RÉPUBLIQUE FRANÇAISE
Liberté
Égalité
Fraternité

ONERA
THE FRENCH AEROSPACE LAB

High-fidelity simulations of turbulent compressible flows in aerodynamics: some typical applications with ONERA CFD codes

C. Content, E. Martin
ONERA/DAAA, Châtillon

MUMPS User Days, Sorbonne University, Paris
June 22-23, 2023

Outline

- Scientific challenge
- Physical modeling and numerics
- Some typical applications
- Krylov iterative solvers for large-scale systems
- Ongoing research activities
- Concluding remarks

Scientific challenge

- Industrial demand for accurate solutions of turbulent compressible flows in aerodynamics
  - Flow features: vorticity, turbulence,…
  - Quantities of interest: lift, drag,…
- High-fidelity simulations often imply
  - Large number of discretization elements to tackle complexity (physics, geometry)
  - A physical modeling of more and more complex phenomena
  - And as a result … increasingly **large** and **ill-conditioned** linear systems !
- **Robust** and **efficient parallel** strategies for linear systems are **mandatory**
  - Solutions must be delivered at a prescribed tolerance if required
- Some properties of the corresponding matrices
  - Matrices are real non-symmetric (values) or complex non-hermitian
  - A block-wise structure and a symmetric pattern

Scientific challenge

Places where linear algebra is involved

- Dealing with **the linearized equations (Jacobian-vector products)**
  - Solve Newton (or pseudo-transient) algorithm
  - Shape optimization
  - Global stability analysis
  - …

- Dealing with **adjoint equations (Transposed Jacobian-vector products)**
  - Shape optimization
  - Goal-oriented mesh adaptation
  - Resolvent analysis
  - Uncertainty quantification
  - Sensitivity
  - …

Physical modeling and numerics – CFD

$$\begin{cases} \dfrac{\partial q}{\partial t} + \nabla \cdot F(q) = S(q, \boldsymbol{x}) \\ q(t = 0) = q_0 \\ q(x \in \partial\Omega) = q_{BC} \end{cases}$$

where

q: a vector of conserved quantities,
$\boldsymbol{x}$: a vector defining the position in space,
F: a tensor of conservative fluxes,
S: a vector of source terms.

Very large number of DoF
… **from 10^5** (simple 2D flows) **up to 10^{10}** (3D flows) !

Physical modeling and numerics – CFD

- Most of the CFD computations require **fixed point evaluation**

$$R(q, X) = 0$$

- **Implicit discrete Navier-Stokes equations**

$$\left(\frac{\Omega}{\lambda \Delta t} I - \frac{\partial R}{\partial q}\right) \Delta q = R(q, X)$$

where

X: the mesh,

Ω: a mass matrix,

Δt: the time step,

λ: the CFL number,

and the explicit residual R supposed C^1

$$R(q, X) = -\nabla \cdot F(q) + S(q, X)$$

Physical modeling and numerics – Stability Analysis

Global stability analysis for oscillatory flows as cylinder (*)

Flow is decompsed as **:** $q = q_b + q'$

Linearized equations $\frac{\partial q'}{\partial t} = \frac{\partial R}{\partial q}|_b q'$

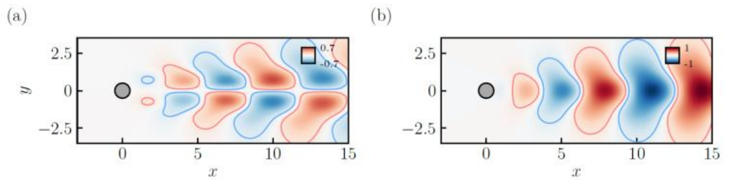


Figure III.12: Real part of streamwise (a) and cross-stream (b) velocity perturbation of the direct unstable mode at Re = 47. Solid lines indicate iso-contours at $\Re(\hat{u}_x) \pm 0.1$ and $\Re(\hat{u}_y) \pm 0.1$.

Searching solution as $q'(\boldsymbol{x}, t) = \hat{q}(\boldsymbol{x})e^{\nu t}$

Eigenvalue problem

$$A_b\, \hat{q} = \sigma \hat{q} \text{ , with } A_b = \frac{\partial R}{\partial q}|_b$$

For each couple $(\sigma_i, \hat{q}_i)$ gives

$\hat{q}_i$: the spatial structure of the i^{th} mode

$Real(\sigma_i)$: its amplification rate (asymptotically unstable if >0)

$Im(\sigma_i)$: its angular frequency

* V. Theofilis. *Progress in aerospace sciences*, 39(4):249–315, 2003.

Physical modeling and numerics – Stability Analysis

Adjoint global stability analysis (, **)*

The adjoint operator $\boldsymbol{A}^*$ of $\boldsymbol{A}$ is defined relatively to a given scalar product $\langle\cdot,\cdot\rangle_Q$

$$\forall \boldsymbol{x}, \boldsymbol{y} : \qquad \langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{y}\rangle_Q = \langle \boldsymbol{x}\boldsymbol{A}^*, \boldsymbol{y}\rangle_Q \;\Rightarrow\; \boldsymbol{A}^* = Q^{-1}\boldsymbol{A}^{\boldsymbol{T}}\, Q$$

Each eigen mode $(\sigma_i, \widehat{q_i})$ has its related adjoint one $(\overline{\sigma_i}, \widehat{q_i}^*)$.

Useful to study receptivity of the direct mode.

* D. Sipp, O. Marquet, P. Meliga, and A. Barbagallo. *Dynamics and control of global instabilities in open-flows: a linearized approach.* Applied Mechanics Reviews, 63(3), 2010.

** F. Giannetti and P. Luchini. *Structural sensitivity of the first instability of the cylinder wake*. Journal of Fluid Mechanics, 581, 2007.

Physical modeling and numerics – Stability Analysis

Resolvent analysis for amplificator flows as the flat plate (,**)*

Due to non-normality of $\boldsymbol{A}$, some globally stable flows may be exposed to instabilities that can grow and break symmetries. The most amplified one can be found by applying a forcing ϕ on linearized equations

$$\frac{\partial q'}{\partial t} = Aq' + \phi$$

Fourier transform: $i\omega t\ \hat{q} = A\hat{q} + \hat{\phi}\ e^{i\omega t}$ <=> $\hat{q} = \boldsymbol{J}\,\hat{\phi}$ with $\boldsymbol{J} = (i\omega I - A)^{-1}$

Searching the maximum gain: $\eta^2(\omega) = \sup\left(\frac{\langle \hat{q},\hat{q}\rangle_{Q1}}{\langle \hat{\phi},\hat{\phi}\rangle_{Q2}}\right) = \sup\left(\frac{\langle \boldsymbol{J}\,\hat{\phi},\boldsymbol{J}\,\hat{\phi}\rangle_{Q1}}{\langle \hat{\phi},\hat{\phi}\rangle_{Q2}}\right)$

Equivalent to solve the following hermitian EVP:

$$\boldsymbol{J}^{\boldsymbol{H}} Q_1 \boldsymbol{J}\,\hat{\phi} = \eta^2 Q_2\,\hat{\phi}$$

* L.N. Trefethen, A.E. Trefethen, S.C. Reddy, T.A. Driscoll. *Hydrodynamic stability without eigenvalues*, Science 261, 578–584,1993
** D. Sipp, O. Marquet. *Characterization of noise amplifiers with global singular modes: the case of the leading-edge flat-plate boundary layer*. Theor. Comput. Fluid Dyn. 27, 617–635, 2013.

Physical modeling and numerics – Stability Analysis

Usual way to perform Stability Analysis

Only a few part of the spectrum is exhibed.

EVP are solved by mean of iterative solver such as the Krylov-Schur (*) solver, an Arnoldi based method which iteratively converges towards eigenvalues of largest magnitudes.

Global modes (Shift and Invert (**)): $(\boldsymbol{A} - s\boldsymbol{I})^{-1}\hat{q} = \tilde{\sigma}\,\hat{q}$ and $\sigma = \tilde{\sigma}^{-1} + s$

Resolvent: $\boldsymbol{J}^{\boldsymbol{H}} Q_1 \boldsymbol{J}\,\hat{\phi} = \eta^2 Q_2\,\hat{\phi}$ or $\boldsymbol{J}\,Q_2^{-1}\boldsymbol{J}^{\boldsymbol{H}} Q_1\,\hat{q} = \eta^2\,\hat{q}$, with $\boldsymbol{J} = (i\omega I - A)^{-1}$

With enough memory, the best practice is the LU factorisation for each operator

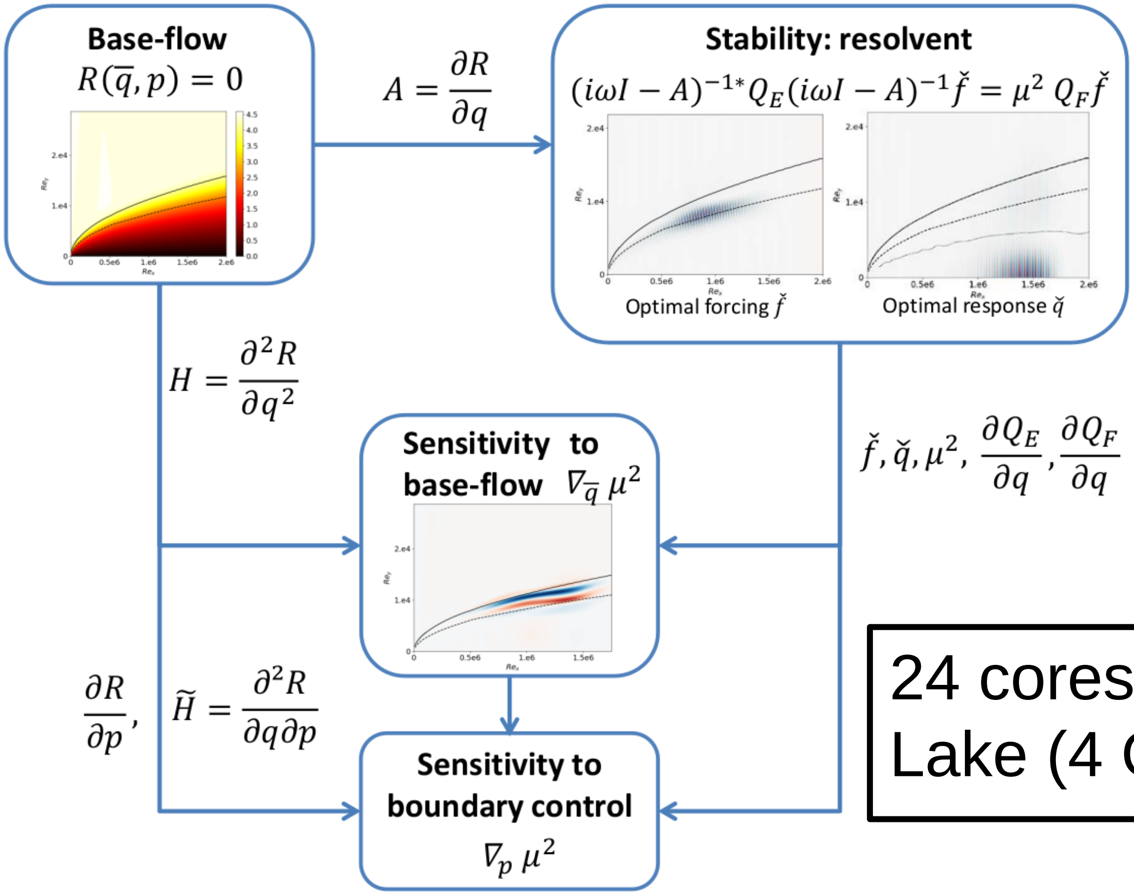
All operators are obtained by mean of A. D. with Tapenade (***)

* G. Stewart. *A Krylov-Schur Algorithm for Large Eigenproblems*. SIMAX, 23(3):601-614, 2002.

** K. N. Christodoulou and L. E. Scriven. *Finding leading modes of a viscous free surface flow: An asymmetric generalized eigenproblem*. J Sci Comput, 3(4):355–406,1988.

*** L. Hascoët, and V. Pascual. The Tapenade automatic differentiation tool : Principles,model, and specification, ACM Trans. Math. Softw. 39(3) : 20 (2013)

Application to flow over flate plate at Mach=4.5
A. Poulain (ONERA/DAAA) (*, **) ; NDoF ~ 10^6



24 cores of a Cascade Lake (4 GB/CPU)

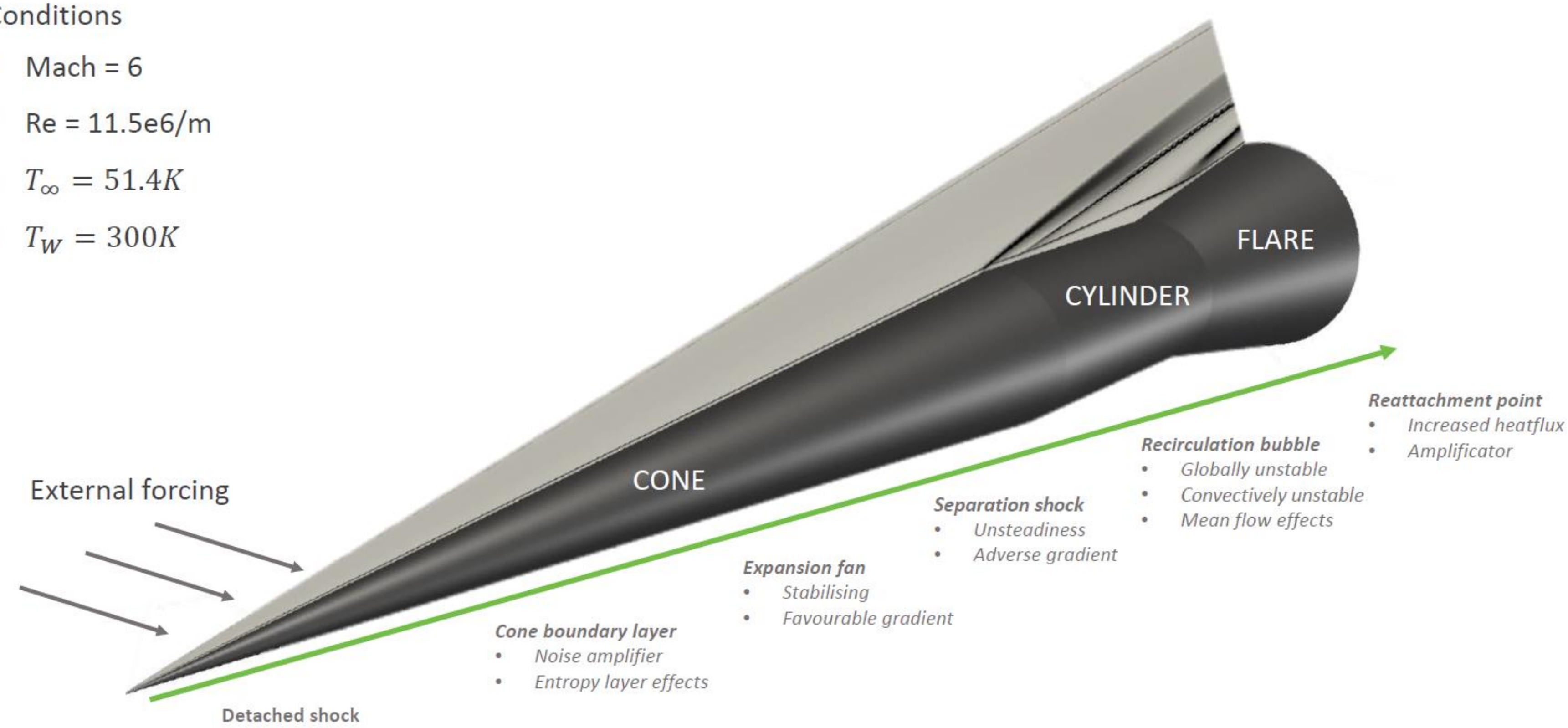
* A. Poulain, C. Content, D. Sipp, G. Rigas, E. Garnier. *BROADCAST: A high-order compressible CFD toolbox for stability and sensitivity using Algorithmic Differentiation*. Computer Physics Communications 283, 108557 (2023).

** A. Poulain, C. Content, D. Sipp, G. Rigas, E. Garnier. *Adjoint-based linear sensitivity of a hypersonic boundary layer to steady wall blowing-suction/heating-cooling*, arXiv 13 June 2023.

Application to flow over Cone-Cylinder-Flare (CCF) at Mach=6
C. Caillaud (CEA-ONERA/DAAA) (*) ; NDoF ~ 10^7

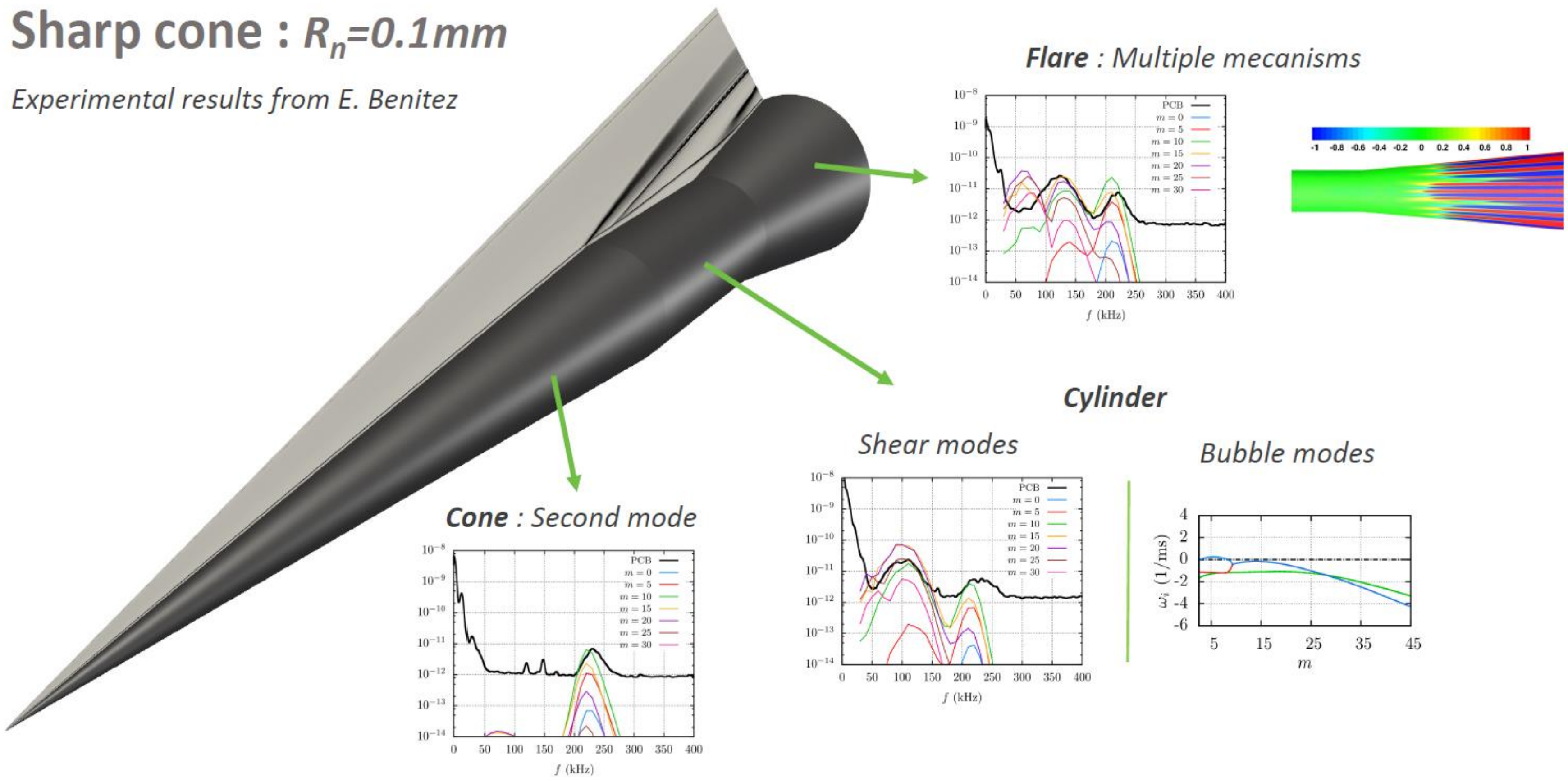
Conditions

- Mach = 6
- Re = 11.5e6/m
- $T_\infty = 51.4K$
- $T_W = 300K$



* C. Caillaud, M. Lugrin, S. Esquieu, C. Content. *Global stability analysis of a hypersonic cone-cylinder-flare geometry.* 57th 3AF International Conference on Applied Aerodynamics, 29-31 March 2023, Bordeaux, France.

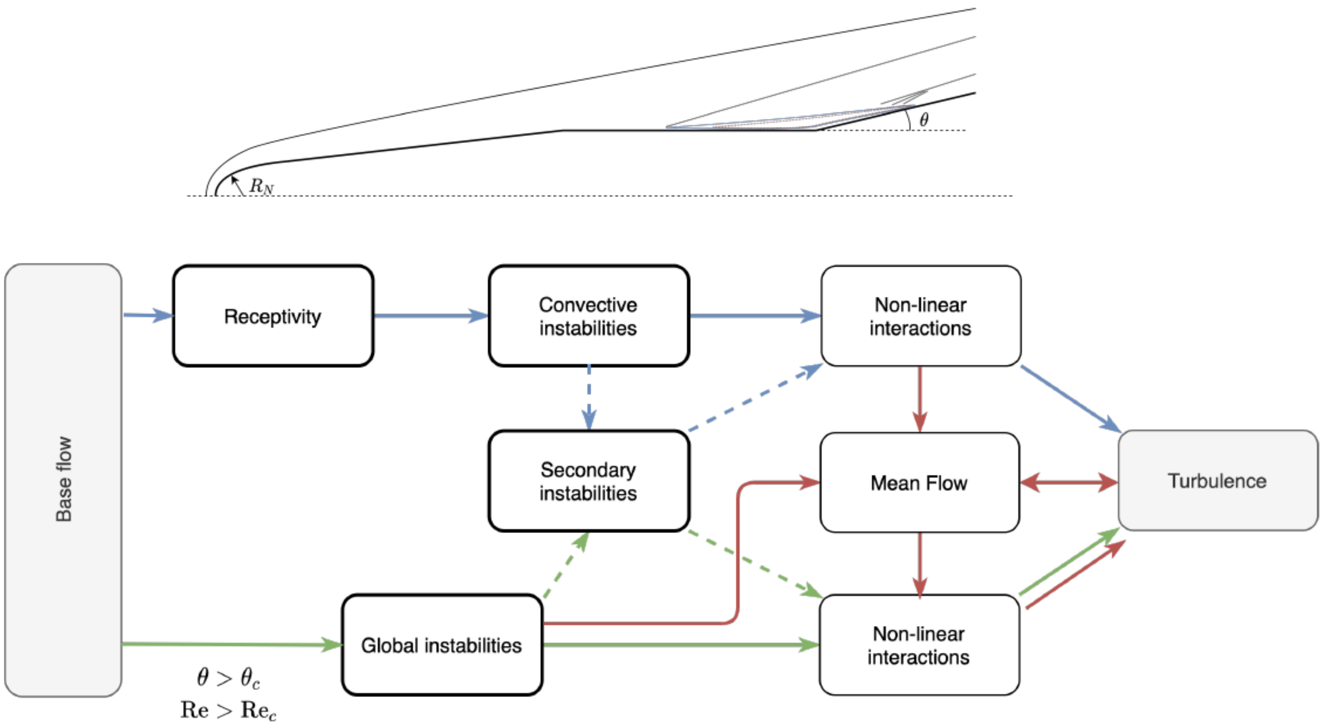
Application to flow over Cone-Cylinder-Flare (CCF) at Mach=6
C. Caillaud (CEA-ONERA/DAAA) (*) ; NDoF ~ 10^7



* C. Caillaud, M. Lugrin, S. Esquieu, C. Content. *Global stability analysis of a hypersonic cone-cylinder-flare geometry.* 57th 3AF International Conference on Applied Aerodynamics, 29-31 March 2023, Bordeaux, France.

Application to flow over Cone-Cylinder-Flare (CCF) at Mach=6
C. Caillaud (CEA-ONERA/DAAA) (*) ; NDoF ~ 10^7

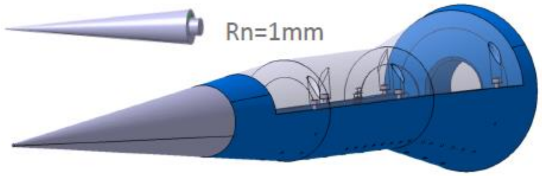
Objective : mapping the linear stability properties of such baseflows



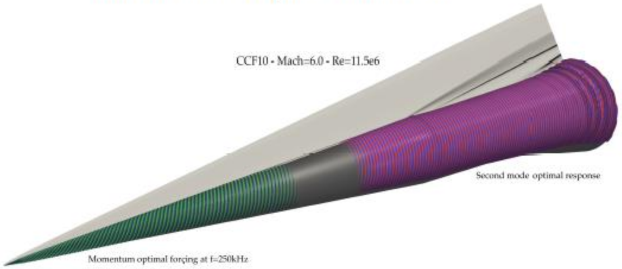
* C. Caillaud, M. Lugrin, S. Esquieu, C. Content. *Global stability analysis of a hypersonic cone-cylinder-flare geometry*. 57th 3AF International Conference on Applied Aerodynamics, 29-31 March 2023, Bordeaux, France.

Application to flow over Cone-Cylinder-Flare (CCF) at Mach=6
C. Caillaud (CEA-ONERA/DAAA) (*) ; NDoF ~ 10^7

CCF experimental model



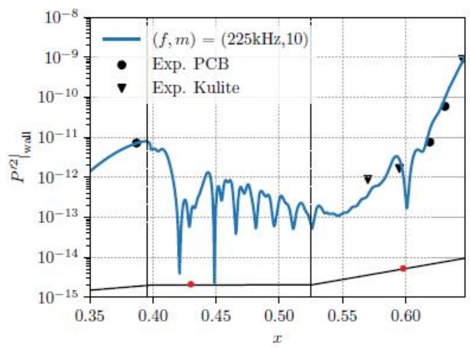
Numerical representation



Rn=0.1mm

- *Pressure signature of the resolvent mode*
- *Amplitude is scaled on the first PCB*

Recovering the experimental dynamics



Run on super-cluster Topaze at CCRT:
3-4 nodes (512 cores)
~1.5 TB RAM

* C. Caillaud, M. Lugrin, S. Esquieu, C. Content. *Global stability analysis of a hypersonic cone-cylinder-flare geometry*. 57th 3AF International Conference on Applied Aerodynamics, 29-31 March 2023, Bordeaux, France.

Scaling up toward industrial applications on unstructured mesh (*)

- A 3D Navier-Stokes example: $N_{eq} = 5$, $N_{cell} = 25$ M ➔ NDoF = 125 M
- ONERA Cluster with Intel Cascade Lake nodes (4 GB/CPU)
- Number of non-zero values of the matrix: NNZ($\boldsymbol{A}$) $\simeq$ stencil X N_{eq} × NDoF
- Finite Volume Spatial Discretization of Order 2 (Stencil $\simeq$ 125)

Storage of $\boldsymbol{A}$ (complex) ~ 1.25 TB

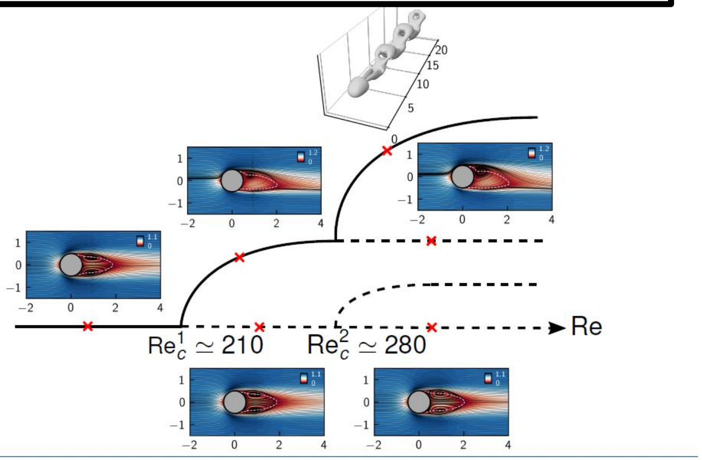


Fig: bifurcation sketch of sphere flow

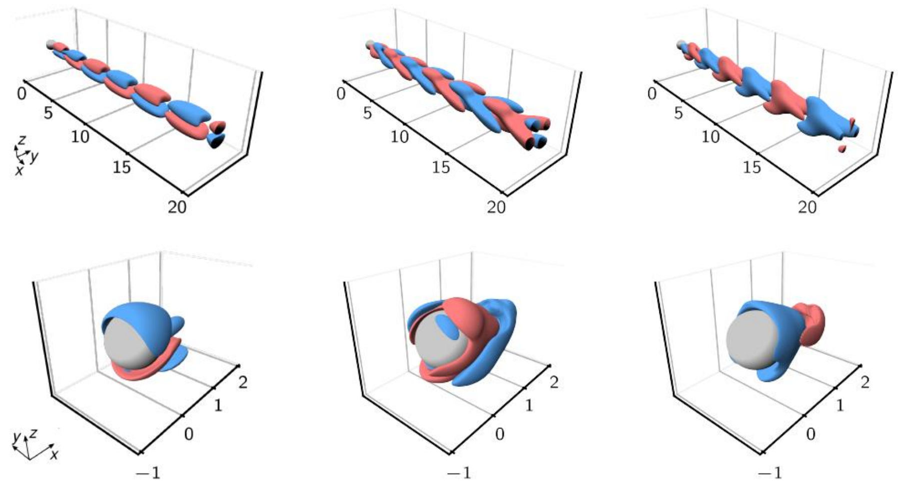


Fig: Resolvent Analysis : optimal response (top)/forcing (bottom)

* V. Fer. *Scale up of efficient global stability tools in order to characterize specific turbomachineries phenomenons,* PhD Thesis, 2022

Scaling up toward industrial applications applications on unstructured mesh (*)

Method	Estimation	Memory	NCPU
LU	$\left(\frac{NNZ(\boldsymbol{A})}{7}\right)^{4/3}$	~1000 TB	>250000
KM-ILU(k)	$\gamma(k) \times NNZ(A) + n_{KM} \times N_{DOF}$	~ 20 TB	~5000

- Memory requirement of direct methods is still a bottleneck for industrial cases
- Krylov iterative Methods (KM) overcome that point
- But the **preconditioning strategy** becomes **the key issue** (***)
  - Classic user parameters: $n_{KM} = 120$, $k = 3$ ($\gamma(3) = 3$)

* V. Fer. *Scale up of efficient global stability tools in order to characterize specific turbomachineries phenomenons*, PhD Thesis, *2022*

** J.Y. L'Excellent, *Multifrontal Methods: Parallelism, Memory Usage and Numerical Aspects*. Hdr, 2012.

*** N. Guilbert. *Amélioration de l'inversion de grands systèmes creux pour la simulation numérique en mécanique des fluides*. *2021.*

Krylov iterative solvers for large-scale systems

- We are looking for **robust** and **efficient parallel** iterative solvers

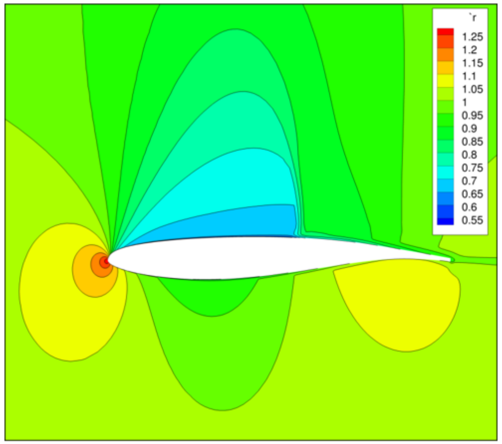
- Evaluations of several numerical algorithms
  - Deflation techniques *GCRO-DR* [*Parks, de Sturler et al. '06*]
  - Flexible preconditioning operator *FGCRO-DR* [*Carvalho, Gratton et al., '11*]
  - Mixed-precision algorithms [*Baboulin et al. '09*] [*Arioli, Duff, '09*]
  - Restricted Additive Schwarz preconditioner [*Cai, Sarkis, '99*]

- Baseline strategy if accurate solutions are required
  - *FGCRO-DR* (m_{outer}, k, $\varepsilon_{outer} = 10^{-9}$) — $\mathbf{A}_{DP}$ global
    - *GMRES* (m_{inner}, $\varepsilon_{inner} = 0.5$) — $\mathbf{A}_{SP}$ global
      - ❑ Restricted Additive Schwarz — Domain coupling
        - ❖ P = Block-ILU(0) — $\mathbf{P}_{SP}$ local

  ($\mathbf{A}_{SP}$ global, Domain coupling, $\mathbf{P}_{SP}$ local: <u>Precond</u>)

Krylov iterative solvers for large-scale systems

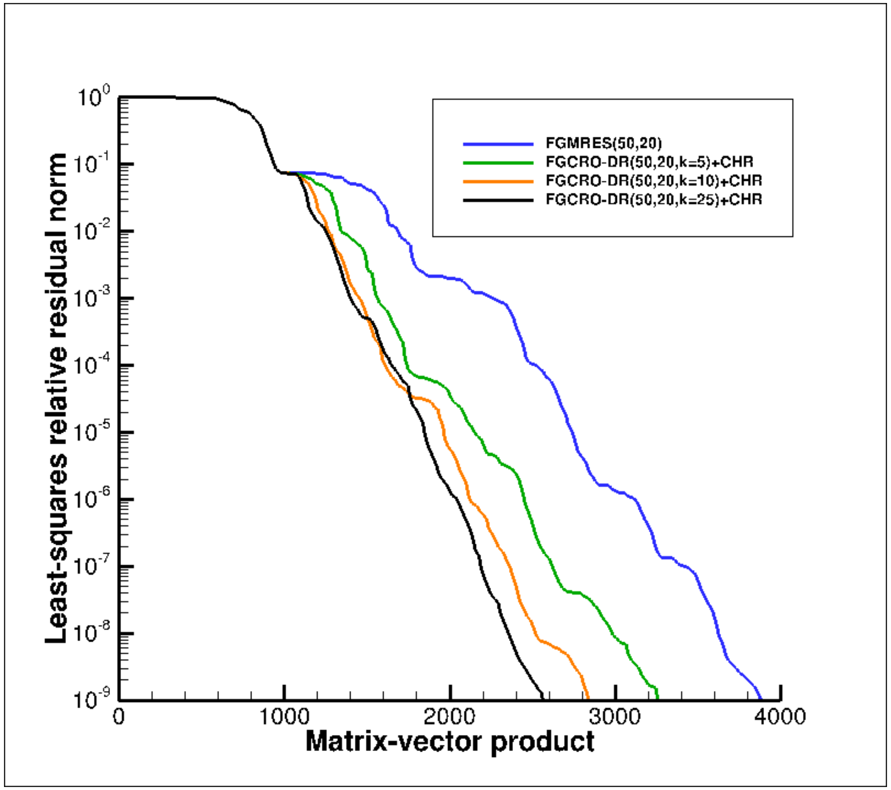
Adjoint solutions with Krylov subspace recycling



OAT15A airfoil

2D compressible (generic) RANS equations
Turbulent transonic flow
Aerodynamic shape optimization problem:
    Minimization of the drag coefficient (only *p* contribution)

DG(*O*4) ; *Aghora* DG code (*)
N ~ 3.2 M ; *NNZ* ~ 802 M
16 MPI ; Intel Broadwell ; Worst case ~ 300 s



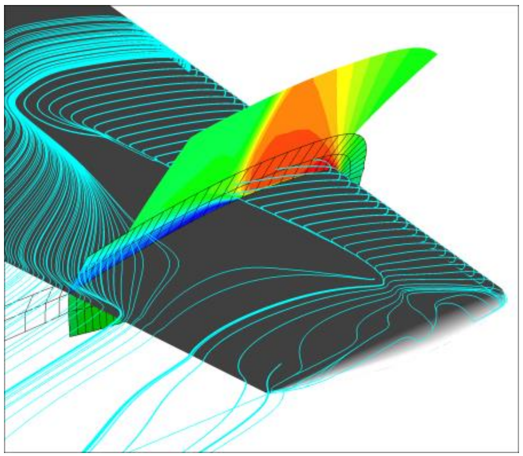
Benefits of recycling varying number k of vectors (CHR)

* F. Renac et al. *Aghora: A High-Order DG Solver for Turbulent Flow Simulations.* IDIHOM: Industrialization of High-Order Methods, Springer book, 2015.

This work is supported by the French project DGAC/LAMA (Direction Générale de l'Aviation Civile) and by the European project NextSim.

Krylov iterative solvers for large-scale systems

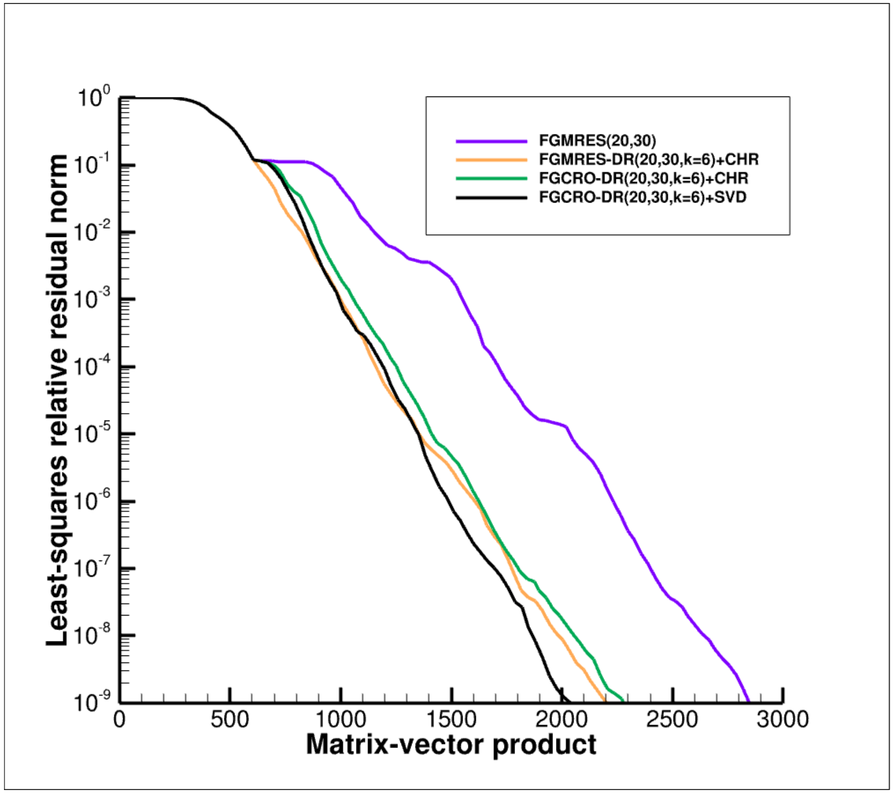
Adjoint solutions with Krylov subspace recycling



ONERA M6 wing

3D compressible (generic) RANS equations
Turbulent transonic flow
Aerodynamic shape optimization problem:
  Minimization of the drag coefficient (only *p* contribution)

DG(*O*4) ; *Aghora* DG code (*)
N ~ 20 M ; *NNZ* ~ 13 B
176 MPI ; Intel Skylake ; Worst case ~ 420 s



Gains of recycling varying solvers and vector type (CHR, SVD)

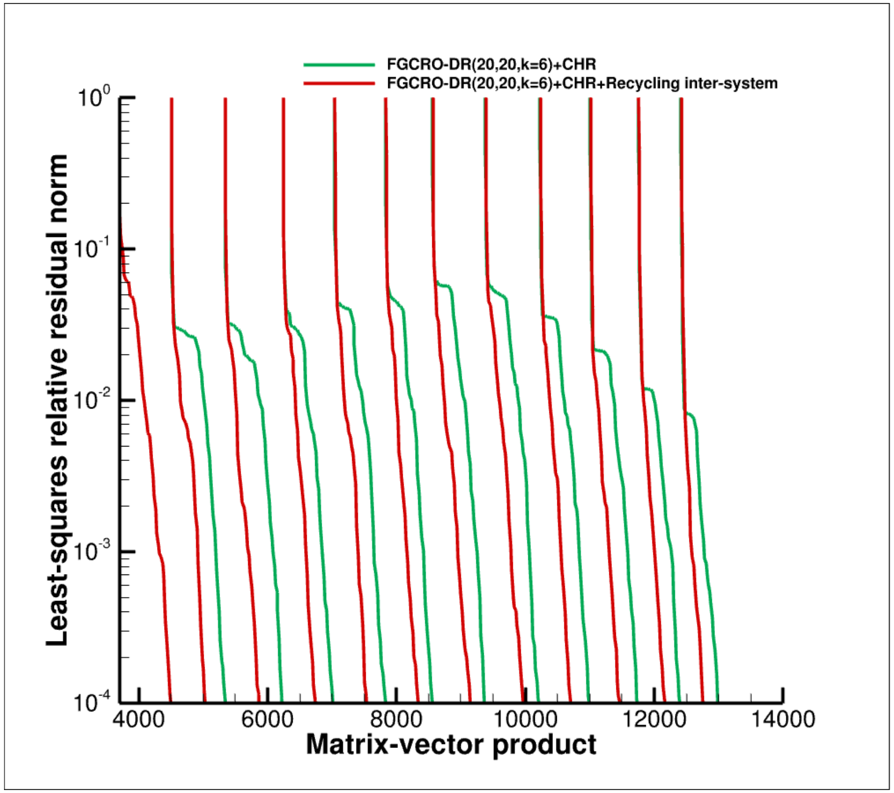
* F. Renac et al. *Aghora: A High-Order DG Solver for Turbulent Flow Simulations.* IDIHOM: Industrialization of High-Order Methods, Springer, 2015.

This work is supported by the French project DGAC/LAMA (Direction Générale de l'Aviation Civile) and by the European project NextSim.

Ongoing research activities

Gains of recycling between consecutive systems

- Strategies to select information
  - When to trigger inter-system recycling
  - Type and quality of the vectors



OAT15A airfoil

2D compressible (generic) RANS equations
Turbulent transonic flow
Sequence of systems from steady-state calculations

DG(O3) ; *Aghora* DG code (*)
N ~ 2 M ; NNZ ~ 288 M
16 MPI ; Intel Broadwell

Recycling starts at the end of the 11^{th} up to the 21^{th}

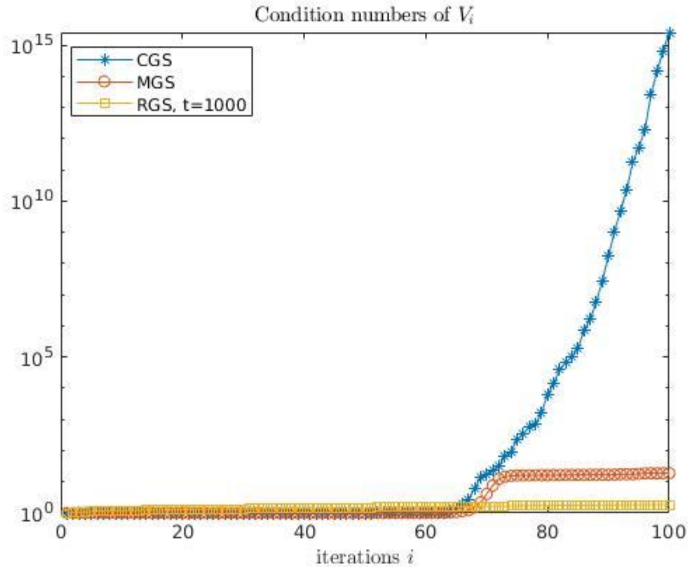
* F. Renac et al. *Aghora: A High-Order DG Solver for Turbulent Flow Simulations.* IDIHOM: Industrialization of High-Order Methods, Springer book, 2015.

This work is supported by the French project DGAC/LAMA (Direction Générale de l'Aviation Civile) and by the European project NextSim.

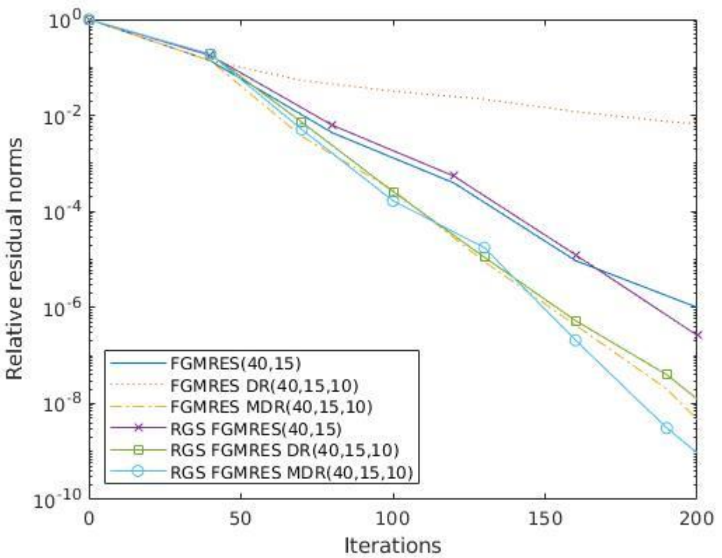
Ongoing research activities

*Randomized Flexible GMRES with Deflated Restarting**

- LS89 test-case: subsonic flow, steady problem (FV(*O*2), RANS, SA-negative)
  - Matrix characteristics: N = 115,368 ; NNZ ~ 6 M ; cond(A) ~10^{14}
  - Preconditioning operator: GMRES + RAS



Stability of Krylov basis varying Gram-Schmidt process



Sensitivity of deflation (CHR,SVD) and GS (CGS, RGS)

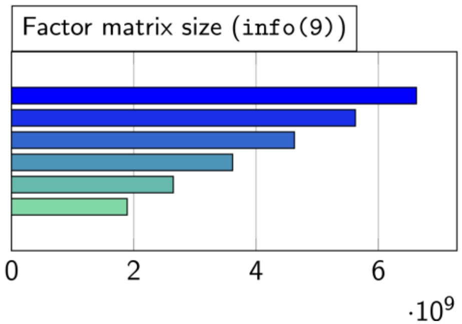
* Y. Jang, L. Grigori, E. Martin, C. Content. *Randomized Flexible GMRES with Deflated Restarting*, 2023, hal-04072873.

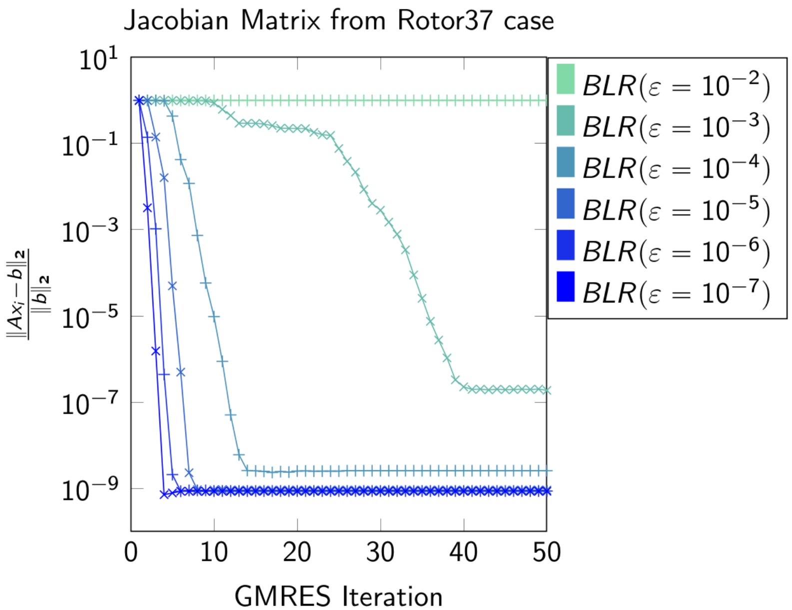
*** This work is funded by DGAC (Direction Générale de l'Aviation Civile) in the frame of the SONICE project.**

Ongoing research activities

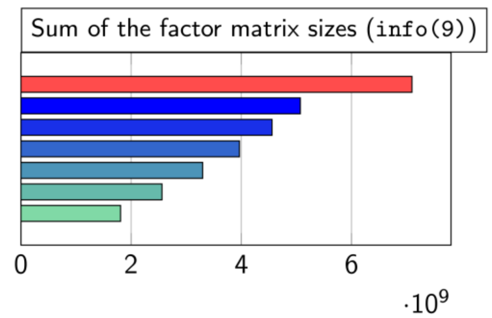
MUMPS-BLR preconditioner for a global strategy with memory constraint

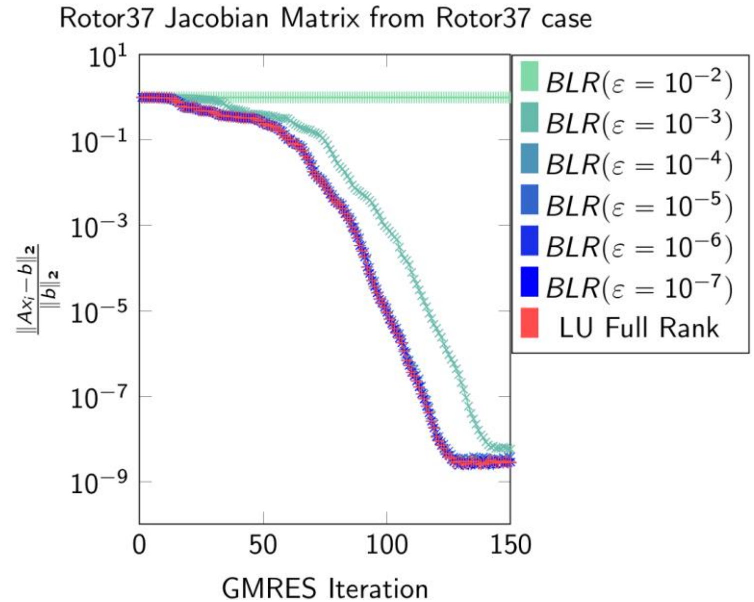
Approach
Global matrix





Approach RAS
10 subdom
Overlap 1





* S. Dubois. *Adaptive preconditioning strategies with data compression in CFD*. ONERA PhD (2022-2025).

Concluding remarks

- Direct methods are used as long as the memory limitation is not reached
- Flexible solvers with Krylov subspace recycling are **a promising alternative**
  - Capability to address larger problem sizes with robustness/efficiency
  - Significant gains are observed on tough problems
  - Random sketching techniques offer a better numerical stability of Krylov basis
  - **Hybrid direct-iterative solvers are of main concern**
  - But **calibration rules** to **leverage costs** are still needed
- Convergence to steady-state of stiff problems remains problematic
  - Limitations of first-level preconditioner (numerical efficiency / memory cost)
    - Data compression: MUMPS BLR feature, mixed-precision algorithms…
  - Coupling between domains plays a significant role
    - One-level RAS preconditioner is not enough
    - Coarse space corrections might be explored
    - Parallel scalability ?

Thank you for your attention !

Any question or remark ?