Solution of larger coupled sparse/dense linear systems in an industrial aeroacoustic context

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Introduction

AIRBUS

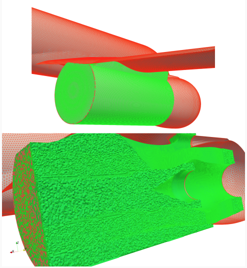
- study the propagation of sound waves emitted by an aircraft
  - acoustic pollution reduction, prototype certification
- discrete model for numerical simulations
  - volume domain v (jet flow)
    - Finite Elements Method (FEM) [19, 16]
  - surface domain s (surface of the aircraft and the volume domain)
    - Boundary Elements Method (BEM) [12, 21]

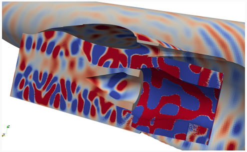
An acoustic wave (blue arrow) emitted by the aircraft's engine, reflected on the wing and crossing the jet flow. Real-life case [20] (left) and a numerical model example (right).

Problem

Global linear system coupling [13, 14] the FEM and the BEM unknowns:

$$\begin{bmatrix} A_{vv} & A_{sv}^T \\ A_{sv} & A_{ss} \end{bmatrix} \times \begin{bmatrix} x_v \\ x_s \end{bmatrix} = \begin{bmatrix} b_v \\ b_s \end{bmatrix}$$





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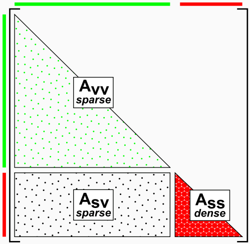
- symmetric coefficient matrices:
  - sparse parts
    - lot of zeros → storing only non-zero values
    - discretization of v with FEM (A_{vv}), s/v interaction (A_{sv})
  - a dense part
    - a few or no zeros → storing all values
    - discretization of s with BEM (A_{ss})



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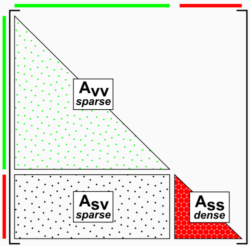
- finer model → larger system
- need for efficient solution methods
  - iterative
    - compute a sequence of terms based on previous ones
    - find a good solution approximation
  - direct
    - using Schur complement [22]



Direct solution

Schur complement

- reduce the problem on boundaries → simplify the system to solve

$$\begin{matrix} R_1 \\ R_2 \end{matrix} \quad \begin{bmatrix} A_{vv} & A_{sv}^T \\ A_{sv} & A_{ss} \end{bmatrix} \times \begin{bmatrix} x_v \\ x_s \end{bmatrix} = \begin{bmatrix} b_v \\ b_s \end{bmatrix}$$

Computation steps

1. eliminate x_v from the second equation → Schur complement S

$$\begin{matrix} R_1 \\ R_2 \leftarrow R_2 - A_{sv} A_{vv}^{-1} \times R_1 \end{matrix} \begin{bmatrix} A_{vv} & A_{sv}^T \\ 0 & \underbrace{A_{ss} - A_{sv} A_{vv}^{-1} A_{sv}^T}_{S} \end{bmatrix} \times \begin{bmatrix} x_v \\ x_s \end{bmatrix} = \begin{bmatrix} b_v \\ b_s - A_{sv} A_{vv}^{-1} b_v \end{bmatrix}$$

2. solve the reduced Schur complement system

$$S x_s = b_s - A_{sv} A_{vv}^{-1} b_v$$

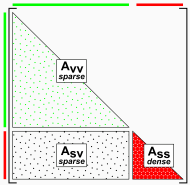
3. determine x_v using x_s

$$x_v = A_{vv}^{-1} (b_v - A_{sv}^T x_s)$$

Numerical computation

Properties of the input linear system

- A_{vv} and A_{ss} are symmetric
  - storing only half of the coefficients
- A_{vv} and A_{sv} are sparse
  - storing only non-zero values



Initial state of A

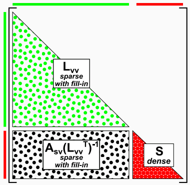
Ideal computation of $S = A_{ss} - A_{sv} A_{vv}^{-1} A_{vs}$

- factorization of A_{vv} into $L_{vv} L_{vv}^T \rightarrow$ fill-in

$$S = A_{ss} - A_{sv} (L_{vv} L_{vv}^T)^{-1} A_{sv}^T$$

- computation of the Schur complement

$$S = A_{ss} - \underbrace{(A_{sv}(L_{vv}^T)^{-1})}_{\text{triangular solve}} \underbrace{(A_{sv}(L_{vv}^T)^{-1})^T}_{\text{implicitly known}}$$



A after computing S

Two-stage implementations

Implementation

- coupling of a sparse direct and a dense direct solver
    - fully-featured community solvers with appealing functionalities
        - low-rank compression
        - out-of-core computation
        - distributed memory parallelism
- two different schemes depending on the way of using the building blocks of the sparse solver
    - *baseline* coupling
    - *advanced* coupling

Vanilla solver couplings

***baseline* coupling**

- separate A_{vv}, A_{sv} and A_{ss}
- *sparse facto.*, *sparse solve*
- *dense facto.*, *dense solve*

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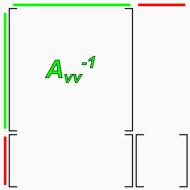

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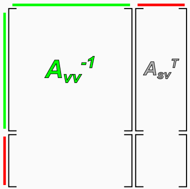

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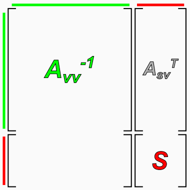

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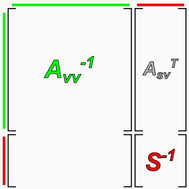

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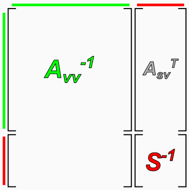
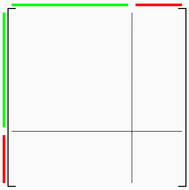


***advanced* coupling**

- A as a whole
- *sparse facto.+Schur*
- *dense facto.*, *dense solve*



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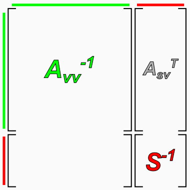

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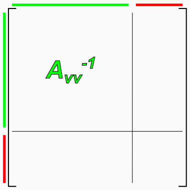

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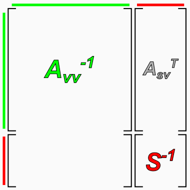

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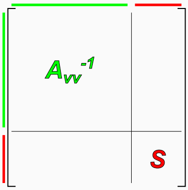

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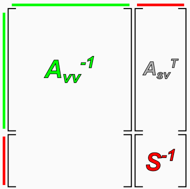

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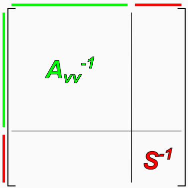

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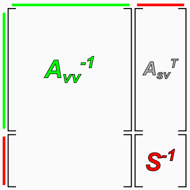

- S non-compressed, dense, entirely stored in RAM
- A_{sv}^T explicitly stored, dense

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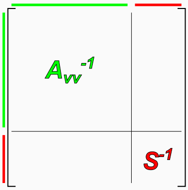

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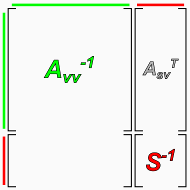

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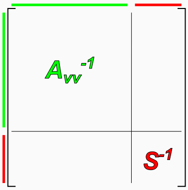

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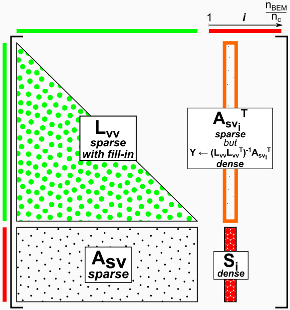
Coping with limitations

- keep using fully-featured well optimized community solvers despite limitations in their API
- two new algorithms for block-wise computation of S
  $\rightarrow$ allow for low-rank compression and out-of-core
  1. multi-solve based on the *baseline* coupling
  2. multi-factorization based on the *advanced* coupling

Multi-solve

$$S_i = A_{ss_i} - A_{sv} \overbrace{(L_{vv} L_{vv}^T)^{-1} A_{sv_i}^T}^{solve \rightarrow Y_i}$$

- 1 *sparse facto.* of the green matrix (symmetric)
- plenty of *sparse solve* involving the orange blocks (result is dense)



WITHOUT compression

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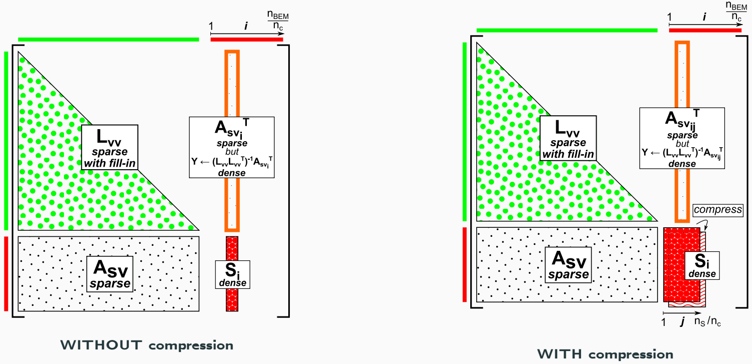
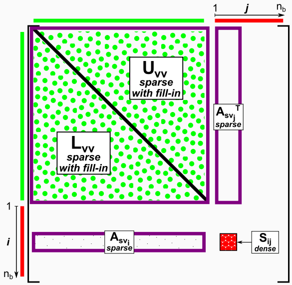


Multi-factorization

$$S_{ij} = A_{ss_{ij}} - \overbrace{A_{sv_i}(L_{vv}U_{vv})^{-1}A_{sv_j}^T}^{used\ \ with\ \ Schur\ \ API}$$

- multiple *sparse facto.+Schur* of the violet matrix (non-symmetric)
- computation of the Schur complement blocks via API



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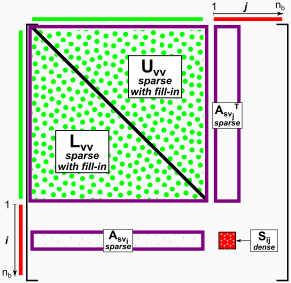

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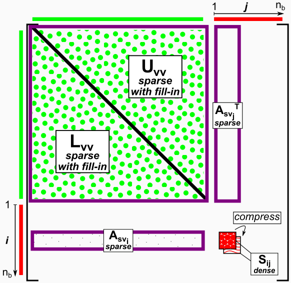


WITH compression

Experimental evaluation

Academic test case [5]

- linear systems close enough to real-life
- arbitrary large FEM/BEM systems

Industrial test case

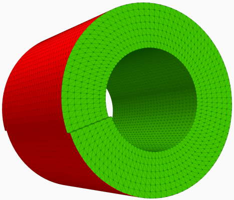
- 2,259,468 unknowns (larger s part)

Solvers

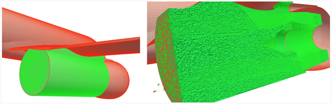
- sparse: MUMPS (compressed) [10]
- dense: SPIDO (non-compressed), HMAT (compressed) [17]

Computation platform

- PlaFRIM [3]



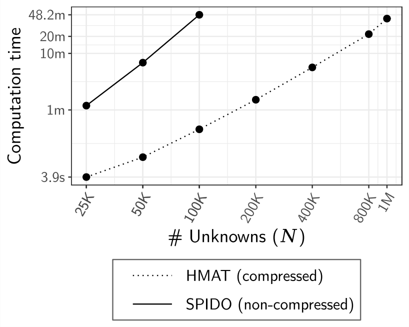
Academic pipe mesh with v and s parts (length: 2 m; radius: 4 m; 20,000 unknowns)

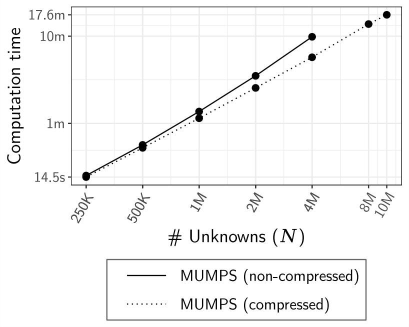


Real-life industrial FEM/BEM mesh

Preliminary comparative study [7]

- single node multi-core benchmarks without out-of-core
- study the solvers separately on sparse FEM and dense BEM systems
  - evaluate the impact of compression
  - identify the best performing parallel configurations
- better understand the behavior on coupled FEM/BEM systems

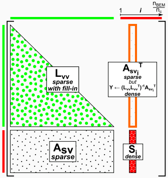




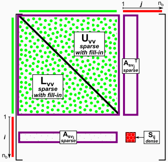
Focus on multi-solve and multi-factorization [8, 9]

- single node multi-core benchmarks without out-of-core
- push the algorithms to their limits (RAM)
- evaluate the impact of compressing the Schur complement S
- study the performance-memory tradeoff for varying block sizes
- validate the algorithms on a real-life industrial case

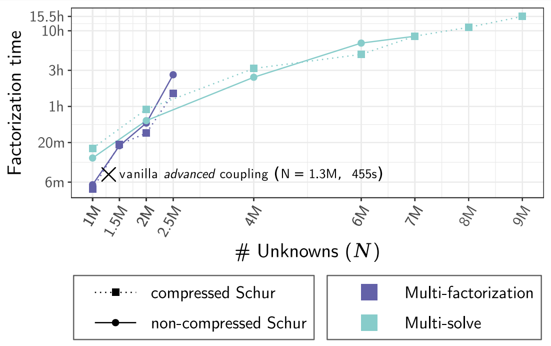
Focus on multi-solve and multi-factorization [8, 9]



multi-solve



multi-factorization



Industrial case

- cannot be processed without our algorithms
- compression of S helps
  - multi-solve: 1.6× faster, 6.4× less RAM
  - multi-factorization: 9.4× faster, 2.0× less RAM

Going further

Energetic profile [6]

- with H. Mathieu (SED), A. Guermouche and B. Tagliaro (STORM)
    - `energy_scope` [18]
- visualize the energy consumption of a complex HPC application
- compare different indicators at once (energy, RAM, flops)
- clues on how to improve the implementation

Out-of-core and distributed memory parallelism (ongoing work)

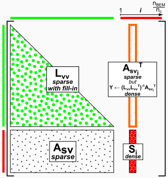
- extends the previous studies of multi-solve and multi-factorization
    1. low-rank compression of S
    2. out-of-core computation of S
    3. scale to multiple computation nodes with MPI

Summary

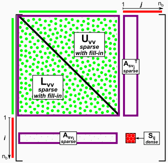
- two algorithms allowing us to:
  - benefit from the most advanced functionalities of fully-featured solvers
  - process larger systems compared to vanilla couplings
    - 9M (multi-solve) and 2.5M (multi-factorization) vs. 1.3M on a single 24-core, 128 GiB RAM workstation
- confirm the advantage of compressing the Schur complement
- validate the algorithms on a real-life industrial case

Single-stage implementations

Towards ideal implementation



multi-solve

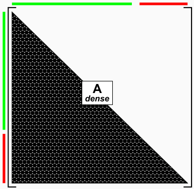


multi-factorization

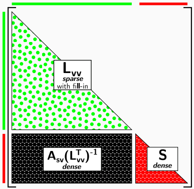
Limitations

- multi-solve: explicit storage of orange blocks in a non-compressed dense matrix
- multi-factorization: superfluous re-factorizations of the sparse submatrix A_{vv}
- two separate stages
  1. Schur complement S assembly
  2. factorization of S and solution of x_s and x_v

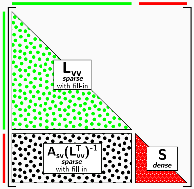
Single-stage schemes



Sparse-oblivious



Partially sparse-aware



Sparse-aware

Sparse-aware single-stage implementation

- with A. Buttari and A. Jego
    - IRIT/ENSEEIHT, Toulouse
- coupling of task based direct solvers
    - sparse: `qr_mumps` [4]
        - no compression, no distributed memory parallelism (ongoing Ph.D.)
    - dense: HMAT
    - relying on the StarPU runtime [11]
        - built-in out-of-core capability
- S is never assembled entirely in memory
- dense solver can start working without waiting for S to be fully assembled

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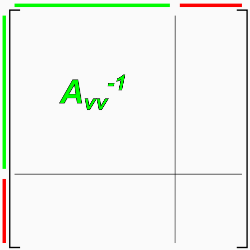

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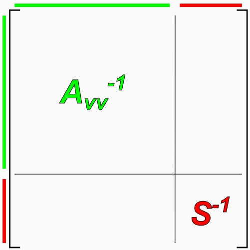

Current status

Done

1. integrate `qr_mumps` into the Airbus solver stack
2. implement multi-solve using `qr_mumps` as sparse solver for matrices with real coefficients
3. implement LL^T factorization for complex symmetric matrices in `qr_mumps` (mission in Toulouse)

Ongoing

4. add a Schur complement API to `qr_mumps`
5. implement multi-factorization using `qr_mumps` as sparse solver

Pending

6. single-stage implementation

Summary

- two-stage multi-solve and multi-factorization allowing us to:
  - benefit from the most advanced functionalities of fully-featured solvers
  - process larger systems compared to vanilla couplings
  - not ideal
- single-stage scheme
  - towards a proof of concept with some sacrifices

Conclusion

Thank you for attending!

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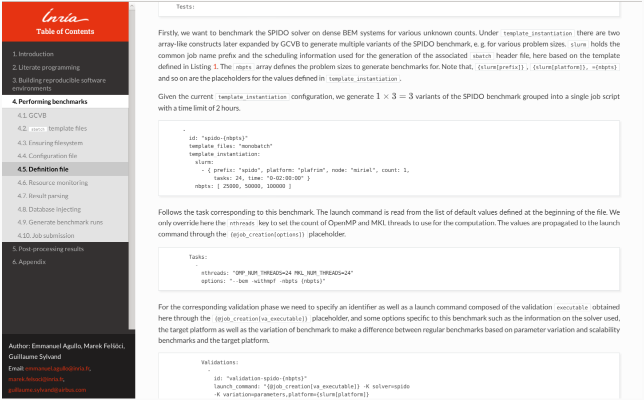
Appendix

Reproducible software envionments with Guix [1]

Guix

- transactional package manager able to co-exist with the primary package manager
- self-contained, executable descriptions of entire software environments
- reproducible accross multiple different machines
    - natively or through container solutions

Reproducible studies with Org mode for Emacs [2, 15]



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```
Tests:
```

Firstly, we want to benchmark the SPIDO solver on dense BEM systems for various unknown counts. Under `template_instantiation` there are two array-like constructs later expanded by GCVB to generate multiple variants of the SPIDO benchmark, e. g. for various problem sizes. `slurm` holds the common job name prefix and the scheduling information used for the generation of the associated `sbatch` header file, here based on the template defined in Listing 1. The `nbpts` array defines the problem sizes to generate benchmarks for. Note that, `{slurm[prefix]}`, `{slurm[platform]}`, `={nbpts}` and so on are the placeholders for the values defined in `template_instantiation`.

Given the current `template_instantiation` configuration, we generate $1 \times 3 = 3$ variants of the SPIDO benchmark grouped into a single job script with a time limit of 2 hours.

```
  -
    id: "spido-{nbpts}"
    template_files: "monobatch"
    template_instantiation:
      slurm:
        - { prefix: "spido", platform: "plafrim", node: "miriel", count: 1,
            tasks: 24, time: "0-02:00:00" }
      nbpts: [ 25000, 50000, 100000 ]
```

Follows the task corresponding to this benchmark. The launch command is read from the list of default values defined at the beginning of the file. We only override here the `nthreads` key to set the count of OpenMP and MKL threads to use for the computation. The values are propagated to the launch command through the `{@job_creation[options]}` placeholder.

```
    Tasks:
      -
        nthreads: "OMP_NUM_THREADS=24 MKL_NUM_THREADS=24"
        options: "--bem -withmpf -nbpts {nbpts}"
```

For the corresponding validation phase we need to specify an identifier as well as a launch command composed of the validation `executable` obtained here through the `{@job_creation[va_executable]}` placeholder, and some options specific to this benchmark such as the information on the solver used, the target platform as well as the variation of benchmark to make a difference between regular benchmarks based on parameter variation and scalability benchmarks and the target platform.

```
        Validations:
          -
            id: "validation-spido-{nbpts}"
            launch_command: "{@job_creation[va_executable]} -K solver=spido
            -K variation=parameters,platform={slurm[platform]}
```

- literate programming paradigm
  - combining formatted text with source code
- exhaustive documentation allowing others to reproduce a study
  - question of proprietary source code, e.g. Airbus

Going further

How to build a reproducible study from scratch with Guix and Org

- `tuto-techno-guix-hpc.gitlabpages.inria.fr/guidelines/`