

PROGRESS WITH VERIFICATION AND STABILIZATION OF REYNOLDS STRESS MODELS USING THE CFD SOFTWARE BY ONERA, DLR, AIRBUS (CODA)

Keerthana Chandrasekar Jeyanthi¹, Tobias Knopp¹, Johannes Löwe¹, Michael Werner²

¹DLR, Institut für Aerodynamik und Strömungstechnik, Abteilung C²A²S²E

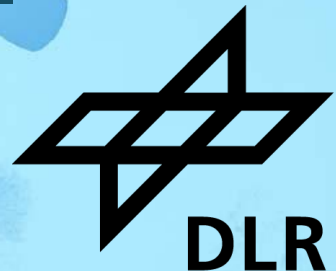
²DLR, Institut für Aerodynamik und Strömungstechnik, Abteilung Hochgeschwindigkeitskonfigurationen,
Bunsenstraße 10, 37073 Göttingen



Co-funded by
the European Union



AIRBUS



INTRODUCTION

Reynolds stress models - RSM

SSG/LRR-In(ω) model



■ What are RSMs?

- A family of RANS models providing transport equations for all the components of the symmetric Reynolds stress tensor.
- **6 transport equations** for the Reynolds stresses (R_{ij}) and **1 additional equation** for the length scale (ω)

■ When do we need RSMs?

- **Accurate representation of anisotropic turbulence** and **complex flow phenomenon** like 3D separation, vortex dominated flows, etc.

$$\frac{\partial(\bar{\rho}\widehat{R}_{ij})}{\partial t} + \frac{\partial(\bar{\rho}U_k\widehat{R}_{ij})}{\partial x_k} = \bar{\rho}P_{ij} + \bar{\rho}\Pi_{ij} - \bar{\rho}\varepsilon_{ij}$$

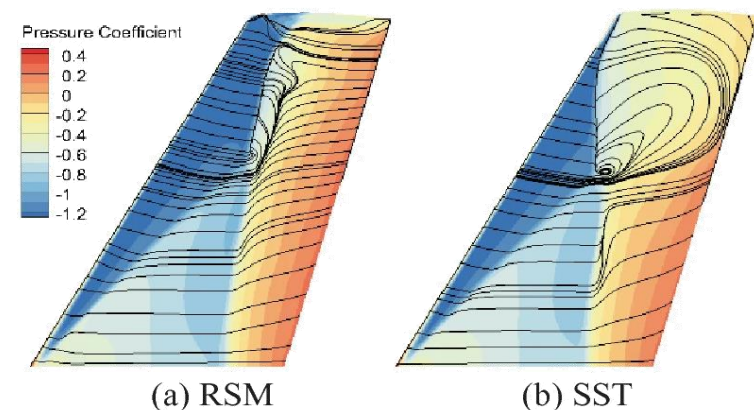
Reynolds stresses equations

Where, $P_{ij} \rightarrow$ Production, $\Pi_{ij} \rightarrow$ Pressure-strain correlation, $\varepsilon_{ij} \rightarrow$ Dissipation tensor

Length scale equation

$$\begin{aligned} \frac{\partial(\bar{\rho}\widehat{\omega})}{\partial t} + \frac{\partial(\bar{\rho}U_k\widehat{\omega})}{\partial x_k} = & \frac{\alpha_{\widehat{\omega}}}{k} \frac{\bar{\rho}P_{kk}}{2} - \beta_{\widehat{\omega}}\bar{\rho}e^{\widehat{\omega}} + \frac{\partial}{\partial x_k} \left[\left(\bar{\mu} + \sigma_{\widehat{\omega}} \frac{\bar{\rho}k}{e^{\widehat{\omega}}} \right) \frac{\partial \widehat{\omega}}{\partial x_k} \right] \\ & + \sigma_d \frac{\bar{\rho}}{e^{\widehat{\omega}}} \max \left(\frac{\partial k}{\partial x_k} \frac{\partial \widehat{\omega}}{\partial x_k}, 0 \right) + \left(\bar{\mu} + \sigma_{\widehat{\omega}} \frac{\bar{\rho}k}{e^{\widehat{\omega}}} \right) \frac{\partial \widehat{\omega}}{\partial x_k} \frac{\partial \widehat{\omega}}{\partial x_k} \end{aligned}$$

$\widehat{\omega} = \ln \omega$, hence, $\omega = e^{\widehat{\omega}}$



Upper-surface flow and C_p distribution comparison of different models for ONERA M6 wing at $Ma = 0.84$, $Re_{MAC} = 11.72 \times 10^6$, $\alpha = 6.06^\circ$.

On the Correction of $k-\omega$ SST Turbulence Model to Three-Dimensional Shock Separated Flow

Challenges with RSMs

SSG/LRR-In(ω) model



■ High non-linearity → dense Jacobian

- Mean flow (S_{ij}, W_{ij}) → Reynolds stresses
- Reynolds stresses ($\partial R_{ij}/\partial x_j$) → Mean flow
- Reynolds stresses (P_{ij}) → Length scale equation
- Length scale equation (ε) → Reynolds stresses
- Reynolds stresses (All source terms, mainly Π_{ij}) ↔ Reynolds stresses

■ Different time scales → Ill conditioning of Jacobian

- $\frac{T_c}{T_s} \sim 10^3 \text{ to } 10^6$, i.e. $T_c \gg T_s$

■ RSM vs Eddy Viscosity Models (SA or SST)

- Less robust
- More iterations
- More memory

$$\frac{\partial(\bar{\rho}\widehat{R}_{ij})}{\partial t} + \frac{\partial(\bar{\rho}U_k\widehat{R}_{ij})}{\partial x_k} = \bar{\rho}P_{ij} + \bar{\rho}\Pi_{ij} - \bar{\rho}\varepsilon_{ij}$$

Production term

$$\bar{\rho}P_{ij} = -\bar{\rho}\widehat{R}_{ik}\frac{\partial\widehat{u}_j}{\partial x_k} - \bar{\rho}\widehat{R}_{ik}\frac{\partial\widehat{u}_j}{\partial x_k}$$

Dissipation term

$$\bar{\rho}\varepsilon_{ij} = \frac{2}{3}\bar{\rho}\varepsilon\delta_{ij}, \quad \varepsilon = C_\mu\widehat{k}\omega, \quad \widehat{k} = \frac{\widehat{R}_{ii}}{2}$$

Pressure-strain correlation term

$$\widehat{a}_{ij} = \frac{\widehat{R}_{ij}}{\widehat{k}} - \frac{2}{3}\delta_{ij}$$

$$\begin{aligned} \bar{\rho}\Pi_{ij} = & -\left(C_1\bar{\rho}\varepsilon + \frac{1}{2}C_1^*\bar{\rho}P_{kk}\right)\widehat{a}_{ij} \\ & + C_2\bar{\rho}\varepsilon\left(\widehat{a}_{ik}\widehat{a}_{kj} - \frac{1}{3}\widehat{a}_{kl}\widehat{a}_{kl}\delta_{ij}\right) \\ & + (C_3 - C_3^*\sqrt{\widehat{a}_{kl}\widehat{a}_{kl}})\bar{\rho}\widehat{k}\widehat{S}_{ij}^* \\ & + C_4\bar{\rho}\widehat{k}\left(\widehat{a}_{ik}\widehat{S}_{jk} + \widehat{a}_{jk}\widehat{S}_{ik} - \frac{2}{3}\widehat{a}_{kl}\widehat{S}_{kl}\delta_{ij}\right) \\ & + C_5\bar{\rho}\widehat{k}\left(\widehat{a}_{ik}\widehat{W}_{jk} + \widehat{a}_{jk}\widehat{W}_{ik}\right) \end{aligned}$$

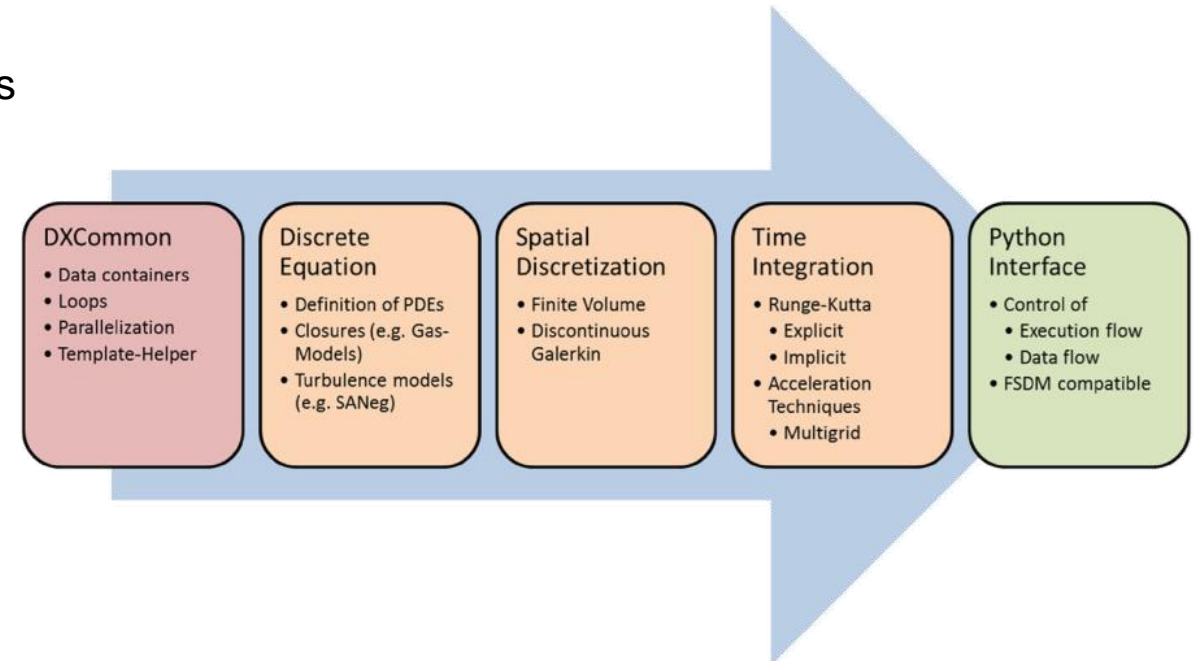
Generalized Gradient Diffusion

$$\bar{\rho}D_{ij} = \frac{\partial}{\partial x_k}\left[\left(\bar{\mu}\delta_{kl} + D\frac{\bar{\rho}\widehat{R}_{kl}}{C_\mu\omega}\right)\frac{\partial\widehat{R}_{kl}}{\partial x_l}\right]$$

CFD software by ONERA, Airbus and DLR (CODA)



- CODA is the CFD software being developed as part of a collaboration between the French Aerospace Lab (ONERA), the German Aerospace Center (DLR), Airbus, and their European research partners. CODA is jointly owned by ONERA, DLR and Airbus.
- Features of CODA:
 - **Cell-centered unstructured fully coupled** solver
 - Common framework for both second order **Finite volume** (FV) and **Discrete Galerkin** (DG) discretizations
 - **Fully implicit** time integration (using Newton method)
 - **Algorithmic differentiation** (AD) for calculating derivatives
 - Modular design to facilitate **highly parallel** simulations
 - Object oriented design using **C++17** with **Python API** to enable coupling to **FlowSimulator** framework
- The main aim of the work is to have a robust implementation of the SSG/LRR-In(ω) RSM model in CODA.



Modular structure of the next generation flow solver (previously) Flucs (now CODA) software

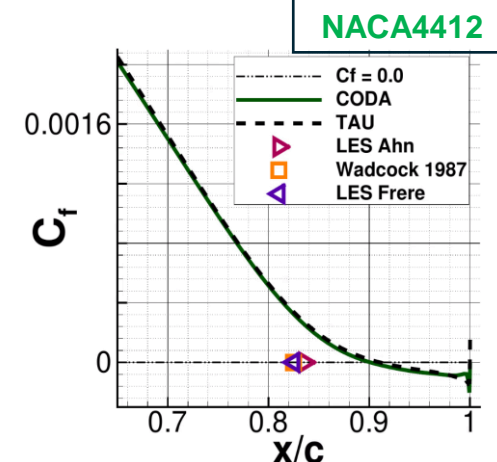
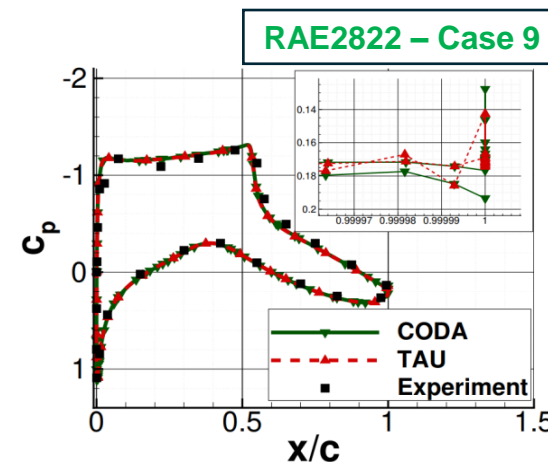
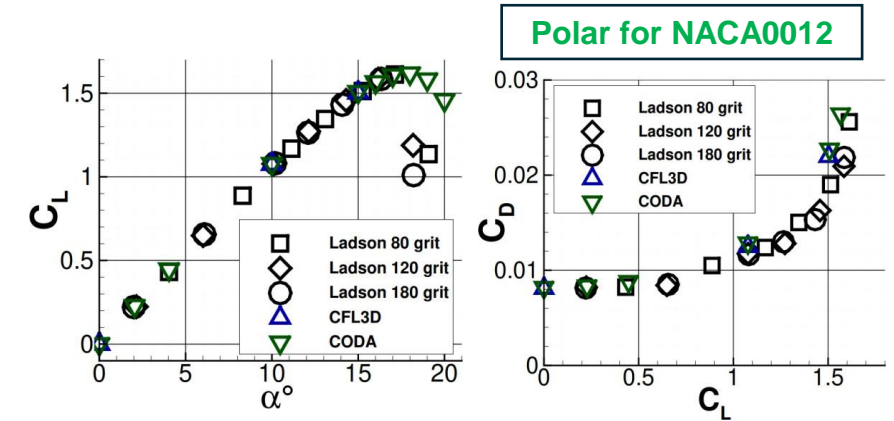
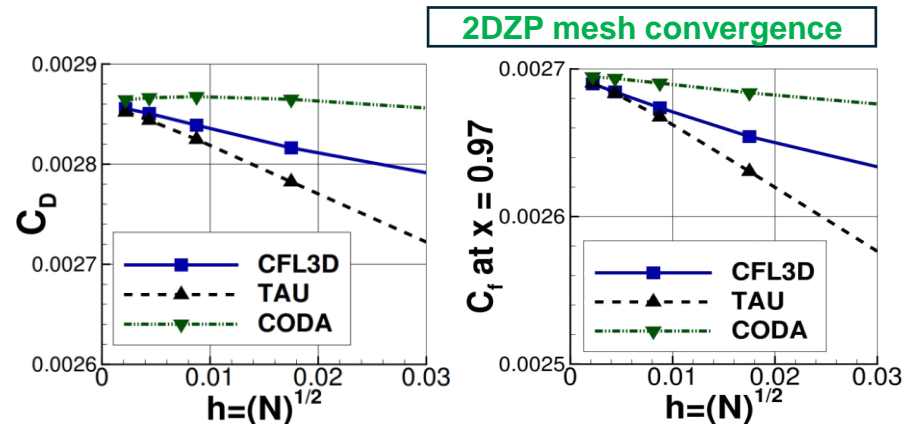


REYNOLDS STRESS MODELS – INITIAL IMPLEMENTATION & PRELIMINARY VERIFICATION

Preliminary verification & validation (V&V) of 2D cases

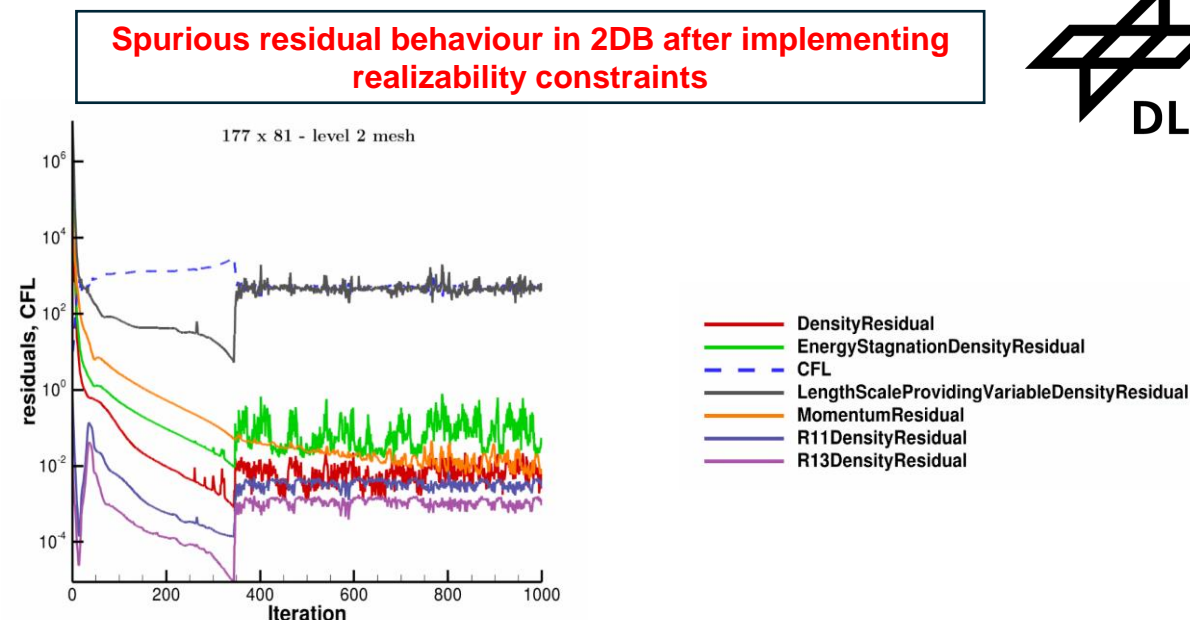


- **Zero pressure gradient flat plate (2DZP):** Very good convergence for all meshes with dependence on CFL ramping
- **Bump in channel (2DB):** Convergence was possible only with simple diffusion (SD) and GGD failed due to realizability violation.
- **RAE2822 – Case 9:** A two stage convergence with first order in the first stage and second order in mean flow during the second stage.
- **NACA0012 – Full Polar:** The simulations converged for the full polar until maximum lift with a two stage approach as well.
- **NACA4412 – Trailing edge separation:** A two stage approach worked well for this case as well.
- The meshes for all the below cases were taken from NASA TMR (except for NACA4412 & RAE2822)



Challenges from initial implementation

- Robustness issues leading to realizability constraints (2DB case)
- Failure of traditional clipping due to AD (differentiability of Reynolds stresses in Jacobian)
- Mesh & parameter studies (NACA4412) – factors affecting convergence:
 - Mesh & Case/Configuration
 - Realizability constraints
 - Gradient reconstruction
 - CFL setting
 - Entropy fix
 - Convection scheme
- Moving to 3D cases like ONERA M6 lead to even more challenges – failure of convergence without realizability constraints.



Mesh & Parameter study for NACA4412

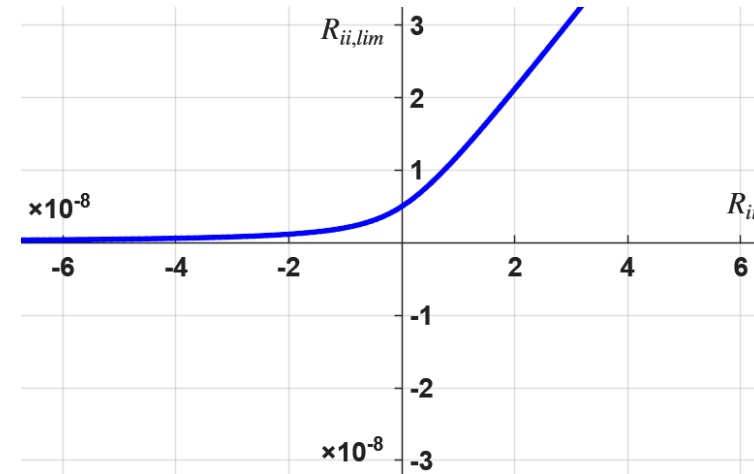
Ma = 0.085, Re = 1.64e6, AoA = 10°, Realizability OFF in Last Stage	Mesh_yp1_blunt_TE	NASA_HexMesh_897x257	Re_1-6Mio_wake_panel_yp1_v1b	Re_1-6Mio_yp1_blunt_TE_v1c_fine
run_1c_composite-scheme_grad-recon-stdGG_Efix-0.2-0.0			Divergence in 2nd Stage (very high residuals, 10 ¹⁰ to 10 ⁴⁰)	Residual stall
run_1c1_composite-scheme_grad-recon-stdGG_Efix-0.2-0.1-0.0		Changing second stage Efix to 0.2 and increasing number of iterations lead to	Inf in 2nd Stage	Residual stall
run_1c2_composite-scheme_grad-recon-stdGG_Efix-0.2-0.1-0.05		Changing second stage Efix to 0.2 and increasing number of iterations lead to	Inf in 2nd Stage	Residual stall
run_2c_composite-scheme_grad-recon-extGG_Efix-0.2-0.0			Divergence in 2nd Stage (very high residuals, 10 ¹⁰ to 10 ⁴⁰)	Residual stall
run_2c1_composite-scheme_grad-recon-extGG_Efix-0.2-0.1-0.0		Residual stall - changing Stage 2 Efix to 0.2 and Stage 3 SER exp to 0.4, integral		Residual stall
run_2c2_composite-scheme_grad-recon-extGG_Efix-0.2-0.1-0.05		Residual stall - changing Stage 2 Efix to 0.2 and Stage 3 SER exp to 0.4, integral	Divergence in 3rd Stage (very high residuals, 10 ¹⁰ to 10 ⁴⁰)	Residual stall
run_7c_composite-scheme_grad-recon-LSQ_Efix-0.2-0.0			Divergence in 2nd Stage (very high residuals, 10 ¹⁰ to 10 ⁴⁰)	Residual stall
run_7c1_composite-scheme_grad-recon-LSQ_Efix-0.2-0.1-0.0				Residual stall
run_7c2_composite-scheme_grad-recon-LSQ_Efix-0.2-0.1-0.05				Residual stall

- Non-physical turbulence can arise due to turbulence modelling and discretization errors affecting convergence - [Schumann](#)
- **Realizability constraints:** Reynolds stress tensor should be Symmetric Positive Semi Definite (SPSD) tensor throughout the simulation.
 - $R_{ij} \geq 0, \forall i = j$
 - $R_{ij} \leq \sqrt{R_{ii}R_{jj}}, \forall i \neq j$
- Several attempts were made to implement the realizability constraints
 - Pure **hard clipping** directly at the source terms: Failed as it is not AD differentiable.
 - Use of **non-linear positivity filter** with eigen value decomposition of Reynolds stress tensor: Eigen decomposition becomes expensive as more cells violate differentiability.
 - **Hard clipping** in the python layer (for testing): Simulations stalled even the ones which may converge otherwise.
 - **Realizability preserving time stepping** (through implicit/explicit linearization of source terms): Worked only for basic test cases, further investigation needed.
 - **Smoothed clipping** of Reynolds stress variables in closure: The **most possible way** which worked for several 2D/3D cases like NACA4412, coarse meshes of ONERA M6 and could be integrated easily to the CODA architecture.

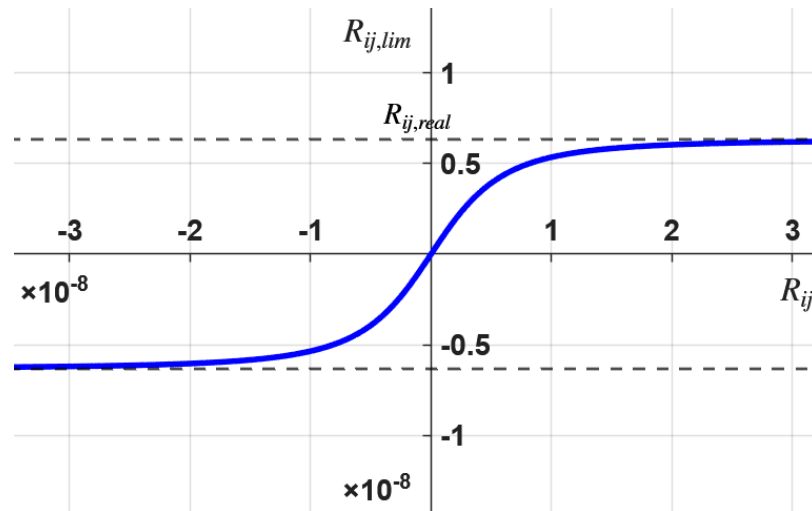
Smooth clipping for realizability constraints

For normal stress, R_{ii} :

- $R_{ii,min}$ → Minimum normal stress
- $R_{ii,lim} = 0.5 (R_{ii} + \sqrt{R_{ii}^2 + R_{ii,min}^2})$



A plot for $R_{ii,lim}$ when $R_{ii,min} = 1 \times 10^{-8}$



A plot for $R_{ij,lim}$ when $R_{ii,lim} = 1 \times 10^{-8}$, $R_{jj,lim} = 4 \times 10^{-9}$

For shear stress, R_{ij} :

$$R_{ij,real} = \sqrt{R_{ii,lim} R_{jj,lim}}$$

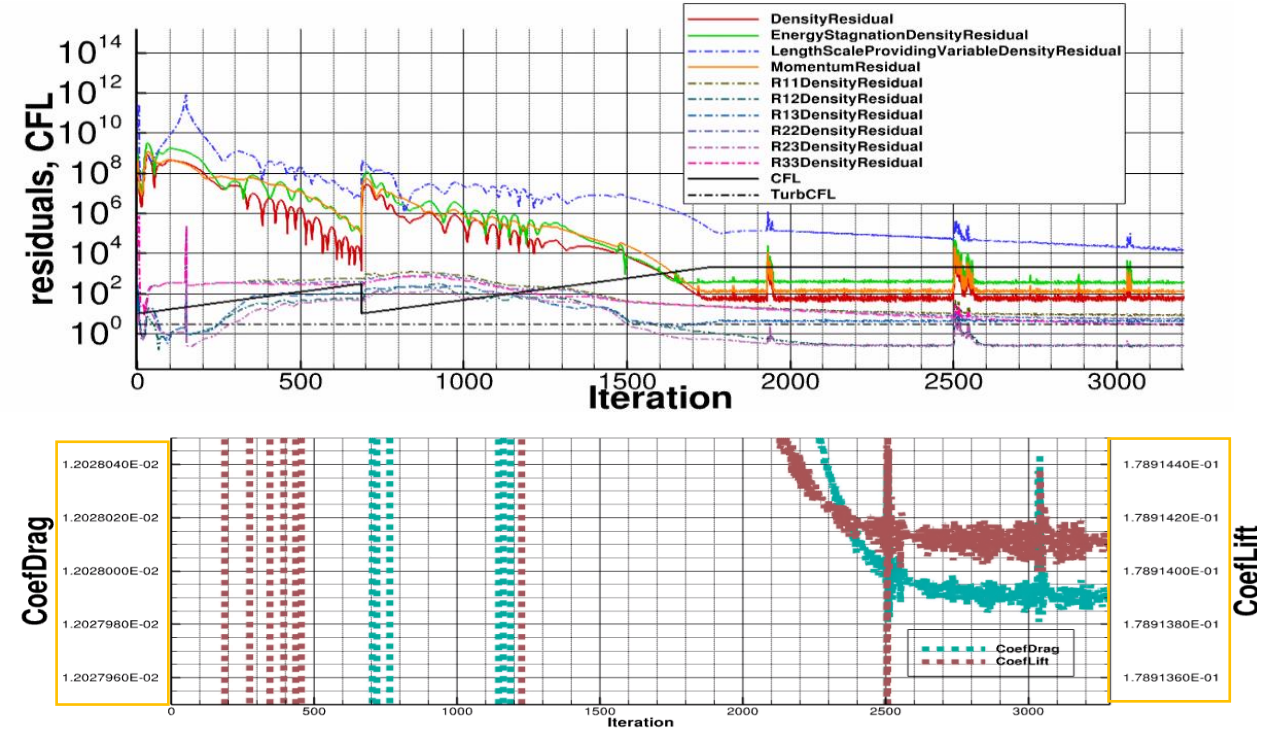
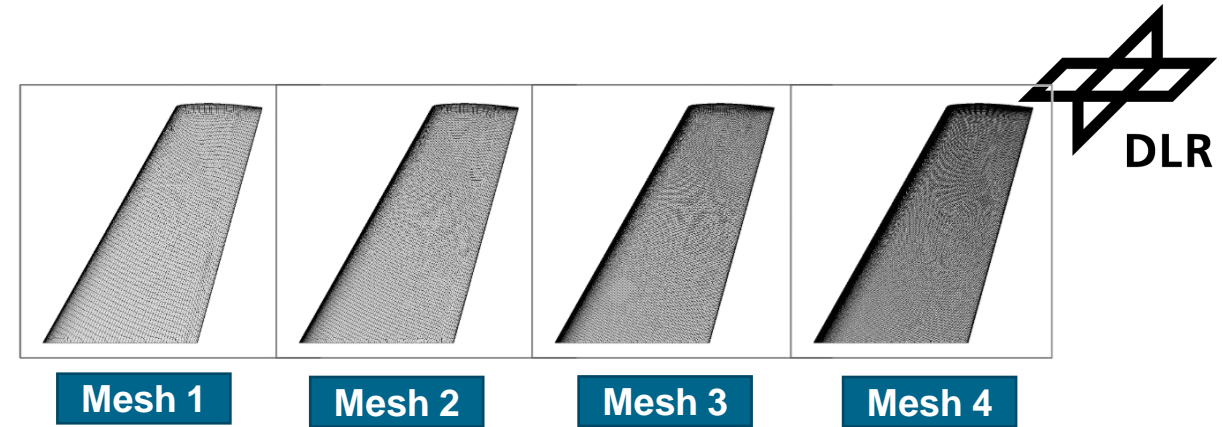
$$R_{ij,lim} = \frac{R_{ij}}{\sqrt{1 + \left(\frac{R_{ij}}{R_{ij,real}}\right)^2}}$$



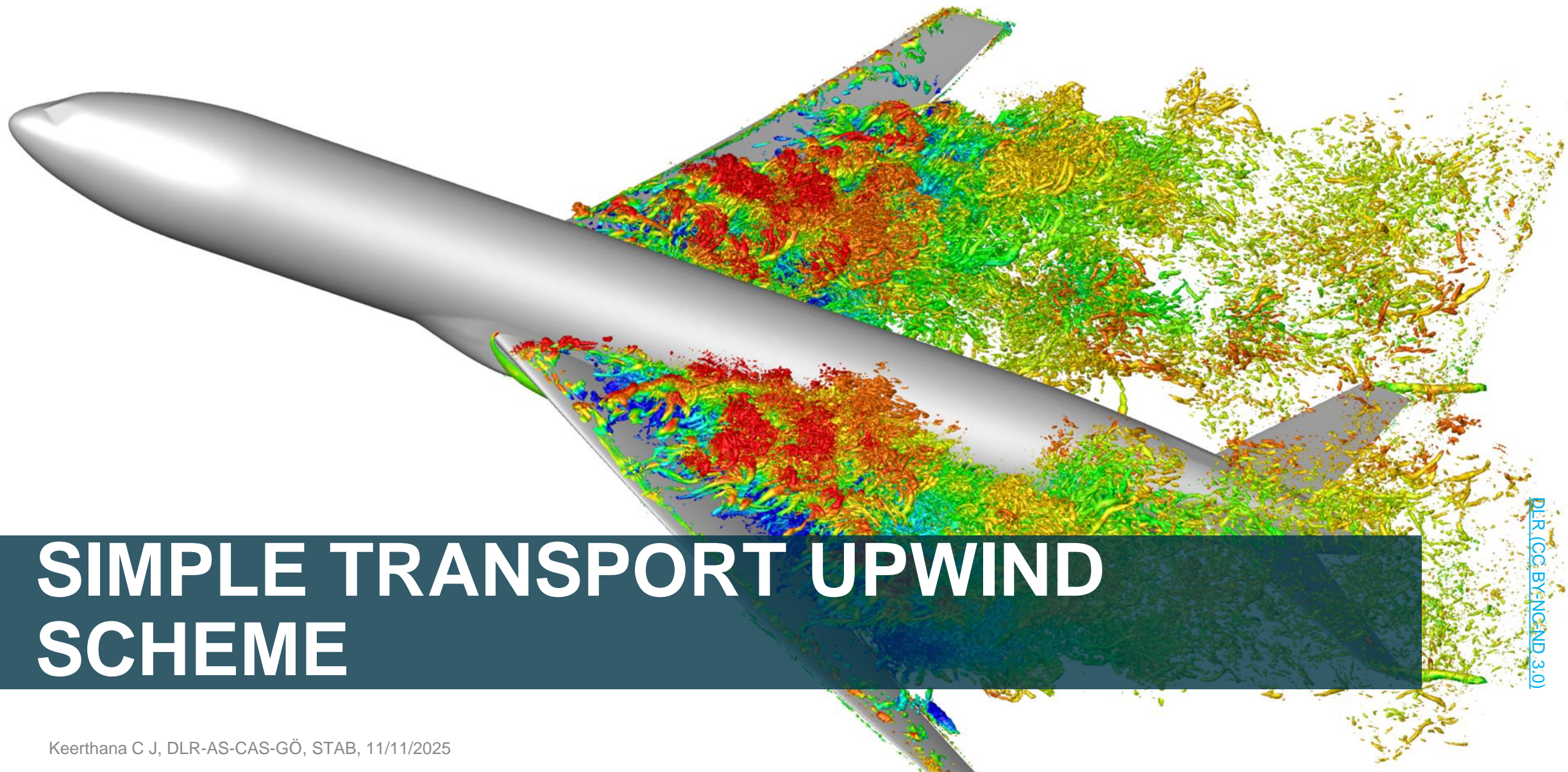
VERIFICATION OF 3D CASES AND WEAK COUPLING OF EQUATIONS

Verification of 3D cases ONERA M6

- Centaur meshes
- **Flow conditions:** $Ma = 0.84$, $\alpha = 3.06^\circ$, $Re = 14.6 \times 10^6$, $L_{Re} = 1$.
- Challenging to converge even with realizability constraints in place.
- Converged only with **LLF Upwinding** scheme for turbulence or with a **weak coupling** of the mean flow and turbulent equations.
- However, weak coupling approach for the equations did not always improve convergence.



Convergence plots for Mesh 1 with weak coupling



SIMPLE TRANSPORT UPWIND SCHEME

Simple upwinding scheme for turbulence equations

Previous Roe scheme for transport eqns. in CODA

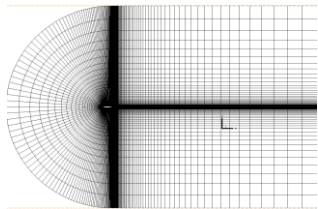
$$flux = \frac{1}{2} \left[(v_L(\rho\varphi)_L + v_R(\rho\varphi)_R) - \left| \left(\frac{(\rho v)_L + (\rho v)_R}{\rho_L + \rho_R} \right) \right|_{max} ((\rho\varphi)_R - (\rho\varphi)_L) \right]$$

Simple upwinding (from DLR-TAU)

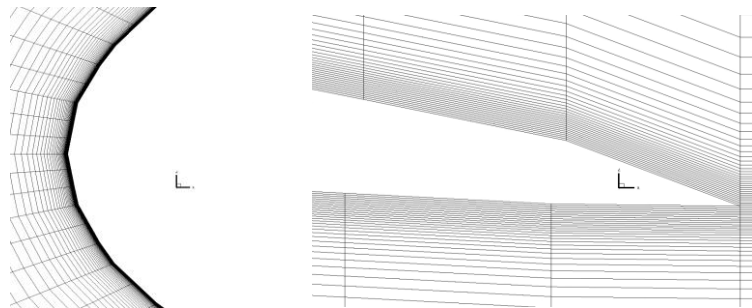
$$flux = \frac{1}{2} [(v_L + v_R)(\rho_L\varphi_L + \rho_R\varphi_R) - |(v_L + v_R)|(\rho_R\varphi_R - \rho_L\varphi_L)]$$

$L, R \rightarrow$ left, right fluxes, $v \rightarrow$ convective velocity, $\varphi \rightarrow$ turbulent variable

RAE2822

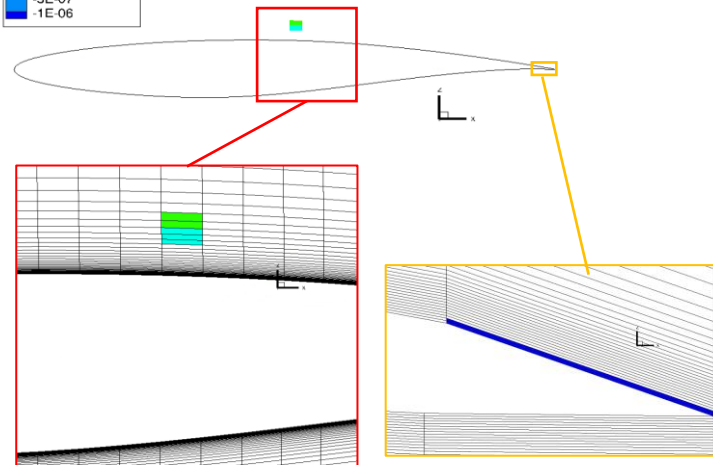
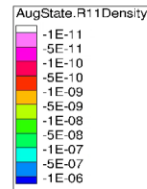


Thanks to Axel Probst for the idea! 😊



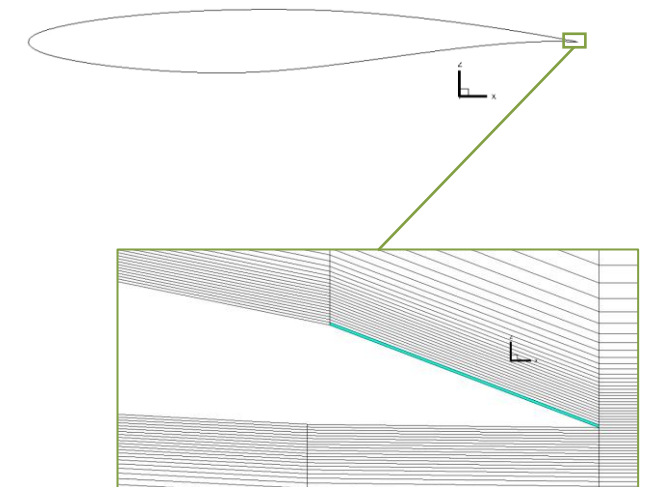
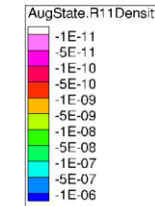
Not a perfect RAE2822 mesh!

Roe



Realizability violations in the shock region

Simple transport upwind

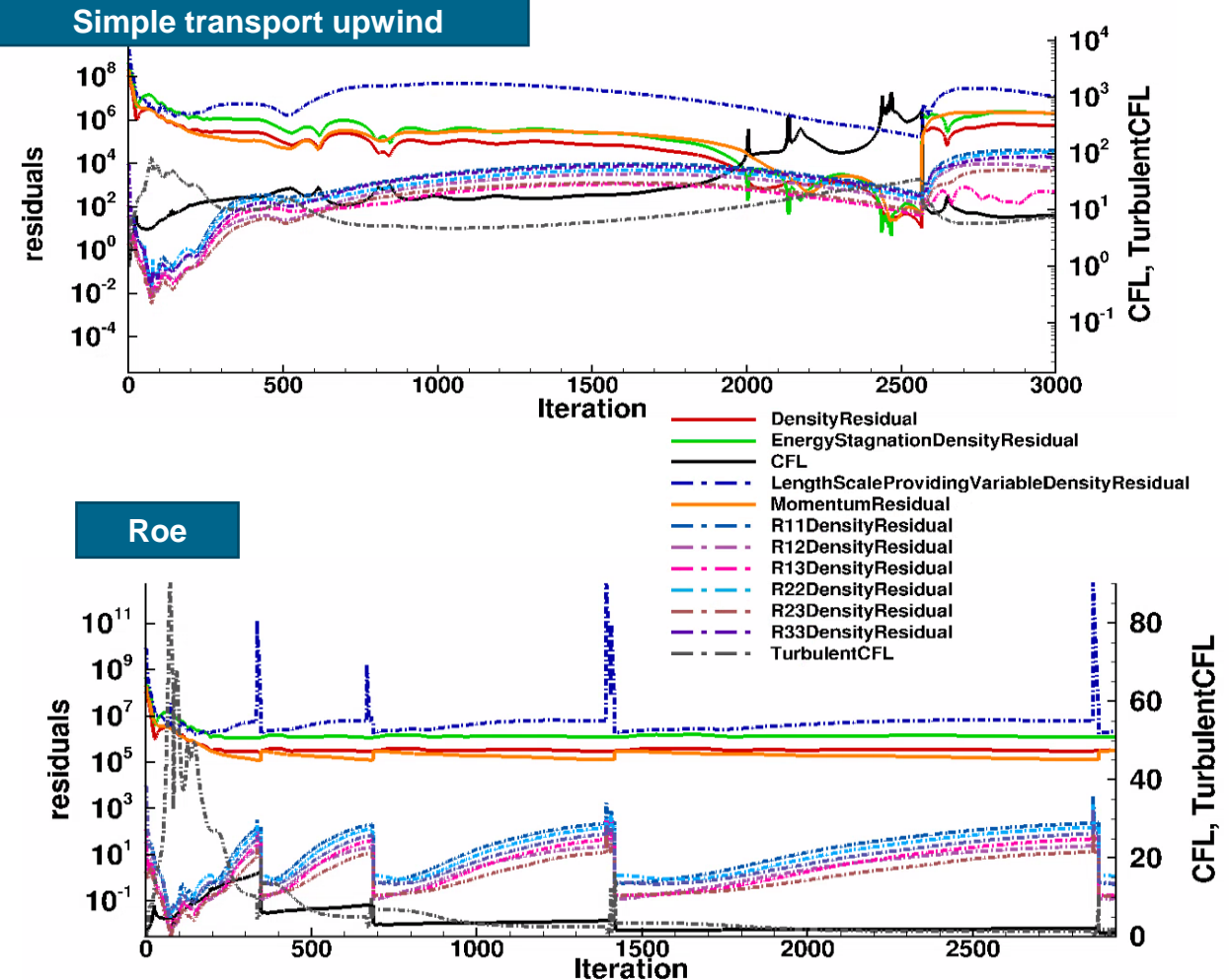


Simple transport upwind scheme

- 2D Bump in Channel converged for the first time with coupled solver approach.
- All the meshes of ONERA M6 converged for the coupled solver and also for second order (except finest mesh)!
- Turbulent CFL numbers can be higher (x2 or x3) compared to Roe scheme.

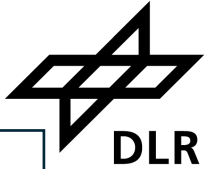
Thanks to Deepak Kunhappan for the combined framework of Simple Upwind scheme 😊

ONERA M6 – Mesh 3



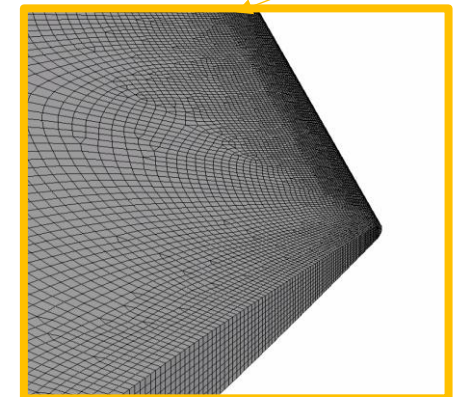
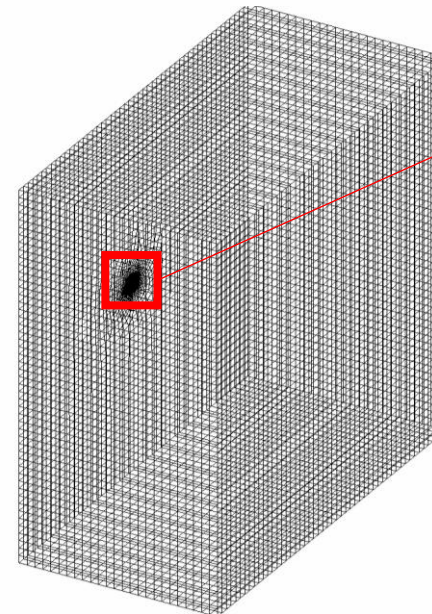
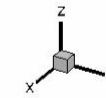
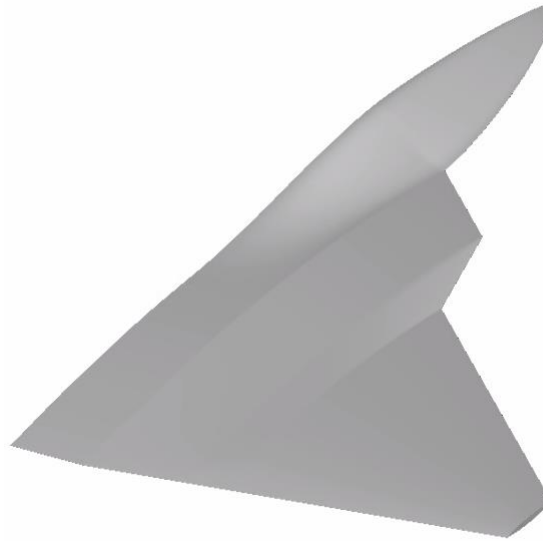
Verification of 3D cases

DLR – F23

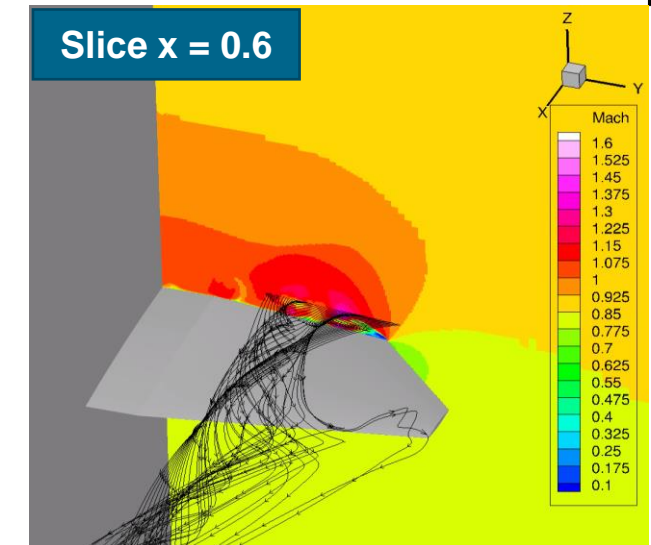
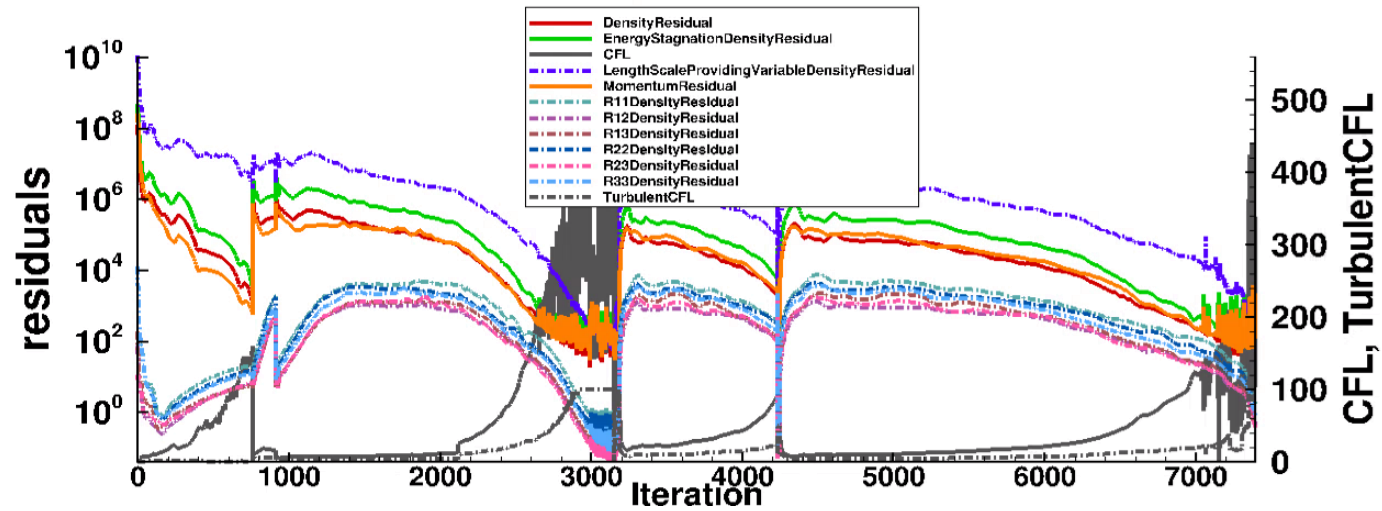


- Case & meshes from Michael Werner (DLR–AS-HGK): **Delta wing** with 32725358 hexas or 36267940 nodes – **ANSA hex-dominant mesh**
- **Flow conditions:** $Ma = 0.85, \alpha = 12^\circ, Re = 3022728.49491777, L_{Re} = 0.382$.
- **Dimensional specs:**
 $p = 37410.7109 \text{ kg/ms}^2, T = 270.8606 \text{ K},$
 $R = 287 \text{ m}^2/\text{Ks}^2, \text{grid unit length} = 0.382 \text{ m}$
- Initially tried to start with $\alpha = 12^\circ$ which failed for any run – weak coupling/coupled, LLF/Roe/Upwind. Restart from $\alpha = 9^\circ$ worked well for upwind scheme.
- For $\alpha = 12^\circ$, stalling of residuals with unsteadiness in the solution – vortex breakdown in the flow.

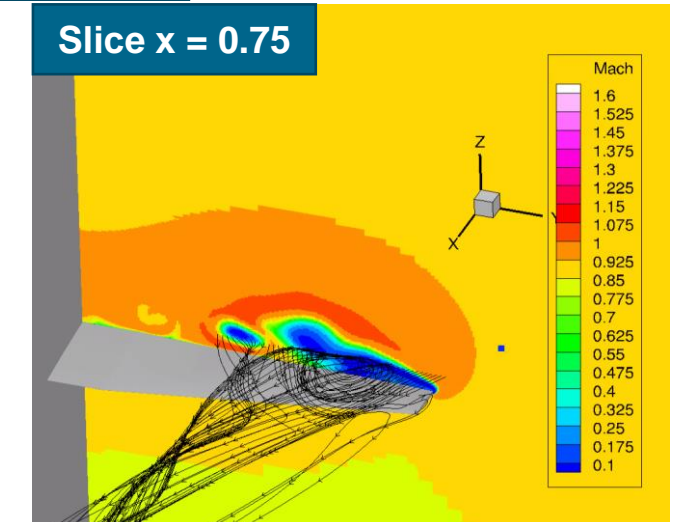
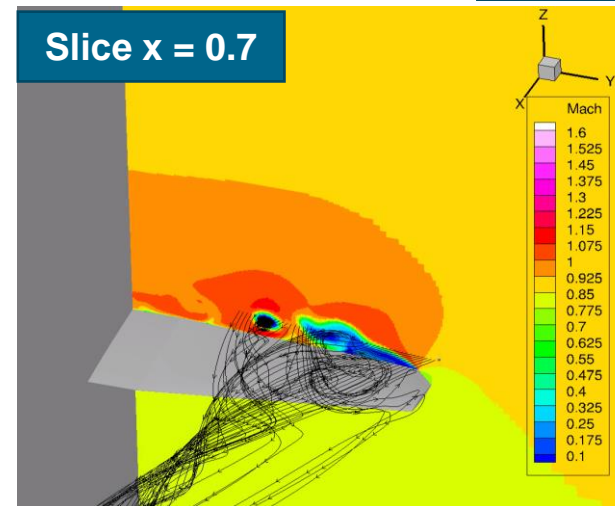
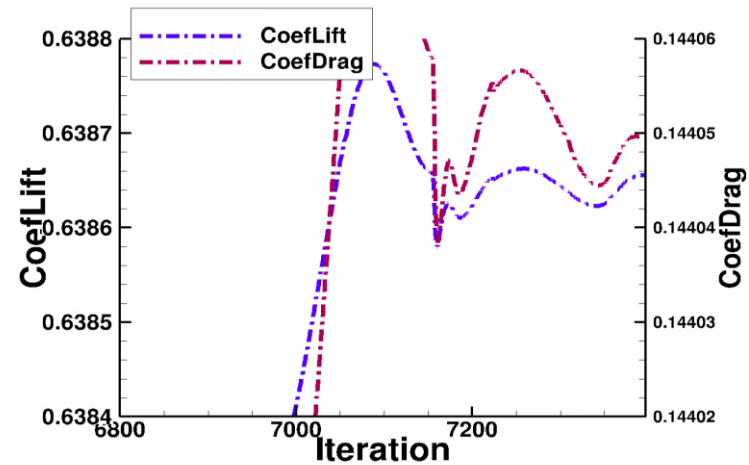
Thanks to Michael Werner for the case, mesh and his inputs for the analysis! ☺



DLR – F23 Results, $\alpha = 12^\circ$

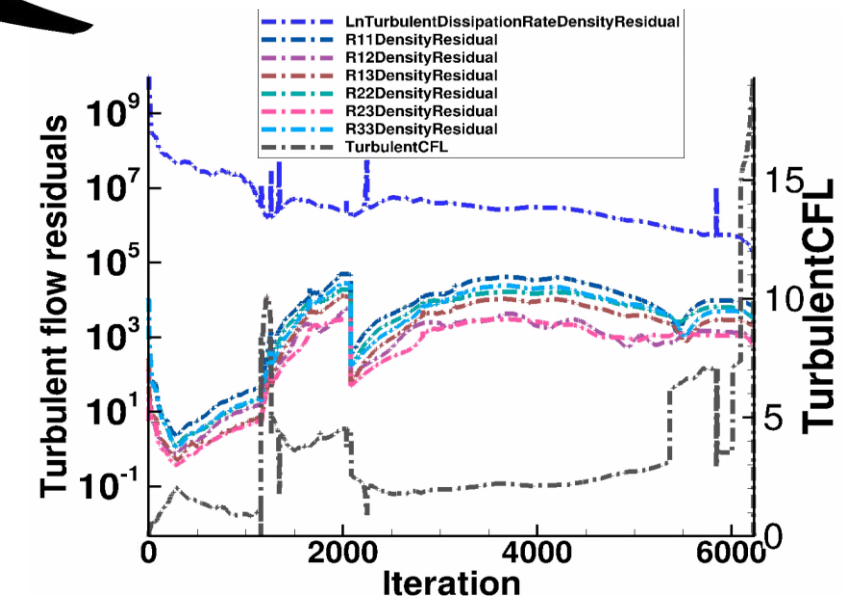
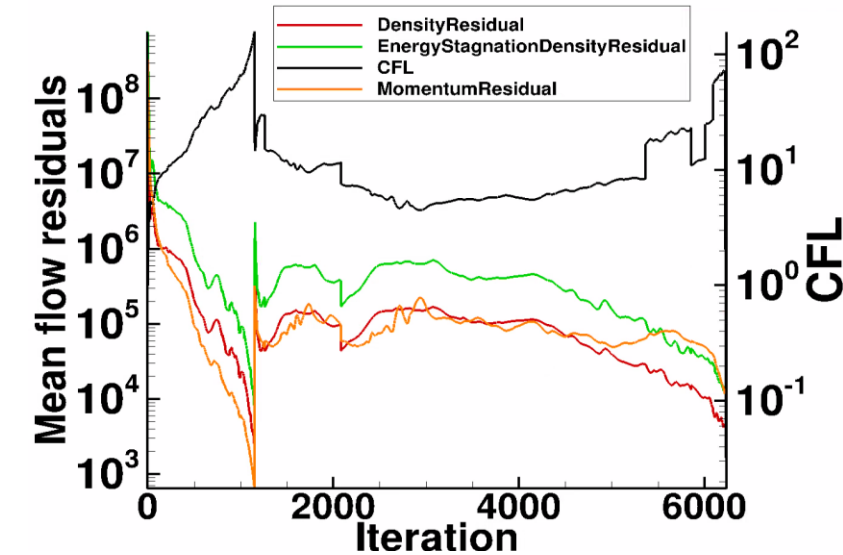
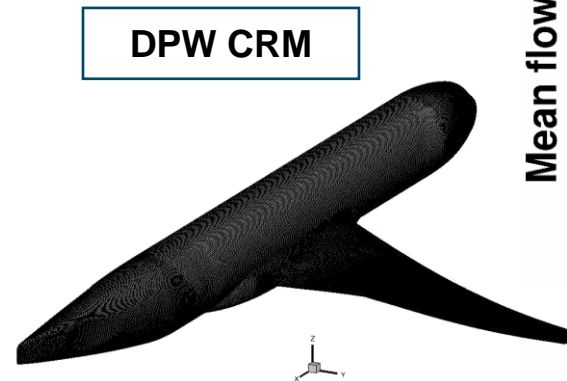


Vortex break down



Cases with convergence issues & challenges yet to be solved

- We may still have meshes/cases which don't converge
- **DPW CRM:** Mesh obtained from Tobias Knopp, results available for Tau for SST and RSM - wing body configuration, solar mesh
- **Flow conditions:** $Ma = 0.85$, $\alpha = 2.5^\circ$, $Re = 5 \times 10^6$, $L_{Re} = 0.18914364$.
- Appearance of **NaN** – Still under investigation!



- With every CODA version, we obtain improvements. A better convergence of RSM has been possible due to several additional improvements like CFL splitting, equations scaling etc. from other developers. Thanks to all CODA developers and verification engineers!
- A textbook implementation can lead to some struggles (Simple upwinding for turbulence).
- Further knowledge of implicit solvers for turbulence models is still needed – stability analysis for RSM in implicit solvers.
- **Appearance of NaN** is of primary concern. Weak coupling may help to improve but further tests are needed.
- **Linearization of source terms:** Previous attempts to linearize source terms were not that successful, a careful linearization may help.
- **Effect of linear solvers:** Algebraic multigrid may help to have better linear system convergence. With integration of Petsc interface, this can be tested.
- **Tackling the issue at discretization level:** Efforts are being undertaken currently for Eddy viscosity models (SST) in CODA, outcomes from these efforts can be extrapolated to RSM.

Special thanks to

- Tobias Knopp, Johannes Löwe for their ideas & support.
- Andreas Krumbein, Axel Probst for their guidance.
- Matthias Lühmann (Airbus) for meshes & verification activities.
- Roberto Sanchez, Deepak Kunhappan for their support with debugging & settings.

THANKS!

Thema: Progress with verification and stabilization of Reynolds stress models using the CFD Software by ONERA, DLR, Airbus (CODA)

Datum: 2023-11-11 (JJJJ-MM-TT)

Autor: Keerthana Chandrasekar Jeyanthi

Institut: DLR-AS-CAS-GÖ

Bildcredits: Alle Bilder „DLR (CC BY-NC-ND 3.0)“, sofern nicht anders angegeben