Accelerating Direct Linear Solvers with Algorithmic and Hardware Advances

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Themes

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- Algorithms with lower arithmetic complexity, lower communication complexity

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  Multilevel algorithms
  - Multigrid
  - Fast Multipole Method (FMM)
  - Hierarchical matrices – algebraic generalization of FMM, (hopefully) applicable to broader classes of problems

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- Algorithms with lower arithmetic complexity, lower communication complexity
  Multilevel algorithms
  - Multigrid
  - Fast Multipole Method (FMM)
  - Hierarchical matrices – algebraic generalization of FMM, (hopefully) applicable to broader classes of problems

- Parallel algorithms and codes for machines with million-way parallelism, hierarchical organization
  - Distributed memory
  - Manycore nodes: 100s of lightweight cores, accelerators, co-processors

Reduce complexity with hierarchical matrix algorithms

Exploit STRUCTURES

1. Sparsity structure: defined by $\{0,1\}$ structure (Graphs).
   LU factorizaion $\sim O(N^2)$ flops, for many 3D discretized PDEs (loosely speaking).

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   Software:

   - SPARSPAK (1981, George and Liu)
   - YSMP (1982, Eisenstat)
   - MA27 multifrontal (1983, Duff and Reid, MA37, MA38, MA47, MA57 etc. in HSL)
   - MUMPS, PaStiX, SuperLU, UMFPACK, WSMP, ...

Exploit STRUCTURES – low rankness

2. On top of (1), can find Data-sparse structure in dense (sub)matrices (approximation)
   $O(N)$ or $O(N\ polylog(N))$ flops for compression, factorization.

   Hierarchical matrices: $\mathcal{H}$- & $\mathcal{H}^2$-matrix (1999, Hackbusch et al.) and their subclasses.

   [Bebendorf, Bini, Börm, Chandrasekaran, Darve, Dewilde, Grasedyck, Gu, Le Borne, Martinsson, Tygert, Van Barel, van der Veen, Vandebril, Xia, ...]

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   Software:

   - HLib (2004, Börm and Grasedyck)
   - HLIBPro (2004, Kriemann)
   - HODLR (2013, Ambikasaran and Darve)
   - MUMPS (2015, Amestoy et al.)
   - STRUMPACK (2015, LBNL)

Hierarchical matrix approximation

- Same mathematical foundation as FMM (Greengard and Rokhlin), put in matrix form:
  - Diagonal block ("near field") represented exactly
  - Off-diagonal block ("far field") approximated via low-rank format

FMM separability of Green's function	Algebraic low rank off-diagonal
$G(x,y) \approx \sum_{\ell=1}^{r} f_\ell(x) g_\ell(y)$	$A = \left[\begin{array}{c\|c} D_1 & U_1 B_1 V_2^T \\ \hline U_2 B_2 V_1^T & D_2 \end{array}\right]$
$x \in X, y \in Y$	

- Algebraic power: matrix multiplication, factorization, inversion, tensors, ...

Multilevel is the key to optimal complexity

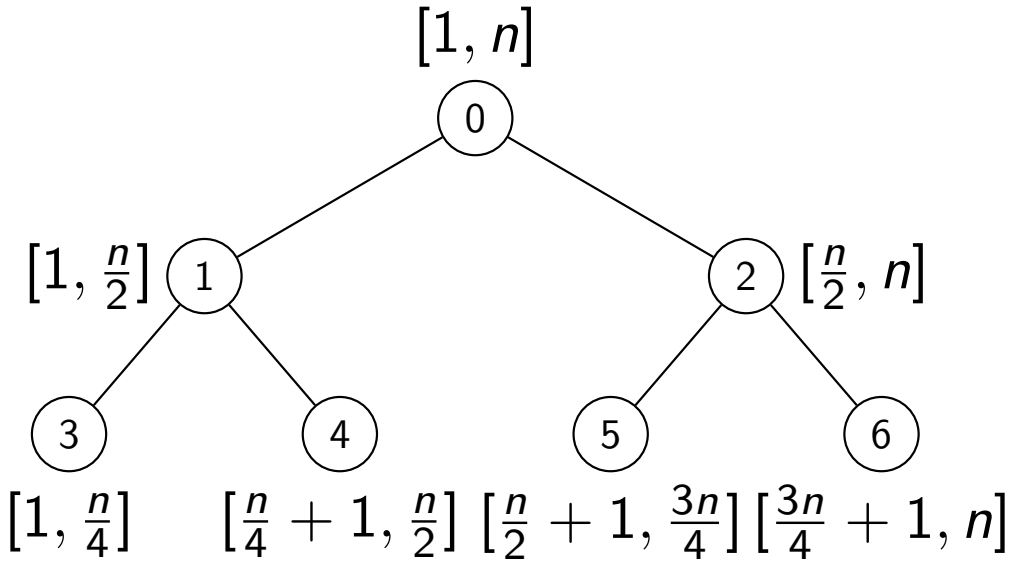
Two hierarchies:

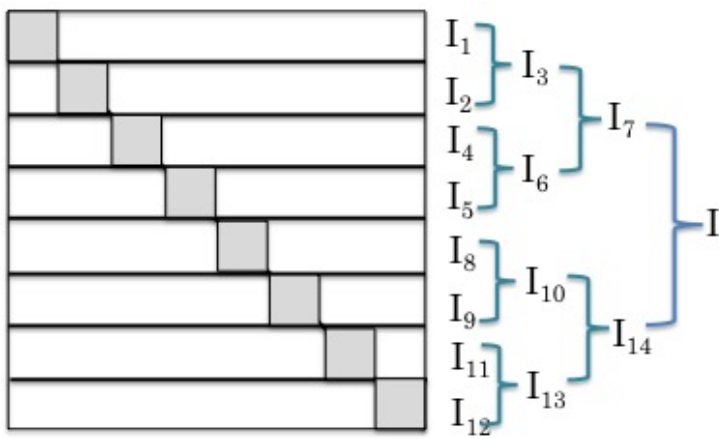
- Hierarchical partitioning using cluster tree
- Hierarchical, nested bases

1. Cluster tree, block cluster tree

Cluster tree $T_{\mathcal{I}}$ defines hierarchical partitioning of the index set $[1, n]$.

- Each node is associated with an interval $\mathcal{I}_\tau$.
- For children ν_1 and ν_2, parent $\mathcal{I}_\tau = \mathcal{I}_{\nu_1} \cup \mathcal{I}_{\nu_2}$, and $\mathcal{I}_{\nu_1} \cap \mathcal{I}_{\nu_2} = \emptyset$





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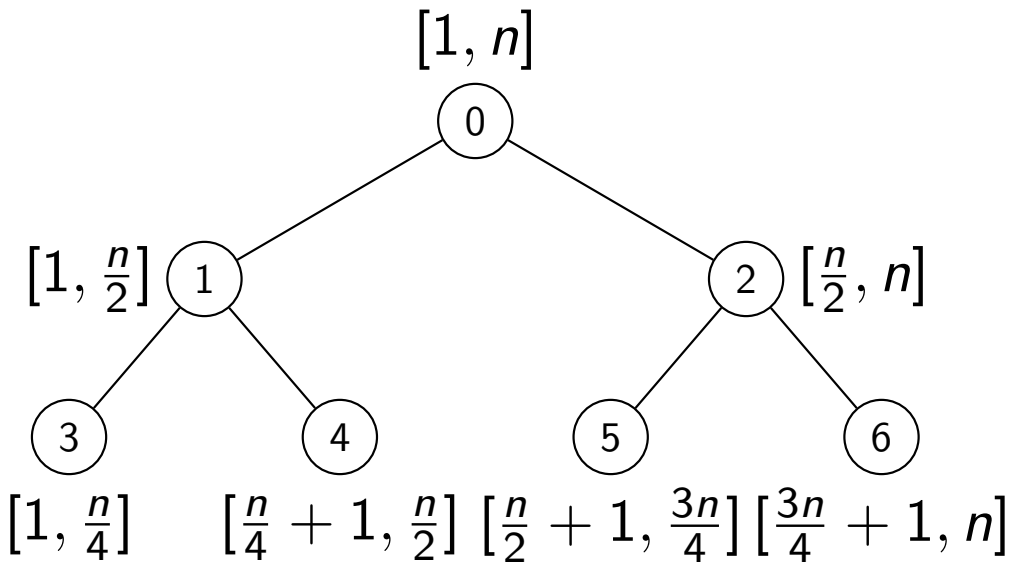

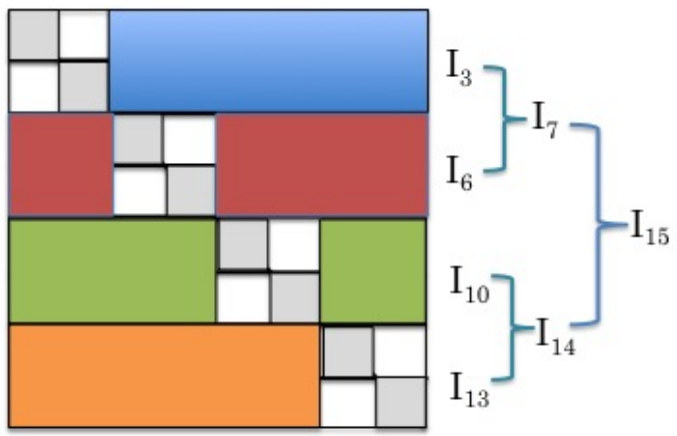

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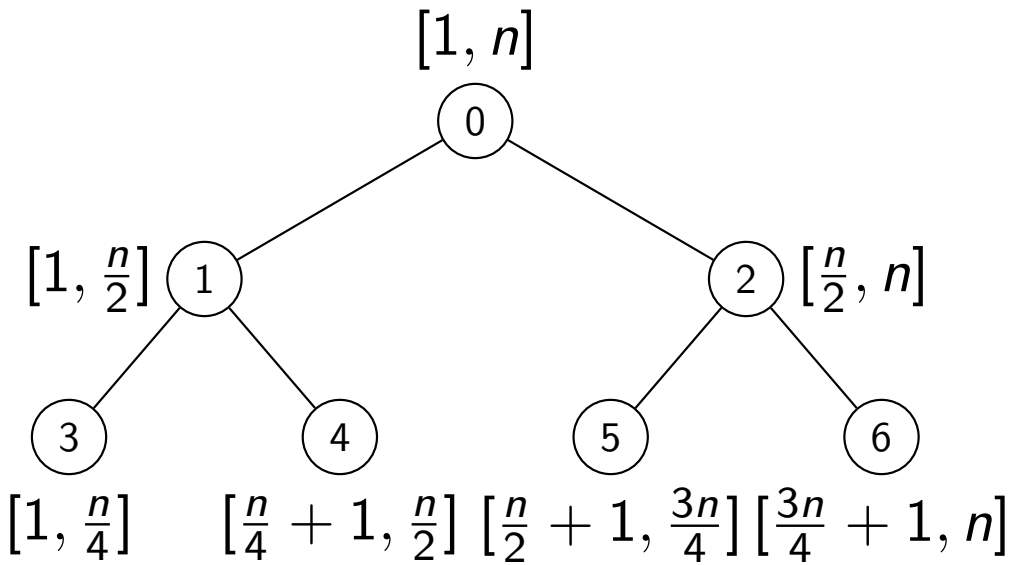

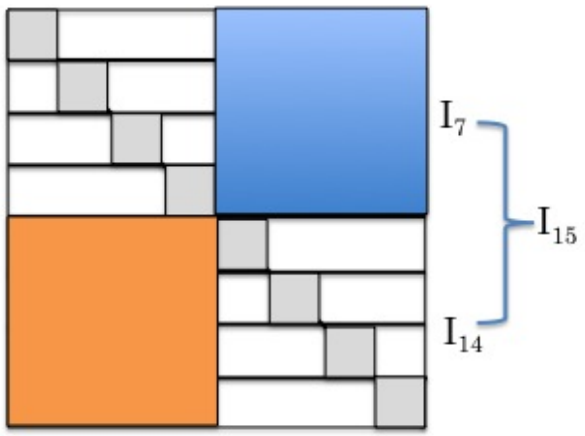

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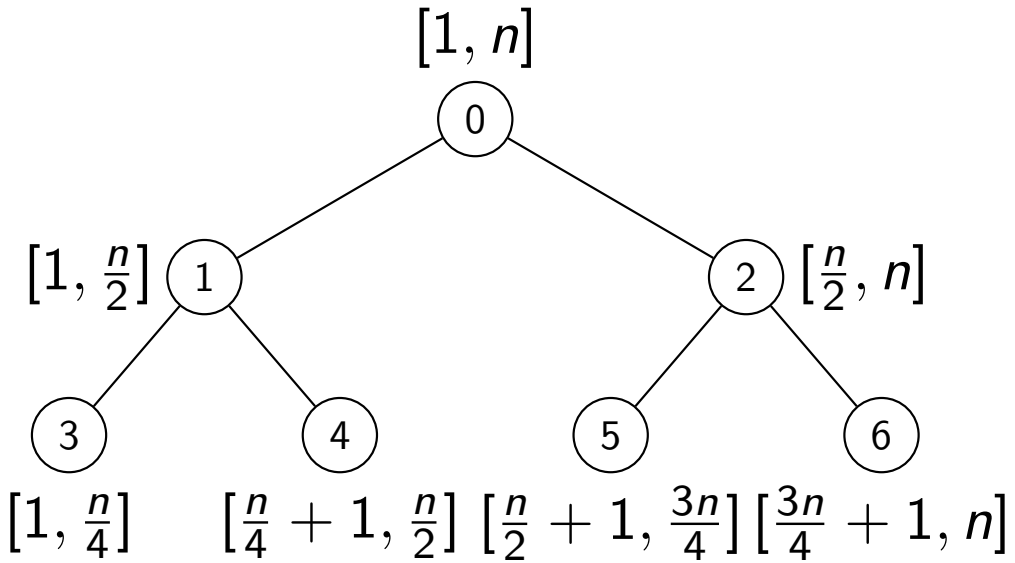
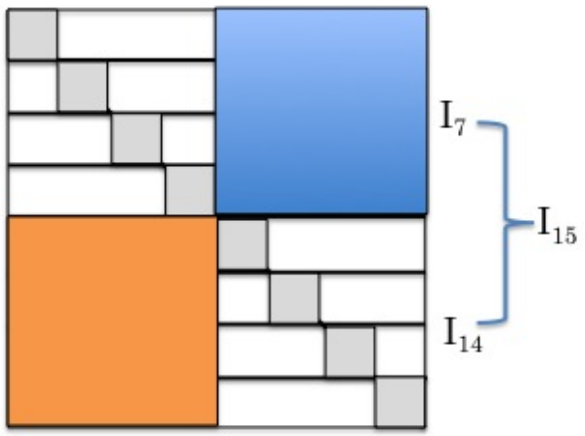


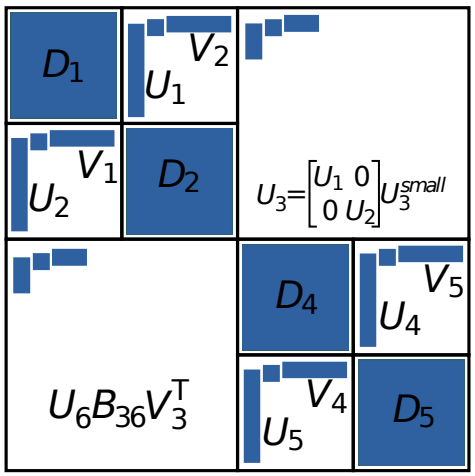


Block cluster tree $T_{\mathcal{I}\times\mathcal{J}}$ defines partitioning of the index set $\mathcal{I} \times \mathcal{J}$, both row- and column-wise.

- Each node corresp. to a matrix block $A(\mathcal{I}_\tau, \mathcal{I}_\sigma)$

2. Nested bases

Example: Hierarchically Semi-Separable matrices (HSS)



- Diagonal blocks are full rank: $D_\tau = A(I_\tau, I_\tau)$
- Off-diagonal blocks as low-rank:

$$A_{\nu_1,\nu_2} = A(I_{\nu_1}, I_{\nu_2}) = U_{\nu_1} B_{\nu_1,\nu_2} V_{\nu_2}^*$$

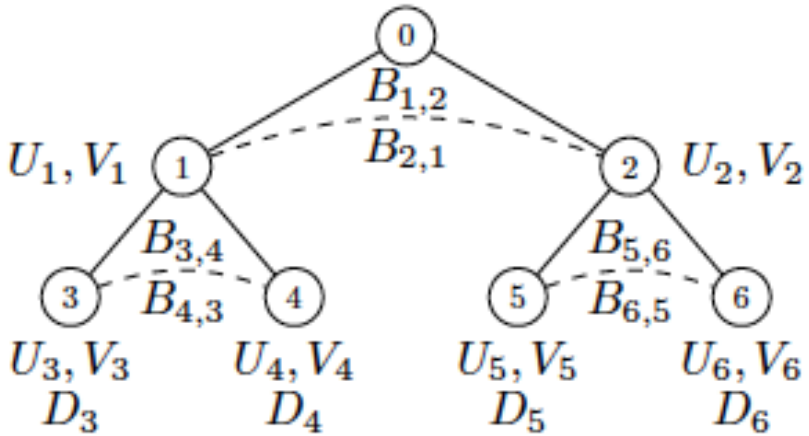
- Column bases U and row bases V^* are nested:

$$U_\tau = \begin{bmatrix} U_{\nu_1} & 0 \\ 0 & U_{\nu_2} \end{bmatrix} U_\tau^{\text{small}}, V_\tau = \begin{bmatrix} V_{\nu_1} & 0 \\ 0 & V_{\nu_2} \end{bmatrix} V_\tau^{\text{small}}$$

HSS matrix – operational view

$$A^{(\ell)} = U^{(\ell)} A^{(\ell-1)} V^{(\ell)^T} + B^{(\ell)}, \qquad \text{levels } \ell = 1, 2, \ldots, L$$

Data structures built on cluster tree (i.e. HSS tree):



- Keep as an unevaluated product & sum
- Operations going up / down the cluster tree

HSS matrix – ULV factorization

ULV-like factored form (U and V^* unitary, L triangular)

$$\Gamma_{1;b\leftrightarrow 2;t}\begin{bmatrix} I & & \\ & \Omega_1 & \\ & & I \\ & & & \Omega_2 \end{bmatrix}\begin{bmatrix} \Gamma_{3;b\leftrightarrow 4;t} & \\ & \Gamma_{5;b\leftrightarrow 6;t} \end{bmatrix}\begin{bmatrix} \Omega_3 & & \\ & \Omega_4 & \\ & & \Omega_5 \\ & & & \Omega_6 \end{bmatrix} A \begin{bmatrix} Q_3^* & & \\ & Q_4^* & \\ & & Q_5^* \\ & & & Q_6^* \end{bmatrix}\begin{bmatrix} \Gamma_{3;b\leftrightarrow 4;t}^T & \\ & \Gamma_{5;b\leftrightarrow 6;t}^T \end{bmatrix}\begin{bmatrix} I & & \\ & Q_1^* & \\ & & I \\ & & & Q_2^* \end{bmatrix}\Gamma_{1;b\leftrightarrow 2;t}^T$$

$$= \left[\begin{array}{|c|c|c|c|c|c|c|}
\hline
L_3 & & & & & & \\
\hline
0 & L_4 & & & & & \\
\hline
(\Omega_1 L_{4,3})_t & (\Omega_1 L_{3,4})_t & L_1 & & & & \\
\hline
\multicolumn{3}{|c|}{0} & L_5 & & & \\
\hline
 & & & 0 & L_6 & & \\
\hline
 & & & (\Omega_2 L_{6,5})_t & (\Omega_2 L_{5,6})_t & L_2 & \\
\hline
(\Omega_1 L_{4,3})_b & (\Omega_1 L_{3,4})_b & W_{1;b} Q_{1;t}^* & \multicolumn{2}{|c|}{B_{1,2} V_2^* \begin{bmatrix} V_5^* Q_{5;t}^* & V_5^* Q_{5;b}^* \\ V_6^* Q_{6;t}^* & V_6^* Q_{6;b}^* \end{bmatrix}\begin{bmatrix} I & \\ & Q_2^* \end{bmatrix}} & & D_0 \\
\hline
\multicolumn{3}{|c|}{B_{2,1} V_1^* \begin{bmatrix} V_3^* Q_{3;t}^* & V_3^* Q_{3;b}^* \\ V_4^* Q_{4;t}^* & V_4^* Q_{4;b}^* \end{bmatrix}\begin{bmatrix} I & \\ & Q_1^* \end{bmatrix}} & (\Omega_2 L_{6,5})_b & (\Omega_2 L_{5,6})_b & W_{2;b} Q_{2;t}^* & \\
\hline
\end{array}\right]$$

Families of $\mathcal{H}$ and $\mathcal{H}^2$ matrices

- Admissibile block (τ, σ): $\max\{\mathrm{diam}(\tau), \mathrm{diam}(\sigma)\} \leq \eta \, \mathrm{dist}(\tau, \sigma)$
- Strong admissibility: blocks next to diagonal not compressed, only compress well separated blocks

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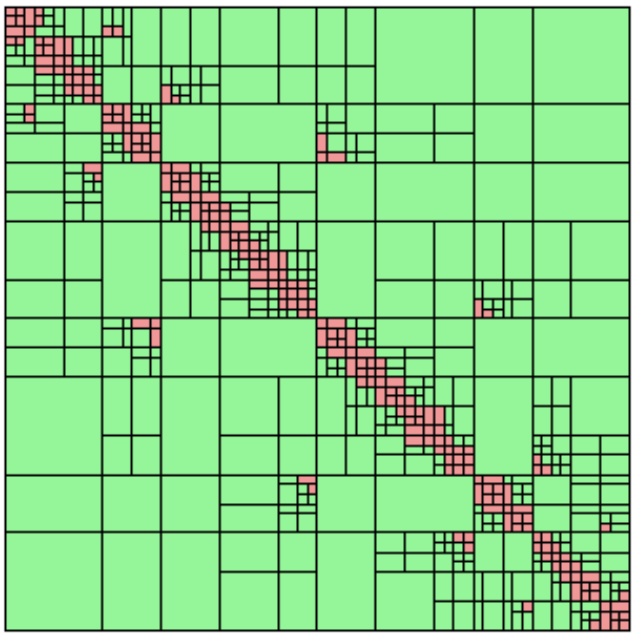
- Strong admissibility: blocks next to diagonal not compressed, only compress well separated blocks

- $\mathcal{H}$: split a node in a block cluster tree if its block is admissible
- $\mathcal{H}^2$: uniform $\mathcal{H}$ partitioning, with nested bases

[Börn/Grasedyck/Hackbusch]

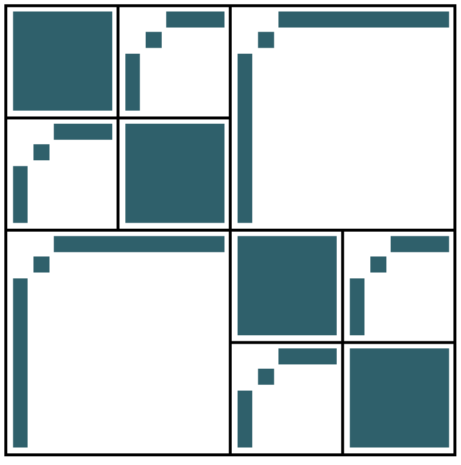


Various data-sparse formats

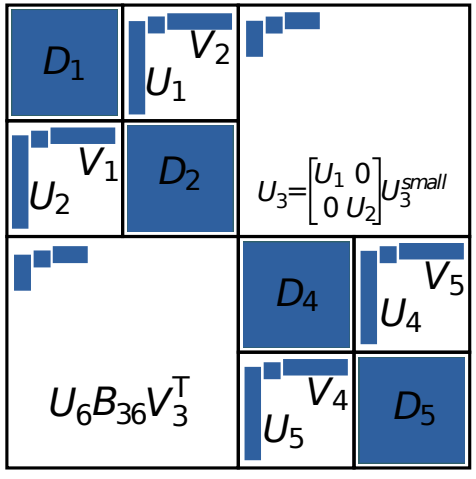
Method	Hier. part.	Nested bases	Admissibility	Family
HODLR	yes	no	weak	$\mathcal{H}$
HSS/HBS	yes	yes	weak	$\mathcal{H}^2$
Barnes-Hut	yes	no	strong	$\mathcal{H}$
FMM	yes	yes	strong	$\mathcal{H}^2$
BLR	no	no	strong	

Various data-sparse formats

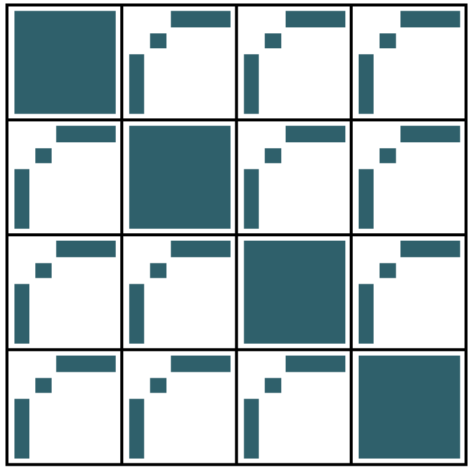
HODLR



HSS

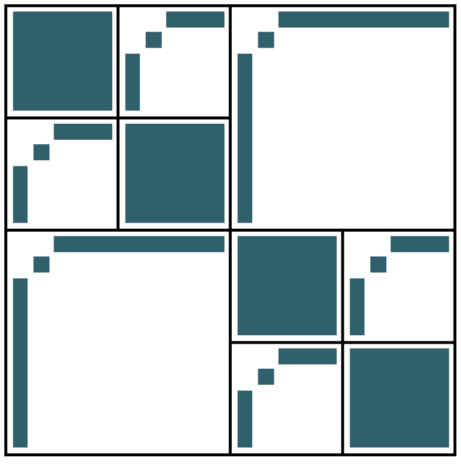


BLR

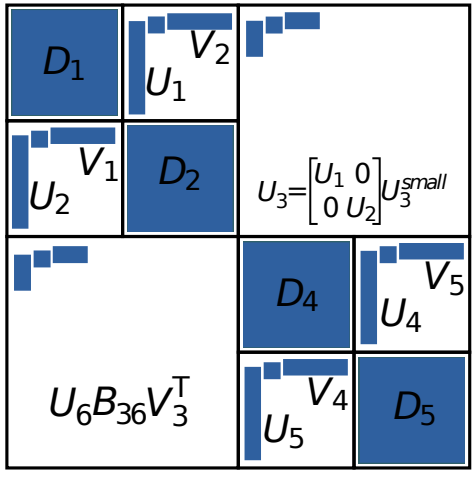


Various data-sparse formats

HODLR



HSS



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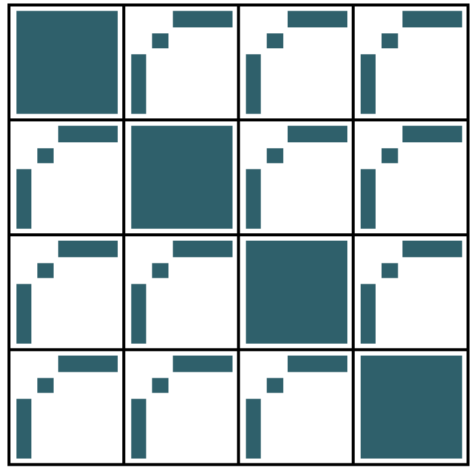
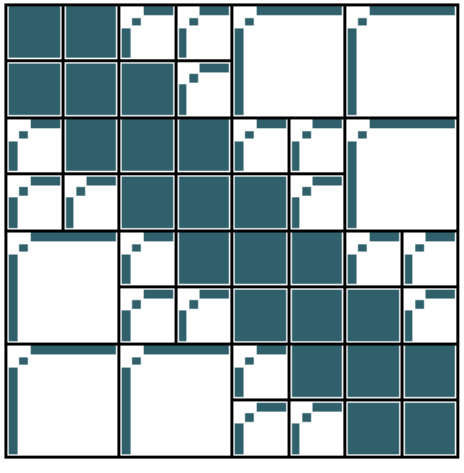
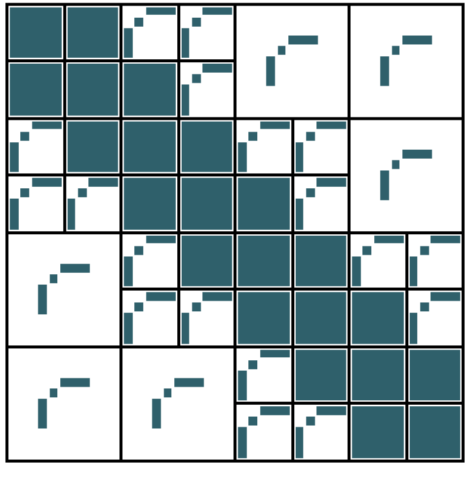


Barnes-Hut



FMM



Practical comparisons ... two other talks

- Francois-Henry Rouet, MS39, Thursday, 11:45-12:10
  "A Comparison of Different Low-Rank Approximation Techniques"

- Rio Yokota, MS45, Thursday, 3:30-3:55
  "Comparison of FMM and HSS at Large Scale"

Low rank compression via randomized sampling

1. Pick random matrix $\Omega_{n\times(k+p)}$, p small, e.g. 10
2. Sample matrix $S = A\Omega$, with slight oversampling p
3. Compute $Q = \text{ON-basis}(S)$

Low rank compression via randomized sampling

1. Pick random matrix $\Omega_{n\times(k+p)}$, p small, e.g. 10
2. Sample matrix $S = A\Omega$, with slight oversampling p
3. Compute $Q =$ ON-basis(S)

- **Accuracy:** with *probability* $\geq 1 - 6 \cdot p^{-p}$,
  $\|A - QQ^*A\| \leq [1 + 11\sqrt{k+p} \cdot \sqrt{\min\{m,n\}}]\sigma_{k+1}$
- **Cost:** $O(kmn)$

N. Halko,P.G. Martinsson, J.A. Tropp, "Finding Structure with Randomness: Probabilistic Algorithms for Constructing Approximate Matrix Decomposition", SIAM Review, Vol.53, pp.217-288, 2011.

RS vs. "direct" methods (RRQR, truncated SVD)

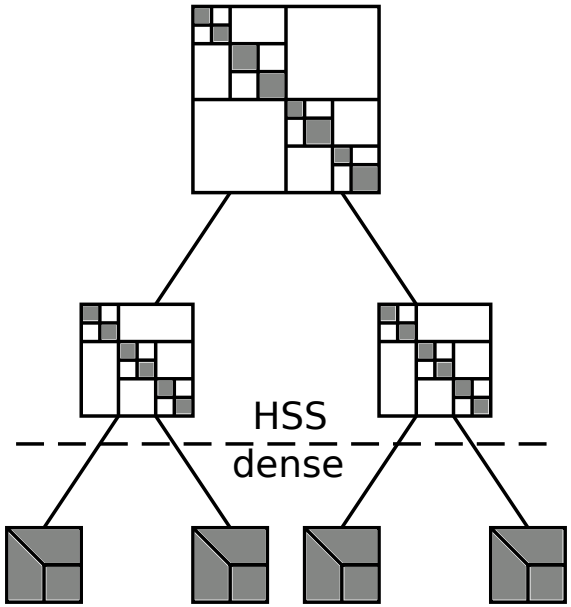
- When using explicit matrix, all have same asymptotic cost.
- RS can be faster when fast matvec available:
  - FMM ($O(kn)$)
  - Structured random matrix, e.g. SRFT (Subsampled Random Fourier Transform) ($O(\log(k)mn)$)
- RS useful when only matvec available (matrix-free).

- **In sparse solver, RS is more appealing ...**

Embedding HSS in multifrontal sparse solver

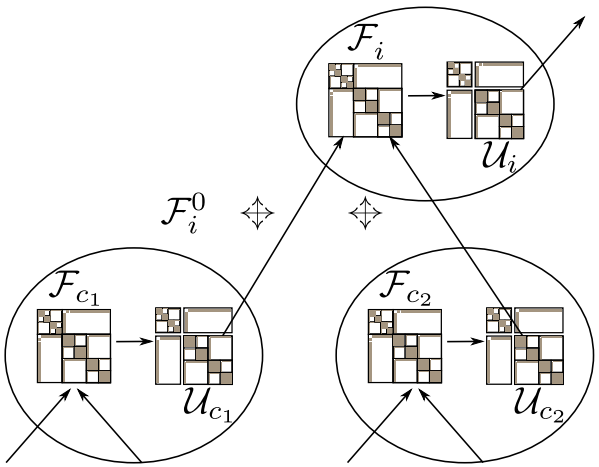
Approximate frontal matrices with HSS

- Only for top ℓ_s levels in the elimination tree, largest frontal matrices
- *ULV* factorization of HSS matrix
- Low-rank Schur complement update



Sparse multifrontal: Extend-Add $\mathcal{F}_j = A_j \boxplus \mathcal{U}_{c_1} \boxplus \mathcal{U}_{c_1}$

$$\mathcal{U}_{c_1} + \mathcal{U}_{c_2} = \begin{pmatrix} a_1 & b_1 & 0 \\ c_1 & d_1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} a_2 & 0 & b_2 \\ 0 & 0 & 0 \\ c_2 & 0 & d_2 \end{pmatrix} = \begin{pmatrix} a_1 + a_2 & b_1 & b_2 \\ c_1 & d_1 & 0 \\ c_2 & 0 & d_2 \end{pmatrix}$$



Main obstacle:
extend-add of two HSS structures

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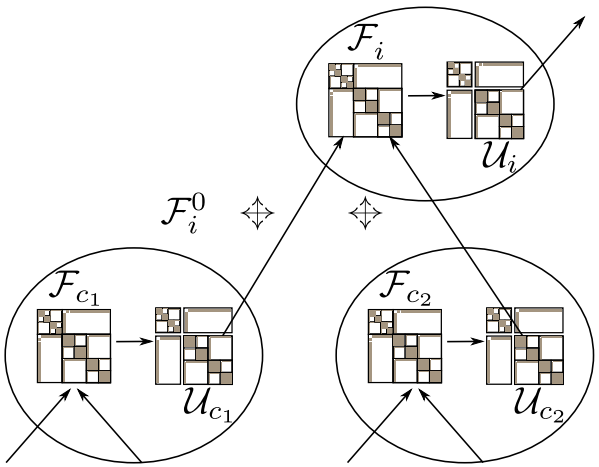

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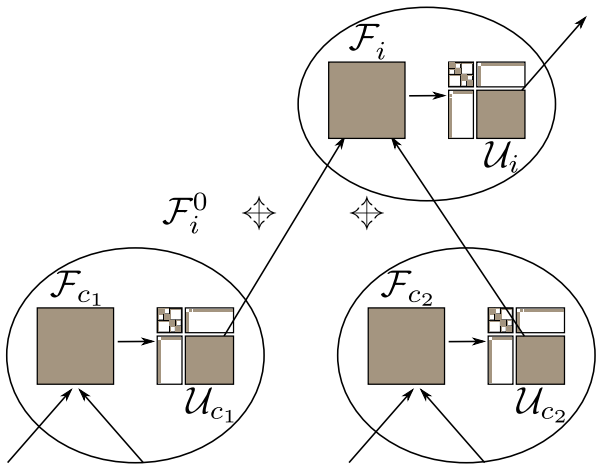
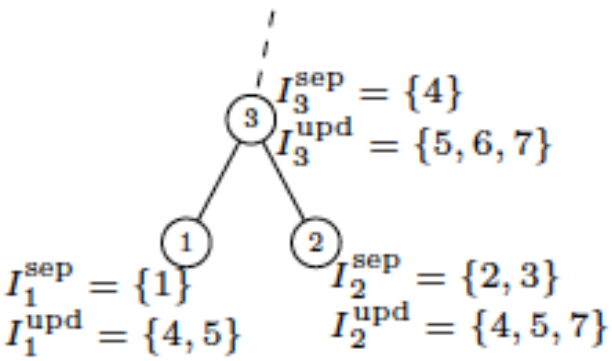


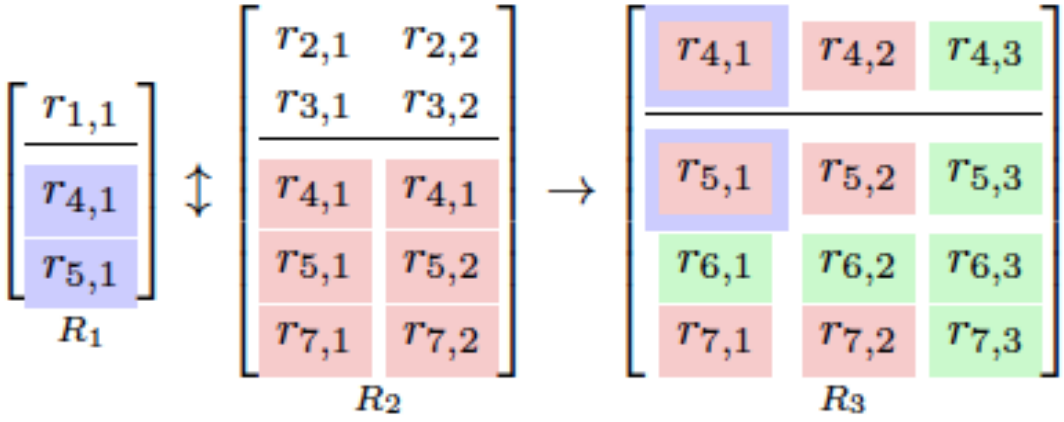
Hsolver [Wang/Rouet/Xia/L. 2013]
Compromise:

- keep update matrix as dense
- extend-add dense

RS simplies frontal extend-add

Skinny extend-merge:





Arithmetic complexities – dense HSS

Let r = HSS rank, i.e., maximum rank found during the different compression steps.

Compression

- Without RS: $O(r\,N^2)$.
- With RS: cost of sampling + $O(r^2 N)$
  - Classical matvec: $O(r\,N^2)$.
  - FFT (e.g., Toeplitz matrix): $O(r\,N \log N)$.
  - FMM: $O(r\,N)$.

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ULV factorization and solve: $O(r\,N)$

Arithmetic complexities – sparse solver w/ HSS embedding

Rank patterns for discretized PDEs on k^d mesh: [Chandrasekaran et al.'10, Enquist/Ying'11, Enquist/Zhao '14]

	2D	3D
Poisson	$O(1)$	$O(k)$
Helmholtz	$O(\log k)$ or $O(k)$	$O(k)$

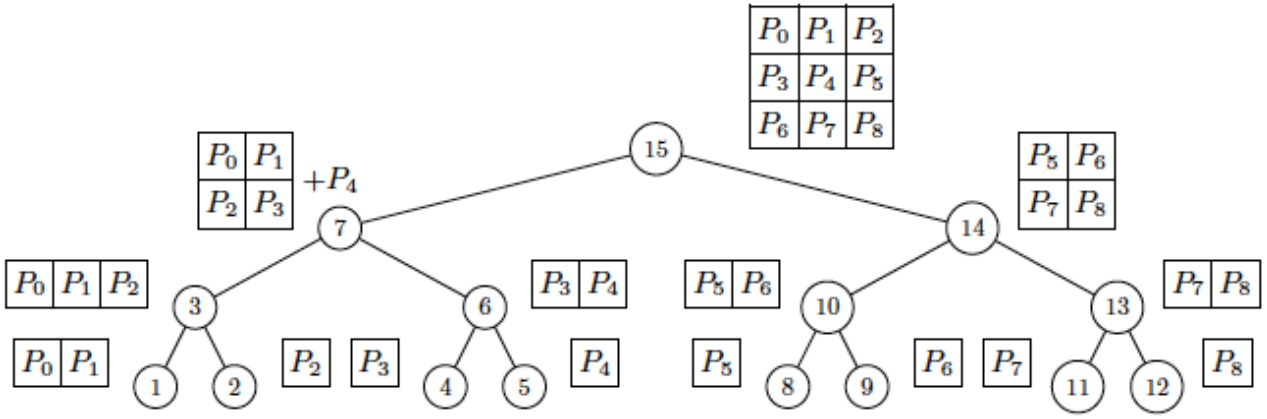
Solver complexities:

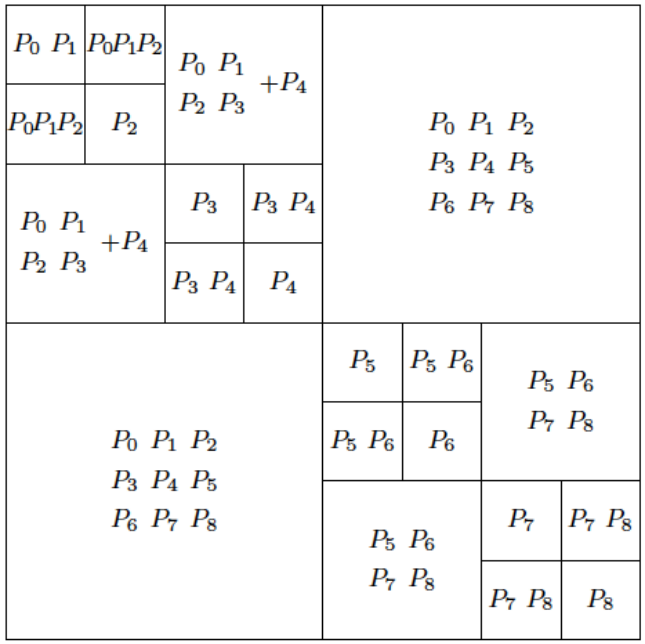
3D Helmholtz cost: [Xia '13] (seems true for many PDEs)

	Mem	Flops
MF-HSS	$O(N \log N)$	$O(N^{4/3} \log N)$
MF-HSS + RS	$O(N)$	$O(N \log N)$

Distributed-memory parallel algorithm

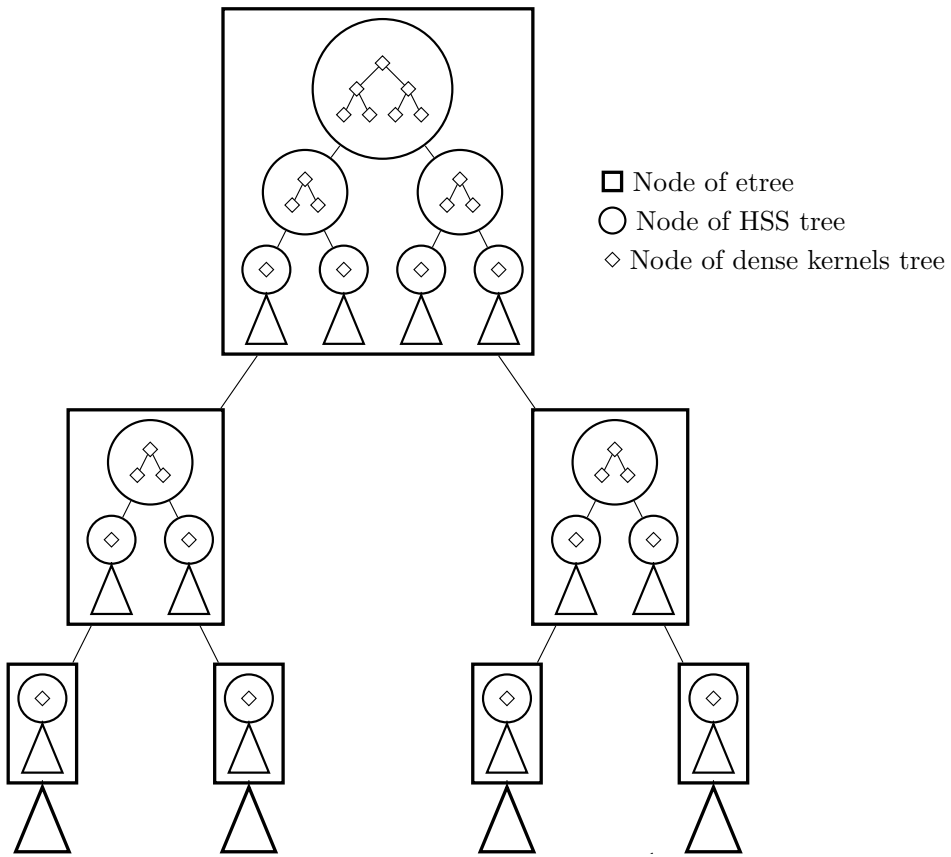
Use HSS tree to help data distribution





Multilevel parallelism in sparse MF-HSS solver

Elimination tree, HSS tree, BLAS tree



Dense – communication analysis

Number of messages and volume of communication on the critical path (for 1 process):

Algorithm	Messages	Words
ScaLAPACK LU	$\mathcal{O}(n \log p)$	$\mathcal{O}\left(n^2 \frac{\log p}{\sqrt{p}}\right)$
Randomized	$\mathcal{O}(p \log p + r \log p + r \log^2 p)$	$\mathcal{O}\left(\frac{n^2}{p} + \frac{rn}{\sqrt{p}} + r^2\right)$
HSS compression	Redist Sampling Tree	Redist Sampling Tree

- Further reduce communication? Lower bound?

STRUMPACK – STRUctured Matrices PACKage

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
  - Sparse matrix in CSR format.
- Can take user input: cluster tree & block partition
- Functions:
  - HSS construction, HSS-vector product, ULV factorization, Solution.
- Public domain, BSD license.

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- Extensible to include other data-sparse formats.

Making software robust

- Adaptive sampling machinery
  - Automatic handling unknown rank patterns: incrementally adjust sample size at any node when rank revealed is too large.
- Non-uniform clustering & partitioning

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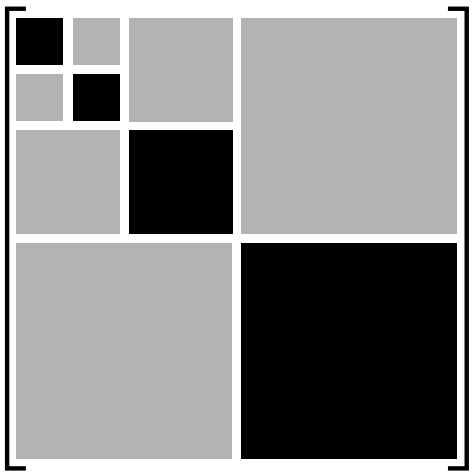
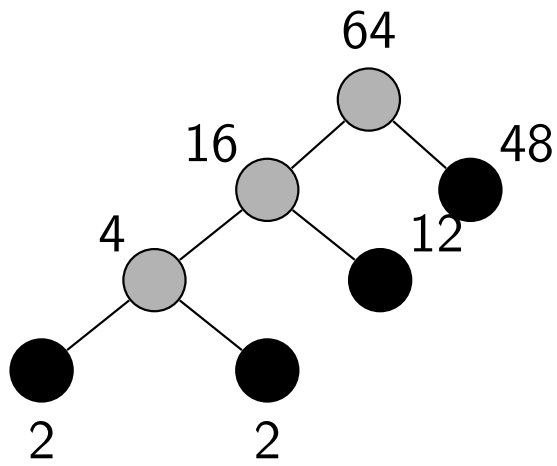


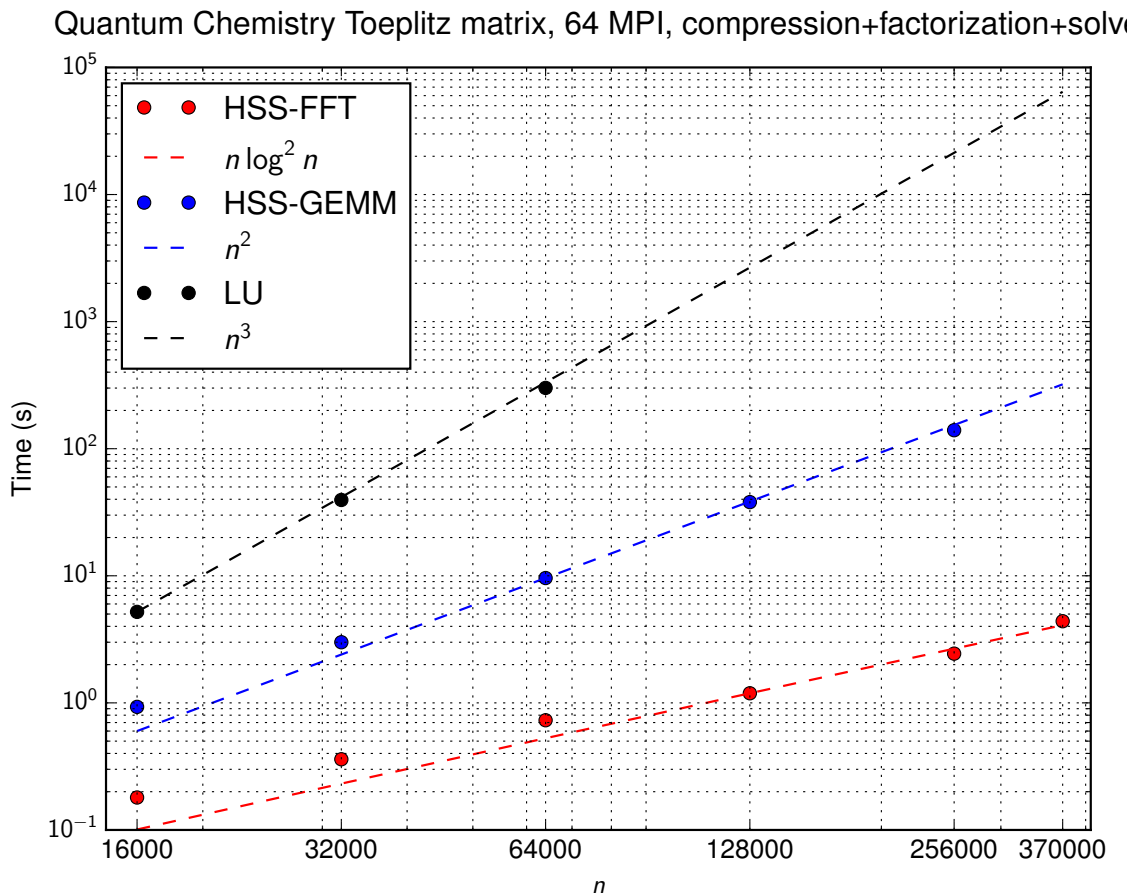
(c) Matrix structure.



(d) Weighted process mapping

Matrix-free interface

- Toeplitz: matvec via FFT
  Quantum chemistry: $a_{i,i} = \frac{\pi^2}{6}$, $a_{i,j} = \frac{(-1)^{i-j}}{(i-j)^2 d^2}$
- Previous best Toeplitz linear solver (e.g. Levinson): $O(n^2)$



Parallel weak scaling

Root node of the multifrontal factorization of a discretized Helmholtz problem (frequency domain, PML boundary, 10Hz).

k (3D mesh: k^3)	100	200	300	400	500
Matrix size ($=k^2$)	10,000	40,000	90,000	160,000	250,000
# Cores	64	256	1,024	4,096	8,192
Maximum rank	313	638	903	1289	1625
Compression time	2.0	13.0	30.6	60.8	133.6
Speed-up over ScaLAPACK	**1.8**	**4.0**	**5.4**	**4.8**	**3.9**
Flops ratio	**0.6**	**18.8**	**132.7**	**626.1**	**1716.7**

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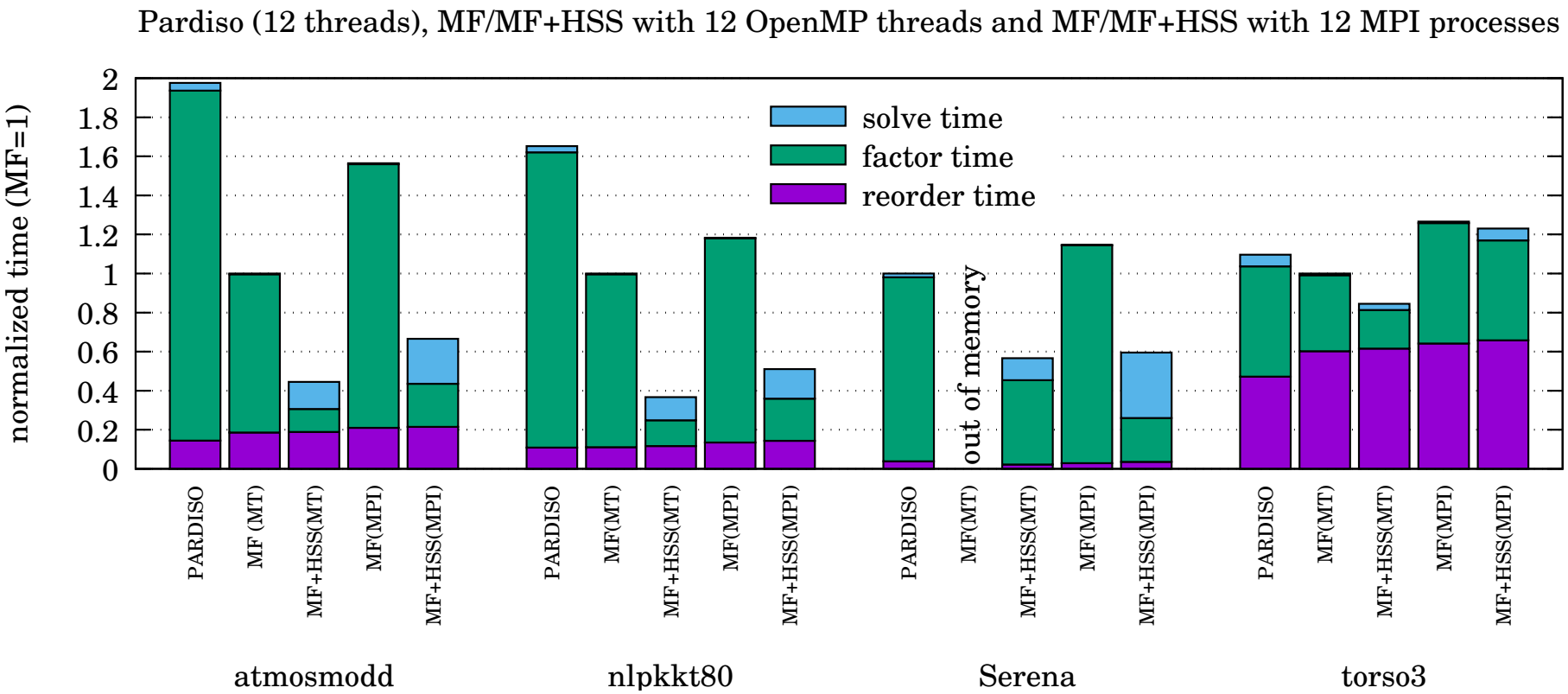
Load imbalance

Parallel performance of sparse MF-HSS solvers

Cray XC30, Edison at NERSC



- Compared to PARDISO in Intel MKL library (12 threads)
- OpenMP (12 threads): MF, MF-HSS
- MPI (12 tasks): MF, MF-HSS

Further details ...

- Pieter Ghysels, MS51, Friday, 11:45-12:10
  "A Parallel Multifrontal Solver and Preconditioner Using Hierarchically Semiseparable Structured Matrices"

New parallel algorithms tracking architecture advances

Evolution of parallel machines, programming

- Vector machines, program with vectorization directives
- Shared memory UMA, program with directives or explicit threading
- Distributed memory machines presented major challenges
  - Data distribution, locality
  - Program with explicit messages, e.g., MPI
- Recently, heterogeneous node architectures, more disruptive
  - NUMA, socket / core / vector unit; accelerator / co-processor (e.g., GPU)
  - Memory per core is small
  - Program with mixed MPI & threads & CUDA ...

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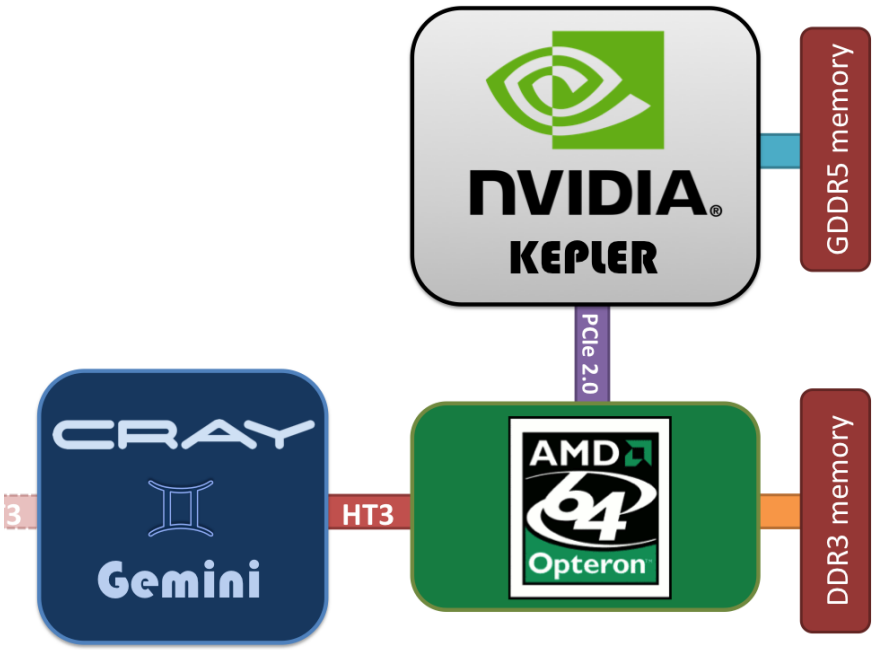
Mixing task parallelism and data parallelism.

Variety of node architectures

Titan at ORNL:
16-core AMD + K20X GPU



Programming:

- Separate CPU/GPU programs
- Transfer data between them

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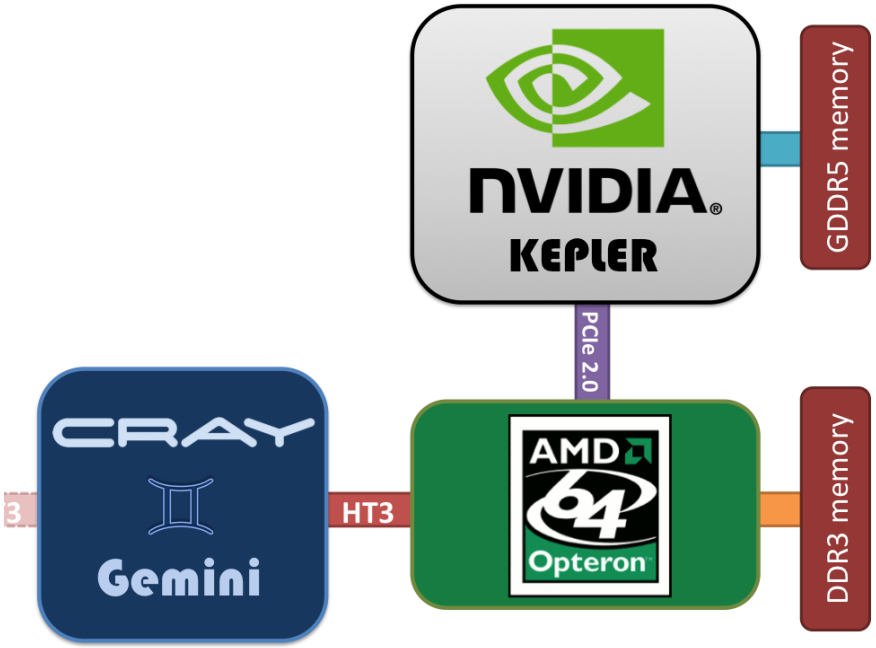

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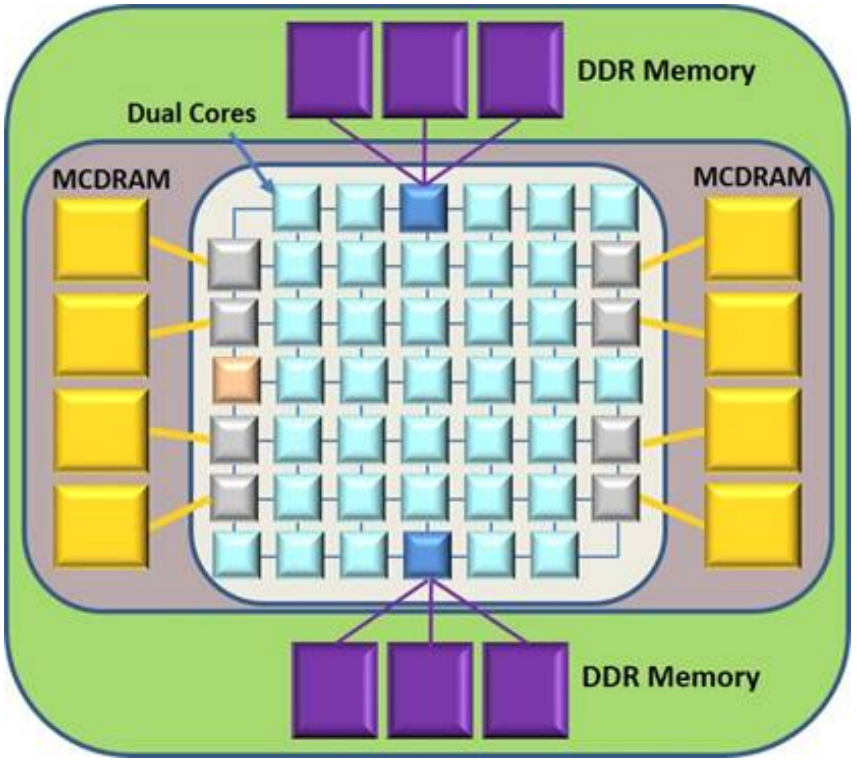
Intel Xeon Phi KNL (2016)

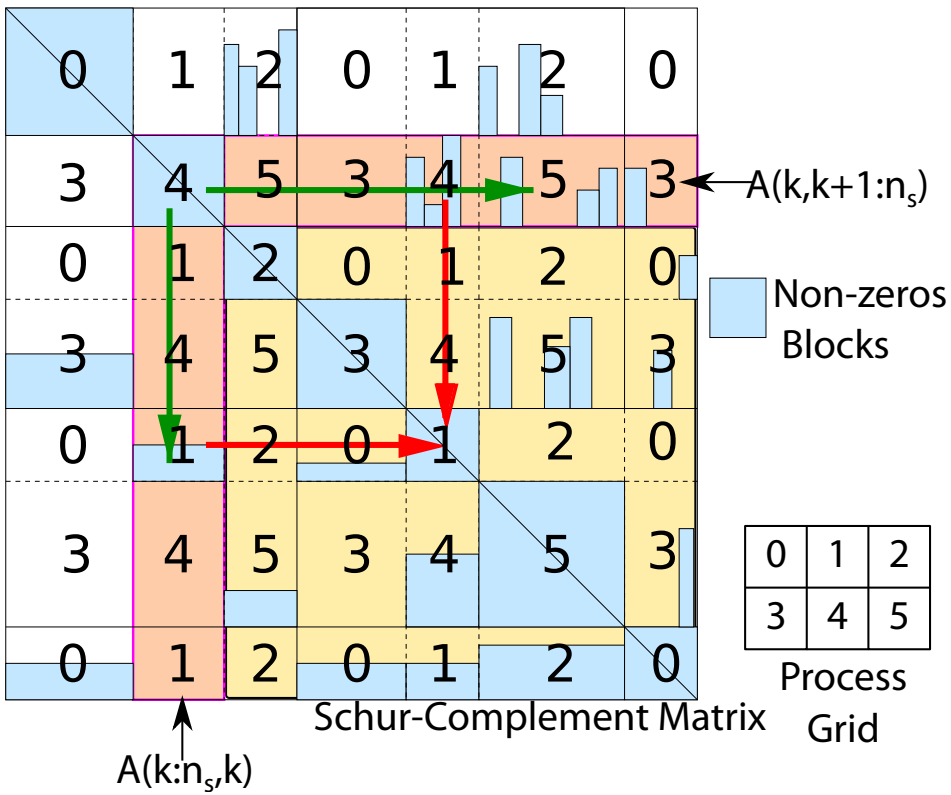


- 72 cores
- 4 threads/core
- 2 512bit vector units/core

SuperLU_DIST

http://crd-legacy.lbl.gov/~xiaoye/SuperLU/

A widely used open-source sparse direct solver library [LBNL/UC Berkeley]



Algorithms

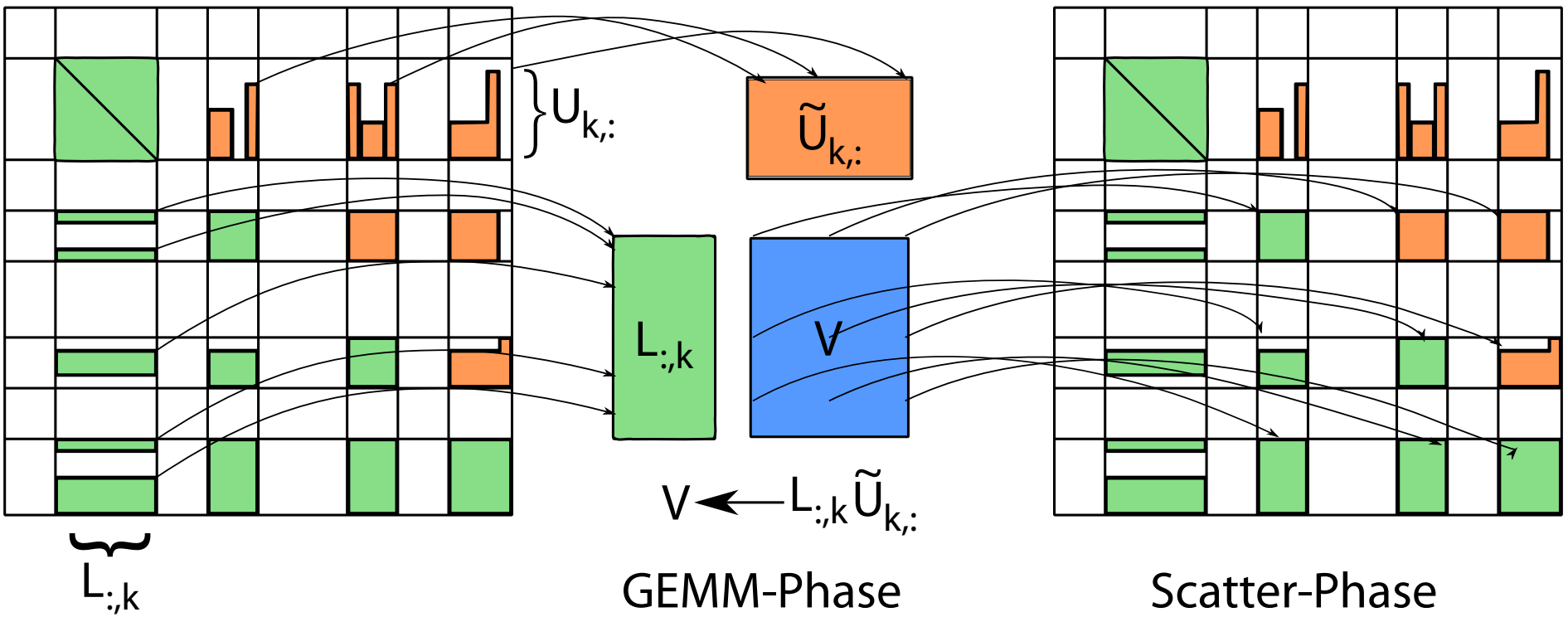
- Right looking
- Static pivoting
- 2D Cyclic data distribution

Two Major computational phases

1. Panel Factorization
2. Schur-Complement Update

Schur-complement udate

- Over 80% factorization time, ample parallelism
- Two operations: GEMM, Gather/Scatter



Design questions for accelerator / co-processor

- Only use accelerator, or use CPU as well?
  Accelerator memory small
  $\rightarrow$ best to use both (offload some computations to GPU)
- What to offload?
  Panel factorization not suitable for fine-grained data-parallel model
  $\rightarrow$ offload only Schur complement update
- Schur complement update: GEMM, and Gather/Scatter?
  - GEMM only compute intensive [Sao/Vuduc/L. 2014]
  - Both GEMM and Gather/Scatter indirect addressing, memory intensive [Sao/Liu/Vuduc/L. 2015]

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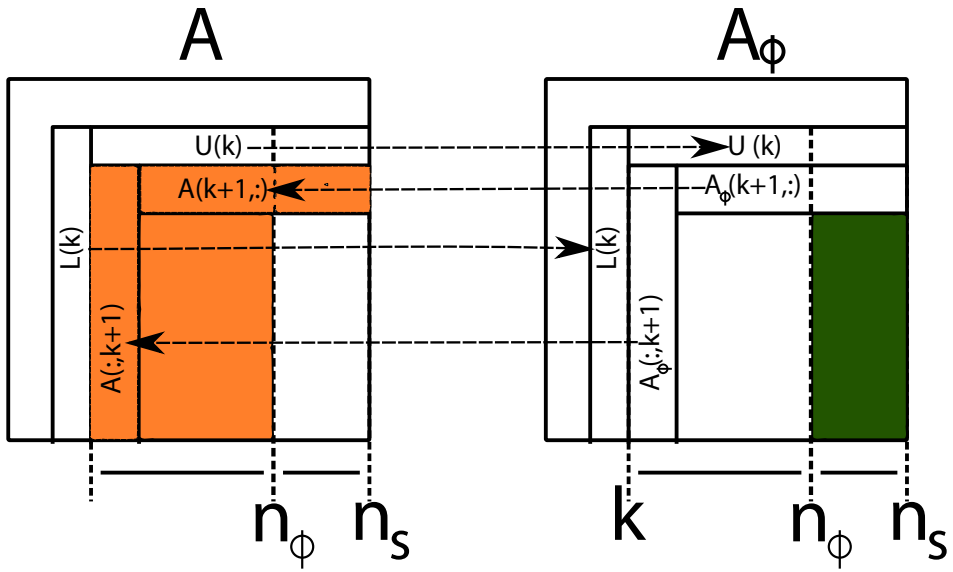
Overlap activities on both CPU/GPU to hide transfer latency over PCIe bus (10-15 microseconds)

HALO algorithm – Highly Asynchronous Lazy Offload

- Maintain two partial sums of Schur-complement on both CPU and GPU, selectively offload Schur updates
  - A_ϕ has the same sparsity structure as A (2x memory duplicate)
  - Part of Schur update on CPU, part on GPU
- Reduce to-be-factorized panel on CPU, absorbing GPU's panel.



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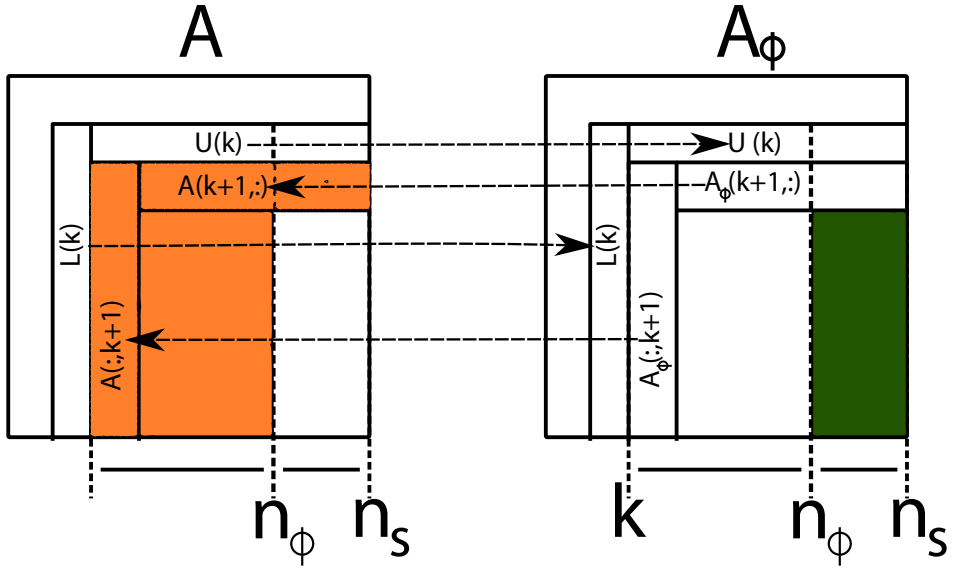

2-3x performance gains on 1000+ nodes GPU cluster Titan at ORNL

2-5x reduction in memory footprint

Further details ...

- Piyush Sao, MS48, Thursday, 4:00-4:25
  "A Sparse Direct Solver for Distributed Memory GPU and Xeon Phi Accelerated Systems"

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Other sparse factorization GPU work:

- PARDISO: left-looking sparse LU, offload BLAS [Schenk/Christen/Burkhart, 2008]
- WSMP: multifrontal sparse Cholesky, offload BLAS [George et al., 2011]
- Multifrontal sparse Cholesky, offload frontal matrix computation [Krawezik and Poole 2009, Vuduc et al. 2011, Yu/Wang/Pierce 2011]
- Threading, offload large frontal matrix computation [Lucas et al., 2010]
- Sparse multifrontal QR: offload subtrees of the assembly tree [Yeralan/Davis/Ranka, 2013]

Summary

- Sparse matrices can be made sparser by combining structural sparsity with data sparsity.
  - Good ordering and hierarchical clustering / partitioning
  - Alternative rank-revealing procedures
  - Dynamic load balancing
- Need redesign known algorithms, refactor existing codes for new architectures.

THANK YOU !