Parallel Fast Direct Solver: $\mathcal{H}$-Matrix. Applications to Uncertainty Management

HPC and Uncertainty Treatment

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Outline

Introduction

Several applications in Statistics lead to large, dense matrices :

- Kriging
- PCA, *etc.*
- Applications using large covariance matrices

Kriging

- Symmetric Positive Definite (SPD) matrix
- Many solves
- Usually,
  - Cholesky decomposition $M = LL^T$
  - Forward - Backward substitutions

Kriging

In a nutshell

Let $Z : \mathbb{R}^d \to \mathbb{R}$ be some ramdom process, stationnary of order 2.
We have N observation points $\{x_i \in \mathbb{R}^d | i = 1, \ldots, N\}$ with values $Z(x_i)$.
Let us assume that the covariance of these points is known and given by a matrix $K \in \mathbb{R}^{N \times N}$, with

$$K_{ij} = Cov(Z(x_i), Z(x_j))$$

An estimation of the mean trajectory is a linear interpolation $\tilde{Z}(x_0)$ of Z at $x_0 \in \mathbb{R}^d$:

$$\tilde{Z}(x_0) = \sum_{i=1}^{N} \alpha_i(x_0) Z(x_i)$$

The weights α_i are solution of

$$\boxed{K\alpha = K_0}$$

with

$$(K_0)_i := Cov(Z(x_i), Z(x_0))$$

Kriging

Writing the systems

- K is SPD (covariance matrix)
- Quite often, K isn't known
  - Modelled as a convolution matrix of a kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to R_+$:

$$K_{ij} := k(x_i, x_j)$$

  - What is k ?
    - Gaussian :

$$k(x, y) = e^{-|x-y|^2/(2\lambda^2)}$$

    - Exponential :

$$k(x, y) = e^{-|x-y|/\lambda}$$

    - Quadratic :

$$k(x, y) = \left(1 + \frac{|x-y|}{2\lambda}\right)^{-2}$$

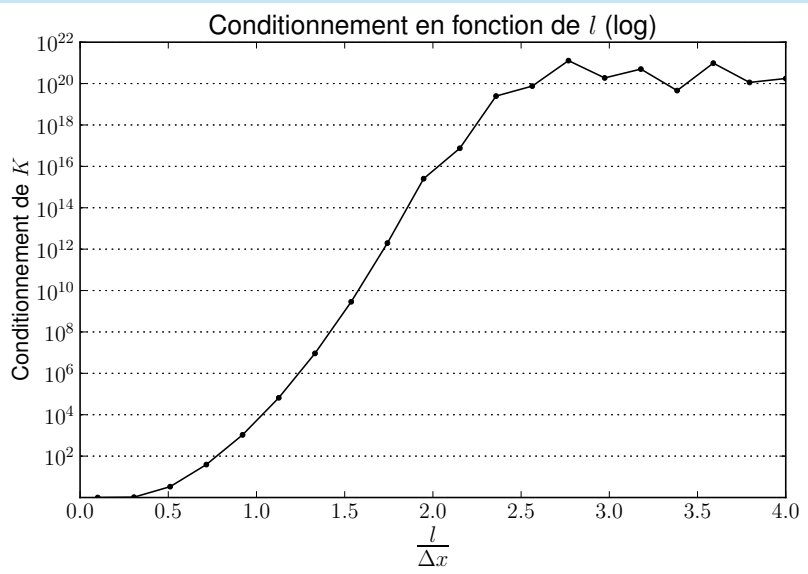
- N can be large. For instance, every node in an FEM discretization
- The interpolation is sought at many points x_0

Kriging

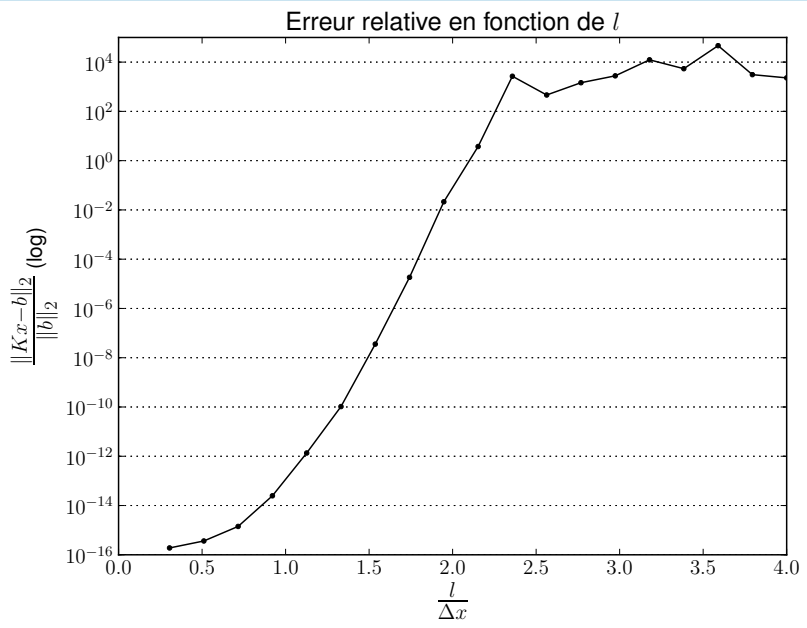
Solving the systems

- K is ill-conditionned [ABW94], many right-hand sides $\Rightarrow$ Direct Solver
- K is SPD $\Rightarrow$ Cholesky

Conditioning



: Condition number



: Relative Error

FIGURE: Condition number and error growth for a gaussian kernel.

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Kriging

Solving the systems

Complexity

- Cholesky Decomposition
  `DPOTRF` $1/3N^3 + 1/2N^2 + 1/6N$ [BD99]
- Solving
  `DPOTRS` $N_{rhs} \times 2N^2$
- Storage : $8N^2/2$

Need of a **fast direct solver** : $\mathcal{H}$-Matrix

Outline

$\mathcal{H}$-Matrices

Broadly speaking,

- Adaptative data-sparse representation of dense matrices
- Hierarchical, adaptative and approximate representation
- Broad range of operations on these compressed matrices (`GEMV`, `AXPY`, `GEMM`, *etc.*). More versatile than the FMM.

2 parts :

- Data-sparse representation of dense matrices
- Approximate operations (*eg* matrix-matrix multiplication) that preserve this representation

$\mathcal{H}$-Matrix

Literature

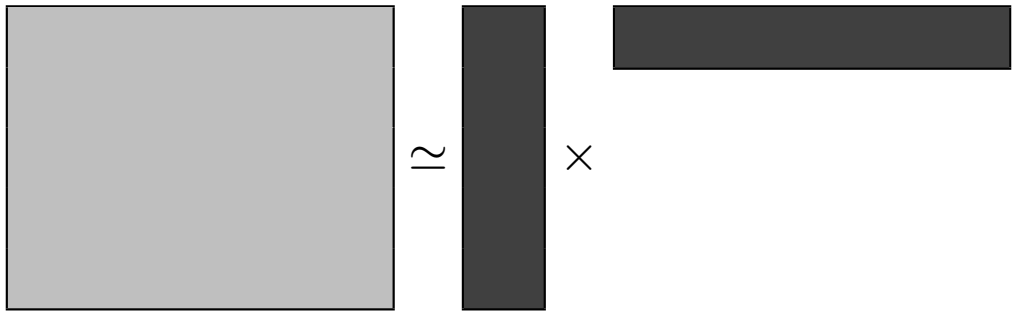
- Genesis in '99, extensions in the 2000s
  [Hac99, HK00, GH03, BGH03, BGH04]
- Several application domains : FEM (elliptical operators), BEM (laplacian, waves)
- Several implementations available
- Recently, $\mathcal{H}^2$-Matrix, close to the Fast Multipole Method

Low-rank approximation

- Hypothesis : it is possible to approximate a matrix by a low-rank one

$$M \simeq AB^T$$

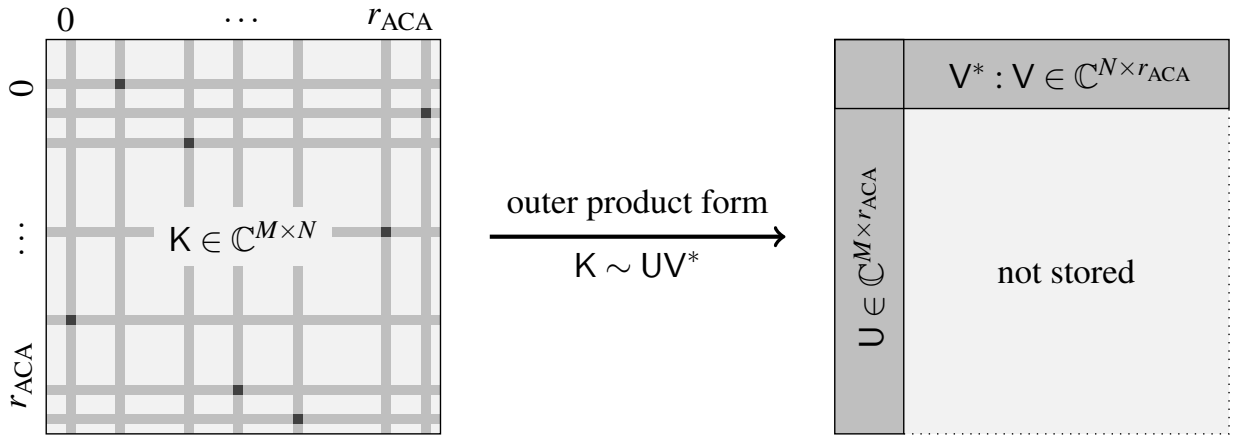
  - $M \in \mathbb{C}^{m \times n}$
  - $A \in \mathbb{C}^{m \times k}$
  - $B^T \in \mathbb{C}^{k \times n}$, $k < \min(m, n)$



Low-rank approximation

Several compression algorithms

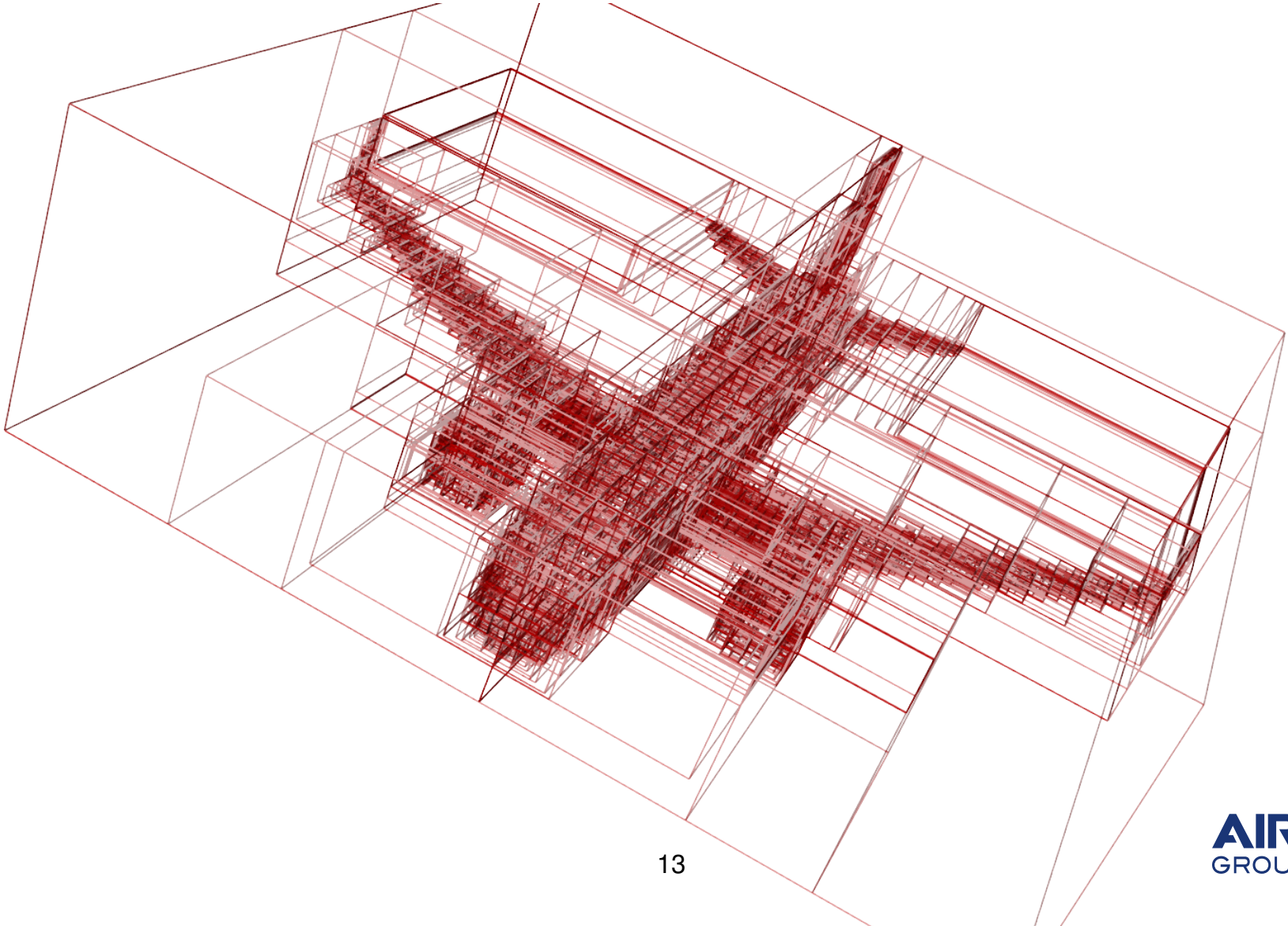
- SVD : $M = U\Sigma V$
  - $U \in \mathbb{C}^{m \times \min(m,n)}$
  - Σ diagonal matrix
  - $V \in \mathbb{C}^{\min(m,n) \times n}$
- Adaptative Cross Approximation (ACA) : Sequence or rank-1 approximations. Heuristics. [Beb11, BR03, Beb00]
  - « Full Pivoting »
  - « Partial Pivoting » (Figure : [Mes12])



Space Partitioning

- Spatial gathering of the degrees of freedom (bounding boxes)
- Binary Space Partitioning :
  - Halves the largest dimension of the bounding box
  - Halves the degrees of freedom in each box along the largest dimension
- Stopping criteria : DoFs in a leaf

A Picture is worth a thousand words



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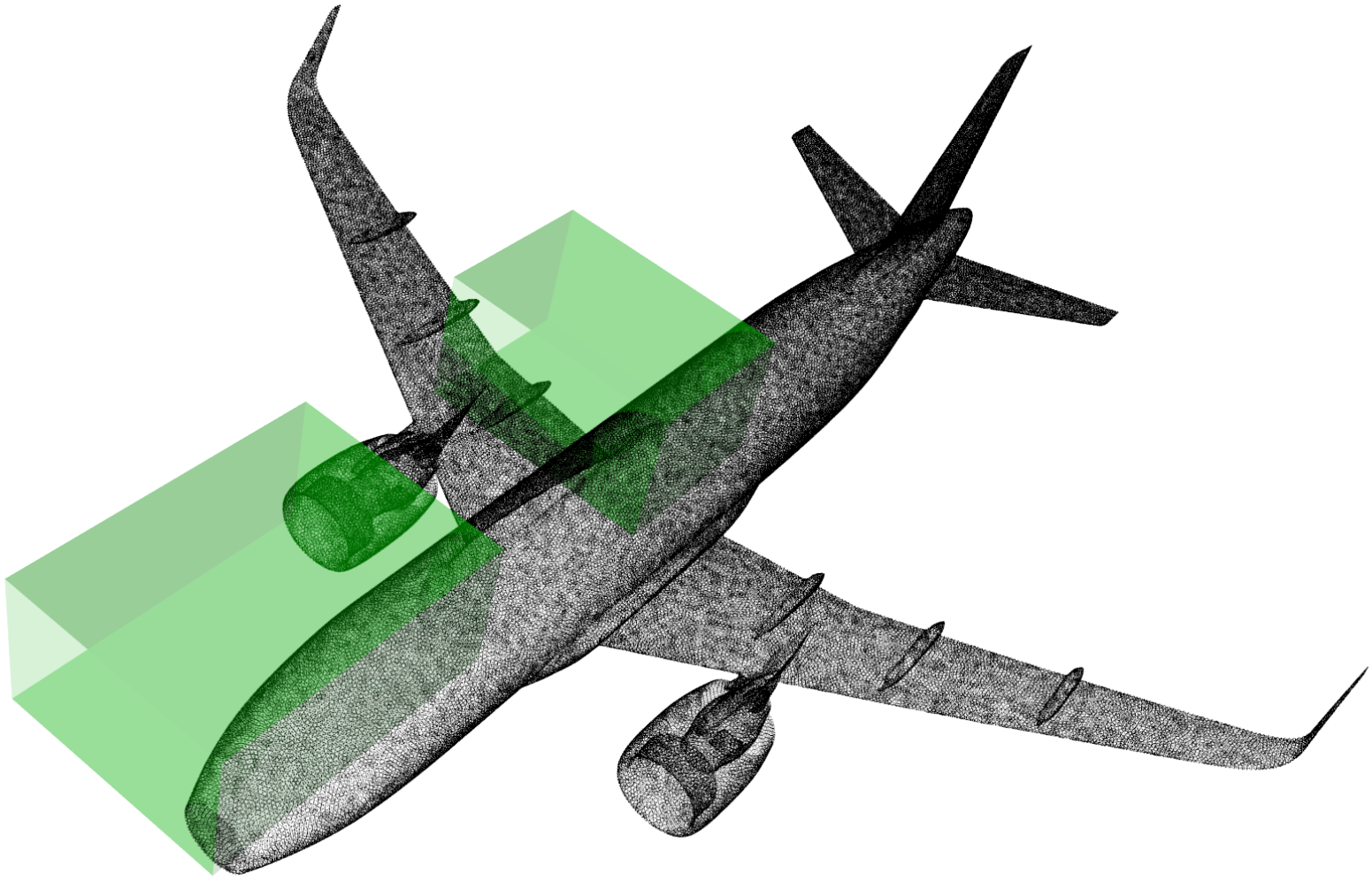

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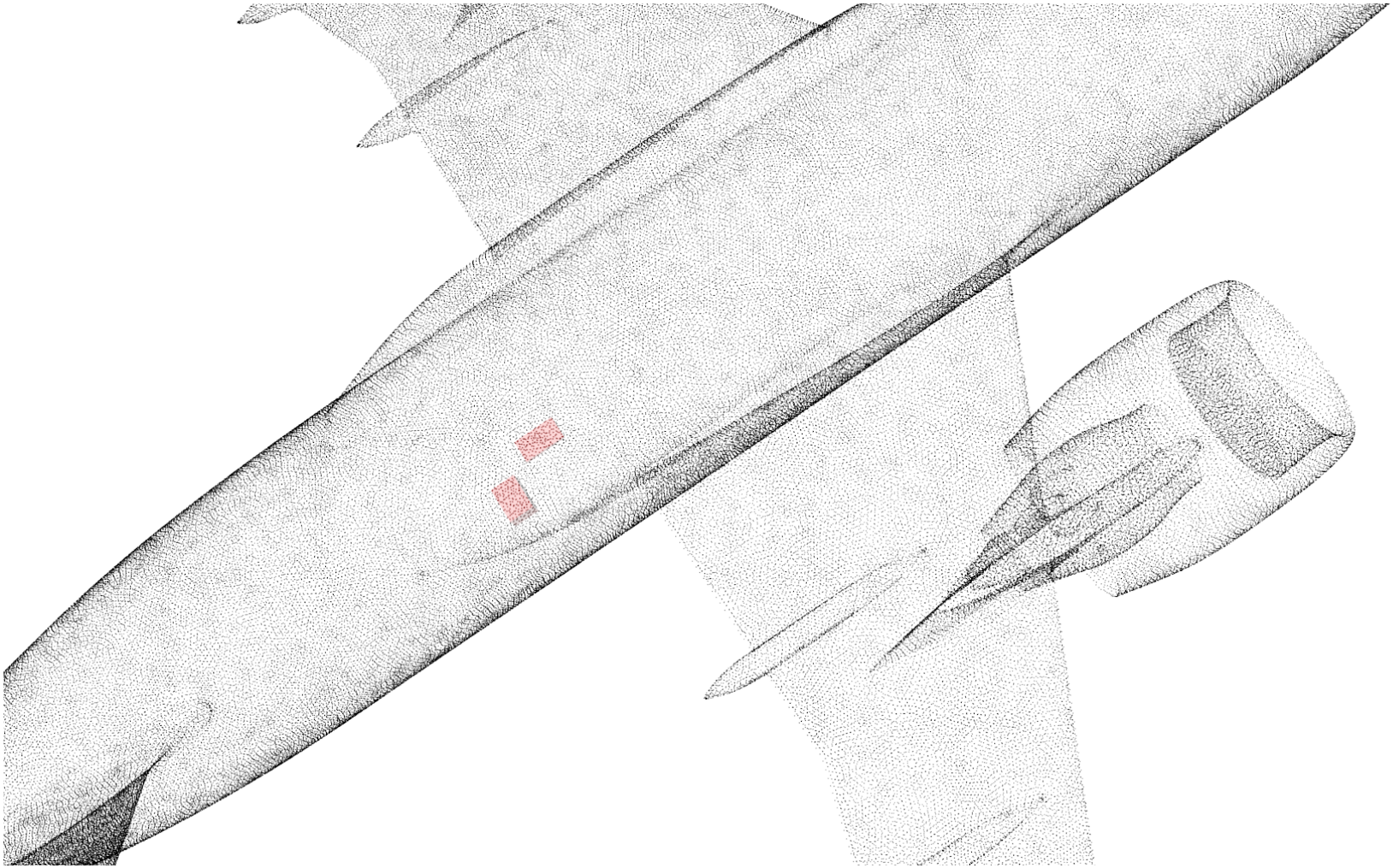

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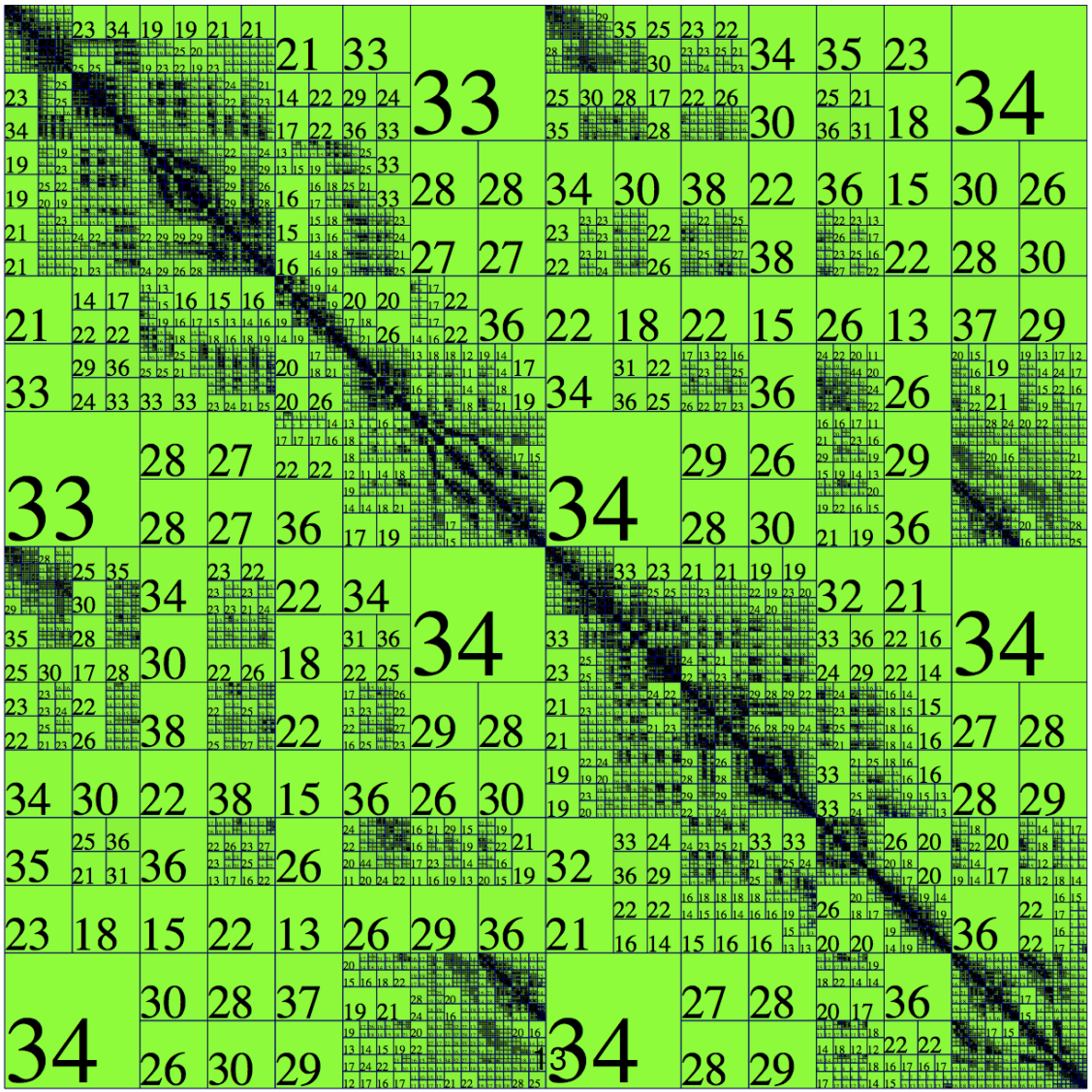

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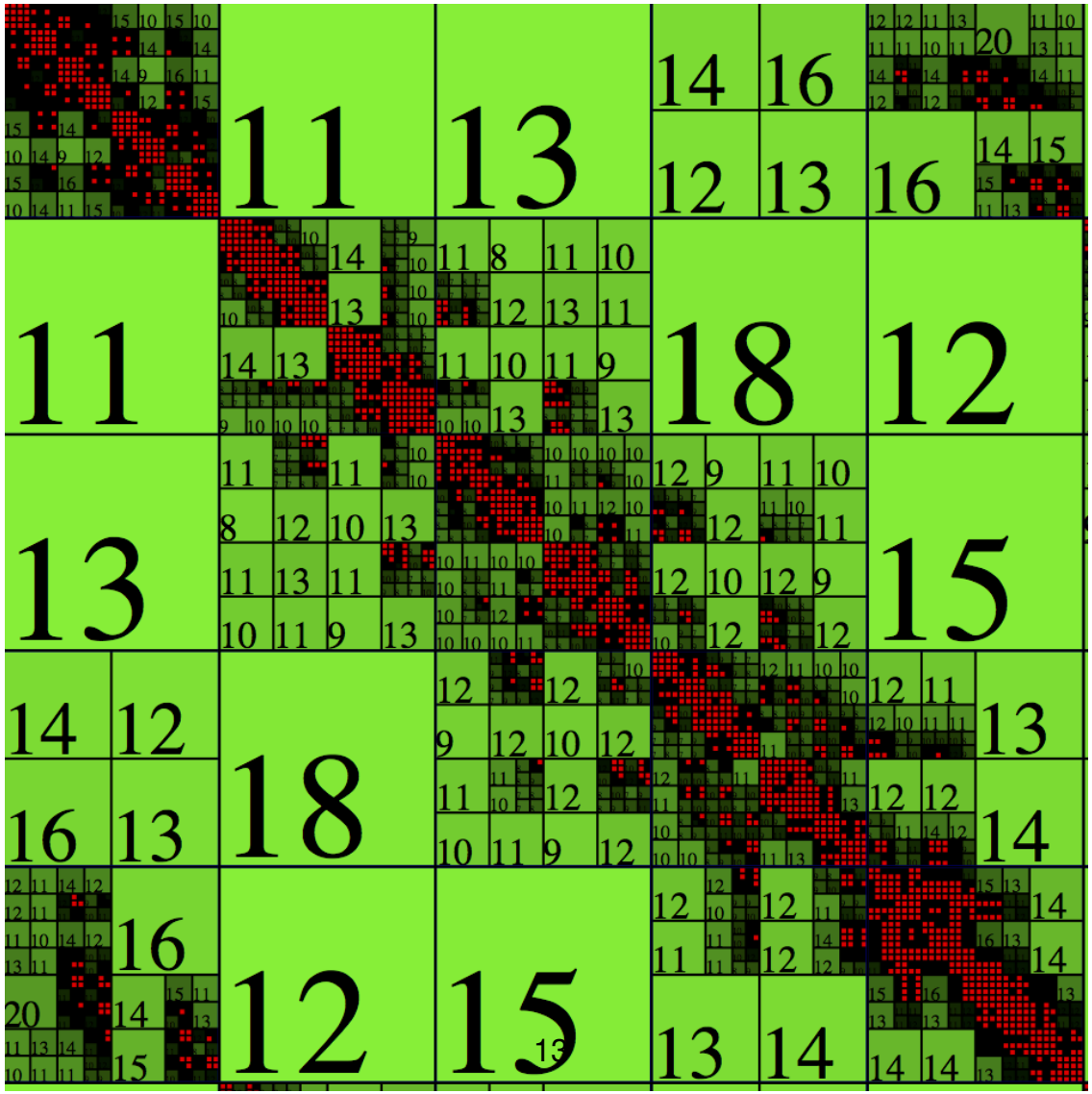

$\mathcal{H}$-Matrix

A $\mathcal{H}$-Matrix is a **quadtree** (with Binary Space Partitioning) :

- Internal nodes : subdivided $\mathcal{H}$-Matrix
- Leaves :
  - Admissible block : $\mathcal{R}k$-Matrix (green)
  - Non-admissible block : full block (red)

Remarks

- Only the leaves carry data
- Big admissible blocks ($10^4 \times 10^4+$)
- Small (and few) non-admissible blocks (100×100)

Operations

3 classes of operations :

$\mathcal{H}-$BLAS1 - $\mathcal{H}-$BLAS2 Assembly, `AXPY`, `GEMV`.
Simple. Operating only on the leaves (adaptative recompression for `AXPY`).

$\mathcal{H}-$BLAS3 `GEMM`, `TRSV`.
More involved. Operations at several levels of the same sub-tree. 27 cases for `GEMM`, 1 recursion case and 26 base cases, hierarchical conversion.

$\mathcal{H}-$LAPACK Inverse, LU, LDL^T.
Uses « BLAS » 2 et 3 operations, harder to implement in parallel.

Base operations

All the operations use BLAS/LAPACK.
Subroutines : SVD, QR, LU, `TRSV`, `GEMM`, `GEMV`

Matrix-Vector Product

GEMV

function VECTORPRODUCT(M, x, y, $\sigma \times \tau$)
  if IsLeaf($\sigma \times \tau$) **then**
    $y|_{\sigma\times\tau} \leftarrow M|_{\sigma\times\tau} x|_{\sigma\times\tau}$ ▷ Full or Compressed
  else
    for all $(\sigma', \tau') \in S(\sigma \times \tau)$ **do**
      VectorProduct(M, x, y, $\sigma' \times \tau'$)
    end for
  end if
end function

Addition

function ADD(M_1,M_2, $\sigma \times \tau$)
  if IsLeaf($\sigma \times \tau$) **then**
    $M_1|_{\sigma\times\tau} \leftarrow M_1|_{\sigma\times\tau} + M_2|_{\sigma\times\tau}$ ▷ Full or Compressed
  else
    for all $(\sigma', \tau') \in S(\sigma \times \tau)$ **do**
      Add(M_1, M_2, $\sigma' \times \tau'$)
    end for
  end if
end function

Remarks

- Adding two $\mathcal{R}k$-Matrices changes the rank (recompression) $\Rightarrow$ unknown final rank
- Costly operation

Multiplication

$$C \leftarrow AB + C$$

- Each operand (A, B, C) can be an internal node, compressed or full leaf
- 27 cases !
- In fact, guided by C structure.

Ideas :

- A, B, C internal nodes : recursive call
- C full leaf : convert A et B in full matrices
- A ou B full or compressed leaf : full or compressed product and recursive formatted add into C
- C compressed leaf : multiplication and hierarchical conversion

Multiplication

function GEMM(C, α, A, B, β, $\sigma \in \mathcal{T}_I$, $\tau \in \mathcal{T}_J$, $\rho \in \mathcal{T}_K$)
  if IsRoot(C) **then**
    $C \leftarrow \beta C$
  end if
  if $\neg$IsLeaf($\sigma \times \tau$) et $\neg$IsLeaf($\sigma \times \rho$) et $\neg$IsLeaf($\rho \times \tau$) **then**
    for all $\sigma' \in S(\sigma)$ **do**
      for all $\tau' \in S(\tau)$ **do**
        for all $\rho' \in S(\rho)$ **do**
          GEMM(C, α, A, B, 1, σ', τ', ρ')
        end for
      end for
    end for
  else
    $C|_{\sigma\times\tau} \leftarrow \alpha A|_{\sigma\times\rho} \cdot B|_{\rho\times\tau} + C|_{\sigma\times\tau}$ ▷ Base Case
  end if
end function

LU

function LUDECOMPOSITION(M)
  if ISLEAF(M) **then**
    $M \leftarrow LU$ ▷ M is full, use LAPACK
  else
    $M := \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}, L := \begin{pmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{pmatrix}, U := \begin{pmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{pmatrix}$
    LUDECOMPOSITION(M_{11}) ▷ $M_{11} \leftarrow L_{11}U_{11}$
    Solve $L_{11}U_{12} = M_{12}$ ▷ Upper Triangular System
    Solve $L_{21}U_{11} = M_{21}$ ▷ Lower Triangular System
    $M_{22} \leftarrow M_{22} - L_{21}U_{12}$
    LUDECOMPOSITION(M_{22}) ▷ $M_{22} \leftarrow L_{22}U_{22}$
  end if
end function

Complexity Estimates

- Most complexity estimates assume a constant rank k for the $\mathcal{R}k$-Matrices
- For ACA with Full Pivoting, $\mathcal{O}(N^2)$, for SVD $\mathcal{O}(N^3)$ (time)
- Assuming a **sparse** Cluster Tree and **almost idemptotent** Block Tree [BGH04]
  - Storage
    $$N_{st}(\mathcal{T}_{I\times I}, k) \leq 2C_{sp}(p+1)\max\{k, N_{leaf}\}N$$
    with $\mathcal{T}_{I\times I}$ the Block Tree of depth $p \propto \log(N)$.
  - Multiplication
    $$N_{\times}(\mathcal{T}_{I\times I}, k) \leq K_5 C_{sp}^3 C_{id}^3 k^3 (p+1)^3 \max\{|I|, |\mathcal{L}(\mathcal{T}_{I\times I})|\}$$

Complexity Estimates

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- Assuming a **sparse** Cluster Tree and **almost idemptotent** Block Tree [BGH04]
  - Storage
    $$\mathcal{O}(N \log_2(N))$$
  - Multiplication
    $$\mathcal{O}(N \log_2^2(N))$$

Computations

Issues

$\mathcal{H}$-Matrix algorithms are not nice for the hardware :

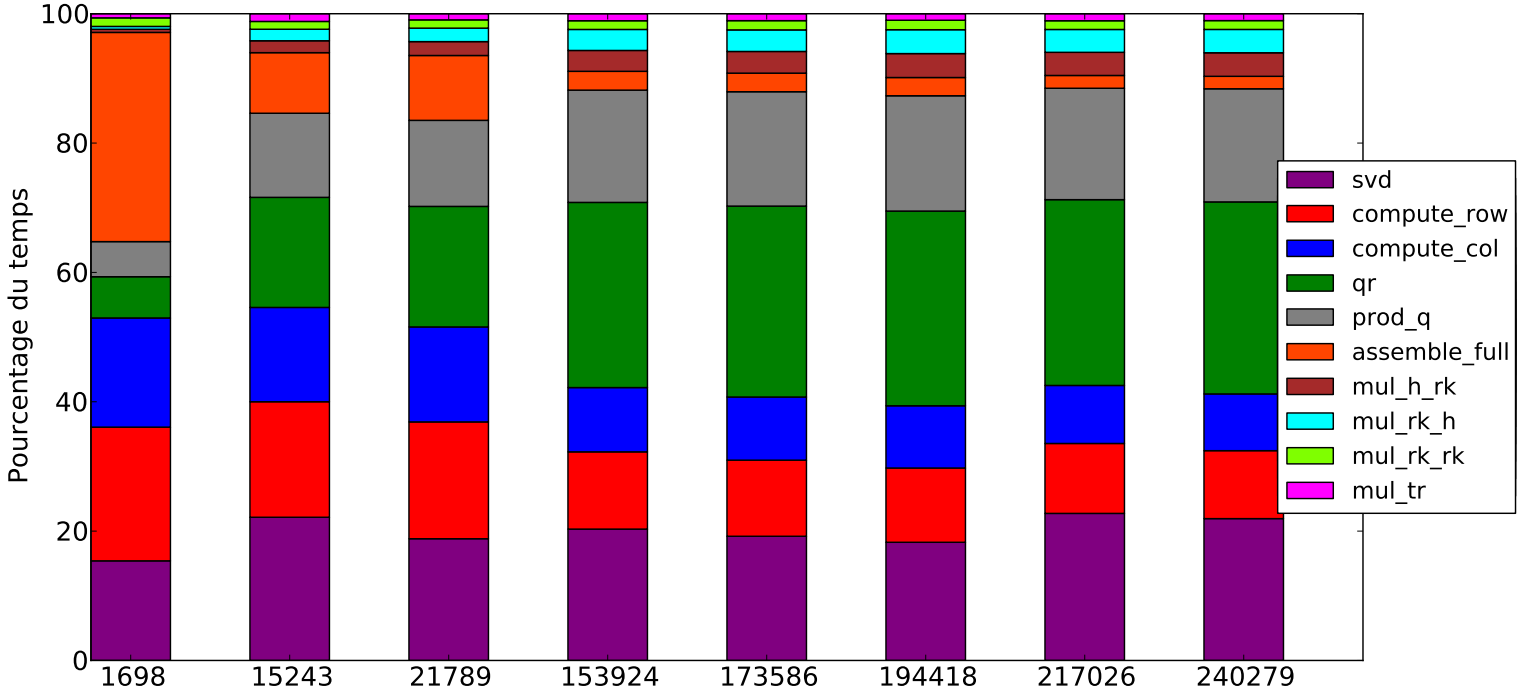
- Very small operations
- Oddly-shaped matrices : « Tall and Skinny »
- High memory bandwidth

Observations

- Most (70-80%) of the time spent in :
  - QR decompositions of T&S matrices (*eg.* $10^4 \times 30$)
  - SVD decompositions of small matrices (*eg.* 30×30)
- BLAS implementations cannot reach the peak performance
- Very high memory bandwidth. Ex : on 12 cores, allocation rate : ~ 1GB/s

Relative cost of operations

LU decomposition, same object (Cone-Sphere), different sizes



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Computations

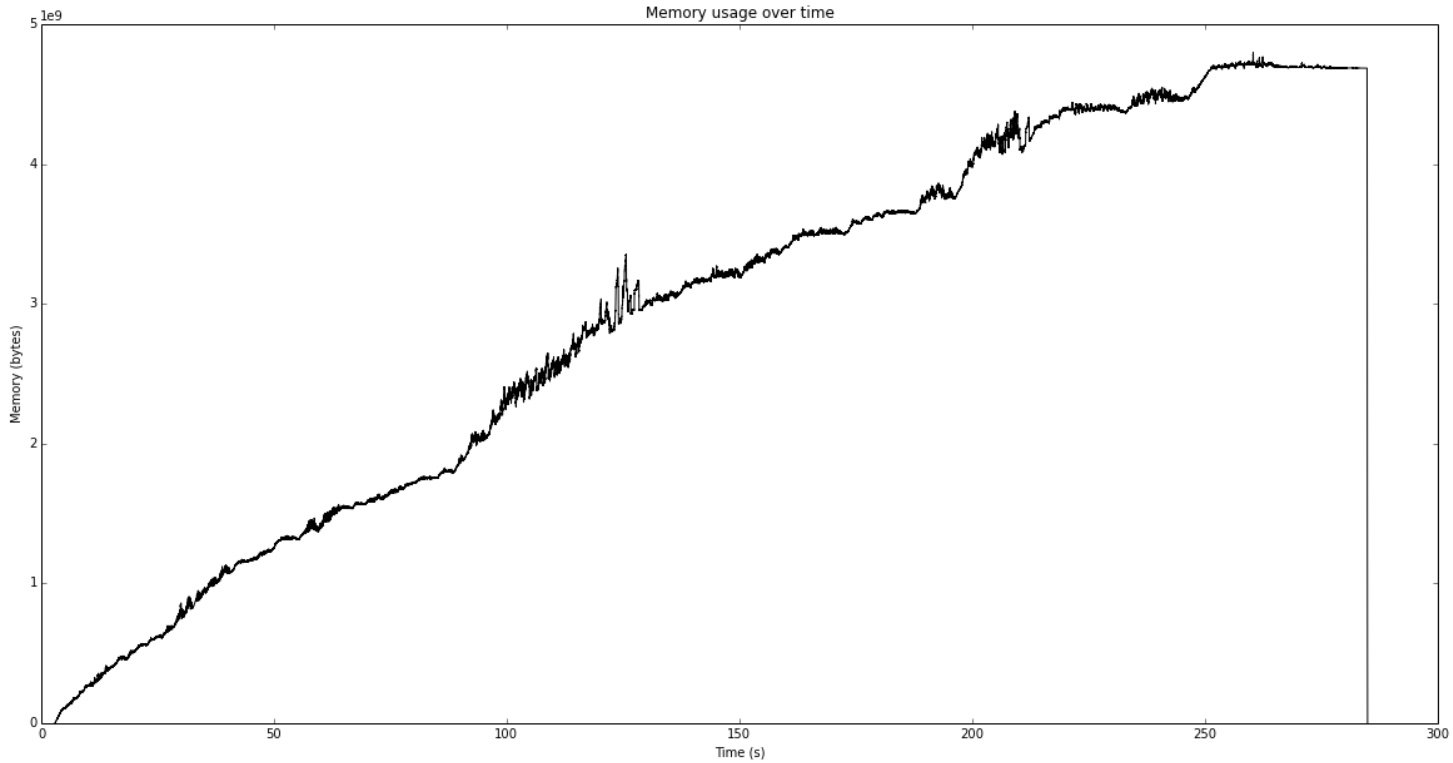
- Exemple : Cone-Sphere, 135 429 unknowns, simple complex, LU
- 2×6 Intel Xeon « Sandy Bridge », 2.3GHz, MKL 11, `icc` 13, Linux
- 205.6s
- 90.8% of the time spent in BLAS/LAPACK
- 148 GFlops (5.36 Flop / cycle)
- ...but requires 217.48$\times$ less operations than a dense solver

Operation	Gflop/s	#Calls	Total Runtime (s)
$M = U\Sigma V^*$	14.09	883 796	814.22
$M = QR$	12.7	1 635 818	708.25
QM	11.7	1 635 818	506.28
MU	13.50	817 909	33.12
$\mathcal{H} \times (AB^T)$	10.72	36437	66.4

Computations

Memory

- 9 974 346 allocations (48 893/s)
- 317 GB (1.55 GB/s)



Outline

Environment

Solver

- Airbus Group Innovations in-house solver
- C++
- Parallel implementation : Enumerated Task Flow (ETF) on top of a runtime system (*eg.* StarPU) [Liz14]
- Shared and distributed memory

Configuration

- 2×6 Intel Xeon « Sandy Bridge », 2.2GHz, 48GB
- Linux, ICC 13, MKL

2D Grid

- x_i are on a regular 2D grid with Δx pitch.
- $\lambda = \Delta x$
- Sequential LDL^T decomposition
- $\varepsilon = 10^{-4}$, $\eta = 3$
- Gaussian, exponential and quadratic kernels

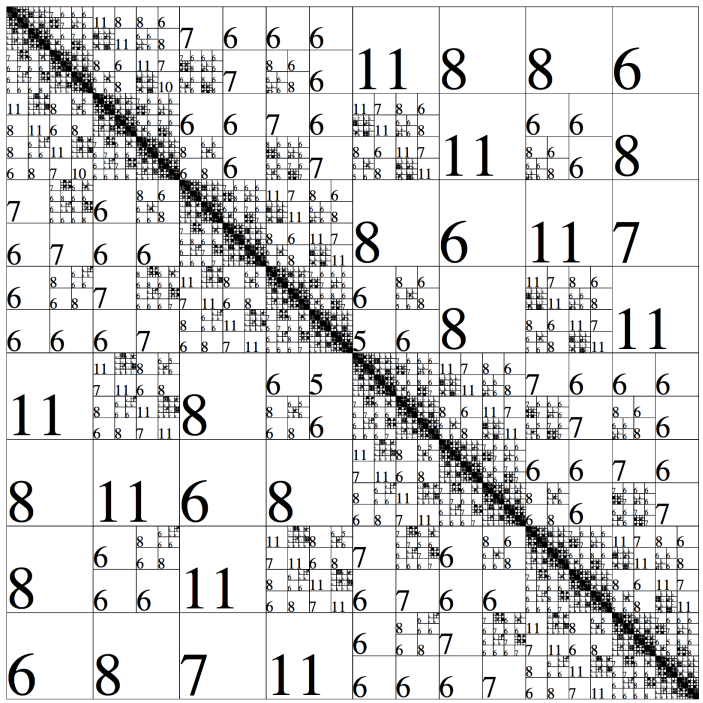
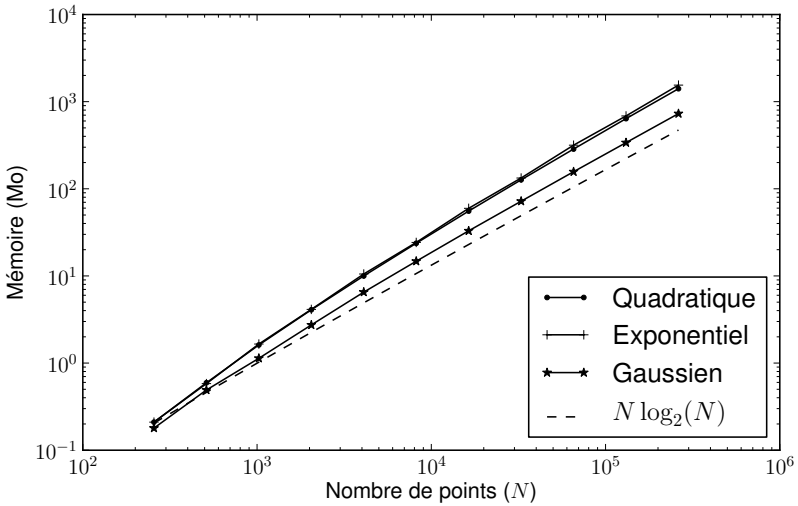
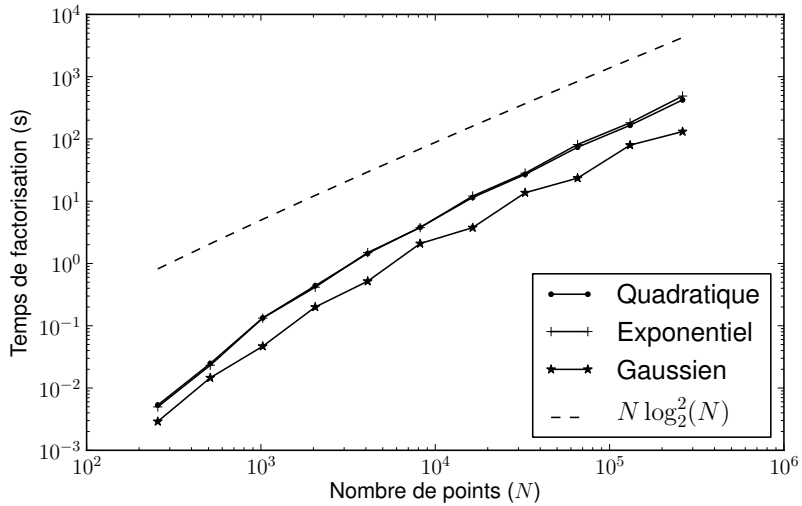


FIGURE: $\mathcal{H}$-Matrix for $N = 2^{18}$ with the quadratic kernel.

2D Grid





: Memory

: Decomposition time

FIGURE: Memory and computation time for several kernels.

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2D Grid

$$\varepsilon_{rel} := \frac{\|Kx - K_0\|_2}{\|K_0\|_2}$$

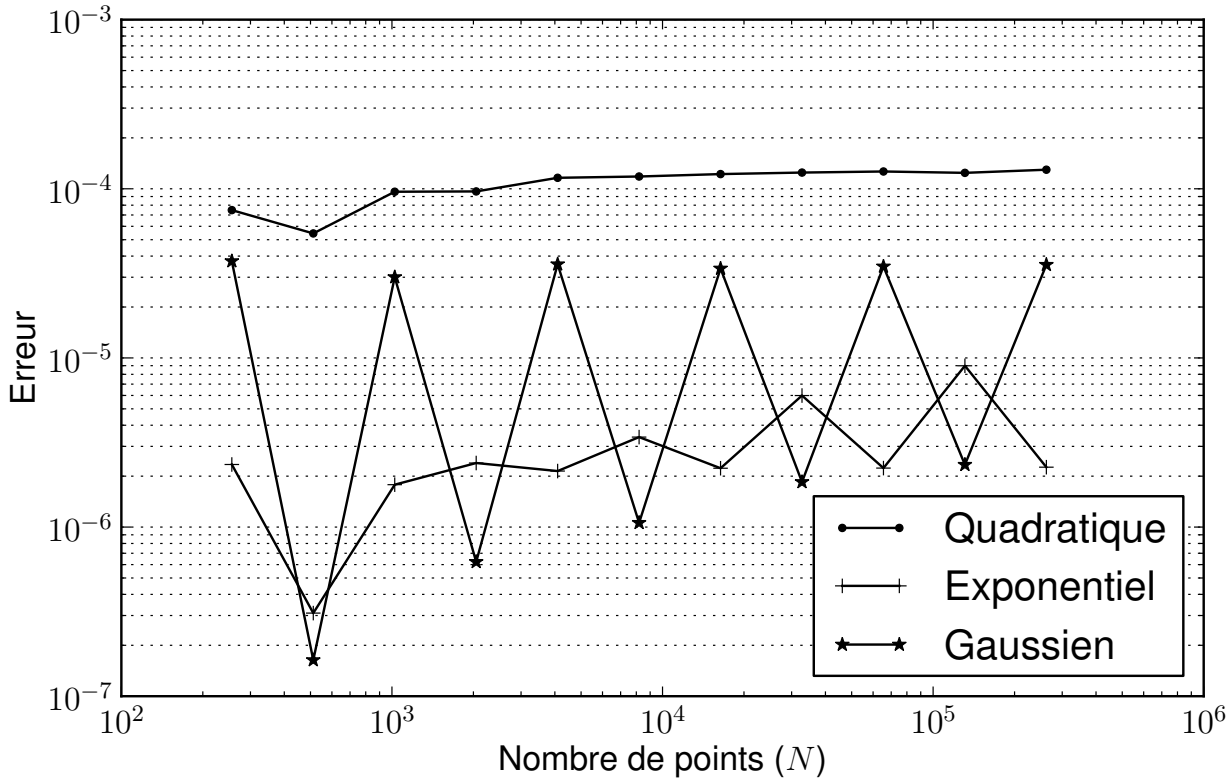

FIGURE: ε_{rel} for several kernels.

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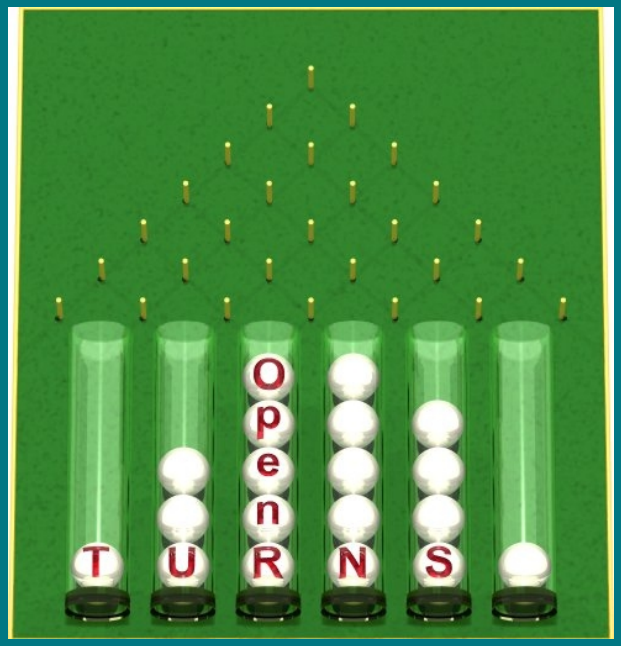
OpenTURNS



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IMACS

❖**The Galton Board** (1822 - 1911) : british explorer, geograph, inventor, meteorologist, proto-geneticist, psychometrician,statistician

The H-Matrices in Open TURNS v1.5

Epsilon	LLt (s)	getRealization (s)	Error	Matrix memory ratio
1e-4	12	0.02	1.4e-5	1 / 8.0
1e-7	25	0.03	3.9e-11	1 / 5.0
1e-10	56	0.05	7.2e-17	1 / 3.1
1e-13	99	0.07	1.2e-22	1 / 2.1
1e-16	400	0.11	2.7e-23	1 / 1.5
LAPACK	30	0.06	0	1

Mesh containing 9644 vertices, machine with 8 cores and 8 GB RAM, opensource HMatrix (sequential)

The H-Matrices in Open TURNS v1.5

Epsilon	LLt (s)	getRealization (s)	Error	Matrix memory ratio
1e-4	16	0.05	1.e-4	1 / 14.1
1e-7	24	0.04	1.e-11	1 / 8.3
1e-10	39	0.05	1.e-16	1 / 5.2
1e-13	60	0.06	1.e-22	1 / 3.5
1e-16	299	0.07	1.e-25	1 / 2.3
LAPACK	175	0.15	-	1

Mesh containing 18292 vertices, machine with 12 cores and 48 GB RAM

The H-Matrices in Open TURNS v1.5

Epsilon	LLt (s)	getRealization (s)	Error	Matrix memory ratio
1e-8	452	0.04	-	1 / 28.6
1e-12	853	0.06	-	1 / 15.6
LAPACK	-	-	-	1

Mesh containing 134331 vertices, machine with 12 cores and 48 GB RAM

Outline

Conclusion

- $\mathcal{H}$-Matrices are an enabler for many statistics problems
- Efficient parallelization is still needed, unfortunately the $\mathcal{H}$-Matrix arithmetic is highly irregular
- At least one order of magnitude for the addressable problem size on a laptop or workstation

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