



# Fast and Scalable Hierarchical Linear Solvers

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### Scientific computing

- Natural phenomenon
- $\Rightarrow$  Modeling
- $\Rightarrow$  Discretization
- $\Rightarrow$  Computer simulation





### Scientific computing needs linear solvers



Linear PDE  $\nabla \cdot (a(x)\nabla u(x)) = f(x)$ 

- Ax = b
- A sparse, SPD

For Newton steps...

- Ax = b
- *A* sparse, unsymmetric





PDE F(x) = 0



For Newton steps...

- Ax = b
- A sparse, SPD

#### Scientific computing needs parallel computing

Even fast algorithms cannot solve problems with 100M+ unknowns...





Three-parts talk



# Sparsified Nested Dissection

Cambier, L., Chen, C., Boman, E. G., Rajamanickam, S., Tuminaro, R. S., & Darve, E. (2020). An algebraic sparsified nested dissection algorithm using low-rank approximations. *SIAM Journal on Matrix Analysis and Applications*, *41*(2), 715-746.

### Why do we want hierarchical solvers?



#### Let's start from direct methods

$$A = \begin{bmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} l_{11} \\ L_{21} & I \end{bmatrix} \begin{bmatrix} I \\ A_{22} - A_{21}a_{11}^{-1}A_{12} \end{bmatrix} \begin{bmatrix} l_{11}^T & L_{21}^T \\ I \end{bmatrix}$$



Matrix graph G = (V, E) $(i, j) \in E \iff A_{ij} \neq 0$ 



A, symmetric, SPD

#### Not all orderings are equal



#### How to minimize fill-in & cost? Nested Dissection!



#### **Block elimination**

Graph of A





#### Fill-in in Nested Dissection

Graph of A







#### Direct methods have a lot of fill-ins



#### Dense blocks take too long to factor



#### Fill-in is dense but low-rank



#### Sparsification: block scaling



#### Sparsification: low-rank approximation

$$\begin{bmatrix} A_{pn} & A_{np}^{T} \end{bmatrix} = \begin{bmatrix} A_{pn_{1}} & A_{pn_{2}} & \dots & A_{n_{1}p}^{T} & A_{n_{2}p}^{T} & \dots \end{bmatrix}$$
$$= \begin{bmatrix} Q_{c} & Q_{f} \end{bmatrix} \begin{bmatrix} W \\ O(\varepsilon) \end{bmatrix} \quad (\text{RRQR, SVD, }\dots)$$
$$= \begin{bmatrix} Q_{f}^{T} \\ Q_{c}^{T} \end{bmatrix} \begin{bmatrix} I & A_{pn} \\ A_{np} & A_{nn} & A_{nw} \\ A_{wn} & A_{ww} \end{bmatrix} \begin{bmatrix} Q_{f} & Q_{c} \end{bmatrix} \quad I \\ I \end{bmatrix}$$
$$= \begin{bmatrix} I \\ W \\ W_{nc} & A_{nn} & A_{nw} \\ A_{wn} & A_{ww} \end{bmatrix}$$

#### Sparsification: low-rank approximation



# Defining interfaces through overlapping separators





### Eliminate $\mapsto$ Scale $\mapsto$ Sparsify $\mathcal{O}$







#### SPD remains SPD

If using Cholesky for elimination and scaling

$$\begin{bmatrix} Q_p^T \\ I \end{bmatrix} \begin{bmatrix} I & A_{pn} \\ A_{np} & A_{nn} \end{bmatrix} \begin{bmatrix} Q_p \\ I \end{bmatrix} = \begin{bmatrix} I & \varepsilon \\ I & W_{cn} \\ W_{nc} & A_{nn} \end{bmatrix}$$
SPD
SPD
(submatrix of SPD)

SPD



Separator sizes decrease  $O\left(N^{\frac{2}{3}}\right) \Rightarrow O\left(N^{\frac{1}{3}}\right)$ "lines" "planes"



### spaND is $O(N \log N)$ in 3D

<u>**If separators**</u> \*  $N^{\frac{2}{3}} \rightarrow N^{\frac{1}{3}}$ 



\* and few other assumptions

#### Orthogonal always works on SPD Scaling improves accuracy

Black = spaND (Orthogonal, scaling) Red = HIF\* (Triangular, scaling)

White = HIF\* (Triangular, no scaling)



#### All >50k SPD problems from SuiteSparse, except 2 that didn't converge in <500

\* Ho, K. L., & Ying, L. (2016). Hierarchical interpolative factorization for elliptic operators: differential equations. *Communications on Pure and Applied Mathematics*, *69*(8), 1415-1451.

#### Ice-Sheet modeling $\kappa(A) > 10^{11}$

		spaND				Direct ILU(0) (Trilinos	
	Ν	t <sub>Fact</sub> (s.)	t <sub>CG</sub> (s.)	n <sub>cg</sub>	size <sub>Top</sub>	t <sub>Fact</sub> +t <sub>Solve</sub> (s.)	t <sub>Solve</sub> (s.)
5 layers	0.6M (16km)	7	3	7	78	19	23
	2.5M (8km)	28	14	8	88	126	286
	10M (4km)	124	89	10	99	1036	7137
10 layers	1M (16km)	23	7	7	137	86	42
	4.6M (8km)	97	34	8	147	725	544
	18.5M (4km)	538	311	10	159	-	18680





 $\mathcal{O}\left(N\right)$ 



Problem from: Tezaur, Irina K., et al. "Albany/FELIX: a parallel, scalable and robust, finite element, first-order Stokes approximation ice sheet solver built for advanced analysis." Geoscientific Model Development (Online) 8.4 (2015). Picture: Tezaur, Irina K., et al. "On the scalability of the Albany/FELIX first-order Stokes approximation ice sheet solver for large-scale simulations of the Greenland and Antarctic ice sheets." Procedia Computer Science 51 (2015): 2026-2035. 27 Thanks to E. Boman, R. Tuminaro, S. Rajamanickam & M. Perego

#### The SPE problem



 $10^9$ 

2M

8M

4M

16M

 $(N^{1/3})$ 

16M

8M

4M

 $10^{2.5}$ 

2M



## Top separator 32 GB $\rightarrow$ 6MB

Problem and picture from: Christie, Michael Andrew, and M. J. Blunt. "Tenth SPE comparative solution project: A comparison of upscaling techniques." *SPE reservoir simulation symposium*. Society of Petroleum Engineers, 2001. Thanks to Bazyli Klockiewicz for the matrix

#### spaND also works on unsymmetric problems 3D advection-diffusion



 $-\nabla \cdot (a(x)\nabla u(x)) + b(x) \cdot \nabla u(x) = f(x)$ , centered FD on  $[0,1]^3$ ,  $a = 10^{-2}$ ,  $b_i = 1$ 

#### Conclusion

spaND is

- Much faster than direct methods
- Never breaks on SPD problems
- Robust and versatile

# TaskTorrent

Cambier, L., Qian, Y. and Darve, E. "TaskTorrent: a Lightweight Distributed Task-Based Runtime System in C++." *To appear in Proceeding of the 2020 Parallel Application Workshop: Alternatives to MPI+X. arXiv preprint arXiv:2009.10697* (2020).

#### Runtime systems

Computations = tasks with dependencies

Runtime systems schedule tasks and

- avoid synchronization
- exploit all resources

```
for (k=0; k<n; k++) {
    POTRF(A[k,k]);
    for (i=k+1; i<n; i++) {
        TRSM(A[k,k],A[i,k]);
    }
    for (i=k+1; i<n; i++) {
        SYRK(A[i,k], A[i,i]);
        for (j=k+1; j<i; j++) {
            GEMM(A[i,k], A[j,k], A[i,j]);
        }
}</pre>
```



#### Two approaches: STF and PTG

Sequential task flow (STF)

```
/** Define tasks **/
void task(A: in, B: out)
/** Register data **/
A = [ ... ]
B = [ ... ]
/** Process DAG **/
for (i ..., j ...)
    task(A[i], B[j])
```

- Data dependencies inferred through data sharing rules

Parametrized task graph (PTG)

```
/** Define DAG using
 * functions of K
 **/
in_deps = (K k) { ... }
task = (K k) { ... }
out_deps = (K k) { ... }
/** Seed tasks **/
for (k in kinit)
    start(k)
```

- Task defined as functions over K
- Computation triggered by seeding initial tasks

#### Existing solutions

Legion/Regent:

- Sequential semantic (STF)
- Custom language
- May need tuning for good performances
- Hard to use within legacy codes

TRSM(k, m)

#### 

BODY trsm(A, C); END

#### PaRSEC:

- Custom language (JDF)
- Cannot use other data structures

### Goals of TaskTorrent

Current adoption of runtime systems is low Wider adoption requires

- Easy to learn API
  - No new language
  - API with predictable behaviors
  - Good OOTB performances
- Good interaction with existing codebases
  - Plays well with MPI and message-passing codes
  - Incremental adoption
  - Standard tools (MPI and C++)
  - Any user data structures
  - Minimal overhead, no task refactoring

#### STF is easier to use but may not scale

Need to enumerate the DAG !



DAG of 20x20 Cholesky (very small)

#### TaskTorrent combines PTG and Active messages

- Lightweight: PTG + AMs
- Message-passing, with MPI and C++ threads
- Any user data structures
- Good performances out-of-the-box



#### How to use TaskTorrent?

- 1. Tasks are functions (K k)
  - Mapping task to threads
  - # incoming deps
  - Computations + fulfill deps
- 2. Communications using AMs
  - Send data + fulfill deps
- 3. Seed + join



/\*\* Initialize structures \*\*/ Communicator comm(MPI\_COMM\_WORLD); Threadpool tp(n\_threads, &comm); Taskflow<int> tf(&tp): /\*\* Create active message \*\*/ am = comm.make\_active\_msg( [&](int d, int k, payload pk) { data[k] = pk;tf.fulfill\_promise(d); }): /\*\* Define Taskflow \*\*/ tf.set\_mapping(mapping) .set\_indegree(n\_deps) .set\_run([&](int k) { compute(k); for (auto d : deps(k)) { int dest = task\_2\_rank(d); if (dest == my\_rank) { tf.fulfill\_promise(d); } else { am->send(dest, d, k, data[k])  $\left( \left\{ \right\} \right)$ /\*\* Start initial tasks \*\*/ for (auto k : initial\_tasks) tf.fulfill\_promise(k); /\*\* Wait for completion \*\*/ tp.join();

#### Detecting completion is non-trivial



#### So what is "completion"?



#### Detecting completion is done in two stages



#### No AM can cross the "envelope" $\Rightarrow$ Idle forever



### Properties of the completion algorithm

Theorem 1:

If the user creates a finite number of messages, the algorithm uses a finite number of messages

 $\Rightarrow$  Finishes even if MPI is unfair

Theorem 2:

The algorithm terminates if and only if completion is reached

 $\Rightarrow$  Correct

#### Benchmarks

We compare

- TaskTorrent
- StarPU (STF)
- Intel ScaLAPACK (MPI + OpenMP)

We show that

- 1. Runtimes outperform bulk-synchronous (ScaLAPACK)
- 2. TTOR (PTG) is competitive with other SOTA runtimes (StarPU, STF)
- 3. TTOR is easy to use
- 4. PTG scales better than STF when tasks are small

### Distributed GEMM

Strong and weak scalings



Block  $\mapsto$  node mapping

$$C_{ij} = \sum_{k} A_{ik} B_{kj}$$

gemm\_Cikj.set\_task([&](int3 ikj){ int i = ikj[0];int k = ikj[1];int i = iki[2]; C\_ij[i + j \* num\_blocks].noalias() +=  $A_ij[i + k * num_blocks] *$  $B_ij\bar{k} + j * num_blocks];$ if(k < num\_blocks-1) {</pre> gemm\_Cikj.fulfill\_promise({i,k+1,j}); } }).set\_indegree([&](int3 ikj) { return (ikj[1] == 0 ? 2 : 3); }).set\_mapping([&](int3 ikj) { return (ikj[0] / nprows + ikj[2] / npcols \* (num\_blocks / nprows)) % n\_threads; });



#### Distributed dense Cholesky

Strong and weak scalings







max block size / average block size

Load balancing test Various average block sizes N=65k, 1024 CPUs

#### Conclusion

- TTOR combines PTG + AMs
- Its design makes it
  - Lightweight, minimal overhead, parallel DAG exploration
  - Easy to use and integrate into an existing code
  - Good out-of-the-box performances

https://github.com/leopoldcambier/tasktorrent

# Task-based distributed spaND

With TaskTorrent

### spaND sparsification is usually sequential

For level k = 1, ..., L

- Eliminate interiors
- Scale interfaces
- Sparsify interfaces

Compute  $Q_p$  (depends on  $A_{pn}$ ,  $A_{np}$  for all n) Update  $A_{nc} \leftarrow A_{np}Q_{pc}$ ,  $A_{pc} \leftarrow Q_{pc}^T A_{pn}$ 



#### Simultaneous sparsification is more concurrent...

For level k = 1, ..., L

- Eliminate interiors
- Scale interfaces
- Sparsify interfaces

For all p, compute  $Q_p$  (w/ original  $A_{pn}$ ,  $A_{np}$ ) Update  $A_{ij}^+ = Q_{ic}^T A_{ij} Q_{jc}$ 



- More concurrent
- More flops
- Less accurate ?



#### ... and as accurate

Sequential sparsification



#### Simultaneous sparsification





#### How to express the DAG?

- 1 block operation  $\Leftrightarrow$  1 task
- Granularity = interfaces
- Level-per-level DAGs

Rank revealing QR...



- Inputs: scaled  $(A_{pn}, A_{np})$  from block scaling
- Task: RRQR,  $Q_p = \text{RRQR}(\begin{bmatrix} A_{pn} & A_{np}^T \end{bmatrix})$
- Output: sends  $Q_p$ , triggers compressions  $Q_p^T A_{pq} Q_q$  and  $Q_q^T A_{qp} Q_p$

Per-level DAG is wide



### Still some limitations in 3D

Since Tasks  $\Leftrightarrow$  Block operation between interfaces







#### Ice-Sheet Ranks are (fairly) uniform throughout the domain



Minimum = 22, Average = 98, Maximum = 350

#### Ice-Sheet: good weak scalings

cores	N		spa	AMG (Hypre)			
		t <sub>fact</sub>	t <sub>app</sub>	n <sub>cg</sub>	t <sub>total</sub>	n <sub>cg</sub>	t <sub>total</sub>
36	1M	6.2	0.14	6	7.1	427	15
144	4M	7.3	0.15	6	8.5	456	16
576	18M	8.9	0.15	7	10.5	527	22
2304	74M	9.8	0.17	8	11.7	627	29
9216	296M	13.2	0.21	12	16.9	623	39

Weak scalings. 36 cores (N=1M) to 9216 cores (N=296M).  $\varepsilon = 10^{-2}$ . CG stops at  $10^{-8}$ . Hypre using Boomer AMG. On Quartz (LLNL) TTOR DAG Eliminations Block scalings Sparsification

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#### spaND in SU2: the NACA airfoil



Ranks from 40 to 296 Strong directionality in the ranks Inviscid flow around a wing Euler equations



SU2: Economon, T. D., Palacios, F., Copeland, S. R., Lukaczyk, T. W., & Alonso, J. J. (2016). SU2: An open-source suite for multiphysics simulation and design. *AIAA Journal*, *54*(3), 828-846. Thanks to Zan Xu and Juan Alonso

#### Some difficulties with irregular ranks

Matrix size (cores)



Weak scalings. 8 cores (N = 250k) to 2048 cores (N = 67M).

 $\varepsilon = 10^{-3}$ . GMRES stops at  $10^{-3}$ . Newton stops at  $10^{-14}$ . On Armstrong (Stanford HPCC)

# Conclusion and perspectives

#### Hierarchical solvers are versatile

spaND

- Can be used on many matrices
- For most problems, complexity is about  $O(N \log N)$
- Guaranteed to work on SPD
- More studies on unsymmetric problems are needed
- Full, general 3D task-based parallel require distributed RRQRs or other sparsification approach

#### Task-based runtimes have to be easy to use

- Runtime systems need to be easy to use for adoption
- A simple approach like TTOR scales well in practice
- It is easy to combine with block algorithms such as spaND and leads to excellent performances

#### References

#### • spaND

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#### Thank you for attending!

Now is a great time to ask questions