SuperLU and STRUMPACK Sparse Direct Solver and Preconditioner

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    - Ichitaro Yamazaki, LBNL
  - STRUMPACK:
    - Pieter Ghysels, Francois-Henry Rouet, Sherry Li, LBNL

SuperLU

Quick installation

- Download site http://crd.lbl.gov/~xiaoye/SuperLU
  - Users' Guide, HTML code documentation
- Gunzip, untar
- Follow README at top level directory
  - Edit make.inc for your platform (compilers, optimizations, libraries, ...) (may move to autoconf in the future)
  - Link with a fast BLAS library
    - The one under CBLAS/ is functional, but not optimized
    - Vendor, GotoBLAS, ATLAS, …
- In the process of creating CMake build system.

Outline of Tutorial

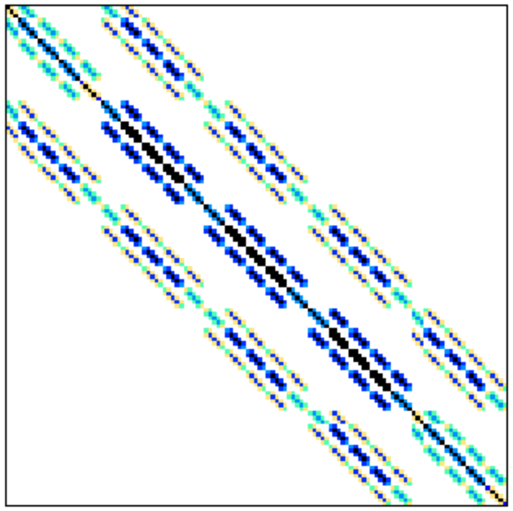
- Functionality
- Sparse matrix data structure, distribution, and user interface
- Background of the algorithms
  - Differences between sequential and parallel solvers
- Examples, Fortran 90 interface

- Hands on exercises

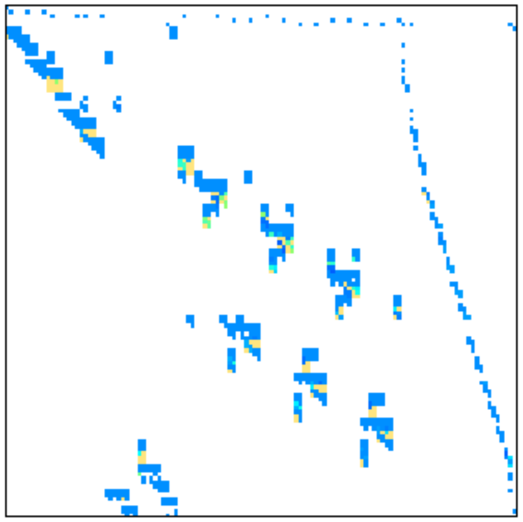
Solve sparse Ax=b : lots of zeros in matrix

- fluid dynamics, structural mechanics, chemical process simulation, circuit simulation, electromagnetic fields, magneto-hydrodynamics, seismic-imaging, economic modeling, optimization, data analysis, statistics, . . .
- Example: A of dimension 10^6, 10~100 nonzeros per row
- Matlab: > spy(A)

Boeing/msc00726 (structural eng.)



Mallya/lhr01 (chemical eng.)



Strategies of sparse linear solvers

- Solving a system of linear equations $Ax = b$
  - Sparse: many zeros in A; worth special treatment
- 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)
  - Harder to optimize and parallelize
  - Numerically robust, but higher algorithmic complexity
- Often use direct method to precondition iterative method
  - Solve an easy system: $M^{-1}Ax = M^{-1}b$

Available direct solvers

- **Survey of different types of factorization codes**

  http://crd.lbl.gov/~xiaoye/SuperLU/SparseDirectSurvey.pdf

  - **LL^T (s.p.d.)**
  - **LDL^T (symmetric indefinite)**
  - **LU (nonsymmetric)**
  - **QR (least squares)**
  - **Sequential, shared-memory (multicore), distributed-memory, out-of-core, few are GPU-enabled …**

- **Distributed-memory codes:**
  - **SuperLU_DIST [Li/Demmel/Grigori/Yamazaki]**
    - **accessible from PETSc, Trilinos, . . .**
  - **MUMPS, PasTiX, WSMP, . . .**

SuperLU Functionality

- LU decomposition, triangular solution
- Incomplete LU (ILU) preconditioner (serial SuperLU 4.0 up)
- Transposed system, multiple RHS
- Sparsity-preserving ordering
  - Minimum degree ordering applied to A^TA or A^T+A [MMD, Liu `85]
  - 'Nested-dissection' applied to A^TA or A^T+A [(Par)Metis, (PT)-Scotch]
- User-controllable pivoting
  - Pre-assigned row and/or column permutations
  - Partial pivoting with threshold
- Equilibration: $D_r A D_c$
- Condition number estimation
- Iterative refinement
- Componentwise error bounds [Skeel `79, Arioli/Demmel/Duff `89]

Software Status

	SuperLU	SuperLU_MT	SuperLU_DIST
Platform	Serial	SMP, multicore	Distributed memory
Language	C	C + Pthreads or OpenMP	C + MPI + OpenMP + CUDA
Data type	Real/complex, Single/double	Real/complex, Single/double	Real/complex, Double
Data structure	CCS / CRS	CCS / CRS	Distributed CRS

- **Fortran interfaces**
- **SuperLU_MT similar to SuperLU both numerically and in usage**

Data structure: Compressed Row Storage (CRS)

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

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

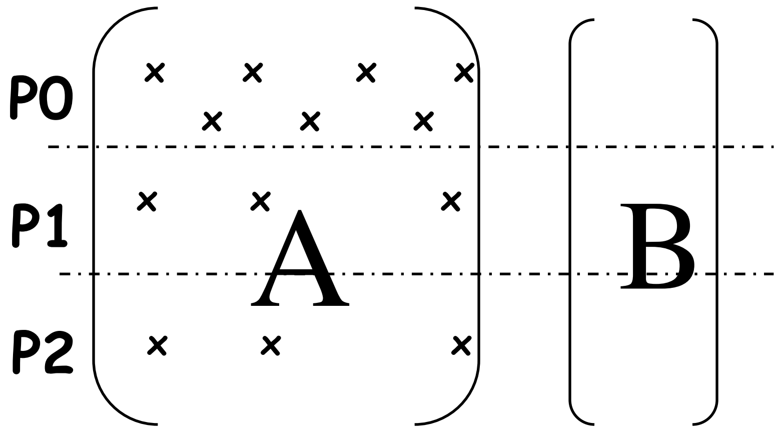
	1	3	5	8	11	13	17	20
nzval	1 a	2 b	c d 3	e 4 f	5 g	h i 6 j	k l 7	
colind	1 4	2 5	1 2 3	2 4 5	5 7	4 5 6 7	3 5 7	

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.

User interface – distribute input matrices

- 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*

  - Natural for users, and consistent with other popular packages: e.g. PETSc

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;
```

Distributed Compressed Row Storage

A is distributed on 2 processors:

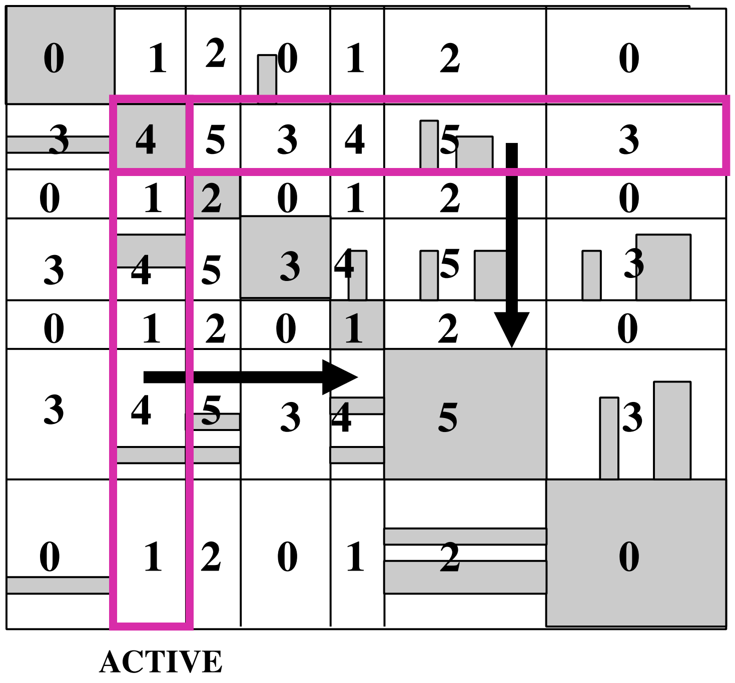
P0	s		u		u
	l	u			
		l	p		
P1				e	u
	l	l			r

- **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 }**

Internal : distributed L & U factored matrices

- 2D block cyclic layout – specified by user
- 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.

Matrix



Process mesh

0	1	2
3	4	5

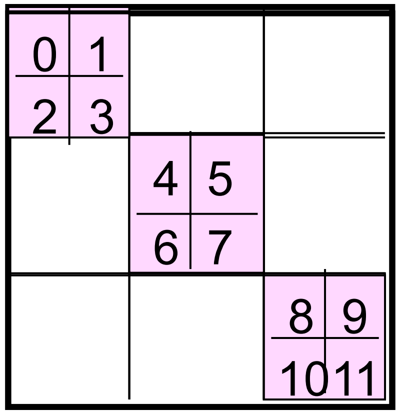
Process grid and MPI communicator

- Example: Solving a preconditioned linear system

  $M^{-1}A\ x = M^{-1}\ b$

  $M = \text{diag}(A_{11}, A_{22}, A_{33})$

  → use SuperLU_DIST for each diagonal block



- Create 3 process grids, same logical ranks (0:3), but different physical ranks
- Each grid has its own MPI communicator

Two ways to create a process grid

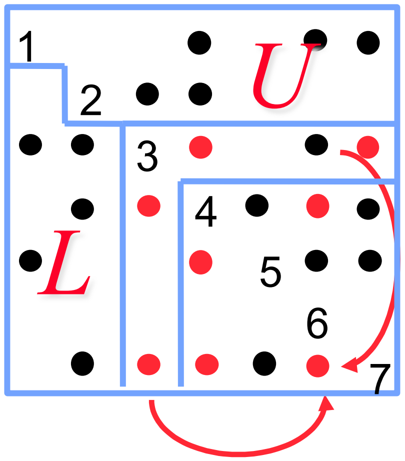
- **superlu_gridinit(MPI_Comm Bcomm, int nprow,**
  int npcol, gridinfo_t *grid);
  - **Maps the first {nprow, npcol} processes in the MPI communicator Bcomm to SuperLU 2D grid**
- **superlu_gridmap(MPI_Comm Bcomm, int nprow,**
  int npcol, int usermap[], int ldumap, gridinfo_t *grid);
  - **Maps an *arbitrary* set of {nprow, npcol } processes in the MPI communicator Bcomm to SuperLU 2D grid. The ranks of the selected MPI processes are given in usermap[] array.**

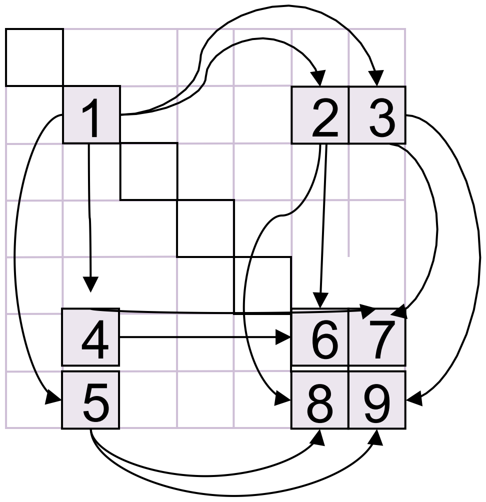
    For example:

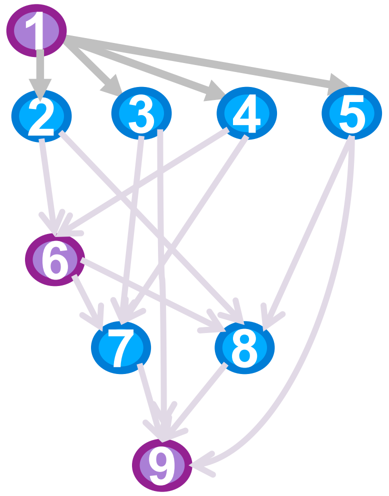
	0	1	2
0	11	12	13
1	14	15	16

Sparse factorization

- Store A explicitly … many sparse compressed formats
- "Fill-in" . . . new nonzeros in L & U
  - Typical fill-ratio: 10x for 2D problems, 30-50x for 3D problems
- Graph algorithms: directed/undirected graphs, bipartite graphs, paths, elimination trees, depth-first search, heuristics for NP-hard problems, cliques, graph partitioning, . . .
- Unfriendly to high performance, parallel computing
  - Irregular memory access, indirect addressing, strong task/data dependency







Algorithmic phases in sparse GE

1. Minimize number of fill-ins, maximize parallelism (~10% time)
   - Sparsity structure of L & U depends on that of 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. Predict the fill-in positions in L & U (~10% time)
   - Symbolic factorization (combinatorial algorithms)

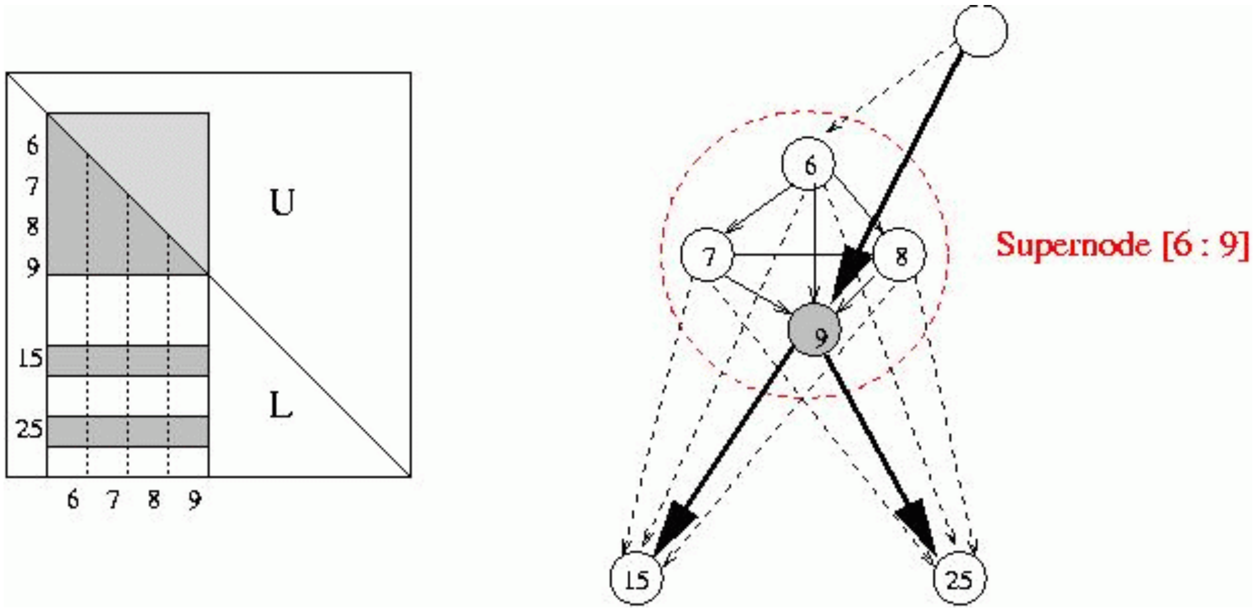
3. Design efficient data structure for storage and quick retrieval of the nonzeros
   - Compressed storage schemes

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 my be interleaved.

General Sparse Solver

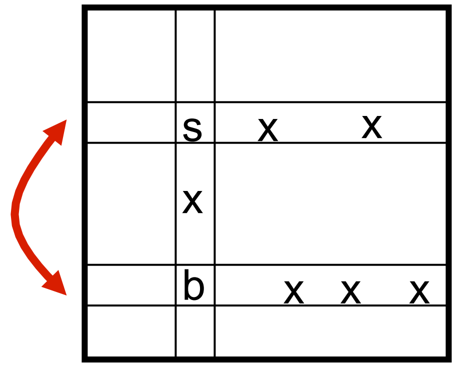
- Use (blocked) CRS or CCS, and any ordering method
  - Leave room for fill-ins ! (symbolic factorization)
- Exploit "supernode" (dense) structures in the factors
  - Can use Level 3 BLAS
  - Reduce inefficient indirect addressing (scatter/gather)
  - Reduce graph traversal time using a coarser graph



Numerical Pivoting

- 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 sequential SuperLU and SuperLU_MT (GEPP)
  - Can force diagonal pivoting (controlled by diagonal threshold)
  - Hard to implement scalably for sparse factorization



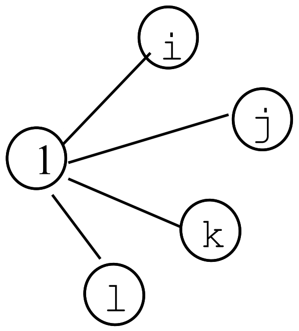
- Static pivoting used in SuperLU_DIST (GESP)
  - Before factor, scale and permute A to maximize diagonal: $P_r D_r A D_c = A'$
  - During factor $A' = LU$, replace tiny pivots by $\sqrt{\varepsilon}\|A\|$, without changing data structures for L & U
  - If needed, use a few steps of iterative refinement after the first solution

➔ quite stable in practice

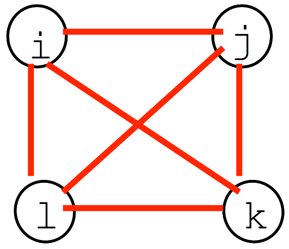
Ordering : Minimum Degree

Local greedy: minimize upper bound on fill-in

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

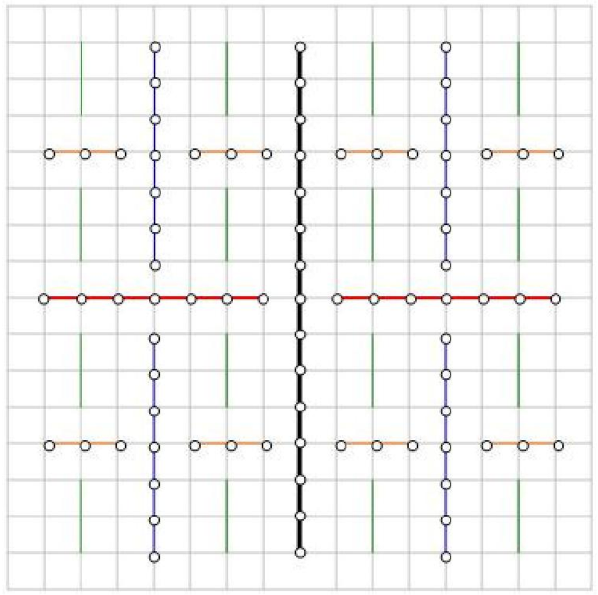


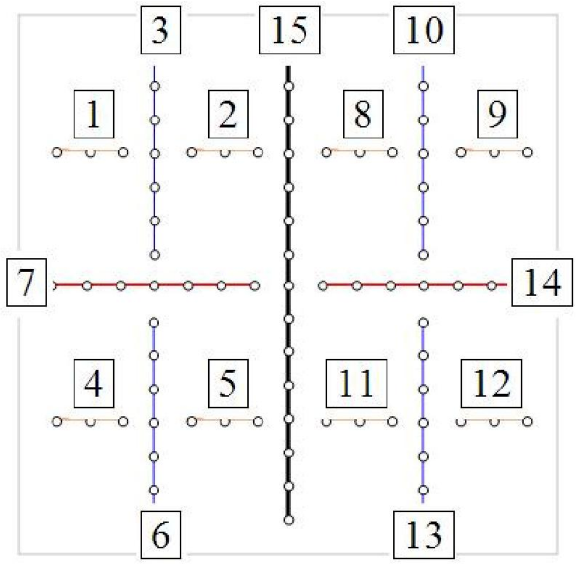
$\xrightarrow{\text{Eliminate 1}}$



Ordering : Nested Dissection

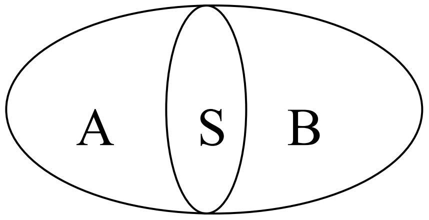
- Model problem: discretized system Ax = b from certain PDEs, e.g., 5-point stencil on n x n grid, $N = n^2$
  - Factorization flops: $O(n^3) = O(N^{3/2})$
- Theorem: ND ordering gives optimal complexity in exact arithmetic [George ' 73, Hoffman/Martin/Rose]





ND Ordering

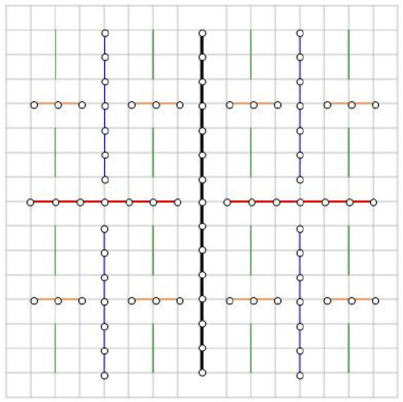
- Generalized nested dissection [Lipton/Rose/Tarjan ' 79]
  - Global graph partitioning: top-down, divide-and-conqure
  - Best for largest problems
  - Parallel codes available: ParMetis, PT-Scotch
  - First level

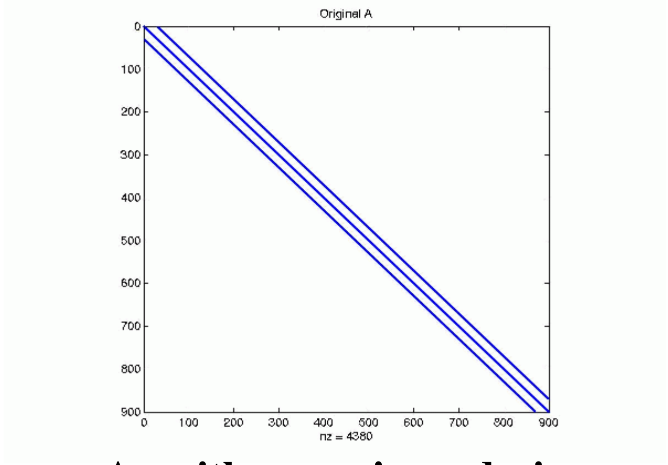


$$\longrightarrow \begin{bmatrix} A & 0 & x \\ 0 & B & x \\ x & x & S \end{bmatrix}$$

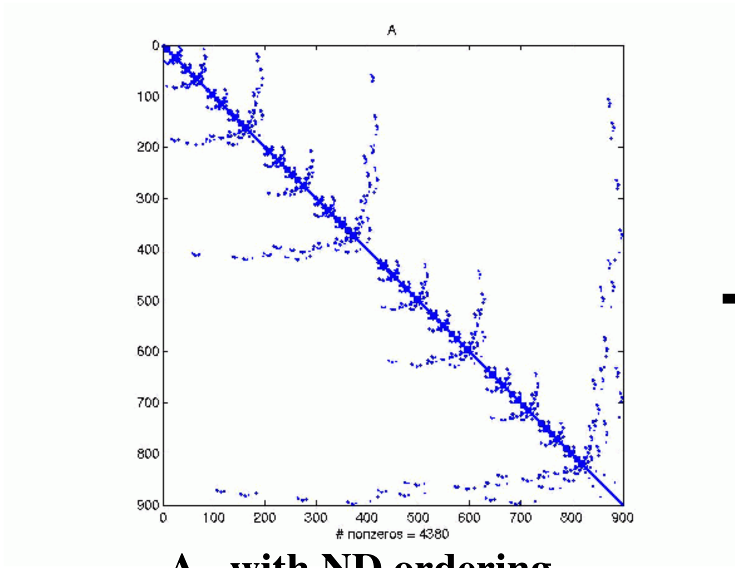
  - Recurse on A and B
- Goal: find the smallest possible separator S at each level
  - Multilevel schemes:
    - Chaco [Hendrickson/Leland `94], Metis [Karypis/Kumar `95]
  - Spectral bisection [Simon et al. `90-`95]
  - Geometric and spectral bisection [Chan/Gilbert/Teng `94]

ND Ordering

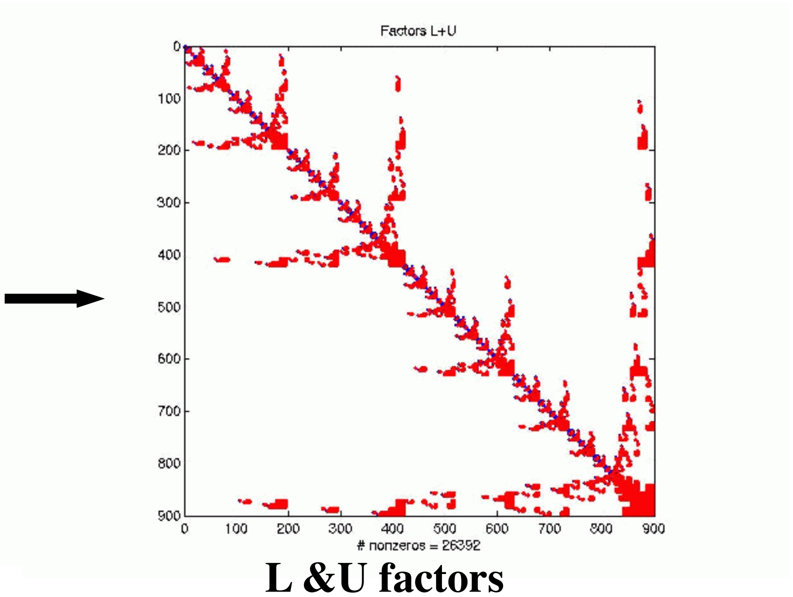

2D mesh



A, with row-wise ordering



A, with ND ordering



L &U factors

Ordering for LU (unsymmetric)

- 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

Ordering Interface in SuperLU

- Library contains the following routines:
  - Ordering algorithms: MMD [J. Liu], COLAMD [T. Davis], (Par)METIS [G. Karypis etc.]
  - Utility routines: form A^T+A , A^TA

- Users may input any other permutation vector (e.g., using Metis, Chaco, etc.)

```
. . .
set_default_options_dist ( &options );
options.ColPerm = MY_PERMC;    // modify default option
ScalePermstructInit ( m, n, &ScalePermstruct );
METIS (  . . . , &ScalePermstruct.perm_c );
. . .
pdgssvx ( &options, . . . , &ScalePermstruct, . . . );
. . .
```

Symbolic Factorization

- **Cholesky** [George/Liu `81 book]
  - **Use elimination graph of L and its transitive reduction (elimination tree)**
  - **Complexity linear in output: O(nnz(L))**

- **LU**
  - **Use elimination graphs of L & U and their transitive reductions (elimination DAGs)** [Tarjan/Rose `78, Gilbert/Liu `93, Gilbert `94]
  - **Improved by symmetric structure pruning** [Eisenstat/Liu `92]
  - **Improved by supernodes**
  - **Complexity greater than nnz(L+U), but much smaller than flops(LU)**

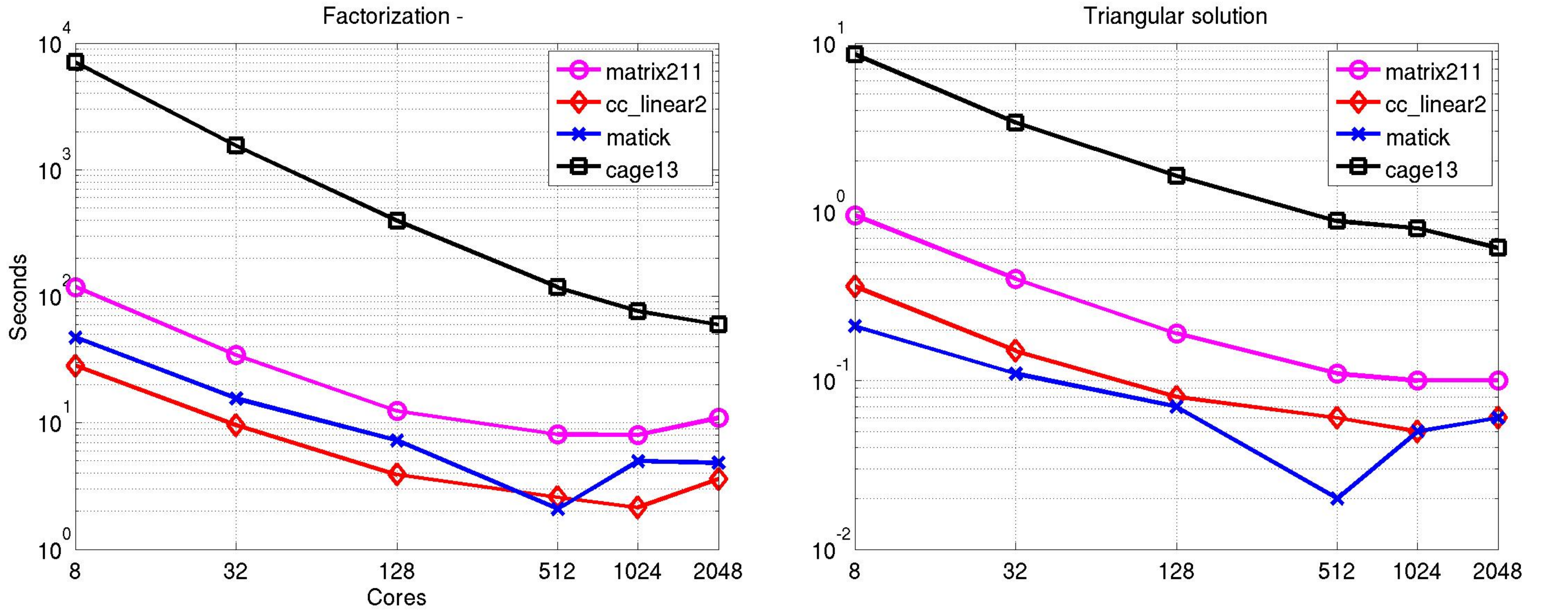
Performance of larger matrices

Name	Application	Data type	N	|A| / N Sparsity	|L\U| (10^6)	Fill-ratio
matrix211	Fusion, MHD eqns (M3D-C1)	Real	801,378	161	1276.0	9.9
cc_linear2	Fusion, MHD eqns (NIMROD)	Complex	259,203	109	199.7	7.1
matick	Circuit sim. MNA method (IBM)	Complex	16,019	4005	64.3	1.0
cage13	DNA electrophoresis	Real	445,315	17	4550.9	608.5

- **Sparsity ordering: MeTis applied to structure of A' +A**

Strong scaling (fixed size): Cray XE6 (hopper@nersc)

- 2 x 12-core AMD 'MagnyCours' per node, 2.1 GHz processor



❖ **Up to 1.4 Tflops factorization rate**

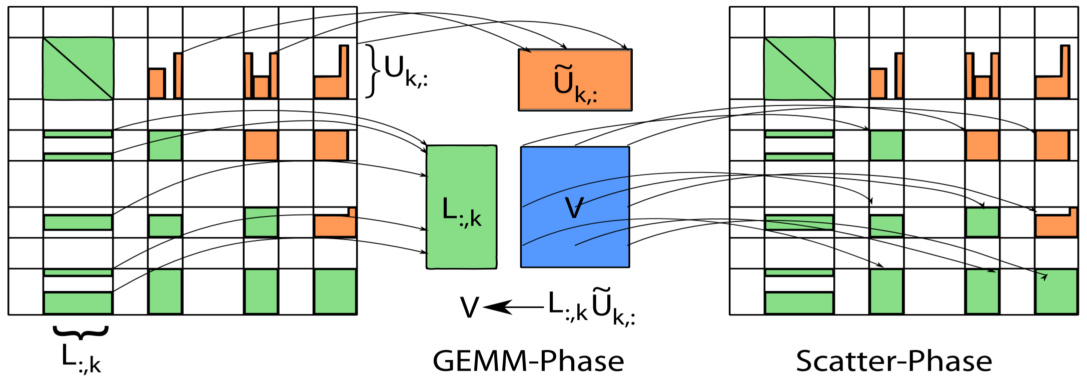
Multicore / GPU-acceleration

- New hybrid programming code: MPI+OpenMP+CUDA, able to use all the CPUs and GPUs on manycore computers.
  - SuperLU_DIST_4.0 release, Aug. 2014.

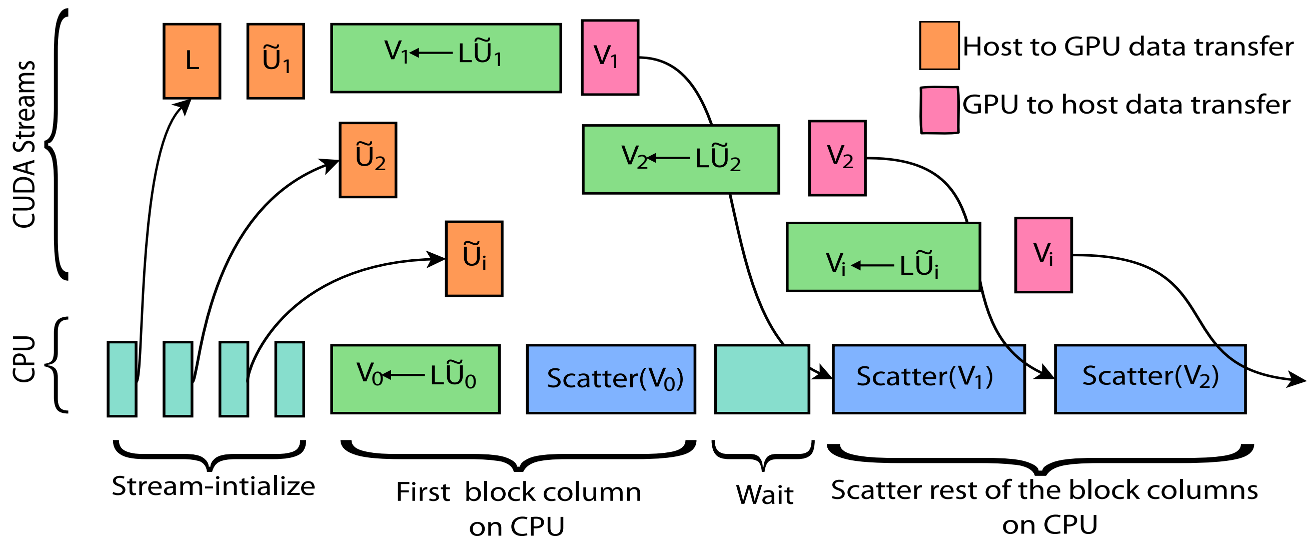
- Algorithmic changes:
  - Aggregate small BLAS operations into larger ones.
  - CPU multithreading Scatter/Gather operations.
  - Hide long-latency operations.

- Results: using 100 nodes GPU clusters, up to 2.7x faster, 2x-5x memory saving.

CPU + GPU algorithm



① *Aggregate small blocks*
② *GEMM of large blocks*
③ *Scatter*



CUDA Streams
CPU
L
$\tilde{U}_1$
$V_1 \leftarrow L\tilde{U}_1$
V_1
Host to GPU data transfer
GPU to host data transfer
$\tilde{U}_2$
$V_2 \leftarrow L\tilde{U}_2$
V_2
$\tilde{U}_i$
$V_i \leftarrow L\tilde{U}_i$
V_i
$V_0 \leftarrow L\tilde{U}_0$
Scatter(V_0)
Scatter(V_1)
Scatter(V_2)
Stream-intialize
First block column on CPU
Wait
Scatter rest of the block columns on CPU

GPU acceleration:
Software pipelining to overlap GPU execution with CPU Scatter, data transfer.

How to use multicore, GPU

- Instructions in top-level README.
- To use OpenMP parallelism:

```
setenv OMP_NUM_THREADS <##>
```

- To enable Nvidia GPU access, need to take the following 2 step:
  1) set the following Linux environment variable:

```
setenv ACC GPU
```

  2) Add the CUDA library location in make.inc: (see sample make.inc)

```
ifeq "${ACC}" "GPU"
   CUDA_FLAGS = -DGPU_ACC
   INCS += -I<CUDA directory>/include
   LIBS += -L<CUDA directory>/lib64 -lcublas -lcudart
endif
```

ILU Interface

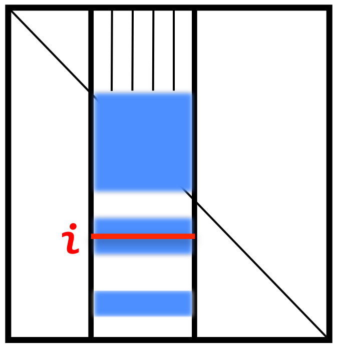
- Available in serial SuperLU 4.0, June 2009
- Similar to ILUTP [Saad]: "T" = threshold, "P" = pivoting
  - among the most sophisticated, more robust than structure-based dropping (e.g., level-of-fill)
- ILU driver: SRC/dgsisx.c

  ILU factorization routine: SRC/dgsitrf.c

  GMRES driver: EXAMPLE/ditersol.c
- Parameters:
  - ilu_set_default_options (&options)
    - options.ILU_DropTol – numerical threshold (τ)
    - options.ILU_FillFactor – bound on the fill-ratio (γ)

Result of Supernodal ILU (S-ILU)

- New dropping rules S-ILU(τ , γ)
  - supernode-based thresholding (τ)
  - adaptive strategy to meet user-desired fill-ratio upper bound (γ)



- Performance of S-ILU
  - For 232 test matrices, S-ILU + GMRES converges with 138 cases (~60% success rate)
  - S-ILU + GMRES is 1.6x faster than scalar ILU + GMRES

Tips for Debugging Performance

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

- Need good BLAS library (vendor, ATLAS, GOTO, . . .)
  - May need adjust block size for each architecture

    (Parameters modifiable in routine sp_ienv())
    - Larger blocks better for uniprocessor
    - Smaller blocks better for parallellism and load balance

  - Open problem: automatic tuning for block size?

Summary

- Sparse LU, ILU are important kernels for science and engineering applications, used in practice on a regular basis
- Performance more sensitive to latency than dense case
- Continuing developments funded by DOE SciDAC projects
  - Integrate into more applications
  - Hybrid model of parallelism for multicore/vector nodes, differentiate intra-node and inter-node parallelism
    - Hybrid programming models, hybrid algorithms
  - Parallel HSS precondtioners
  - Parallel hybrid direct-iterative solver based on domain decomposition

Exercises of SuperLU_DIST

- Instruction

https://redmine.scorec.rpi.edu/anonsvn/fastmath/docs/ATPESC_2015/Exercises/Exercises/superlu/README.html

- On vesta:

/projects/FASTMath/ATPESC-2015/examples/superlu

/projects/FASTMath/ATPESC-2015/install/superlu

Examples in EXAMPLE/

- **pddrive.c**: Solve one linear system
- **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.

SuperLU_DIST Example Program

- EXAMPLE/pddrive.c

- Five basic steps
  1. Initialize the MPI environment and SuperLU process grid
  2. Set up the input matrices A and B
  3. Set the options argument (can modify the default)
  4. Call SuperLU routine PDGSSVX
  5. Release the process grid, deallocate memory, and terminate the MPI environment

Fortran 90 Interface in FORTRAN/

- **All SuperLU objects (e.g., LU structure) are opaque for F90**
  - **They are allocated, deallocated and operated in the C side and not directly accessible from Fortran side.**
- **C objects are accessed via handles that exist in Fortran's user space**
- **In Fortran, all handles are of type INTEGER**
- **Example: FORTRAN/f_5x5.f90**

$$A = \begin{bmatrix} s & & u & u & \\ l & u & & & \\ & l & p & & \\ & & & e & u \\ l & l & & & r \end{bmatrix}, \quad s = 19.0,\ u = 21.0,\ p = 16.0,\ e = 5.0,\ r = 18.0,\ l = 12.0$$

STRUMPACK – STRUctured Matrices PACKage

STRUMPACK

- http://portal.nersc.gov/project/sparse/strumpack/
- C++, OpenMP, MPI
- Support both real & complex datatypes, single & double precision (via template), and 64-bit indexing.
- Input interfaces
  - Dense matrix in standard format.
  - Matrix-free – user provides matvec multiplication routine, and routine for selecting some matrix entries.
  - Sparse matrix in CSR format.
- Two components:
  - Dense – applicable to Toeplitz, Cauchy, BEM, integral equations, etc.
  - Sparse – aim at matrices discretized from PDEs.
- Functions:
  - HSS construction, HSS-vector product, ULV factorization, Solution.

Hierarchical matrix approximation

- Algebraic generalization to FMM, independent of Green's function.
  - Matrix multiplication, factorization, inversion, etc.
- Applications:
  - Integral equations, BEM, statistics, acoustic and electromagnetic scattering theory, rational interpolation, …
  - General discretized PDEs
- Exploit low-rank submatrices.
  - If A has numerical low rank k (called epsilon-rank):

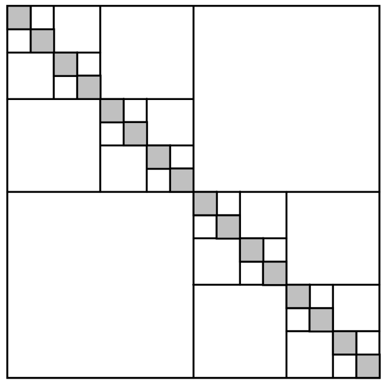
$$A = U\Sigma V^T \approx A_k := U\Sigma_k V^T, \Sigma = diag(\sigma_1, ..., \sigma_k, \sigma_{k+1}, \ldots, \sigma_n)$$

$$\Sigma_k = diag(\sigma_1, ..., \sigma_k, 0, ..., 0), \quad \text{with } \sigma_k > \varepsilon$$

  - Algorithms
    - **Truncated SVD**
    - **Rank-revealing QR (RRQR)**
    - **Randomized sampling (+ Interpolative Decomposition (ID) via RRQR)**

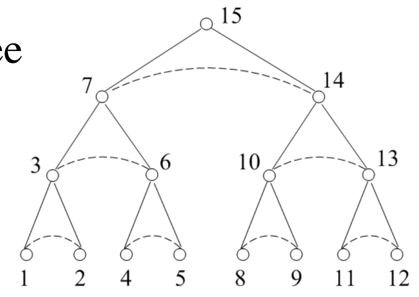
HSS factorization

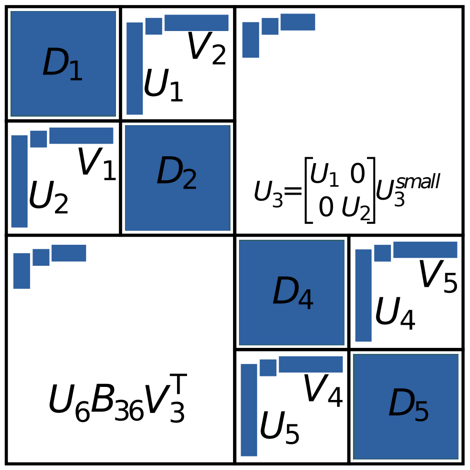
- Dense (but data-sparse): hierarchically semi-separable structure
  - Off-diagonal blocks are rank deficient: BEMs, Integral equations, PDEs with smooth kernels
  - Recursion leads to hierarchical partitioning
  - Key to low complexity: nested bases



$$A = \left[\begin{array}{c|c} \begin{array}{c|c} D_1 & U_1B_1V_2^T \\ \hline U_2B_2V_1^T & D_2 \end{array} & U_3B_3V_6^T \\ \hline U_6B_6V_3^T & \begin{array}{c|c} D_4 & U_4B_4V_5^T \\ \hline U_5B_5V_4^T & D_5 \end{array} \end{array}\right]$$

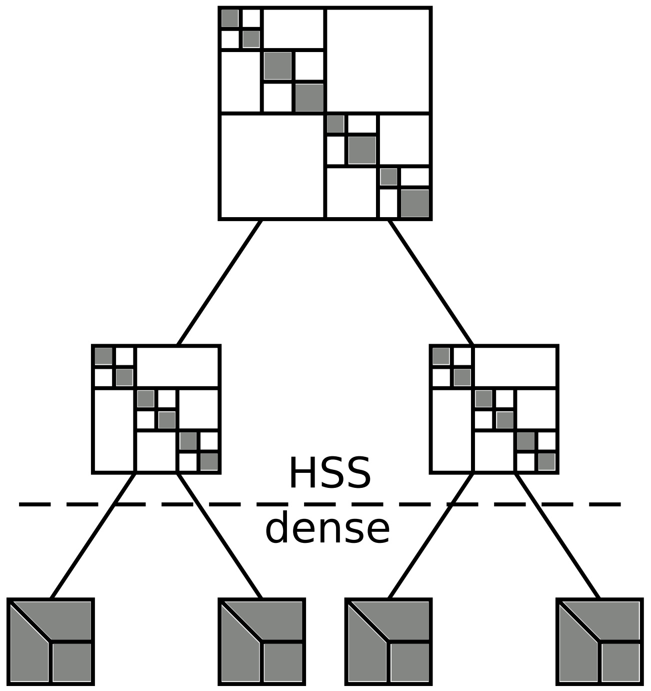
HSS tree





HSS-embedded sparse multifrontal factorization

- Frontal matrices are dense, can be approximated by HSS
- Only for top levels (l_s) in the elimination tree, with largest frontal matrices.
  - ULV factorization of HSS matrix
  - Low-rank Schur complement update

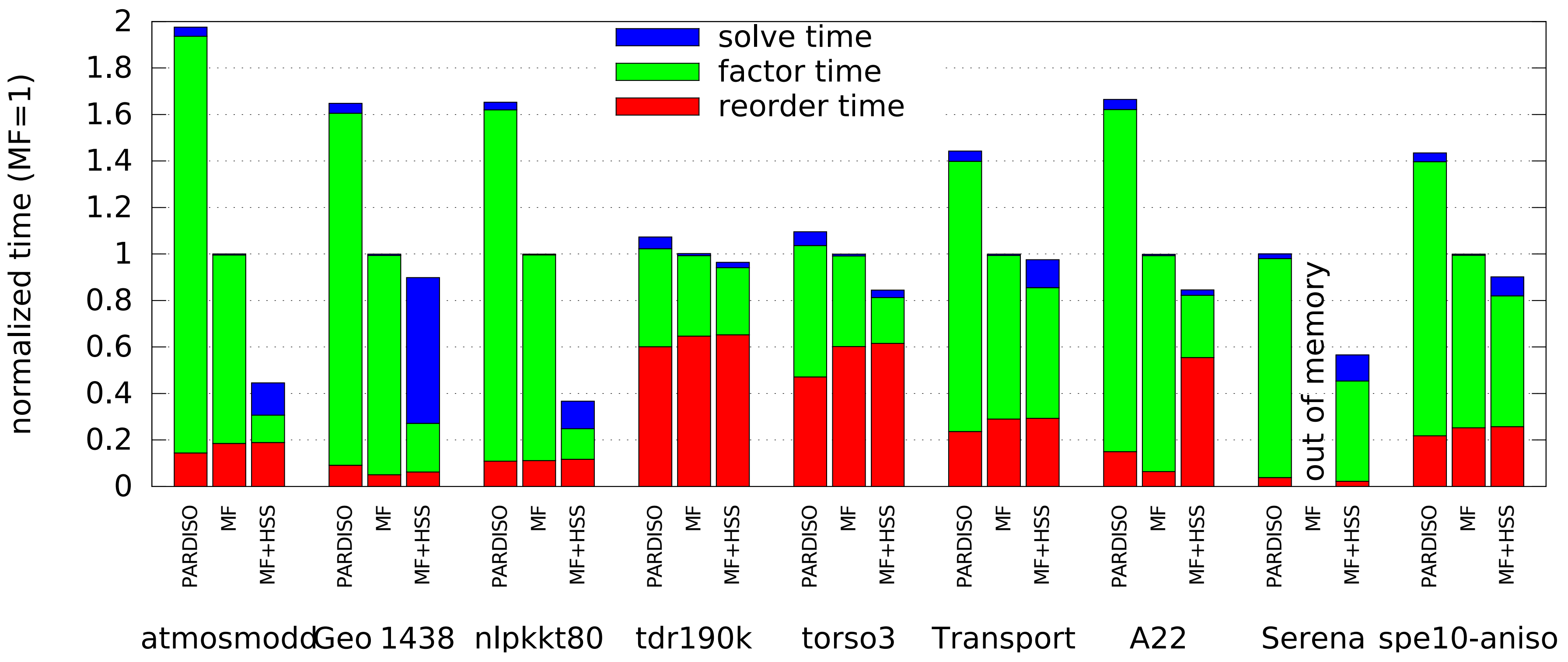


STRUMPACK-dense: parallel weak scaling

- Root node of the multifrontal factorization of a discretized Helmholtz problem (frequency domain, PML boundary, 10Hz).
- For many PDEs on mesh KxKxK, max. off-diagonal rank O(K).

K (mesh: K^{3})	**100**	**200**	**300**	**400**	**500**
Matrix size K^2	10,000	40,000	90,000	160,000	250,000
MPI tasks	64	256	1,024	4,096	8,192
Max. rank	313	638	903	1289	1625
Speedup over ScaLAPACK LU	1.8	4.0	5.4	4.8	3.9

STRUMPACK-Sparse: Compare to Intel MKL PARDISO



- 9 matrices: DOE SciDAC Accelerator, Fusion simulations; Oil reservoir, UF collection
- HSS-enabled sparse solver:
  - Factorization cost decreases.
  - Solve cost (and GMRES iterations) increases.