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Sparse supernodal solver with low-rank compression for solving the frequency-domain Maxwell equations discretized by a high order HDG method

November 20th, 2017 - JJC

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Introduction

PaStiX: Sparse Direct Solver

- Originally designed for distributed heterogeneous architectures
- Recent works introduced low-rank compression to reduce the burden on time and memory complexities

HORSE: HDG solver

- Solve a reduced system on faces instead of elements
- Lead to a sparse system smaller than the one using CG or DG
- Domain-Decomposition is then used
- Use a sparse direct solver on each subdomain

Objective for this talk: evaluate the impact of using low-rank compression to enhance subdomains' factorization in HORSE.

Outline

1. Background on Sparse Direct Solvers
2. Block Low-Rank Operations
3. Numerical Experiments
4. Case study: PASTIX inside a HDG method

1

Background on Sparse Direct Solvers

PaStiX: a sparse direct solver

Current sparse direct solvers for 3D problems

- $\Theta(n^2)$ time complexity
- $\Theta(n^{\frac{4}{3}})$ memory complexity
- BLAS 3 operations: efficient operations

Block Low-Rank solver

- In many applications, the machine precision is not required
- **Minimal Memory** strategy allows to save memory
- **Just-In-Time** strategy allows to reduce time-to-solution

Objective: build an algebraic low-rank solver following the supernodal approach of PASTIX, with block-data structures

Sparse Direct Solvers approach

Problem: solve $Ax = b$

- Cholesky: factorize $A = LL^t$ (symmetric pattern ($A + A^t$) for LU)
- Solve $Ly = b$
- Solve $L^t x = y$

PaStiX steps

1. Order unknowns to minimize the fill-in
2. Compute a symbolic factorization to build L structure
3. Factorize the matrix in place on L structure
4. Solve the system with forward and backward triangular solves

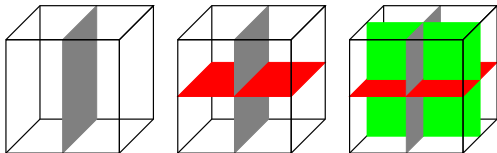
Ordering with Nested Dissection

Entry graph $G = (V, E, \sigma_p)$

V : vertices, E : edges, σ_p : unknowns permutation

Algorithm to compute σ_p

1. Partition $V = A \cup B \cup C$
2. Order C with larger numbers: $V_A < V_C$ and $V_B < V_C$
3. Apply the process recursively on A and B



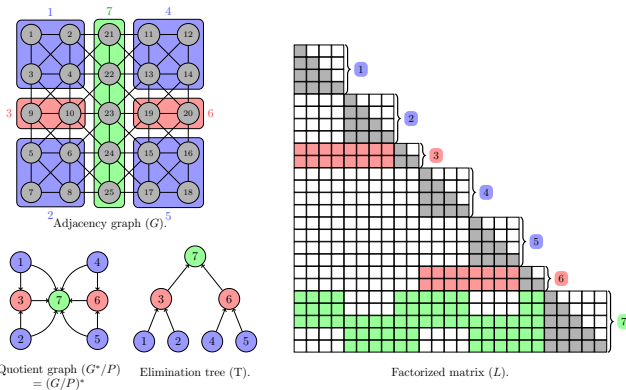
Three-levels of nested dissection on a regular cube.

Metis and Scotch are mostly used to perform this partitioning.

Symbolic Factorization

General approach

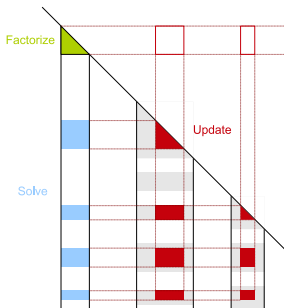
1. Build a partition with the nested dissection process
2. Compress information on data blocks
3. Compute the block elimination tree using the block quotient graph



Numerical Factorization

Algorithm to eliminate the column block k

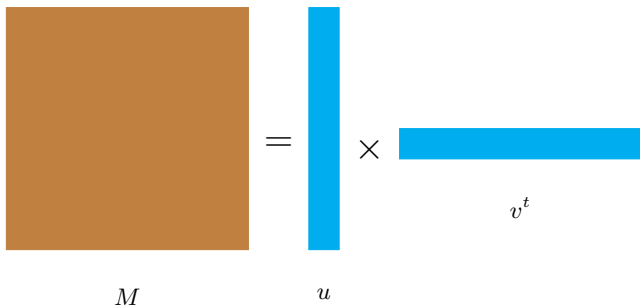
1. **Factorize** the diagonal block (POTRF/GETRF)
2. **Solve** off-diagonal blocks in the current column (TRSM)
3. **Update** the trailing matrix with the column's contribution (GEMM)



2

Block Low-Rank Operations

Low-Rank Compression

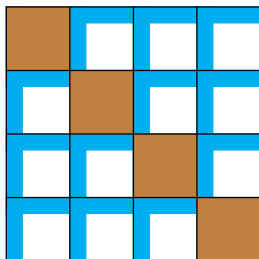


$$M \in \mathbb{R}^{n \times n}; u, v \in \mathbb{R}^{n \times r}$$

Memory Consumption reduced: $2nr$ instead of n^2
Several methods can be used: SVD, RRQR, BDLR, ACA...

The objective is to compute \hat{A} such that $\|A - \hat{A}\|_2 < \tau$

Block Low-Rank Compression for a dense matrix



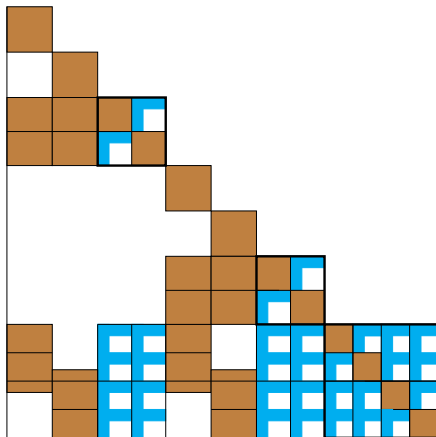
■ Full Rank

■ Low Rank

Some related works for dense matrices

- LSTC
- Airbus (hmat-oss)
- CEA

Block Low-Rank Compression – Symbolic Factorization



Large off-diagonal are low-rank, in the form uv^t

Some Related Works

Sparse Block Low-Rank solver: BLR-MUMPS

- They introduced an approach to reduce the time-to-solution
- The main difference is the difference between multifrontal and supernodal

Some other approaches for sparse

- Strumpack HSS by Ghysels et al. uses randomized sampling to perform an efficient extend-add
- HODLR by Darve et al. uses pre-selection of rows and columns (BDLR)
- \mathcal{H} -LU by Hackbusch et al. does not fully exploit the symbolic factorization
- HODLR/HSS like method by Chadwick et al. uses estimation of ranks and the geometry of the problem

Block Low-Rank Algorithm

Approach

- Large supernodes are partitioned into a set of smaller supernodes
- Large off-diagonal blocks are represented as low-rank blocks

Operations

- Diagonal blocks are dense
- TRSM are performed on low-rank off-diagonal blocks
- GEMM are performed between low-rank off-diagonal blocks. It creates contributions to dense or low-rank blocks: this is the extend-add problem

Compression techniques

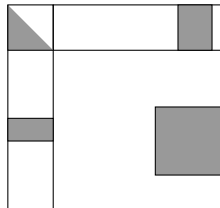
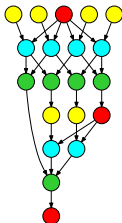
- SVD, RRQR for now
- Possible extension to any algebraic method: ACA, randomized techniques...

Strategy Just-In-Time

Compress L

1. Eliminate each column block
 - 1.1 Factorize the dense diagonal block
Compress off-diagonal blocks belonging to the supernode
 - 1.2 Apply a TRSM on LR blocks (cheaper)
 - 1.3 LR update on dense matrices (**LR2GE** extend-add)
2. Solve triangular systems with low-rank blocks

Yellow	Compression
Red	GETRF (Facto)
Cyan	TRSM (Solve)
Purple	LR2LR (Update)
Green	LR2GE (Update)

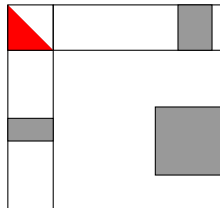
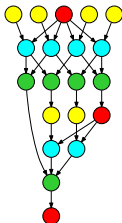


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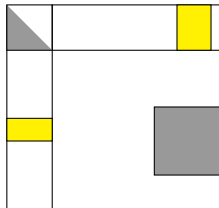
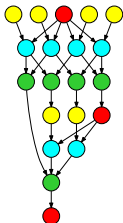


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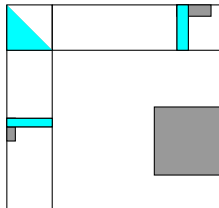
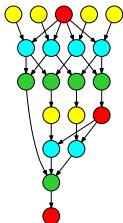


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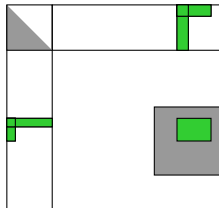
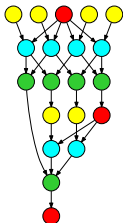


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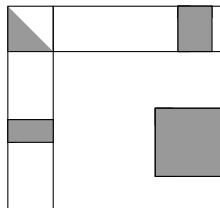
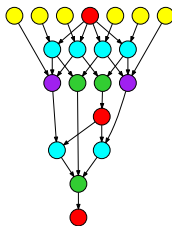


Strategy Minimal Memory

Compress A

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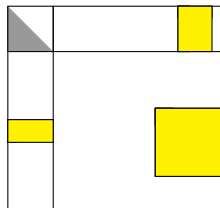
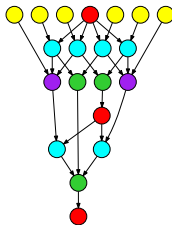


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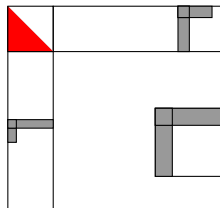
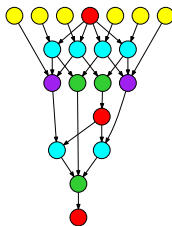


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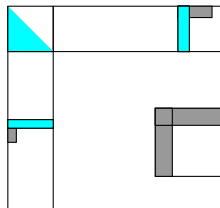
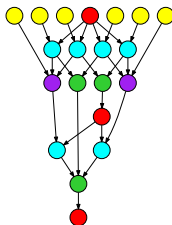


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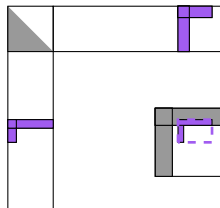
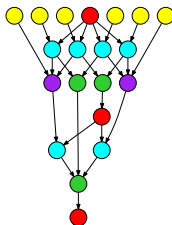


Strategy Minimal Memory

Compress A

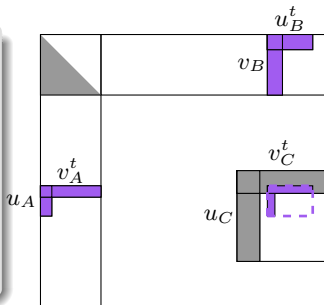
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Focus on the LR2LR kernel: build the $u_{AB}v_{AB}^t$ contribution

- Update of C with contribution from blocks A and B
- The low-rank matrix $u_{AB}v_{AB}^t$ is added to $u_C v_C^t$
- $u_{AB}v_{AB}^t = (u_A(v_A^t v_B))u_B^t$ or $u_{AB}v_{AB}^t = u_A((v_A^t v_B)u_B^t)$
- Eventually, recompression of $(v_A^t v_B)$



Focus on the LR2LR kernel: add the contribution into $u_C v_C^t$

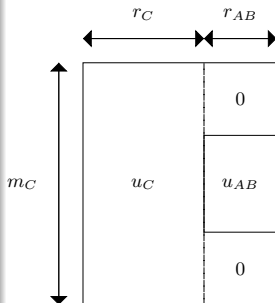
A low-rank structure $u_C v_C^t$ receives a low-rank contribution $u_{AB} v_{AB}^t$.

Algorithm

$$A = u_C v_C^t + u_{AB} v_{AB}^t = ([u_C, u_{AB}]) \times ([v_C, v_{AB}])^t$$

- QR: $[u_C, u_{AB}] = Q_1 R_1 \quad \Theta(m(r_C + r_{AB})^2)$
- QR: $[v_C, v_{AB}] = Q_2 R_2 \quad \Theta(n(r_C + r_{AB})^2)$
- SVD: $R_1 R_2^t = u \sigma v^t \quad \Theta((r_C + r_{AB})^3)$

$$A = (Q_1 u \sigma) \times (Q_2 v)^t$$



Optimizations using RRQR to reduce complexity to $\Theta(n(r_C + r_{AB})r_C^*)$

Comparison of both strategies

Memory consumption

- **Minimal Memory** strategy really saves memory
- **Just-In-Time** strategy reduces the size of L' factors, but supernodes are allocated dense at the beginning: no gain in pure **right-looking**

Low-Rank extend-add

- **Minimal Memory** strategy requires expensive extend-add algorithms to update (recompress) low-rank structures with the **LR2LR** kernel
- **Just-In-Time** strategy continues to apply dense update at a smaller cost through the **LR2GE** kernel

3

Numerical Experiments

Experimental setup

Machine: 2 INTEL Xeon E5 – 2680v3 at 2.50 GHz

- 128 GB
- 24 cores

3D Matrices from The SuiteSparse Matrix Collection

- **Audi**: structural problem (943 695 DoFs)
- **Atmosmodj**: atmospheric model (1 270 432 DoFs)
- **Geo1438**: geomechanical model of earth (1 437 960 DoFs)
- **Hook**: model of a steel hook (1 498 023 DoFs)
- **Serena**: gas reservoir simulation (1 391 349 DoFs)
- + Laplacian: Poisson problem (7-points stencil)

Parallelism is obtained with PASTIX static scheduling for multi-threaded architectures

Parameters

Entry parameters

- Tolerance τ : absolute parameter (normalized for each block)
- Compression method: SVD or RRQR
- Compression strategy: **Minimal Memory** or **Just-In-Time**
- Blocking sizes: between 128 and 256 in following experiments
- Compression sizes: 128 for width and 20 for height

Strategy **Minimal Memory**

- Blocks are compressed at the beginning
- Each contribution implies a recompression

Strategy **Just-In-Time**

- Blocks are compressed just before a supernode is eliminated
- Those blocks are never uncompressed

Costs distribution on the Atmosmodj matrix with $\tau = 10^{-8}$

	Complete	Just-In-Time	Minimal Memory
		RRQR	RRQR
Factorization time (s)			
Compression	-	3.4e+01	5.6+00
Block factorization (GETRF)	7.2e-01	7.3e-01	7.6e-01
Panel solve (TRSM)	1.7e+01	7.4e+00	7.9e+00
Update			
Formation of contribution	-	-	4.2e+01
Addition of contribution	-	-	7.3e+02
Dense update (GEMM)	4.6e+02	9.7e+01	2.4e+01
Total	4.7e+02	1.4e+02	8.1e+02
Solve time (s)	6.3e+00	3.0e+00	3.2e+00
Factors final size (GB)	16.3	7.49	7.31
Memory peak (GB)	16.3	16.3	7.31

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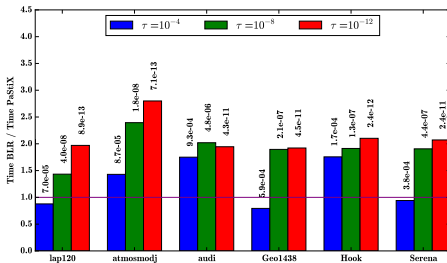
Costs distribution on the Atmosmodj matrix with $\tau = 10^{-8}$

	Complete	Just-In-Time	Minimal Memory
		RRQR	RRQR
Factorization time (s)			
Compression	-	3.4e+01	5.6+00
Block factorization (GETRF)	7.2e-01	7.3e-01	7.6e-01
Panel solve (TRSM)	1.7e+01	7.4e+00	7.9e+00
Update			
Formation of contribution	-	-	4.2e+01
Addition of contribution	-	-	7.3e+02
Dense update (GEMM)	4.6e+02	9.7e+01	2.4e+01
Total	4.7e+02	1.4e+02	8.1e+02
Solve time (s)	6.3e+00	3.0e+00	3.2e+00
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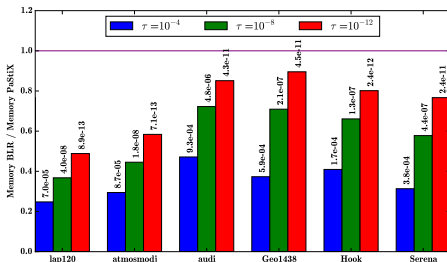
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Behaviour of RRQR/Minimal Memory

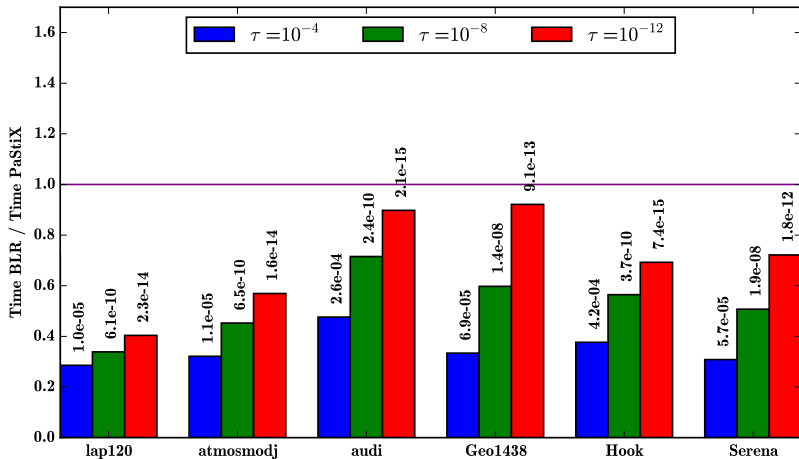


Performance

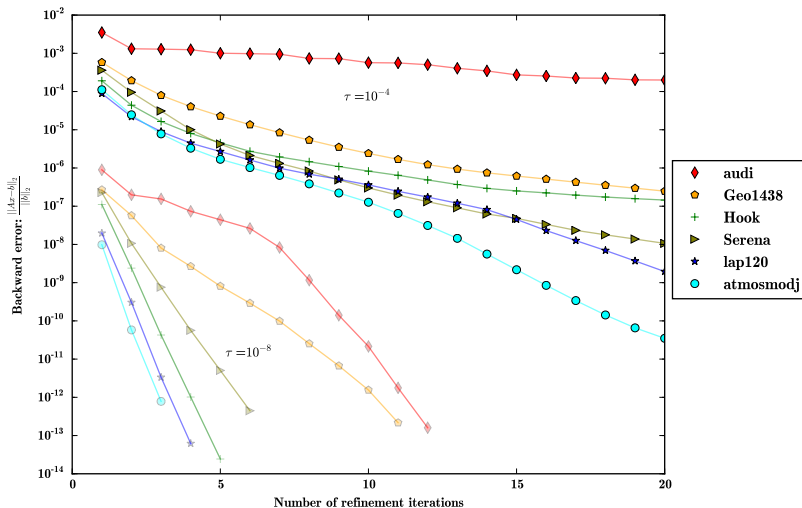


Memory footprint

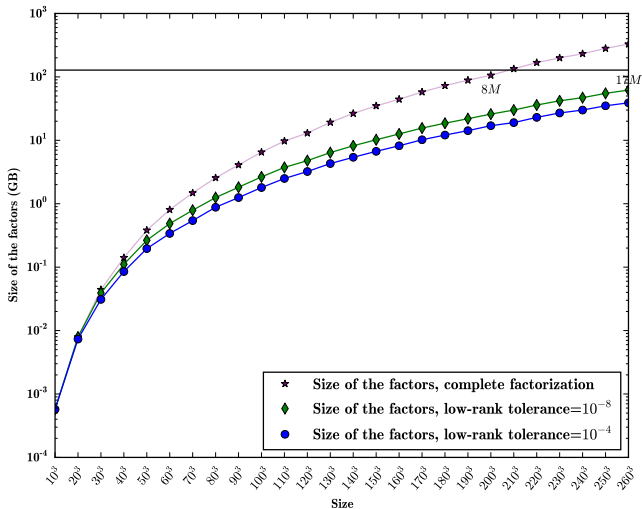
Performance of RRQR/Just-In-Time



Convergence of RRQR/Minimal Memory



Scaling on Laplacians: size of the factors using RRQR/Minimal Memory



4

Case study: PASTIX inside a HDG method

HORSE

Method

- Introduce an hybrid variable to solve a system smaller than the one obtained through DG
- Perform Domain-Decomposition to solve this system
- Use a direct solver for subdomains

Solve 3D frequency-domain Maxwell's equations

- $i\omega\epsilon_r \mathbf{E} - \mathbf{curl} \mathbf{H} = -\mathbf{J}$, in Ω
- $i\omega\mu_r \mathbf{H} + \mathbf{curl} \mathbf{E} = 0$, in Ω
- $\mathbf{n} \times \mathbf{E} = 0$, on Γ_m
- $\mathbf{n} \times \mathbf{E} + \mathbf{n} \times (\mathbf{n} \times \mathbf{H}) = \mathbf{n} \times \mathbf{E}^{inc} + \mathbf{n} \times (\mathbf{n} \times \mathbf{H}^{inc})$, on Γ_a

The challenge with DG for frequency-domain problems

Classical DG formulation

- Naturally adapted to heterogeneous media and discontinuous solutions
- Can easily deal with unstructured, possibly non-conforming meshes (h -adaptivity)
- High order with compact stencils and non-conforming approximations (p -adaptivity)
- Usually rely on polynomial interpolation but can also accommodate alternative functions (e.g. plane waves)
- Well-suited for efficient parallelization
- But leads to larger problems compared to continuous finite element methods

Hybridizable DG method in 3D

Principles of a HDG formulation

- Keep the advantages of classical DG methods
- Introduce an hybrid variable to decouple local problems defined at the element level
- Solve a reduced linear system for the hybrid variable unknowns only

Complexity: number of globally coupled degrees of freedom

- Classical DG method with \mathbb{P}_p interpolation

$$(p + 1)(p + 2)(p + 3)N_e \quad , \quad N_e \text{ is the \# of elements}$$

- HDG method with \mathbb{P}_p interpolation

$$(p + 1)(p + 2)N_f \quad , \quad N_f \text{ is the \# of faces}$$

- Continuous finite element formulation based on Nedelec's first family of face/edge elements in a simplex (tetrahedron): $\frac{p(p + 2)(p + 3)}{2} N_e$

Hybridizable DG method in 3D

ANR TECSER project (May 2014 - April 2017)

Funded by DGA (French armament procurement agency)

<http://www-sop.inria.fr/nachos/projects/tecseser>

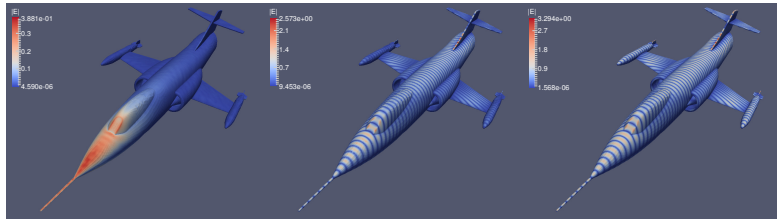
- Implementation of HDG for arbitrary high order interpolation
- Local definition (element-wise and face-wise) of the interpolation degree
- Extension of the formulation to a non-conforming hybrid hexahedral/tetrahedral mesh
- Scalability improvement
PDE-based Schwartz domain decomposition algorithm
PaStiX as a local (subdomain) solver
- Coupling with a BEM for an accurate treatment of far field radiation
- HORSE software
High Order solver for Radar cross Section Evaluation

Hybridizable DG method in 3D

Scattering of a plane wave by a jet

- Unstructured tetrahedral mesh: 1,645,874 elements / 3,521,251 faces
- Frequency: 600 MHz, Wavelength: $\lambda \simeq 0.5$ m, Penalty parameter: $\tau = 1$

HDG method	# DoF Λ field	# DoF EM field
HDG- \mathbb{P}_1	21,127,506	39,500,976
HDG- \mathbb{P}_2	42,255,012	98,752,440
HDG- \mathbb{P}_3	70,425,020	197,504,880



Contour line of $|E|$ - HDG- \mathbb{P}_1 to HDG- \mathbb{P}_3

Practical example

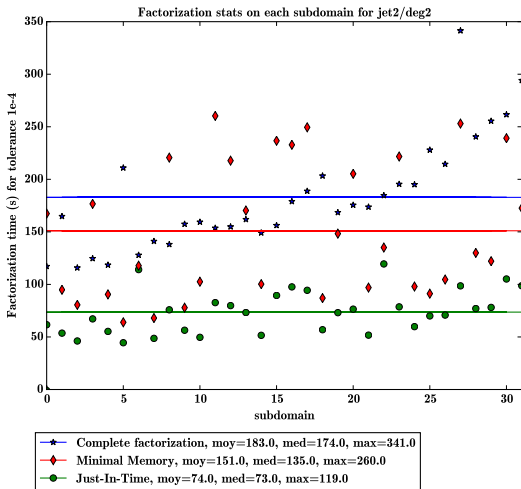
Study case

- Jet with \mathbb{P}_2 interpolation
- 42 255 012 unknowns for Λ
- A single factorization is performed on each subdomain
- There may be several solves for iterative refinement between subdomains

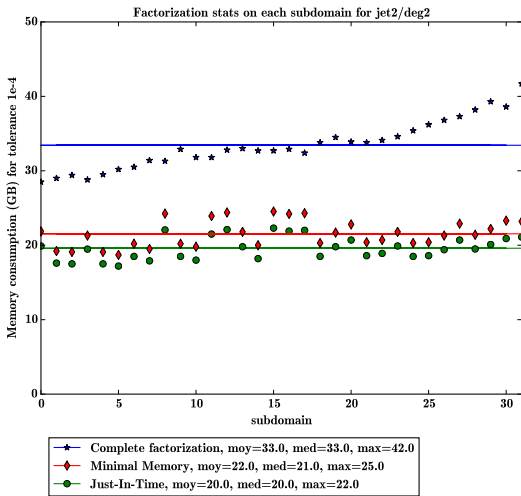
Machine

- Occigen: 24-cores nodes with 128 GB
- Each MPI process is hold on a socket with 12 cores
- In next experiments, we use 32, 48 or 64 subdomains
- Subdomains are ordered accordingly to the number of operations for the complete factorization

Factorization on each subdomain – 32 processes with $\tau = 1e-4$



Memory Consumption on each subdomain – 32 processes with $\tau = 1e-4$



Impact on HORSE

Subs	τ	Method	Fact(s)	Nb. of iters	Refinement (s)	HDGM (s)	Memory (GB)
32	-	Complete-Factorization	526.0	9	254.5	814.0	41.7
	1e-4	Just-In-Time	209.3	9	164.8	405.8	41.7 (22.3)
		Minimal-Memory	516.7	15	273.2	822.0	24.5
	1e-8	Just-In-Time	325.2	9	192.9	550.4	41.7 (29.4)
		Minimal-Memory	600.1	9	193.2	825.8	30.5
48	-	Complete-Factorization	237.3	8	118.6	374.6	24.9
	1e-4	Just-In-Time	112.2	9	106.1	237.1	24.9 (14.1)
		Minimal-Memory	229.3	13	159.7	407.5	15.3
	1e-8	Just-In-Time	171.5	8	105.8	296.1	24.9 (18.1)
		Minimal-Memory	319.4	8	109.8	447.9	18.8
64	-	Complete-Factorization	179.8	9	104.7	298.3	17.4
	1e-4	Just-In-Time	79.7	10	91.1	184.1	17.4 (10.0)
		Minimal-Memory	138.1	13	120.7	272.2	11.0
	1e-8	Just-In-Time	124.6	9	90.0	228.2	17.4 (12.9)
		Minimal-Memory	239.2	9	91.5	344.5	13.7

Conclusion

Block Low-Rank solver

- Exploits the symbolic structure
- Demonstrate the extend-add issues in a supernodal context
- The version presented follows the parallelism of PaStiX
- On-going work to implement efficiently this approach over runtime systems

PaStiX in HORSE

- Low-rank compression is useful to reduce memory footprint and/or time-to-solution
- Future work: study load imbalance between subdomains
- Future work: impact with $\mathbb{P}_3/\mathbb{P}_4$ interpolation

PASTIX 6.0.0alpha is now available!

<http://gitlab.inria.fr/solverstack/pastix>

- Support shared memory with different schedulers:
 - ▶ sequential
 - ▶ static scheduler
 - ▶ PaRSEC runtime system
- Low-rank support
- Cholesky and LU factorizations

Thank you.