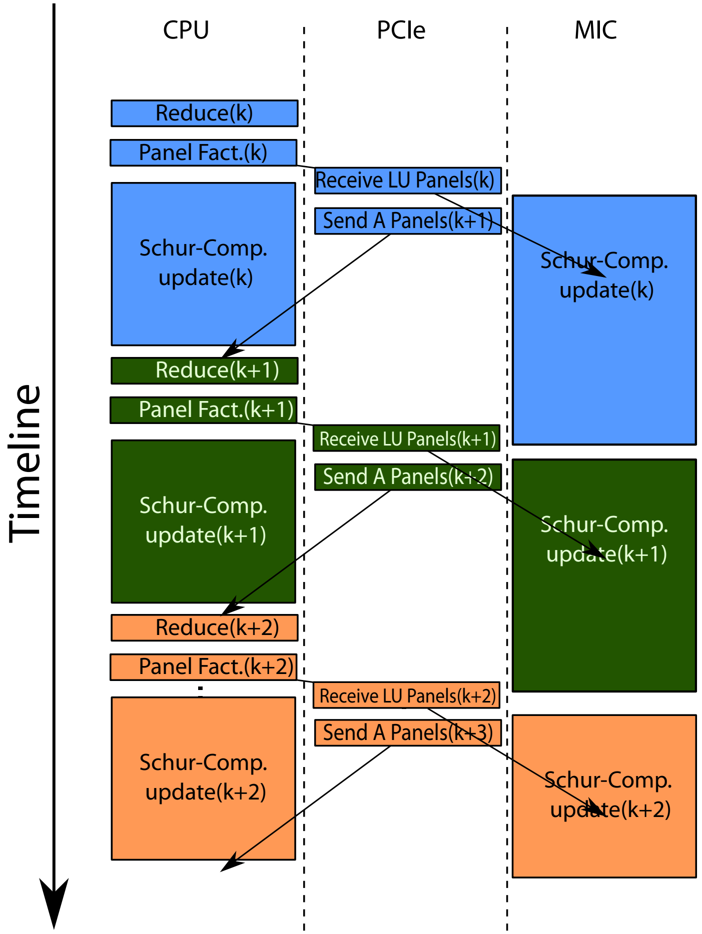
Offload more to GPU

- Offload Schur-complement update to GPU

Sao, Liu, Vuduc, Li, IPDPS 2015

GPU variable: MAX_BUFFER_SIZE





SpLU tiime on ThetaGPU (AMD EPYC 7742, NVIDIA A100)

export matdir=/grand/ATPESC2022/usr/MathPackages/datafiles

export OMP_NUM_THREADS=1

- 2D algorithm: mpiexec -n 2 pddrive -r 1 -c 2 ${matdir}/<matrix file>
  - Only offload GEMM
- 3D algorithm: mpiexec -n 2 pddive3d -r 1 -c 1 -d 2 ${matdir}/<matrix file>
  - Offload GEMM and Scatter in Schur-complement, panel factor still on CPU

		2D proc grid: 1x1	1x2	3D proc grid: 1x1x1	1x1x2
torso3	CPU (SUPERLU_ACC_OFFLOAD=0) +GPU	21.2 18.1	12.2 10.8	24.4 6.3	14.3 5.2
Li4244	CPU (SUPERLU_ACC_OFFLOAD=0) +GPU	259.5 175.1	140.6 98.2	298.5 31.1	179.8 28.2

User-controllable options in SuperLU_DIST

For stability and efficiency, need to solve transformed linear system:

$$P_c\,(\,P_r\,(D_r\,A\,D_c)\,)\,P_c^T\,P_c\,D_c^{-1}\,x = P_c\,P_r\,D_r\,b$$

“Options” fields with C enum constants:

- Equil: { NO, **YES** }
- RowPerm: { NOROWPERM, **LargeDiag_MC64**, LargeDiag_HWPM, MY_PERMR }
- ColPerm: { NATURAL, MMD_ATA, MMD_AT_PLUS_A, COLAMD, **METIS_AT_PLUS_A,** PARMETIS, ZOLTAN, MY_PERMC }

Call set_default_options_dist(&options) to set default values.

Tips for Debugging Performance

- Check sparsity ordering
- Diagonal pivoting is preferable
  - **E.g., matrix is diagonally dominant, . . .**

- Need good BLAS library (vendor, OpenBLAS, ATLAS)
  - **May need adjust block size for each architecture**
    (Parameters modifiable by environment variables)
    - **Larger blocks better for uniprocessor**
    - **Smaller blocks better for parallellism and load balance**

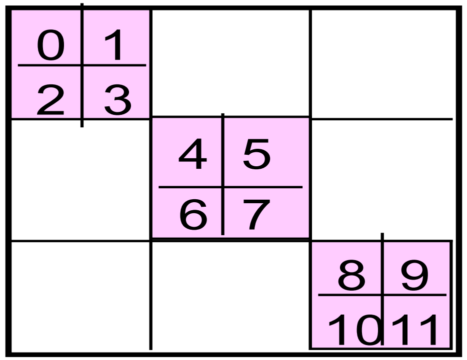
- **GPTune:** ML algorithms for selection of best parameters
  - https://github.com/gptune/GPTune/

SuperLU_DIST other examples

superlu_dist/EXAMPLE

See README file (e.g. mpiexec -n 12 ./pddrive1 -r 3 -c 4 stomach.rua)

- pddrive1.c: Solve the systems with same A but different right-hand side at different times.
  - **Reuse the factored form of A.**
- pddrive2.c: Solve the systems with the same pattern as A.
  - **Reuse the sparsity ordering.**
- pddrive3.c: Solve the systems with the same sparsity pattern and similar values.
  - **Reuse the sparsity ordering and symbolic factorization.**
- pddrive4.c: Divide the processes into two subgroups (two grids) such that each subgroup solves a linear system independently from the other.



Block Jacobi preconditioner

Algorithm complexity (in bigO sense)

- Dense LU: $O(N^3)$
- Model PDEs with regular mesh, nested dissection ordering

	2D problems $N = k^2$			**3D problems** $N = k^3$		
	Factor flops	Solve flops	Memory	Factor flops	Solve flops	Memory
Exact sparse LU	$N^{3/2}$	N log(N)	N log(N)	N^2	$N^{4/3}$	$N^{4/3}$
STRUMPACK with low-rank compression	N	N	N	N^α polylog(N) ($\alpha < 2$)	N log(N)	N log(N)

Code	Technique	Scope	Contact	
Serial platforms (possibly on GPU				
CHOLMOD	Left-looking	SPD	Davis	[8]
GLU3.0	Left-looking	Unsym (GPU)	Peng	[36]
KLU	Left-looking	Unsym	Davis	[11]
MA57	Multifrontal	Sym	HSL	[19]
MA41	Multifrontal	Sym-pat	HSL	[1]
MA42	Frontal	Unsym	HSL	[20]
MA67	Multifrontal	Sym	HSL	[17]
MA48	Right-looking	Unsym	HSL	[18]
Oblio	Left/right/Multifr.	sym, Out-core	Dobrian	[14]
SPARSE	Right-looking	Unsym	Kundert	[32]
SPARSPAK	Left-looking	SPD, Unsym, QR	George et al.	[22]
SPOOLES	Left-looking	Sym, Sym-pat, QR	Ashcraft	[5]
SSIDS	Multifrontal	Sym (GPU)	Hogg	[28]
SuperLLT	Left-looking	SPD	Ng	[35]
SuperLU	Left-looking	Unsym	Li	[12]
UMFPACK	Multifrontal	Unsym	Davis	[9]
Shared memory parallel machines (possibly on GPU)				
BCSLIB-EXT	Multifrontal	Sym, Unsym, QR	Ashcraft et al.	[6]
Cholesky	Left-looking	SPD	Rothberg	[31]
MF2	Multifrontal	Sym, Sym-pat, Out-core (GPU)	Lucas	[34]
MA41	Multifrontal	Sym-pat	HSL	[2]
MA49	Multifrontal	QR	HSL	[4]
PanelLLT	Left-looking	SPD	Ng	[24]
PARASPAR	Right-looking	Unsym	Zlatev	[41]
PARDISO	Left-Right looking	Sym-pat	Schenk	[39]
SPOOLES	Left-looking	Sym, Sym-pat	Ashcraft	[5]
SuiteSparseQR	Multifrontal	Rank-revealing QR	Davis	[10]
SuperLU_MT	Left-looking	Unsym	Li	[13]
TAUCS	Left/Multifr.	Sym, Unsym, Out-core	Toledo	[7]
WSMP	Multifrontal	SPD, Unsym	Gupta	[25]
Distributed memory parallel machines				
Clique	Multifrontal	Sym (no pivoting)	Poulson	[37]
MF2	Multifrontal	Sym, Sym-pat, Out-core, GPU	Lucas	[34]
DSCPACK	Multifrontal	SPD	Raghavan	[26]
MUMPS	Multifrontal	Sym, Sym-pat	Amestoy	[3]
PARDISO	Left-Right looking	Sym-pat, Unsym	Schenk	[39]
PaStiX	Left-Right looking	SPD, Sym, Sym-pat	Ramet	[29]
PSPASES	Multifrontal	SPD	Gupta	[23]
SPOOLES	Left-looking	Sym, Sym-pat, QR	Ashcraft	[5]
STRUMPACK	Multifrontal	Unsym, Sym-pat (GPU)	Ghysels	[40]
SuperLU_DIST	Right-looking	Unsym (GPU)	Li	[33]
symPACK	Left-Right looking	SPD	Jacquelin	[30]
S+	Right-looking†	Unsym	Yang	[21]
WSMP	Multifrontal	SPD, Unsym	Gupta	[25]

Table 1: Software to solve sparse linear systems using direct methods.

Survey of sparse direct solver codes

portal.nersc.gov/project/sparse/superlu/SparseDirectSurvey.pdf

References

- Short course, “Factorization-based sparse solvers and preconditioners”, 4th Gene Golub SIAM Summer School, 2013.https://archive.siam.org/students/g2s3/2013/index.html
  - 10 hours lectures, hands-on exercises
  - Extended summary: http://crd-legacy.lbl.gov/~xiaoye/g2s3-summary.pdf

    (in book “Matrix Functions and Matrix Equations”, https://doi.org/10.1142/9590)

- SuperLU: portal.nersc.gov/project/sparse/superlu
  - Users guide, papers, …

Rank Structured Solvers for Dense Linear Systems

EXASCALE COMPUTING PROJECT

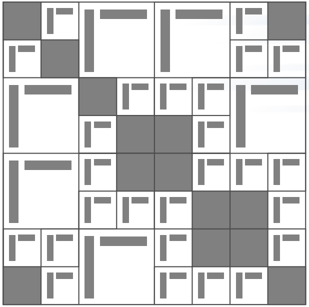
Hierarchical Matrix Approximation

$\mathcal{H}$-matrix representation [1]

- Data-sparse, rank-structured, compressed

Hierarchical/recursive 2×2 matrix blocking, with blocks either:

- Low-rank: $A_{IJ} \approx UV^{\top}$
- Hierarchical
- Dense (at lowest level)

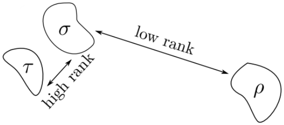


Use cases:

- Boundary element method for integral equations
- Cauchy, Toeplitz, kernel, covariance, ... matrices
- Fast matrix-vector multiplication
- $\mathcal{H}$-LU decomposition
- Preconditioning

Hackbusch, W., 1999. *A sparse matrix arithmetic based on $\mathcal{H}$-matrices. part I: Introduction to $\mathcal{H}$-matrices.* Computing, 62(2), pp.89-108.

Admissibility Condition

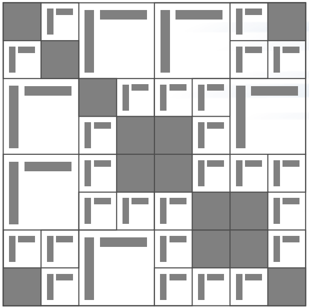


- Row cluster σ
- Column cluster τ
- $\sigma \times \tau$ is compressible $\Leftrightarrow$

$$\frac{\max(\text{diam}(\sigma), \text{diam}(\tau))}{\text{dist}(\tau, \sigma)} \leq \eta$$

  - diam(σ): diameter of physical domain corresponding to σ
  - dist(σ, τ): distance between σ and τ

- Weaker interaction between clusters leads to smaller ranks
- Intuitively larger distance, greater separation, leads to weaker interaction
- Need to cluster and order degrees of freedom to reduce ranks



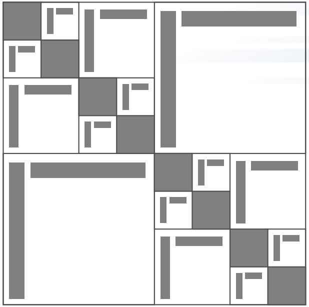
Hackbusch, W., 1999. *A sparse matrix arithmetic based on $\mathcal{H}$-matrices. part i: Introduction to $\mathcal{H}$-matrices.* Computing, 62(2), pp.89-108.

HODLR: Hierarchically Off-Diagonal Low Rank

- Weak admissibility

$$\sigma \times \tau \text{ is compressible } \Leftrightarrow \sigma \neq \tau$$

  Every off-diagonal block is compressed as low-rank, even interaction between neighboring clusters (no separation)



Compared to more general $\mathcal{H}$-matrix

- Simpler data-structures: same row and column cluster tree
- More scalable parallel implementation
- Good for 1D geometries, e.g., boundary of a 2D region discretized using BEM or 1D separator
- Larger ranks

HSS: Hierarchically Semi Seperable

- Weak admissibility
- Off-diagonal blocks

$$A_{\sigma,\tau} \approx U_\sigma B_{\sigma,\tau} V_\tau^\top$$

- Nested bases

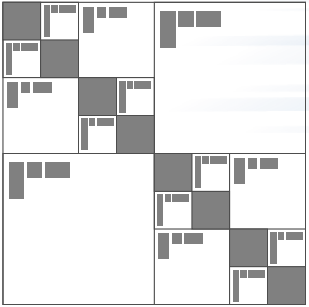
$$U_\sigma = \begin{bmatrix} U_{\nu_1} & 0 \\ 0 & U_{\nu_2} \end{bmatrix} \hat{U}_\sigma$$

with ν_1 and ν_2 children of σ in the cluster tree.

- At lowest level

$$U_\sigma \equiv \hat{U}_\sigma$$

- Store only $\hat{U}_\sigma$, smaller than U_σ
- Complexity $\mathcal{O}(N) \leftrightarrow \mathcal{O}(N \log N)$ for HODLR
- HSS is special case of $\mathcal{H}^2$: $\mathcal{H}$ with nested bases



$$\begin{bmatrix} \begin{matrix} D_0 & U_0 B_{0,1} V_1^* \\ U_1 B_{1,0} V_0^* & D_1 \end{matrix} & \color{red}{U_2 B_{2,5} V_5^*} \\ \color{red}{U_5 B_{5,2} V_2^*} & \begin{matrix} D_3 & U_3 B_{3,4} V_4^* \\ U_4 B_{4,3} V_3^* & D_4 \end{matrix} \end{bmatrix}$$

HSS: Hierarchically Semi Seperable

- Weak admissibility
- Off-diagonal blocks

$$A_{\sigma,\tau} \approx U_\sigma B_{\sigma,\tau} V_\tau^\top$$

- Nested bases

$$U_\sigma = \begin{bmatrix} U_{\nu_1} & 0 \\ 0 & U_{\nu_2} \end{bmatrix} \hat{U}_\sigma$$

  with ν_1 and ν_2 children of σ in the cluster tree.
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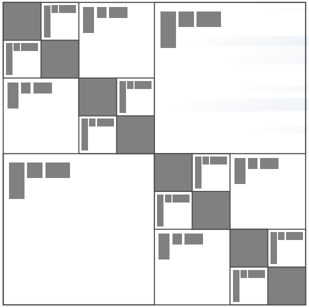
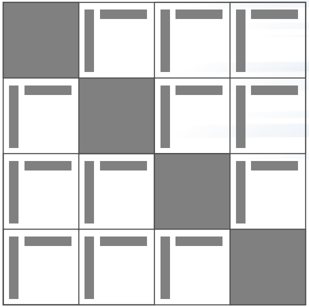


$$\begin{bmatrix} \begin{matrix} D_0 & U_0 B_{0,1} V_1^* \\ U_1 B_{1,0} V_0^* & D_1 \end{matrix} & \begin{bmatrix} U_0 & 0 \\ 0 & U_1 \end{bmatrix} \hat{U}_2 B_{2,5} \hat{V}_5^* \begin{bmatrix} V_3^* & 0 \\ 0 & V_4^* \end{bmatrix} \\ \begin{bmatrix} U_3 & 0 \\ 0 & U_4 \end{bmatrix} \hat{U}_5 B_{5,2} \hat{V}_2^* \begin{bmatrix} V_0^* & 0 \\ 0 & V_1^* \end{bmatrix} & \begin{matrix} D_3 & U_3 B_{3,4} V_4^* \\ U_4 B_{4,3} V_3^* & D_4 \end{matrix} \end{bmatrix}$$

EXASCALE COMPUTING PROJECT

BLR: Block Low Rank [1, 2]

- Flat partitioning (non-hierarchical)
- Weak or strong admissibility
- Larger asymptotic complexity than $\mathcal{H}$, HSS, . . .
- Works well in practice



Mary, T. (2017). *Block Low-Rank multifrontal solvers: complexity, performance, and scalability.* (Doctoral dissertation).

Amestoy, Patrick, et al. (2015). *Improving multifrontal methods by means of block low-rank representations.* SISC 37.3 : A1451-A1474.

Data-Sparse Matrix Representation Overview

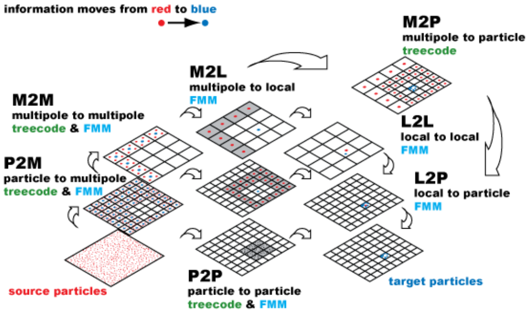
$\mathcal{H}$ HODLR HSS BLR

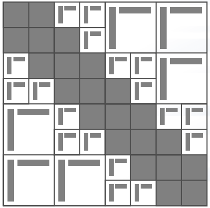
- Partitioning: **hierarchical** ($\mathcal{H}$, HODLR, HSS) or **flat** (BLR)
- Admissibility: **weak** (HODLR, HSS) or **strong** ($\mathcal{H}$, $\mathcal{H}^2$)
- Bases: **nested** (HSS, $\mathcal{H}^2$) or **not nested** (HODLR, $\mathcal{H}$, BLR)

Fast Multipole Method [1]

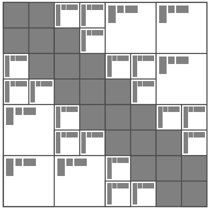
Particle methods like Barnes-Hut and FMM can be interpreted algebraically using hierarchical matrix algebra

- Barnes-Hut $\mathcal{O}(N \log N)$
- Fast Multipole Method $\mathcal{O}(N)$





Barnes-Hut

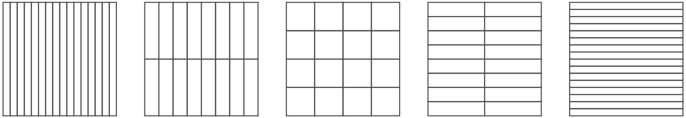


FMM

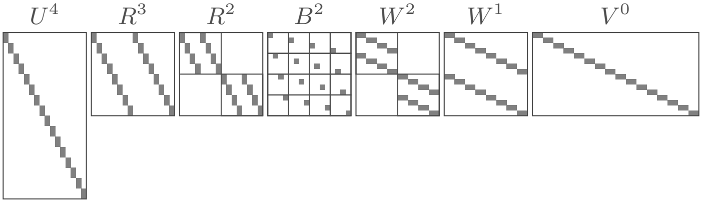
Greengard, L., and Rokhlin, V. *A fast algorithm for particle simulations.* Journal of computational physics 73.2 (1987): 325-348.

Butterfly Decomposition [1]

Complementary low rank property: sub-blocks of size $\mathcal{O}(N)$ are low rank:



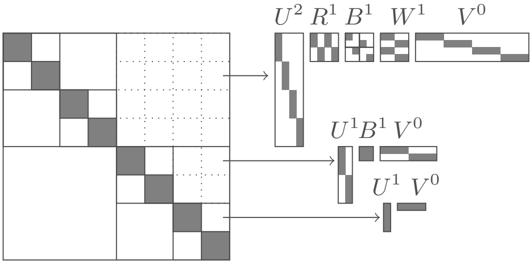
Multiplicative decomposition:



- Multilevel generalization of low rank decomposition
- Based on FFT ideas, motivated by high-frequency problems

Michielssen, E., and Boag, A. *Multilevel evaluation of electromagnetic fields for the rapid solution of scattering problems.* Microwave and Optical Technology Letters 7.17 (1994): 790-795.

HODBF: Hierarchically Off-Diagonal Butterfly



- HODLR but with low rank replaced by Butterfly decomposition
- Reduces ranks of large off-diagonal blocks

EXASCALE COMPUTING PROJECT

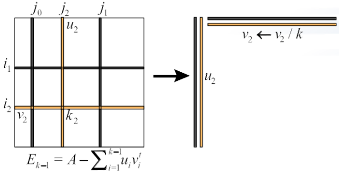
Low Rank Approximation Techniques

Traditional approaches need entire matrix

- Truncated Singular Value Decomposition (TSVD): $A \approx U \Sigma V^T$
  - Optimal, but expensive
- Column Pivoted QR: $AP \approx QR$
  - Less accurate than TSVD, but cheaper

Adaptive Cross Approximation

- No need to compute every element of the matrix
- Requires certain assumptions on input matrix
- Left-looking LU with rook pivoting



Randomized algorithms [1]

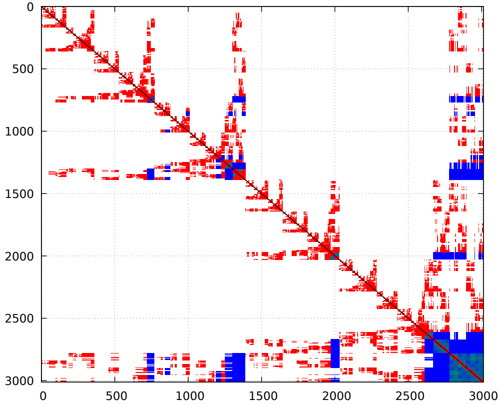
- Fast matrix-vector product: $S = A\Omega$
  Reduce dimension of A by random projection with Ω
- E.g., operator is sparse or rank structured, or the product of sparse and rank structured

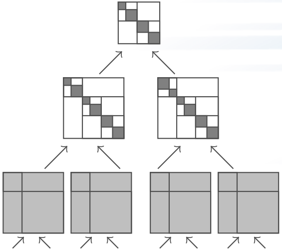
Halko, N., Martinsson, P.G., Tropp, J.A. (2011). *Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions.* SIAM Review, 53(2), 217-288.

Approximate Multifrontal Factorization

Sparse Multifrontal Solver/Preconditioner with Rank-Structured Approximations

L and U factors, after nested-dissection ordering,
compressed blocks in blue



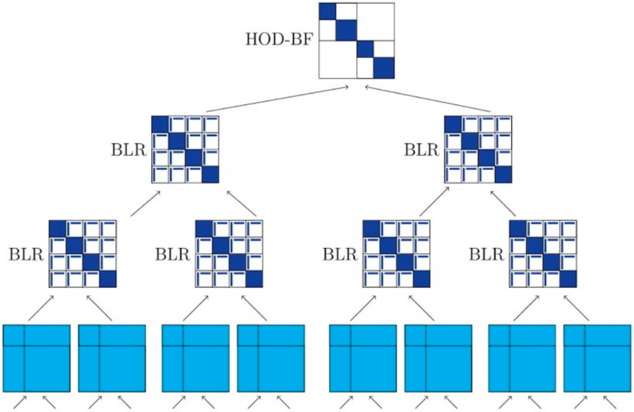


Only apply rank structured compression to largest fronts (dense sub-blocks), keep the rest as regular dense

Combining Block Low Rank and Hierarchically Off-Diagonal Butterfly

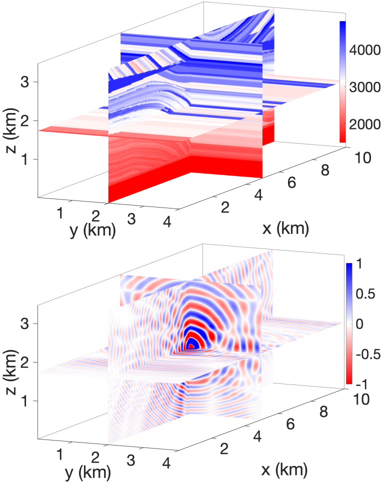
Rank-structured compression of largest dense blocks in the multifrontal/assembly tree

- Largest: HOD-BF
- Medium: BLR
- Smaller: dense

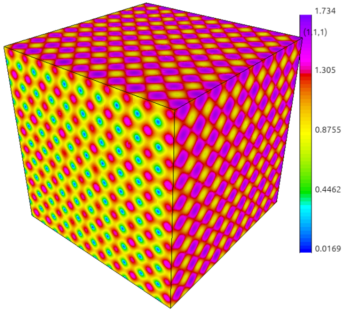


High Frequency Helmholtz and Maxwell

Regular $k^3 = N$ grid, fixed number of discretization points per wavelength



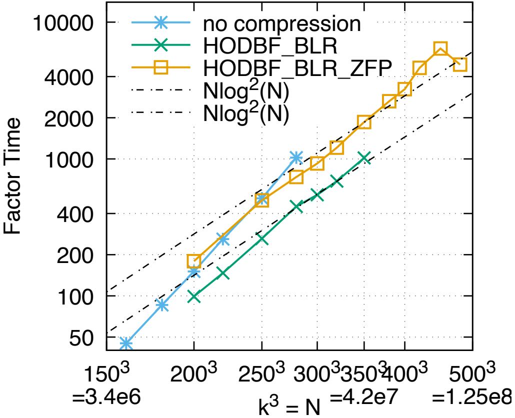
Marmousi2 geophyical elastic dataset

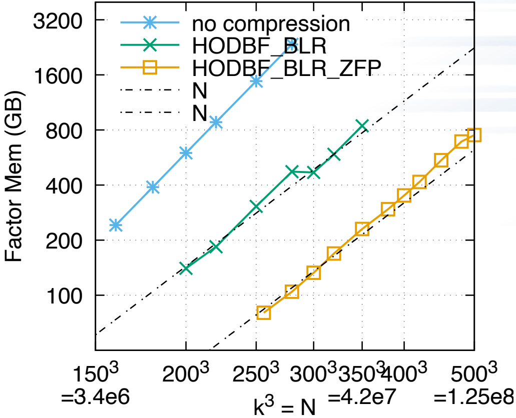


Indefinite Maxwell, using MFEM

STRUMPACK Preconditioners for High Frequency Helmholtz and Maxwell

Sparse multifrontal solver with hybrid ZFP, BLR and HODBF compression





- Highly oscillatory problems are hard for iterative solvers
- Typically solved with sparse direct solvers, but scale as $\mathcal{O}(N^2)$

Software: ButterflyPACK

- Butterfly
- Hierarchically Off-Diagonal Low Rank (HODLR)
- Hierarchically Off-Diagonal Butterfly (HODBF)
- Hierarchical matrix format ($\mathcal{H}$)
  - Limited parallelism

- Fast compression, using randomization
- Fast multiplication, factorization & solve
- Fortran2008, MPI, OpenMP

`https://github.com/liuyangzhuan/ButterflyPACK`

EXASCALE COMPUTING PROJECT

Software: STRUMPACK

STRUctured Matrix PACKage

- Fully algebraic solvers/preconditioners
- Sparse direct solver (multifrontal LU factorization)
- Approximate sparse factorization preconditioner
- Dense
  - HSS: Hierarchically Semi-Separable
  - BLR: Block Low Rank
  - ButterflyPACK integration/interface:
    - Butterfly
    - HODLR
    - HODBF

- C++, MPI + OpenMP + CUDA, real & complex, 32/64 bit integers
- BLAS, LAPACK, Metis
- Optional: MPI, ScaLAPACK, ParMETIS, (PT-)Scotch, cuBLAS/cuSOLVER, SLATE, ZFP

`https://github.com/pghysels/STRUMPACK`
`https://portal.nersc.gov/project/sparse/strumpack/master/`

Other Available Software

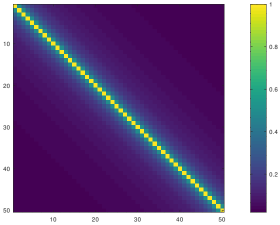
HiCMA	`https://github.com/ecrc/hicma`
HLib	`http://www.hlib.org/`
HLibPro	`https://www.hlibpro.com/`
H2Lib	`http://www.h2lib.org/`
HACApK	`https://github.com/hoshino-UTokyo/hacapk-gpu`
MUMPS	`http://mumps.enseeiht.fr/`
PaStiX	`https://gitlab.inria.fr/solverstack/pastix`
ExaFMM	`http://www.bu.edu/exafmm/`

See also:
`https://github.com/gchavez2/awesome_hierarchical_matrices`

STRUMPACK Hands-On Session

HODLR Compression of Toeplitz Matrix $T(i,j) = \frac{1}{1+|i-j|}$

track-5-numerical/rank_structured_strumpack/build/testHODLR



- See `track-5-numerical/rank_structured_strumpack/README`
- Get a compute node:
```
qsub -I -n 1 -t 30 -A ATPESC2022 -q single-gpu
```
- Set OpenMP threads:
```
export OMP_NUM_THREADS=1
```
- Run example:
```
mpiexec -n 1 ./build/testHODLR 2000
```
- With description of command line parameters:
```
mpiexec -n 1 ./build/testHODLR 2000 --help
```
- Vary leaf size (smallest block size) and tolerance:
```
mpiexec -n 1 ./build/testHODLR 2000 --structured_rel_tol 1e-4 --structured_leaf_size 16
mpiexec -n 1 ./build/testHODLR 2000 --structured_rel_tol 1e-4 --structured_leaf_size 12
```
- Vary number of MPI processes:
```
mpiexec -n 12 ./build/testHODLR 2000 --structured_rel_tol 1e-8 --structured_leaf_size 1
mpiexec -n 12 ./build/testHODLR 2000 --structured_rel_tol 1e-8 --structured_leaf_size 1
```

HODLR Compression of Toeplitz Matrix $T(i,j) = \frac{1}{1+|i-j|}$

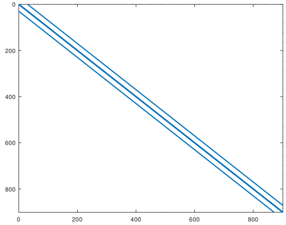
track-5-numerical/rank_structured_strumpack/build/testHODLR

```
OMP_NUM_THREADS=1 mpiexec -n 16 ./testHODLR 20000 --structured_rel_tol 1e-4

dense (2DBC) 20000 x 20000 matrix
  - memory(T2d) = 201.925 MByte

 Compression from matrix elements
HODLR
  - total_nonzeros(H) = 297121
  - total_memory(H) = 2.37697 MByte
  - maximum_rank(H) = 12
  - ||T-H||_F/||T||_F = 1.95816e-06
  - ||X-T\(T*X)||_F/||X||_F = 2.90269e-06
GMRES it. 0 res =      140.258 rel.res =            1  restart!
GMRES it. 1 res =  0.000378084 rel.res =  2.69563e-06
GMRES it. 2 res =  7.45695e-09 rel.res =  5.31659e-11
  - ||X-A\(A*X)||_F/||X||_F = 5.24893e-11
```

Solve a Sparse Linear System with Matrix `pde900.mtx`

track-5-numerical/rank_structured_strumpack/build/testMMdouble{MPIDist}

- See `track-5-numerical/rank_structured_strumpack/README`
- Get a compute node:
  `qsub -I -n 1 -t 30 -A ATPESC2022 -q single-gpu`
- Set OpenMP threads: `export OMP_NUM_THREADS=1`



- Run example:
  `mpiexec -n 1 ./build/testMMdouble pde900.mtx`
- With description of command line parameters:
  `mpiexec -n 1 ./build/testMMDouble pde900.mtx --help`
- Enable/disable GPU off-loading:
  `mpiexec -n 1 ./build/testMMDouble pde900.mtx --sp_disable_gpu`
- Vary number of MPI processes:
  `mpiexec -n 1 ./build/testMMdouble pde900.mtx`
  `mpiexec -n 12 ./build/testMMdoubleMPIDist pde900.mtx`
- Other sparse matrices, in matrix market format:
  NIST Matrix Market: `https://math.nist.gov/MatrixMarket`
  SuiteSparse: `http://faculty.cse.tamu.edu/davis/suitesparse.html`

GPU Performance for SuiteSparse Problems

track-5-numerical/rank_structured_strumpack/build/testMMdouble

See `/grand/ATPESC2022/usr/MathPackages/datafiles/`

```
OMP_NUM_THREADS=16 ./testMMdouble torso3.mtx
OMP_NUM_THREADS=16 ./testMMdouble torso3.mtx --sp_disable_gpu
```

			time (seconds)		GFlop/s	
matrix	N	nnz	GPU A100	16 CPU	GPU A100	16 CPU
torso3	259,156	4,429,042	0.81	2.18	505.4	174.7
Geo_1438	1,437,960	60,236,322	9.54	147.72	3618.7	233.7
nlpkkt80	1,062,400	28,192,672	7.97	133.58	4056.6	242.0

Table: Numerical factorization time (seconds) and performance in terms of floating point operations per second.

Solve 3D Poisson Problem

track-5-numerical/rank_structured_strumpack/build/testPoisson3d{MPIDist}

- See `track-5-numerical/rank_structured_strumpack/README`
- Get a compute node: `qsub -I -n 1 -t 30 -A ATPESC2022 -q single-gpu`
- Set OpenMP threads: `export OMP_NUM_THREADS=1`
- Solve 40^3 Poisson problem:

```
mpiexec -n 1 ./build/testPoisson3d 40 --help --sp_disable_gpu
```

- Enable BLR compression:

```
mpiexec -n 1 ./build/testPoisson3d 40 --sp_compression BLR --help
mpiexec -n 1 ./build/testPoisson3d 40 --sp_compression BLR --blr_rel_tol 1e-2
mpiexec -n 1 ./build/testPoisson3d 40 --sp_compression BLR --blr_rel_tol 1e-4
mpiexec -n 1 ./build/testPoisson3d 40 --sp_compression BLR --blr_leaf_size 128
mpiexec -n 1 ./build/testPoisson3d 40 --sp_compression BLR --blr_leaf_size 256
```

- Parallel, with HSS/HODLR compression:

```
mpiexec -n 12 ./build/testPoisson3dMPIDist 40
mpiexec -n 12 ./build/testPoisson3dMPIDist 40 --sp_compression HSS \
     --sp_compression_min_sep_size 1000 --hss_rel_tol 1e-2
mpiexec -n 12 ./build/testPoisson3dMPIDist 40 --sp_compression HODLR \
     --sp_compression_min_sep_size 1000 --hodlr_leaf_size 128
```

Rank Structured Preconditioning

track-5-numerical/rank_structured_strumpack/build/testPoisson3d

```
export OMP_NUM_THREADS=16
./testPoisson3d 50  --sp_compression none --sp_disable_gpu
./testPoisson3d 100 --sp_compression none --sp_disable_gpu

./testPoisson3d 50  --sp_compression blr  --blr_rel_tol 1e-2
./testPoisson3d 100 --sp_compression blr  --blr_rel_tol 1e-2
```

compression	NONE		BLR	
mesh size	50^3	100^3	50^3	100^3
factor time (sec)	1.11	51.59	0.59	17.20
factor memory (MB)	902	16,477	533	5,190
compression	-	-	59%	31%
peak memory (MB)	2,316	43,956	1,366	16,809
solve time (sec)	0.05	0.78	0.17	2.32
GMRES its	1	1	7	12

Table: Multifrontal solver with block low rank compression for 3D Poisson equation, using compression tolerance $\varepsilon = 10^{-2}$. GMRES relative tolerance is 10^{-6}.

Rank Structured Preconditioning

track-5-numerical/rank_structured_strumpack/build/testMMdouble

```
export OMP_NUM_THREADS=16
./testMMdouble torso3.mtx --sp_compression NONE --sp_disable_gpu
./testMMdouble torso3.mtx --sp_compression BLR  --blr_rel_tol 1e-2
```

matrix	torso3		Geo_1438		nlpkkt80	
compression	NONE	BLR	NONE	BLR	NONE	BLR
factor time (sec)	2.17	1.10	147.81	50.10	140.21	38.19
factor memory (MB)	1,855	1,281	38,523	17,999	30,199	10,128
compression	100%	70.1%	100%	46.7%	100%	33.5%
peak memory (MB)	5,505	3,694	109,741	45,603	89,171	40,775
solve time (sec)	0.09	0.14	1.80	10.69	1.46	5.54
GMRES its	1	2	1	18	1	15

Table: Multifrontal solver with block low rank compression for several SuiteSparse linear systems, using compression tolerance $\varepsilon = 10^{-2}$. GMRES relative tolerance is 10^{-6}.

EXASCALE COMPUTING PROJECT