Towards the scalable inversion of structured matrices with standard admissibility conditions

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Overview

1. Why do Green's functions from certain second-order elliptic equations have numerically low-rank long-range interactions? *(Nested applications of Poincaré and Caccioppoli inequalities)*
2. Why is general dense $\mathcal{H}$-matrix factorization not effectively parallelizable? *(Long critical path)*
3. Why is Newton-Schulz inversion tempting? *(Each iteration is $\mathcal{H}$-matrix composition, which can be fast and parallel)*
4. Why is a good initial guess for Newton-Schulz needed? *(Otherwise, interior iterates will not be cheaply approximable)*
5. What is a reasonable initial guess that can be computed scalably? *(An inverse of a weakly-admissible $\mathcal{H}^2$-matrix)*
6. Some results on scalable $\mathcal{H}$-matrix composition and a discussion of future work

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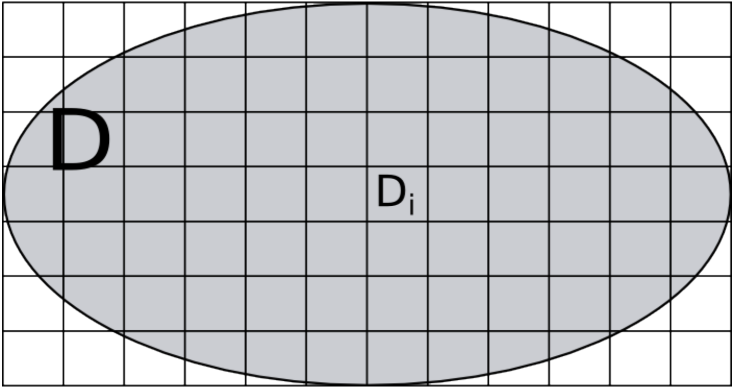
(Projected) piecewise-constant approximation

[Bebendorf/Hackbusch-2002]
For convex $D \subset \mathbb{R}^d$, use Poincaré over convex covering $\{D_i\}_{i=0}^{\ell^d}$:

$$\|u - \bar{u}\|_{L^2(D_i)} \leq \frac{1}{\pi}\mathrm{diam}(D_i)\|\nabla u\|_{L^2(D_i)}, \quad u \in H^1(D),$$

and $\bar{u}$ can be replaced with its $L^2(D)$ projection onto $H^1(D)$ with the same bound.



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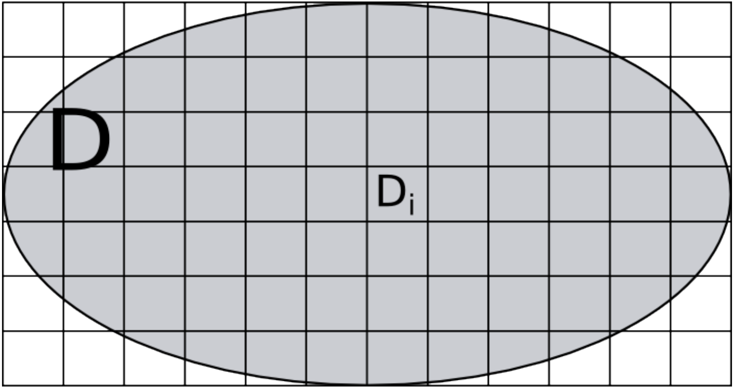
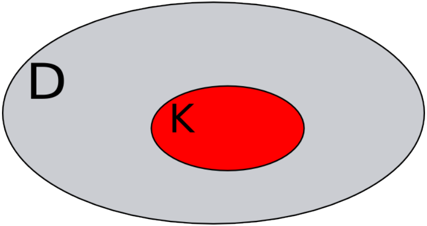


Bounding the gradient via Caccioppoli

[Bebendorf/Hackbusch-2002]
Let $u \in H_1(D)$, $D \subset \Omega$, be $C_0^\infty(D)$-weakly L-harmonic with respect to $Lv = -\sum_{i,j=1}^{d} \partial_j (c_{ij} \partial_i v)$, where $C = C(x) = (c_{ij})_{ij}$, $c_{ij} \in L^\infty(\Omega)$, is symmetric with condition number bound κ_C.
Then, for $K \subset D$,

$$\|\nabla u\|_{L^2(K)} \leq \frac{4\sqrt{\kappa_C}}{\mathrm{dist}(K, \partial D)} \|u\|_{L^2(D)}.$$



Combined with the previous result, we can bound the (projected) piecewise constant approximation of u in K with respect to $\|u\|_{L^2(D)}$.

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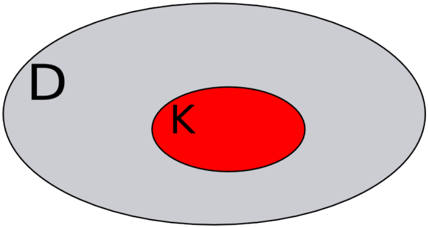

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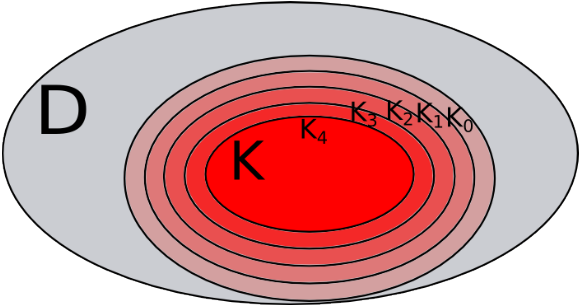
Exponential convergence via nested Caccioppoli

[Bebendorf/Hackbusch-2002]
Poincaré combined with Caccioppoli of K w.r.t. D yields the ℓ^d-dim. approx:

$$\|u - \bar{u}\|_{L^2(K)} \leq \frac{\gamma \,\mathrm{diam}(K)}{\mathrm{dist}(K, \partial D)\ell} \|u\|_{L^2(D)}, \quad \gamma \equiv \frac{2^{2+1/d}\sqrt{\kappa_C}}{\pi},$$

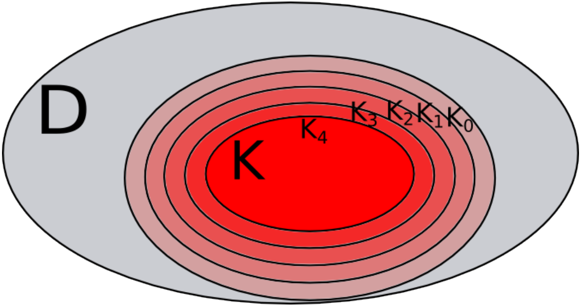
where $u \in H^1(D)$ is weakly L-harmonic. Key point: **recursive application exponentiates bound but only multiplies subspace dimension**



Exponential convergence via nested Caccioppoli

[Bebendorf/Hackbusch-2002]
Let $r_j = (1 - j/i)\mathrm{dist}(K, \partial D)$ and $K_j = \{x \in D : \mathrm{dist}(x, K) \le r_j\}$.
Setting $\rho \equiv \mathrm{dist}(K, \partial D)/\mathrm{diam}(K)$, $u_0 \equiv u$, and
$u_{j+1} \equiv u_j|_{K_{j+1}} - \bar{u}_j$, then we have the $(j+1)\ell^d$-dim. approx. error:

$$\|u_{j+1}\|_{L^2(K_{j+1})} \le \frac{i\gamma(1+2\rho)}{\rho\ell}\|u_j\|_{L^2(K_j)} \le \left(\frac{i\gamma(1+2\rho)}{\rho\ell}\right)^j \|u\|_{L^2(K_0)}$$



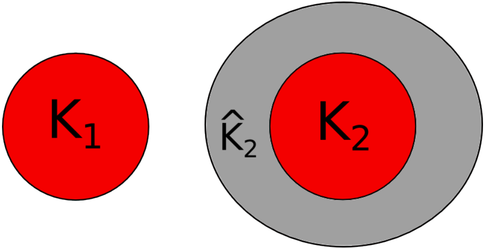
Approximating the Green's function

[Bebendorf/Hackbusch-2002]
Let $K_1, K_2 \subset \Omega$ such that $\mathrm{dist}(K_1, K_2) \geq \rho\,\mathrm{diam}(K_2) > 0$. Then, for any $\epsilon \in (0, 1)$, there is an approximation

$$G_k(x, y) = \sum_{i=1}^{k} u_i(x) v_i(y) \ \text{ with } k = O(\log(\frac{1}{\epsilon})^{d+1}), \ \text{ and}$$

$$\|G(x, \cdot) - G_k(x, \cdot)\|_{L^2(K_2)} \leq \epsilon \|G(x, \cdot)\|_{L^2(\hat{K}_2)}, \ \text{ for all } x \in K_1,$$

where $\hat{K}_2 \equiv \{y \in \Omega : \mathrm{dist}(y, K_2) \leq \frac{\rho}{2}\,\mathrm{diam}(K_2)\}$.



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Low-rank approximations

Why $\mathcal{H}$-matrix factorization is problematic

The promise of Newton-Schulz inversion

The need for a good initial guess

Parallel weakly-admissible $\mathcal{H}^2$ inversion

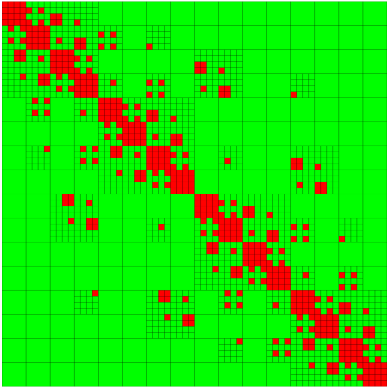
Some distributed $\mathcal{H}$-matrix composition results

Future work

Factoring (dense) $\mathcal{H}$-matrices

Four-level 2D $\mathcal{H}$-matrix with standard admissibility:

$$\min(\mathrm{diam}(K_1), \mathrm{diam}(K_2)) \leq \rho\, \mathrm{dist}(K_1, K_2)$$



- Critical path generally $\Omega(N)$; (approximate) factorization requires $O(N \lg^2 N)$ work, so $O(\lg^2 N)$ parallel speedup...
- Multifrontal techniques boil sparse factorization down to dense interface problems [Grasedyck et al.-2009,Xia et al.-2009]

Outline

Newton-Schulz inversion

Applying Newton's method to

$$f(X) = X^{-1} - A$$

yields the iteration

$$X_{k+1} := (2I - X_k A) X_k$$

Suggested for parallel $\mathcal{H}$-matrix inversion by [Kriemann-2004] as alternative to $\mathcal{H}$-matrix factorization.

Ideally $O(\lg(\kappa(A)))$ approximate $\mathcal{H}$-matrix compositions are required, each involving $O(N \lg^2 N)$ operations

$\mathcal{H}$-matrix composition is highly parallelizable, and so, if the $\mathcal{H}$-matrix approximations are all valid, the problem is solved

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Truncated Newton-Schulz

For large classes of equations (see, e.g., [Hackbusch/Bebendorf-2003]), A and A^{-1} are known to be representable as $\mathcal{H}$-matrices with low ranks.

But what about the intermediate iterates?

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Approximate matrix iterations studied in [Hackbusch/Khoromskij/Tyrtyshnikov-2007]

Their conclusion: Intermediate iterates typically **NOT** representable, but with a sufficiently good initial guess, $\mathcal{H}$-matrix Newton-Schulz converges.

An unanswered question: How should one efficiently construct the initial guess in parallel?

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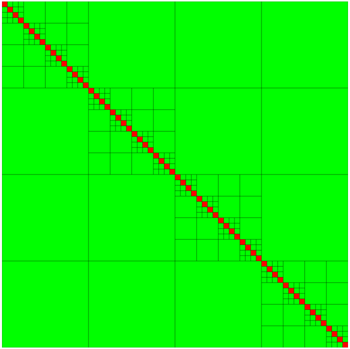
Parallel weakly-admissible $\mathcal{H}^2$-matrix factorization

Weakly-admissible $\mathcal{H}^2$-matrices can be scalably factored in parallel (see, e.g., [Wang et al.-2012]) via ULV decompositions [Chandrasekaran/Gu/Pals-2006].

$K_1 \cap K_2 = \varnothing$



Weak admiss. and shared bases are crucial for the parallelization!

Is the rank needed for initializing a convergent Newton-Schulz sufficiently lower than required for accurate direct inversion?

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Bulk synchronous $\mathcal{H}$-matrix composition

Can vastly generalize three-stage $\mathcal{H}$-matrix/vector multiplication scheme of [Kriemann-2004] to handle composition.[1]

Main idea: Aggressively combine phases of all $\mathcal{H}$-matrix application suboperations, resulting in $O(1)$ communication/computation phases.

[1] Cf. [Izadi-2012]

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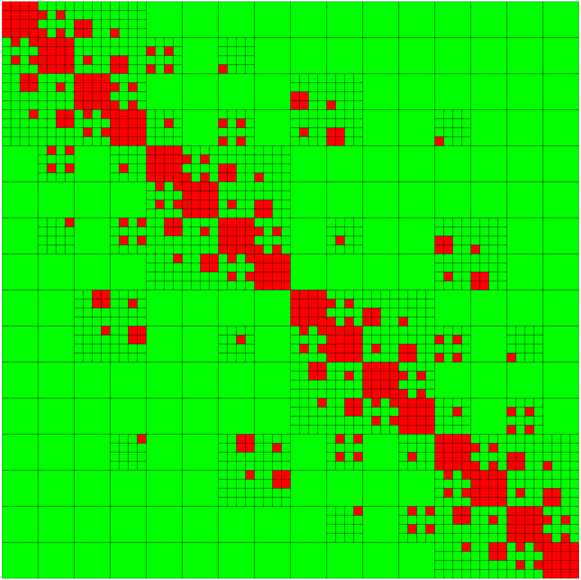
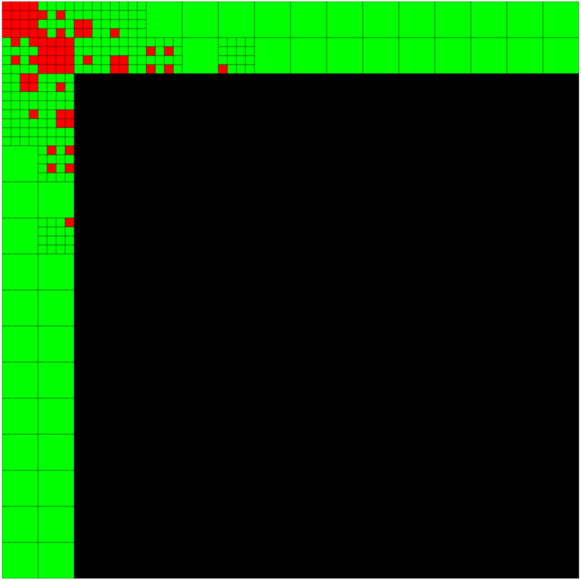
2D standard admissibility



2D standard admissibility (Process 0/8)



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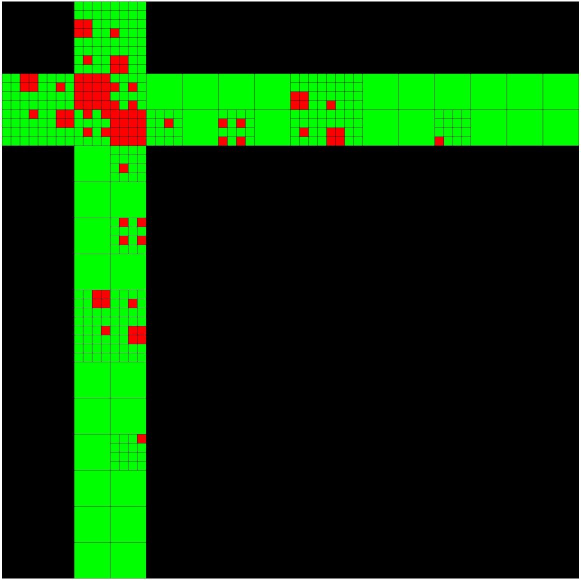
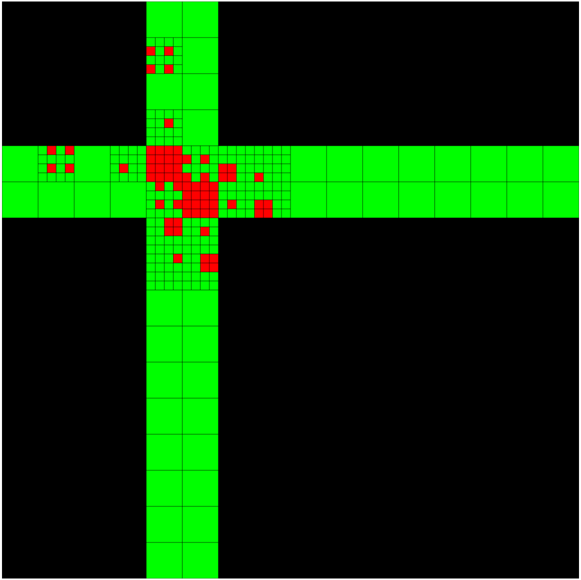
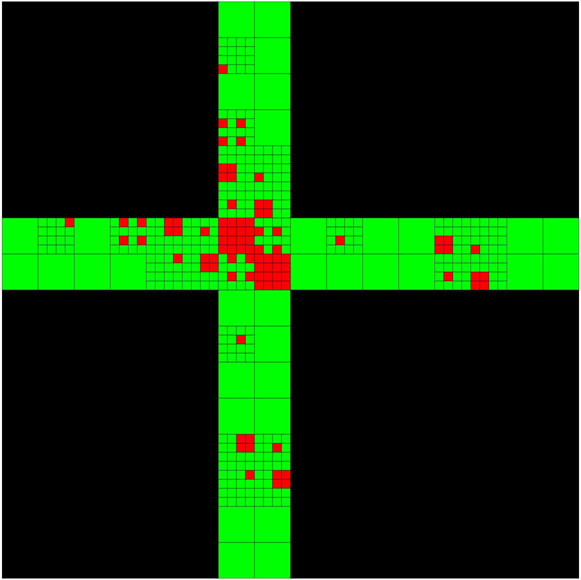


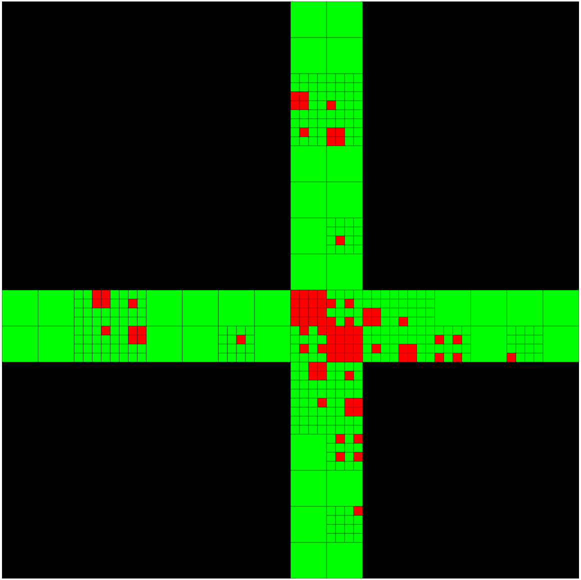
2D standard admissibility (Process 2/8)



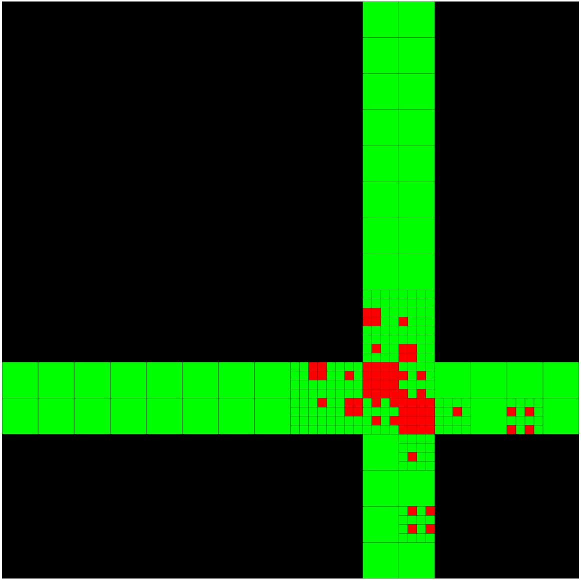
2D standard admissibility (Process 3/8)



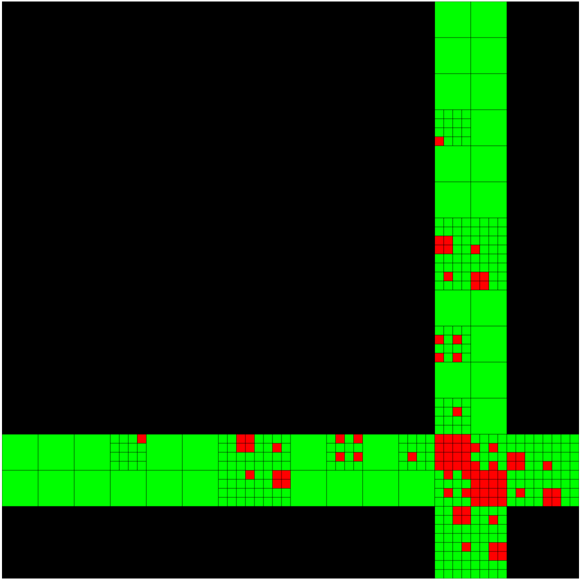
2D standard admissibility (Process 4/8)



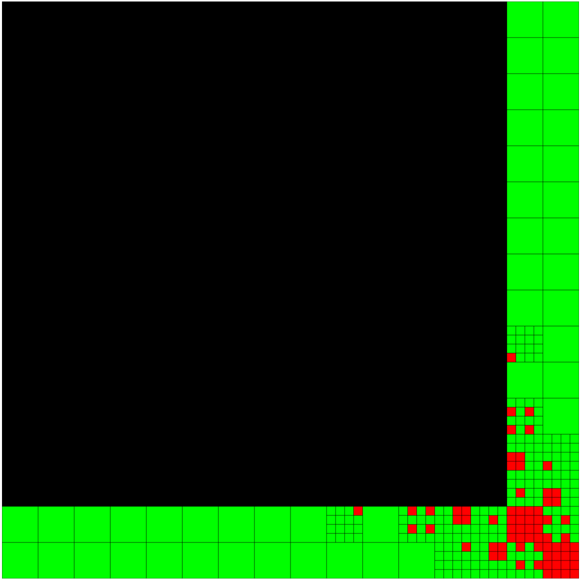
2D standard admissibility (Process 5/8)



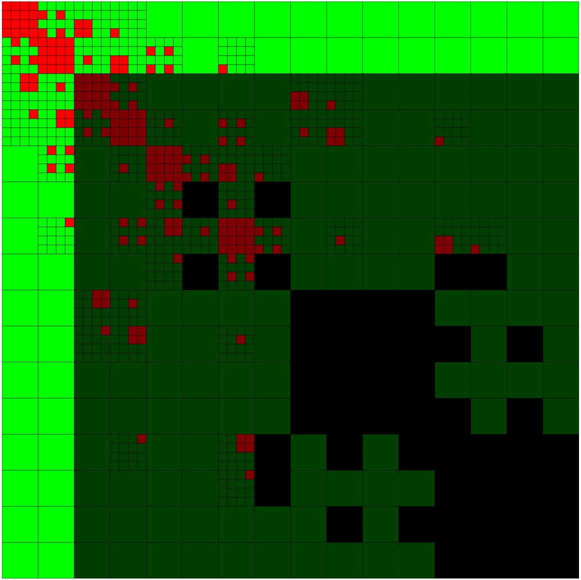
2D standard admissibility (Process 6/8)



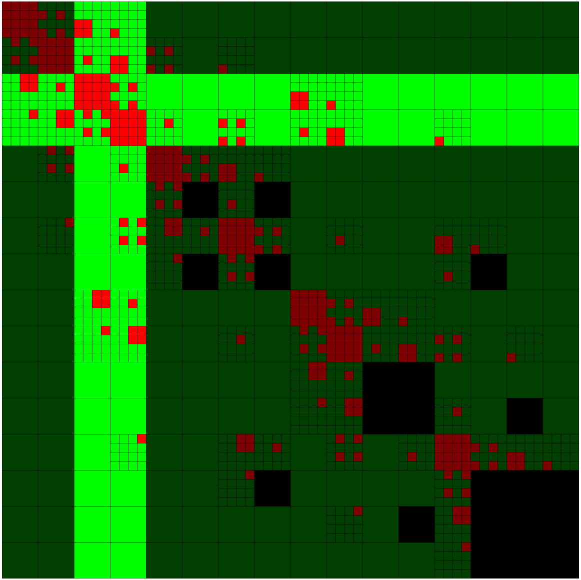
2D standard admissibility (Process 7/8)



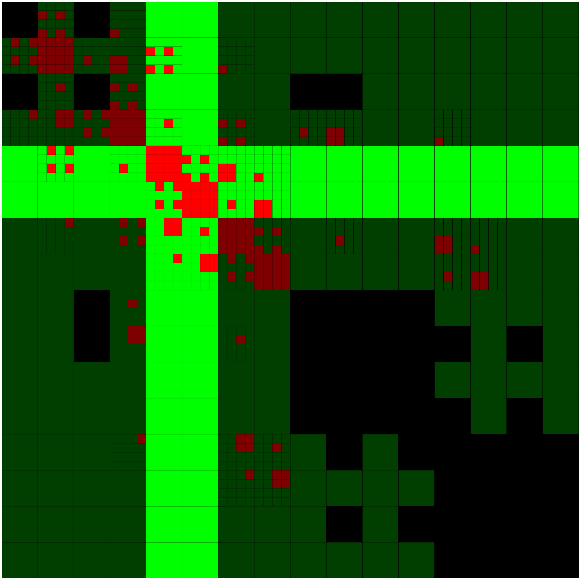
Ghosted 2D standard admissibility (Process 0/8)



Ghosted 2D standard admissibility (Process 1/8)



Ghosted 2D standard admissibility (Process 2/8)



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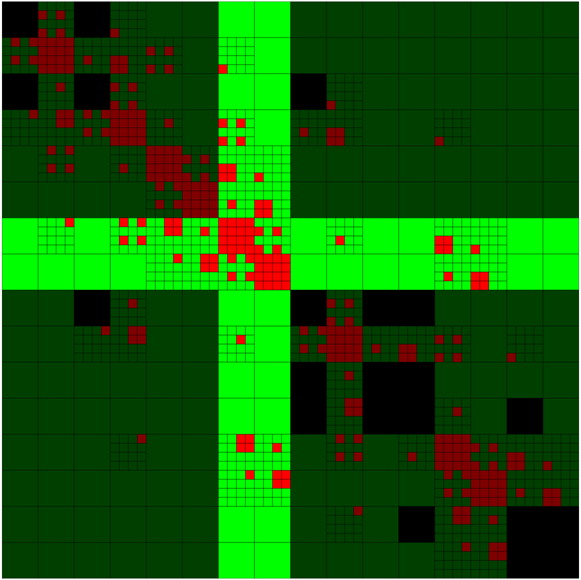
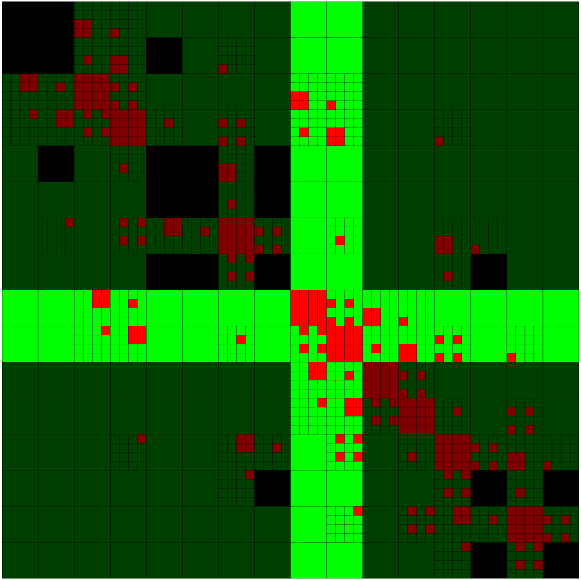


Ghosted 2D standard admissibility (Process 4/8)



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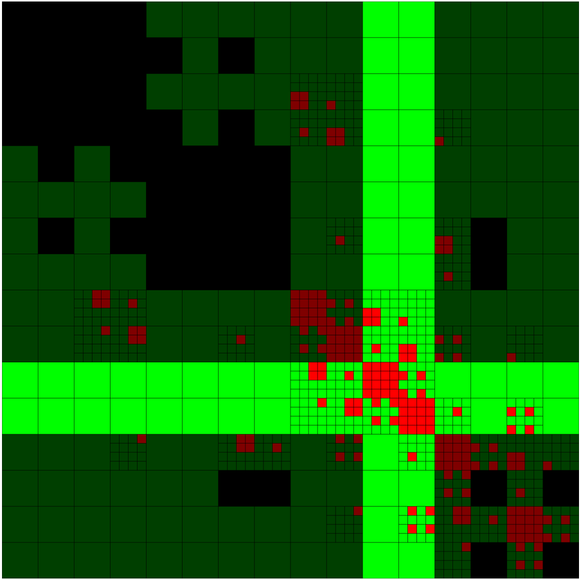

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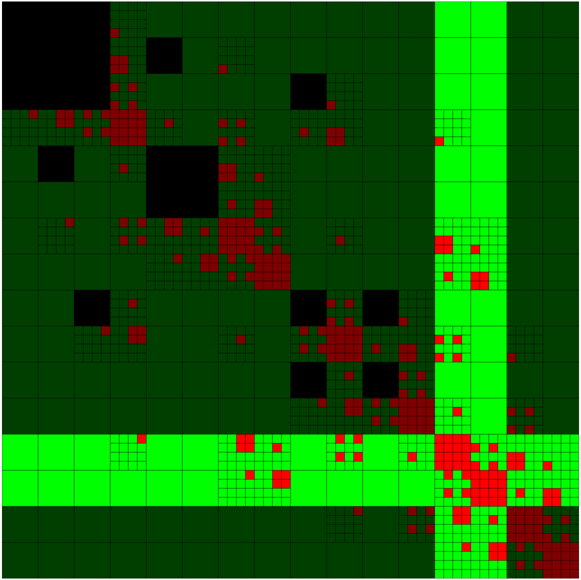

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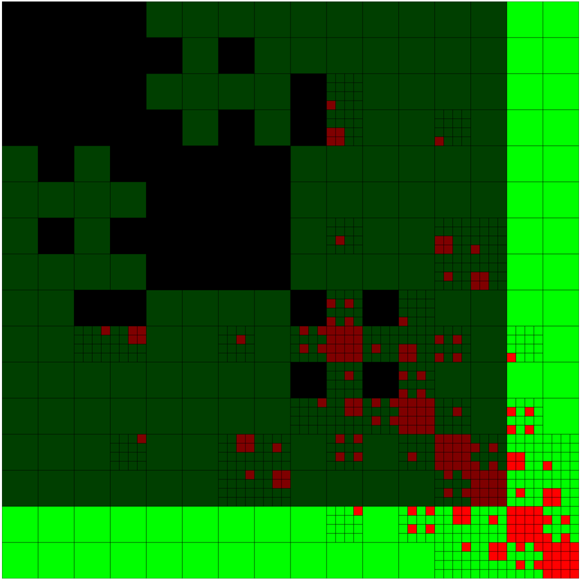
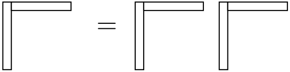
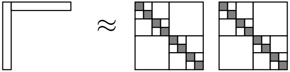


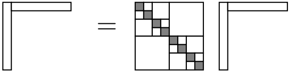
Communication phases for low-rank accumulation



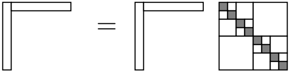
(a) Type FFF



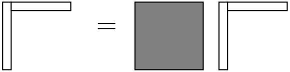
(b) Type FHH



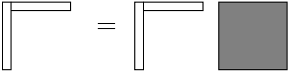
(c) Type FHF



(d) Type FFH



(e) Type FDF



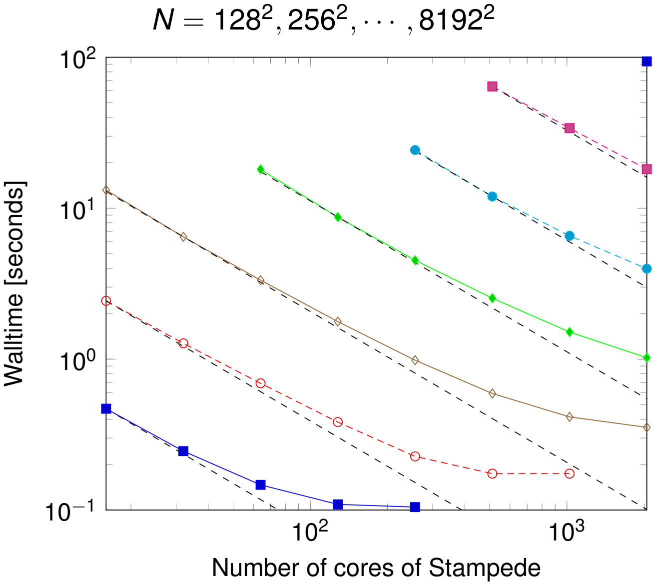
(f) Type FFD

Type FFF	Reduce → Pass → Broadcast
Type FHH	Reduce → Pass → Broadcast → Reduce → Pass → Broadcast
Type FHF	Reduce → Pass → Broadcast
Type FFH	Reduce → Pass → Broadcast
Type FDF	Pass
Type FFD	Pass

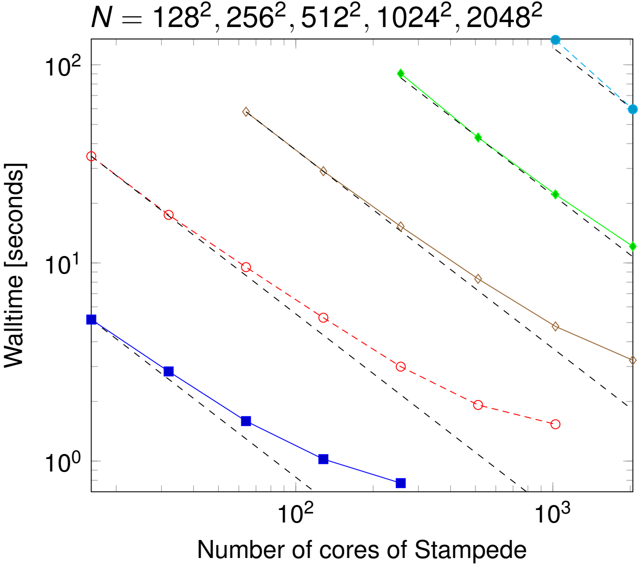
Cost analysis

	Method	γ	α	β
Full	Householder QR	$O(r^2 \frac{N}{p} \lg^3 N)$	$O(r \lg^2 p)$	$O(r^2 \lg^4 p + r^2 \frac{N}{p})$
	TSQR	$O(r^3 \lg^5 p + r^2 \frac{N}{p} \lg^3 N)$	$O(\lg p)$	$O(r^2 \lg^4 p + r^2 \frac{N}{p})$
	CholeskyQR (SVD)	$O(r^3 \lg^4 p + r^2 \frac{N}{p} \lg^3 N)$	$O(\lg p)$	$O(r^2 \lg^4 p + r^2 \frac{N}{p})$
k levels	Householder QR	$O(kr^2 \frac{N}{p} \lg^2 N)$	$O(r \lg^2 p)$	$O(kr^2 \lg^3 p + r^2 \frac{N}{p})$
	TSQR	$O(k^2 r^3 \lg^3 p + kr^2 \frac{N}{p} \lg^2 N)$	$O(\frac{\lg^2 p}{k})$	$O(kr^2 \lg^3 p + r^2 \frac{N}{p})$
	CholeskyQR (SVD)	$O(kr^2 \lg^3 p + kr^2 \frac{N}{p} \lg^2 N)$	$O(\frac{\lg^2 p}{k})$	$O(kr^2 \lg^3 p + r^2 \frac{N}{p})$
Single level	Householder QR	$O(r^2 \frac{N}{p} \lg^2 N)$	$O(r \lg^2 p)$	$O(r^2 \lg^3 p + r^2 \frac{N}{p})$
	TSQR	$O(r^3 \lg^3 p + r^2 \frac{N}{p} \lg^2 N)$	$O(\lg^2 p)$	$O(r^2 \lg^3 p + r^2 \frac{N}{p})$
	CholeskyQR (SVD)	$O(r^2 \lg^3 p + r^2 \frac{N}{p} \lg^2 N)$	$O(\lg^2 p)$	$O(r^2 \lg^3 p + r^2 \frac{N}{p})$

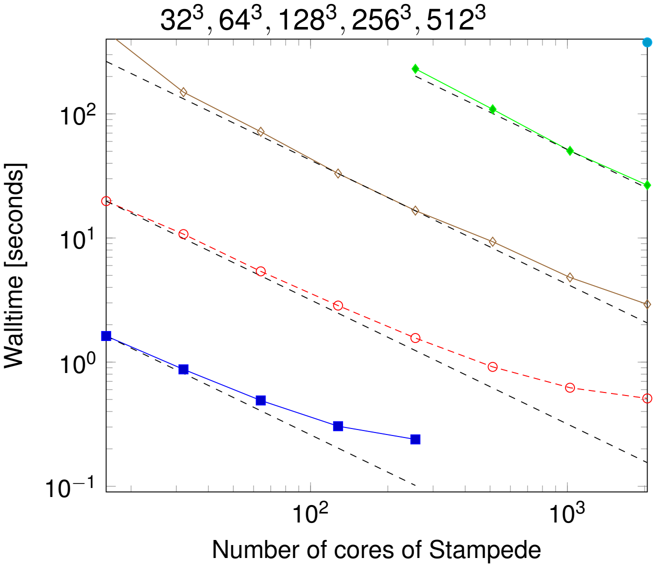
2D composition with weak admissibility ($r = 8$)



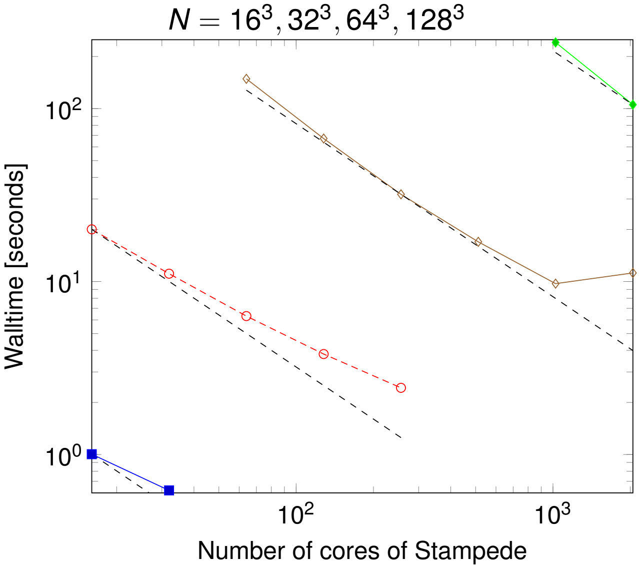
2D composition with standard admissibility ($r = 8$)



3D composition with weak admissibility ($r = 8$)



3D composition with edge admissibility ($r = 8$)



Outline

Future directions

- Efficient parallel conversion of a weakly-admissible $\mathcal{H}^2$ ULV factorization to $\mathcal{H}$-matrix form [Lin/Lu/Ying-2009,Martinsson-2011]
- Probing for the minimum viable $\mathcal{H}^2$ rank
- Large-scale dense inversion tests
- Extend the above to structured multifrontal method with standard admissibility
- Improving data locality for $\mathcal{H}$-matrix application
- Support for more general topologies
- Hierarchical Interpolative Factorizations [Ho/Ying-2013,cf. Gillman et al.] instead of HSS ULV?

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Acknowledgments and Availability

Funding

Computational resources

The organizer
Lenya Ryzhik

Availability
Prototype implementations available at
`bitbucket.org/poulson/dmhm`

Questions?

Memory usage

Update Method	Sequential Memory	Parallel Memory
Full	$O(rN\lg^2 N)$	$O(r^2\lg^3 p + r^2 \frac{N}{p}\lg^3 N)$
k levels	$O(krN\lg N)$	$O(k^2 r^2\lg p + k^2 r^2 \frac{N}{p}\lg N)$
Single level	$O(rN\lg N)$	$O(r^2\lg p + r^2 \frac{N}{p}\lg N)$