STAB Workshop, Göttingen, 5th November 2019

LU-SGS preconditioned Newton-Krylov solver applied to industrial relevant test cases

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DLR

Overview

- Objective
- Description of solution methods
- Numerical results
- Outlook

DLR-TAU Code

- Finite volume method with node centered scheme on unstructured meshes.
- Available solvers/accelerators: single grid (SG), multigrid (FAS), full multigrid (FMG), grid sequencing (GSeq).
- Primarily used solver/smoother is LU-SGS.
- TAU is used by various research institutions, universities and industry (Airbus,….)

Objective of this work

Improvement of the robustness and the efficiency of the TAU code for stationary RANS simulations of various aircraft configurations.

- Improvement of the stability of the multigrid method.
- Improvement of the nonlinear multigrid smoother.
- Implementation of the developments in the central TAU version.
- Demonstration of the efficiency and robustness improvements of the TAU code on specific test cases.

Backward-Euler method and LUSGS iteration

Discretized flow equations:

$$M\frac{dW}{dt} + R(W) = 0, \qquad M = \mathrm{diag}(vol(\Omega_i))$$

Backward-Euler method:

$$\left(\frac{M}{\Delta t} + \mathrm{J}\right)\Delta W = -R(W), \qquad W = W + \Delta W$$

with $A = \frac{M}{\Delta t} + \mathrm{J}$ and Jacobian matrix $J = \frac{dR}{dW}$. Recovers Newton‘s method for $\Delta t \rightarrow \infty$.

LUSGS iteration:

Replace exact Jacobian J by approximate $\tilde{J}$ including flux differences and eigenvalues:

$$\tilde{A} = \frac{M}{\Delta t} + \tilde{J} = \mathrm{L} + \mathrm{D} + \mathrm{U}$$

- Forward sweep: $(D + L)\Delta W^* = -R(W)$
- Backward sweep: $(D + U)\Delta W = D\Delta W^*$

Backward-Euler with LUSGS preconditioned GMRes

$$\left(\frac{M}{\Delta t} + \mathrm{J}\right)\Delta W = -R(W)$$

- Solve $Ax = b$ for x using the GMRes method.
- Use LUSGS (or an iterated version of it) as (linear) preconditioner of GMRes.

Matrix-free approximation to the Jacobian matrix:

Replace matrix-vector multiplication Jx by finite difference (FD) approximation:

$$Jx \approx \frac{R(W + hx) - R(W)}{h}$$

Advantages:

- (Hand-differentiated) Jacobian matrix not required
  - ➢ Significantly simpler implementation and lower memory requirements
- Same formula/code for all turbulence models

(Possible) disadvantage:

- FD gives an approximation only to J. Is it sufficiently good?
- Influence of step size h

FD for matrix-free Jacobian matrix-vector multiplication

$$Ax = \left(\frac{M}{\Delta t} + J\right)x$$

Approximation by forward difference:

$$Ax \approx \frac{M}{\Delta t}x + \frac{R(W + hx) - R(W)}{h}$$

$$h = \epsilon \cdot \frac{\left|\left|W\right|\right|_{l^2}}{\left|\left|x\right|\right|_{l^2}}$$

$$\epsilon = 10^{-8}$$

Switch-Evolution Relaxation (SER)

$$CFL = min\left\{CFL_{max}, CFL_{init} * CFL_{factor} * \left(\frac{\left\|R^{n,ref}\right\|_{l_2}}{\|R^n\|_{l_2}}\right)^{\alpha}\right\}$$

where

- $\alpha = \begin{cases} 1, & 2D\ laminar\ flows \\ 0.6, & 2D\ turbulent\ flows \\ 0.4, & 3D\ turbulent\ flows \end{cases}$
- CFL_{max} is the maximum allowed CFL value
- CFL_{init} is the initial CFL
- CFL_{factor} has default value = 1, might be reduced to $\frac{1}{2}, \frac{1}{4}$... in case of solver recovery
- $\|R^n\|_{l_2}$ is the l_2-norm of the residual computed after the nth nonlinear iteration
- $\left\|R^{n,ref}\right\|_{l_2} = \|R^{\infty}\|_{l_2}$ is the l_2-norm of the freestream residual on the (currently finest) grid

Residual Smoothing [Mavripilis]

- Smooth transition
  - from an explicit iteration scheme (known to provide good initial convergence)
  - to an increasingly implicit scheme (Backward Euler / Newton method).
- Ensure smooth residual field, thus producing smooth updates to the solution vector.

$$\left(\frac{M}{\Delta t}+\frac{\partial R(W^n)}{\partial W}\right)\Delta W^n = -R(W^n)$$

$$\left(\frac{M}{\Delta t}+\frac{\partial R(W^n)}{\partial W}\right)\Delta W^n = -R(W^n) - P^{-1}\frac{M}{\Delta t}R(W^n)$$

$$\left(\frac{M}{\Delta t}+\frac{\partial R(W^n)}{\partial W}\right)\Delta W^n = -\left[I + P^{-1}\frac{M}{\Delta t}\right]R(W^n)$$

$P - preconditioning\ matrix$

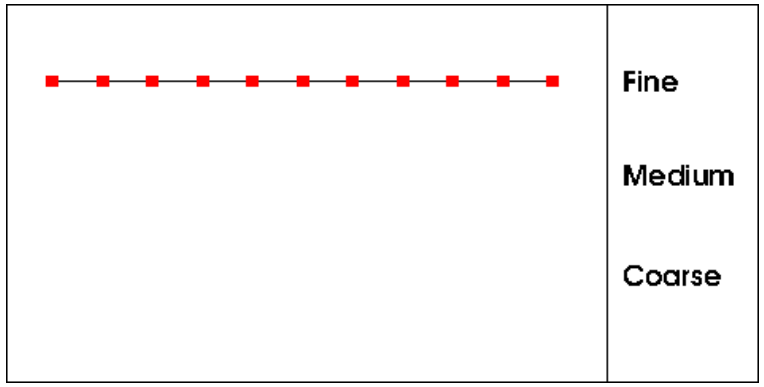
$M - mass\ matrix$

- Left hand side Jacobian of the systems remains identical.
  - implementation is relatively straight-forward.
- Choice of preconditioners (explicit or slightly implicit iteration schemes)
  - Runge-Kutta, **LU-SGS**, **SGS**, nonlinear multigrid.

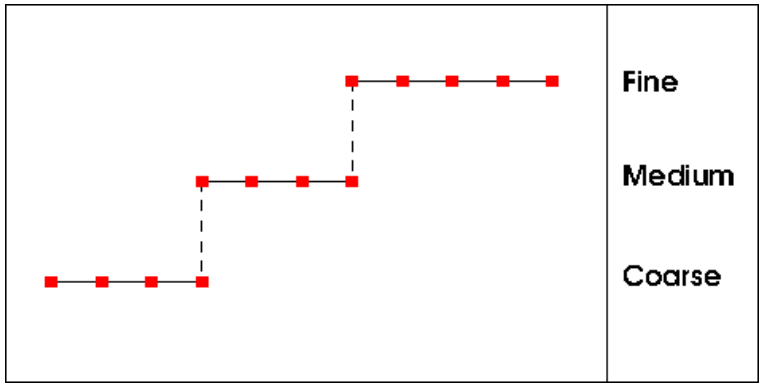
Mavriplis, D. J., A Residual Smoothing Strategy for Accelerating Newton Method Continuation, arXiv:1805.03756v1, May 2018.

Backward-Euler as SG solver or FAS smoother

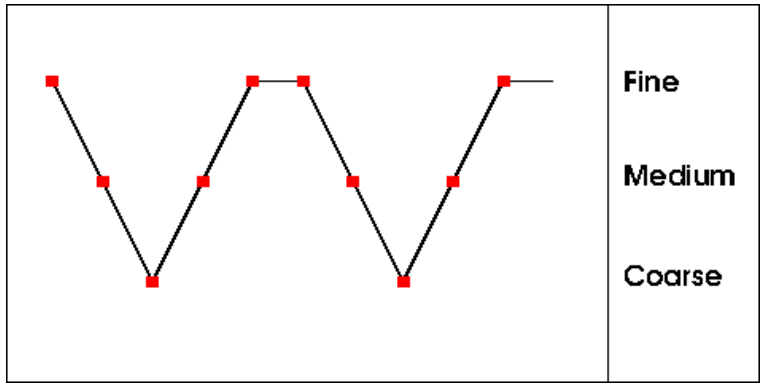
Single grid, SG



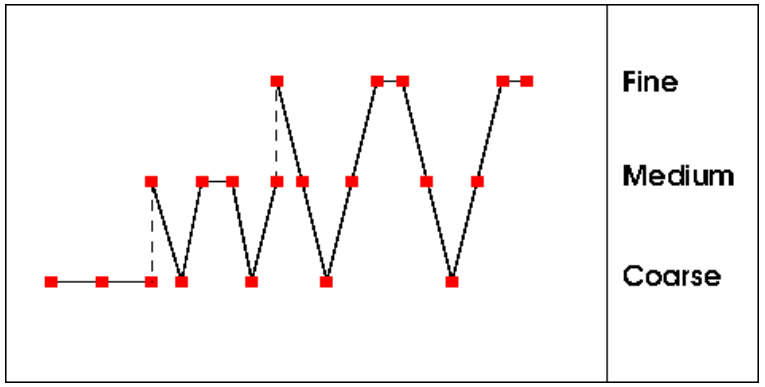
Grid sequencing, GSeq



Nonlinear multigrid
Full approximation scheme, FAS



Full multigrid, FMG (= GSeq x FAS)



Complex geometry, SA-neg: Grid 2 (~63e6 points) mesh

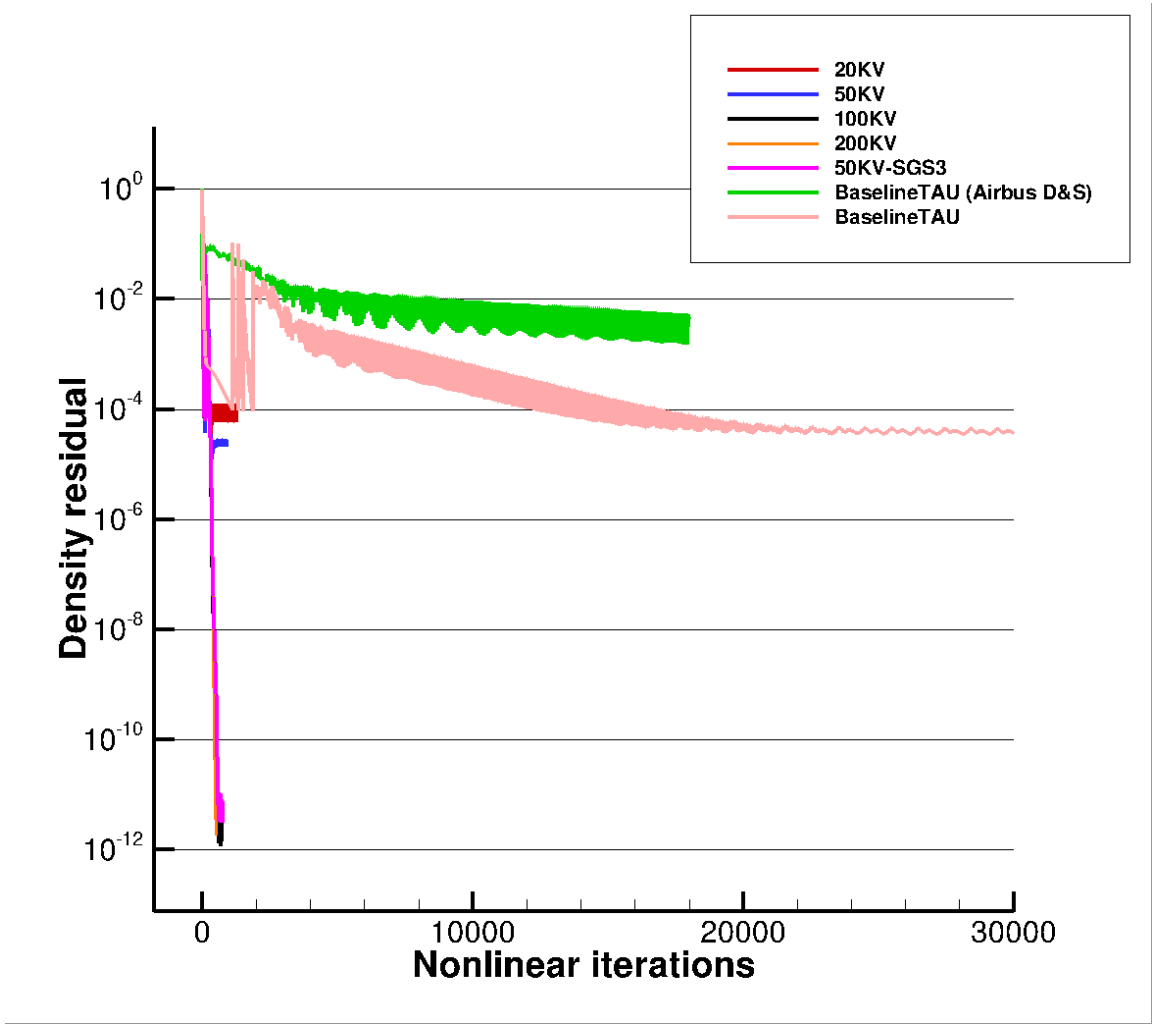
Complex geometry, SA-neg: Case description

		CFL ramping	
Flow equations	$RANS$	CFL_max	10^6
Turbulence model	$SA - neg$	α	0.4
Flow Conditions		**Residual tolerances**	
Reynolds Number (Re)	$3.4 \cdot 10^6$	$fine\ grid$	$10^{-11}\ (Grid\ 1)$ $10^{-8}\ (Grid\ 2)$
Angle of Attack (AoA)	20°	$coarse\ grids\ (in\ multigrid)$	10^{-3}
Mach number (M)	0.15	$linear\ solver\ (GMRes)$	10^{-8}
		Preconditioner	$LUSGS, SGS$

Complex geometry, SA-neg:

	Grid 1 (~23e6 points) $\mathrm{CFL_{init}}$= 1.2 FMGV5	Grid 2 (~63e6 points) $\mathrm{CFL_{init}}$= 1.2 FMGV5
	Iterations till convergence	**Iterations till convergence**
Baseline TAU	Stalled (1e-4)	-
20, 80	Stalled (1e-4)	-
50, 200	519 (SGS 3)	-
100, 400	487	Stalled (1e-6)
200, 800	447	548

Complex geometry, SA-neg: Grid 1 (~23e6 points)



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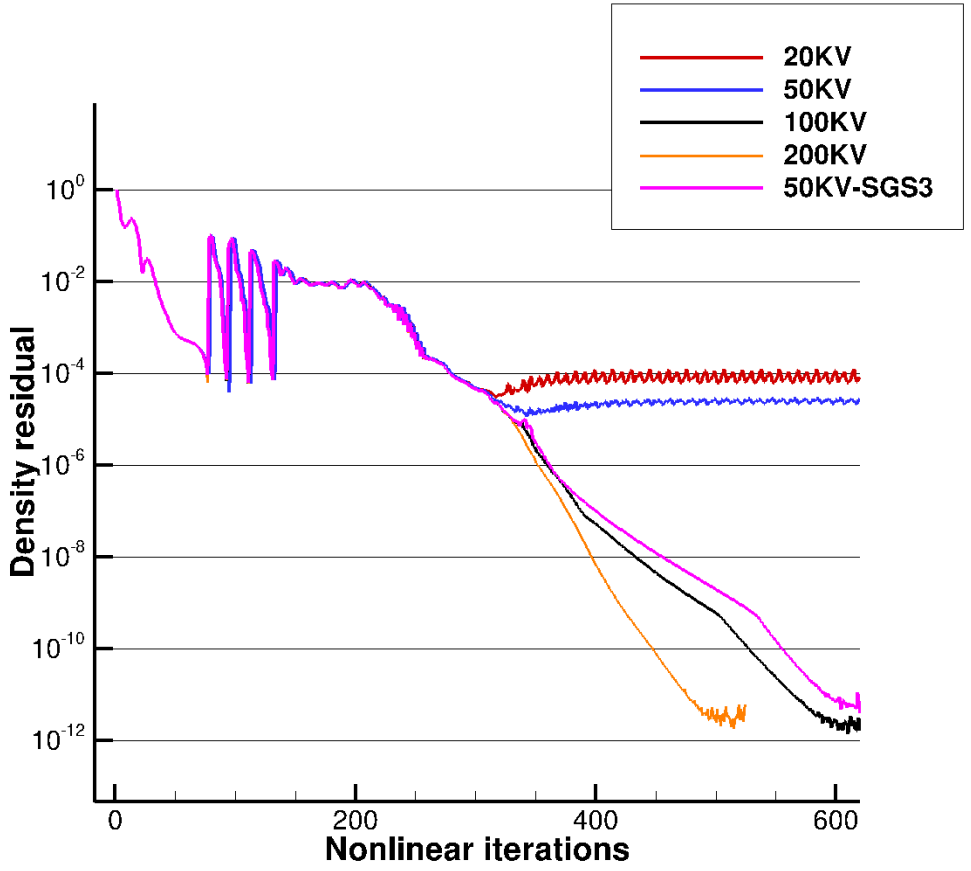
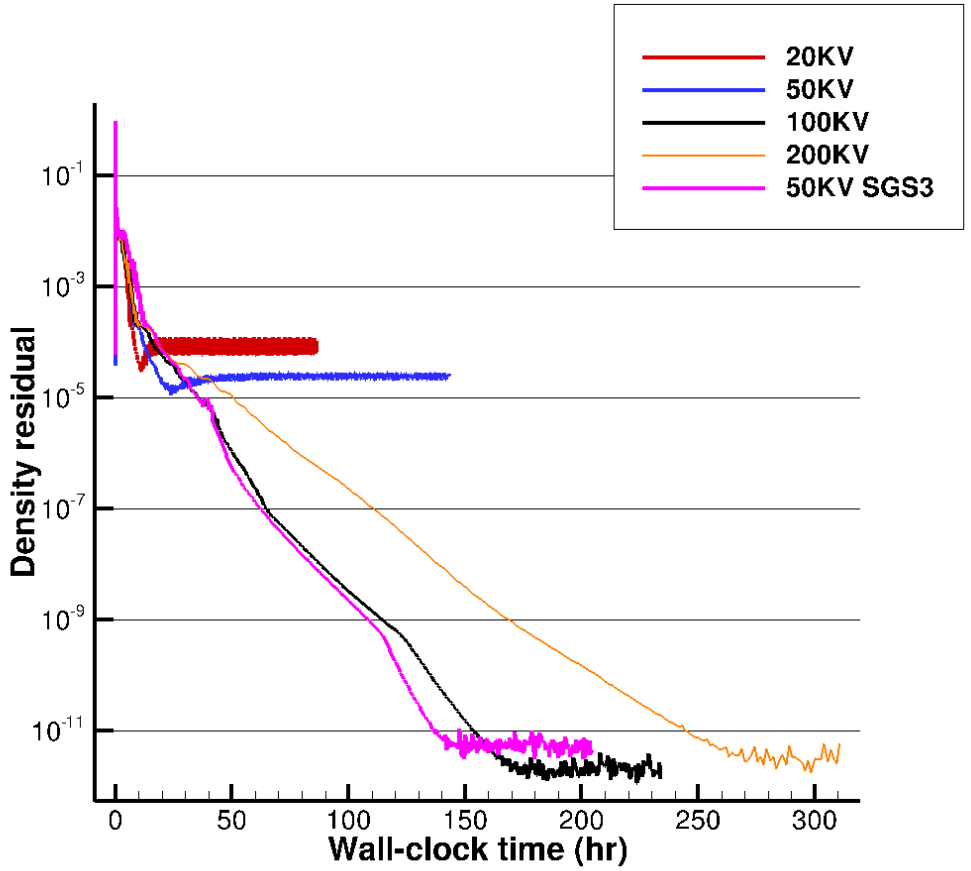
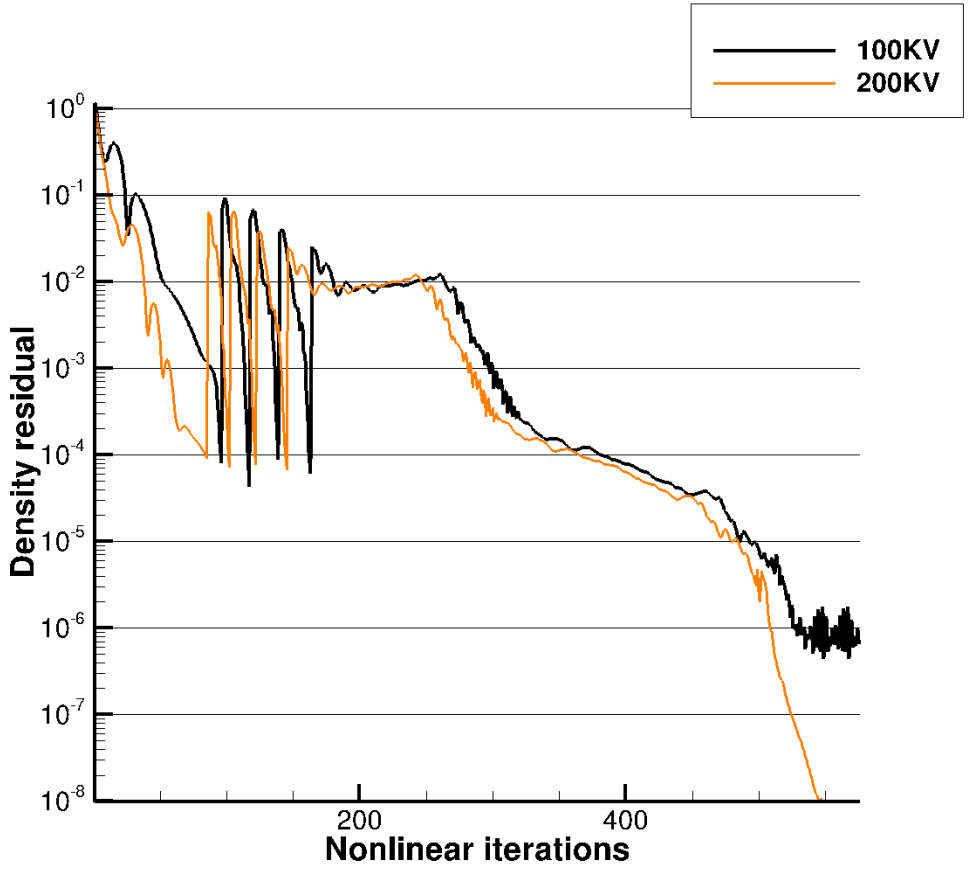
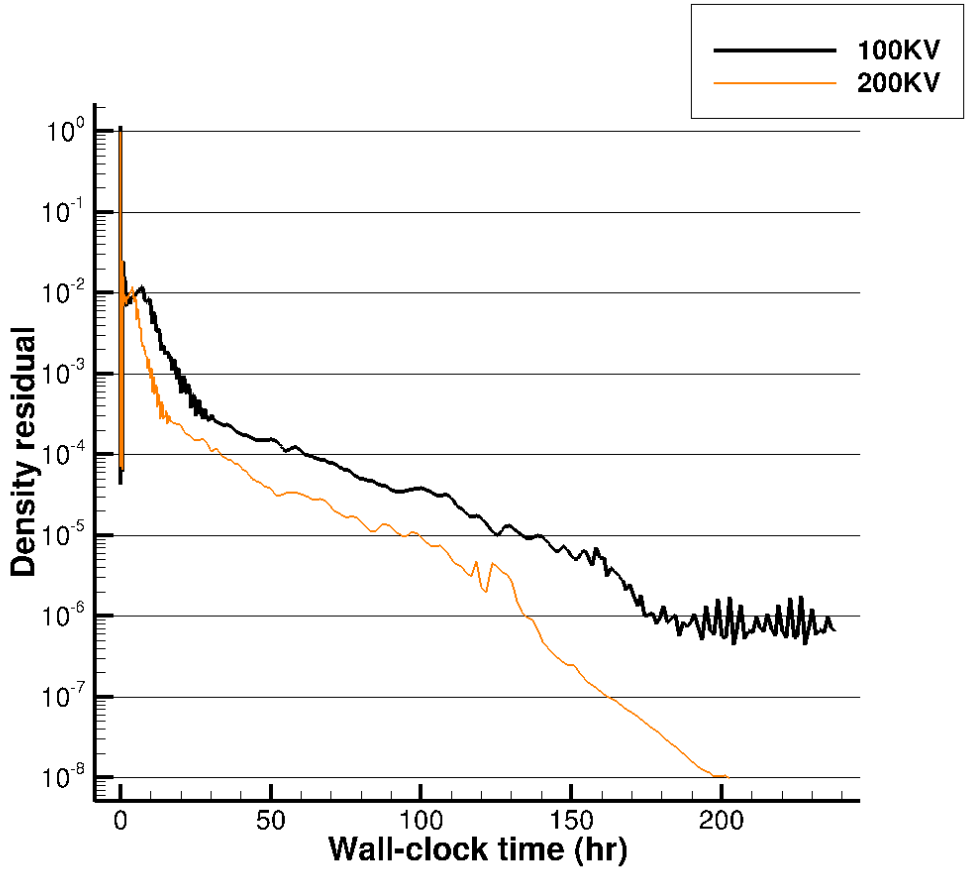


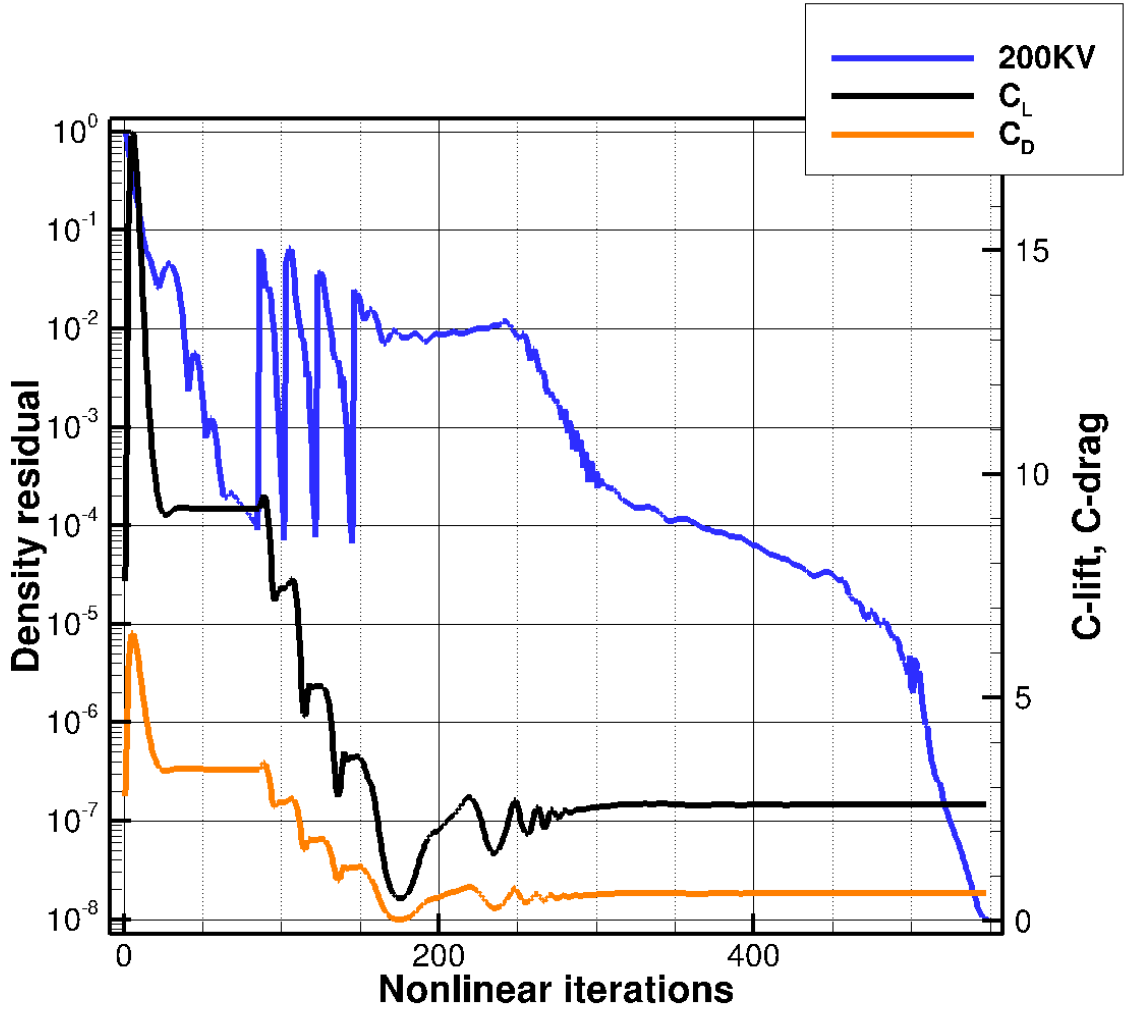


Complex geometry, SA-neg: Grid 2 (~63e6 points)

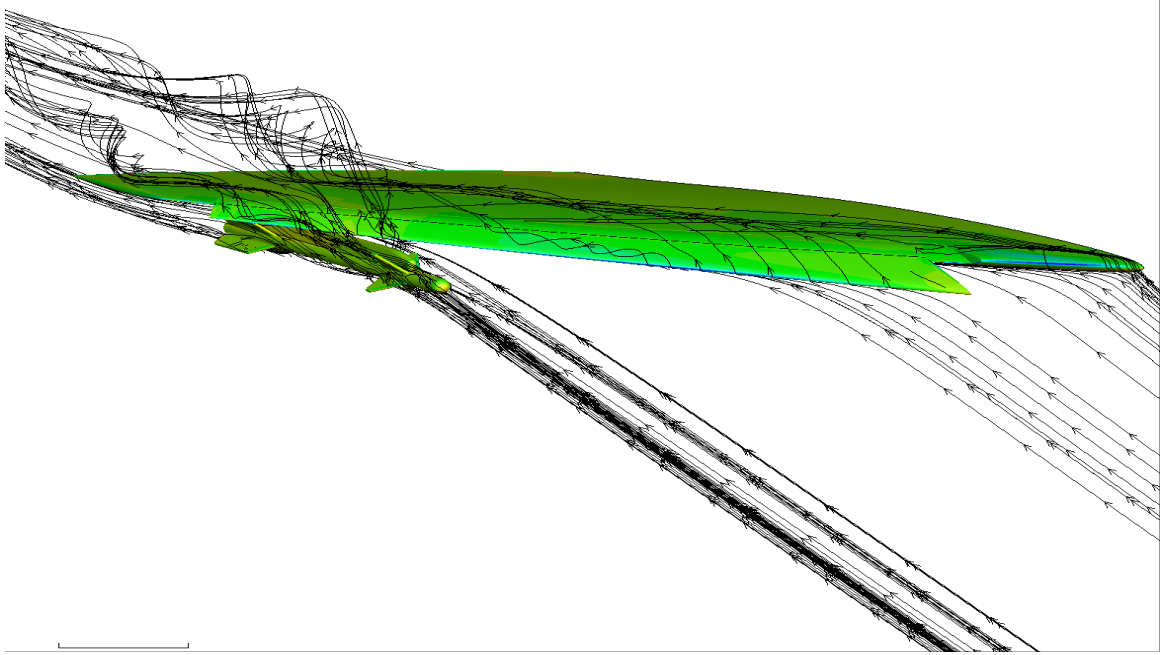


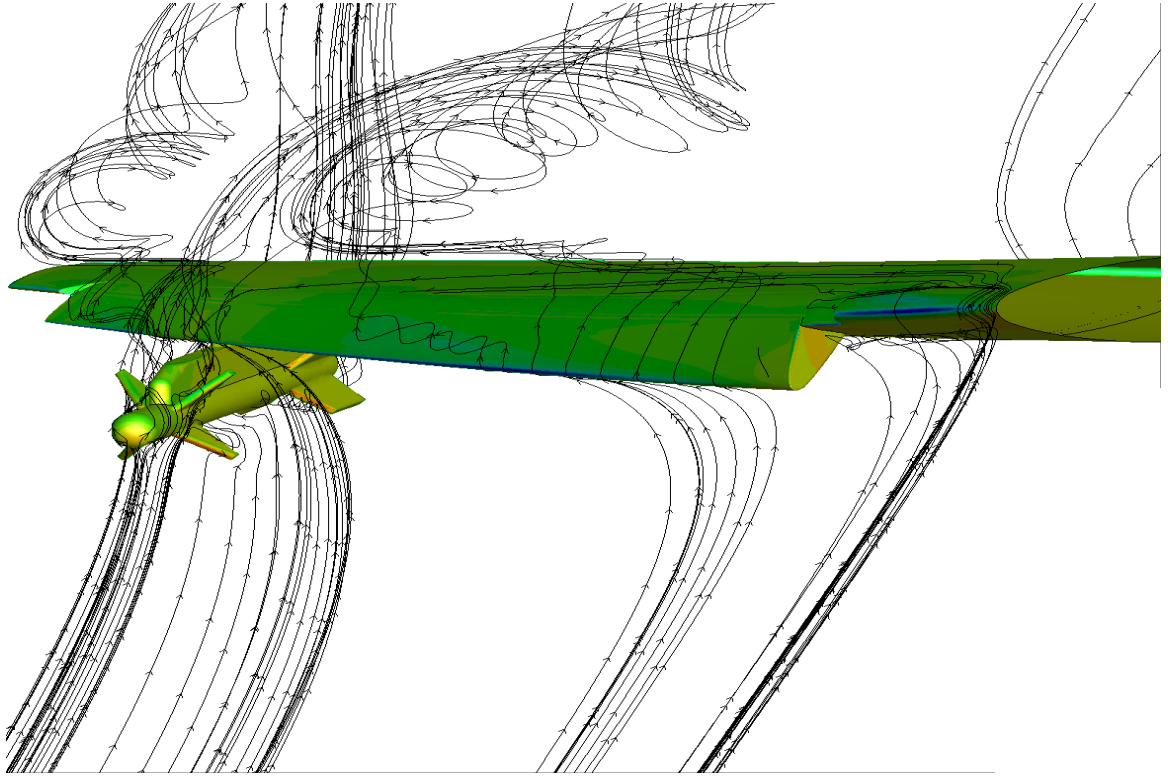


Complex geometry, SA-neg: Grid 2 (~63e6 points)



Complex geometry, SA-neg: Grid 2 (~63e6 points)





VFE-2, SA-neg: Grid 4 (~10e6 points): mesh

VFE-2, SA-neg: Case description

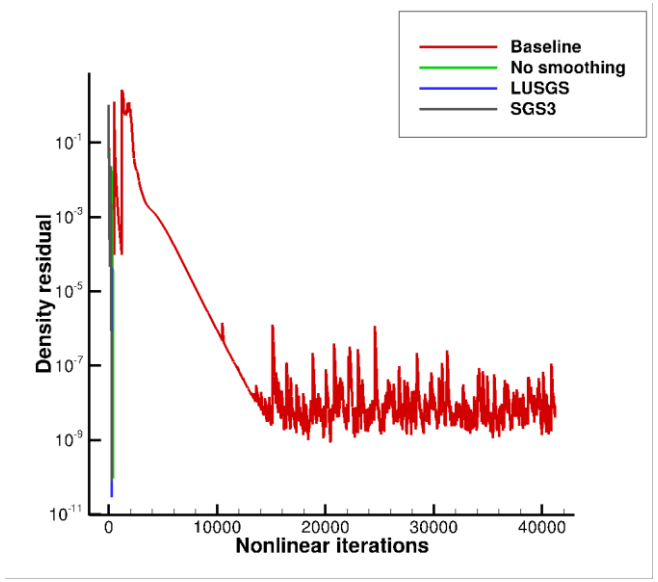
		CFL ramping	
Flow equations	$RANS$	CFL_max	10^6
Turbulence model	$SA - neg$	α	0.4
Flow Conditions		**Residual tolerances**	
Reynolds Number (Re)	$59.5 \cdot 10^6$	$fine\ grid$	10^{-10}
Angle of Attack (AoA)	24.7°	$coarse\ grids\ (in\ multigrid)$	10^{-3}
Mach number (M)	0.869	$linear\ solver\ (GMRes)$	10^{-8}
		Preconditioner	$LUSGS$

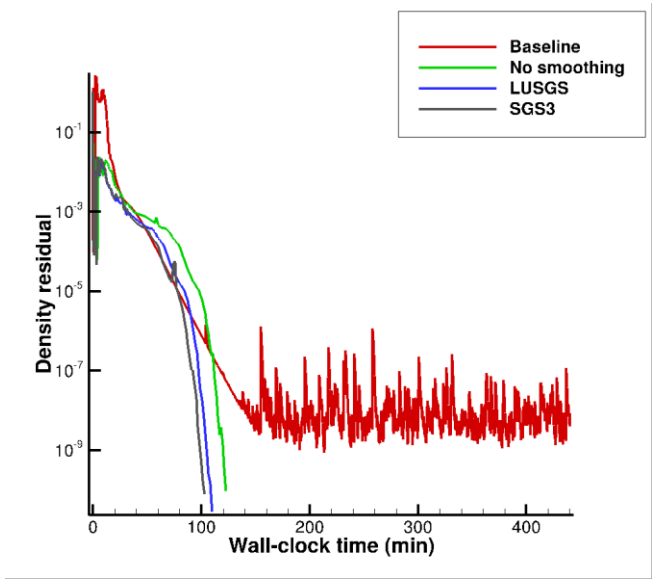
VFE-2, SA-neg:

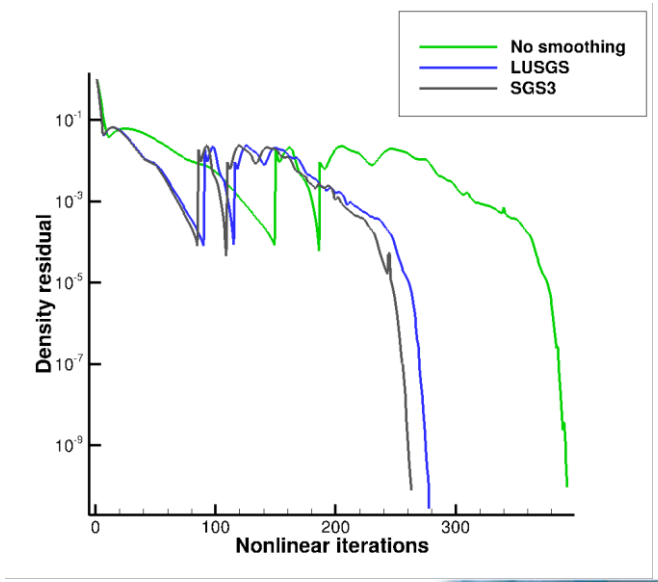
		Grid 1 (~208K points) FMGV3	Grid 2 (~802K points) FMGV3	Grid 3 (~4.6e6 points) FMGV5	Grid 4 (~10e6 points) FMGV5	Grid 5 (~30.9e6 points) FMGV5
		CFL_{init}=1	CFL_{init}= 1	CFL_{init}= 1	CFL_{init}= 1	CFL_{init}= 1
		50 Krylov vectors, 200 GMRes iterations				
Baseline TAU	No. of iterations	~	~	~	~	~
No smoothing		393	647	1854	19594	45670
LUSGS smoother		278	438	568	1819	11140
SGS 3 smoother		263	677	532	10207	4964
SGS 6 smoother		182 (diverged)	403	1232	729	13133

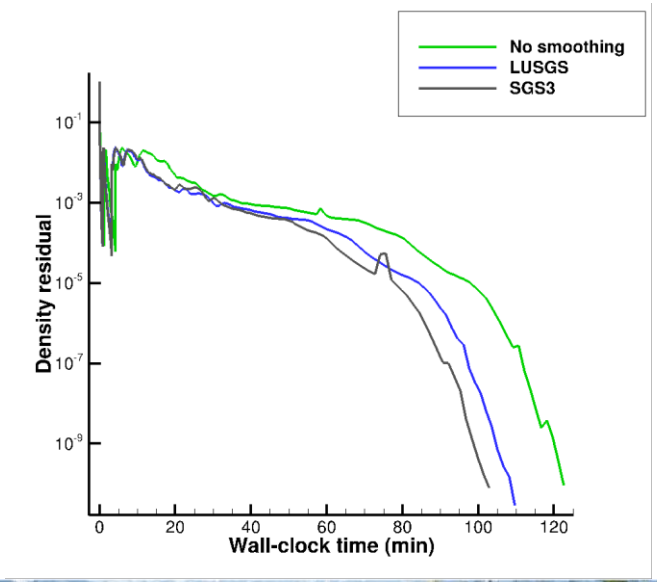
- Residual smoothing helps in all the computations.
- Smoother best practice: unclear.

VFE-2, SA-neg: Grid 1 (~208k points): Residual smoothing

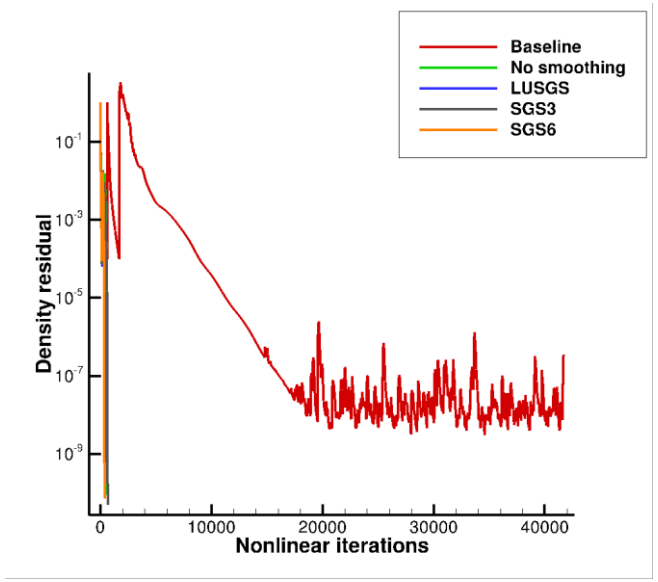


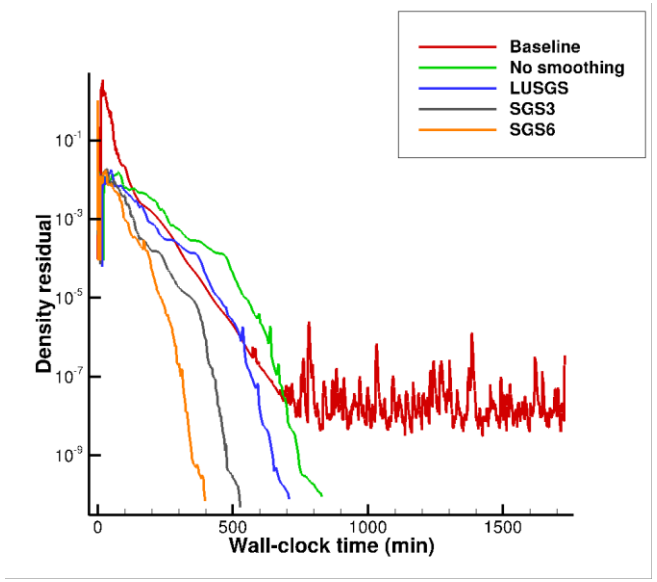


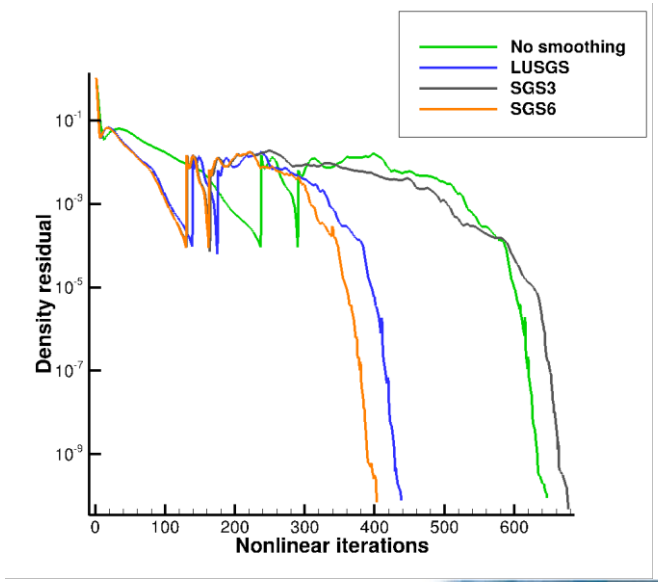


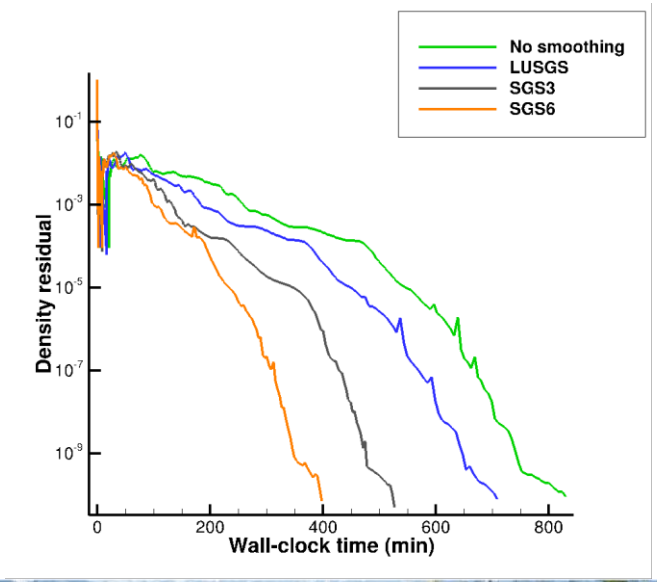


VFE-2, SA-neg: Grid 2 (~802k points): Residual smoothing

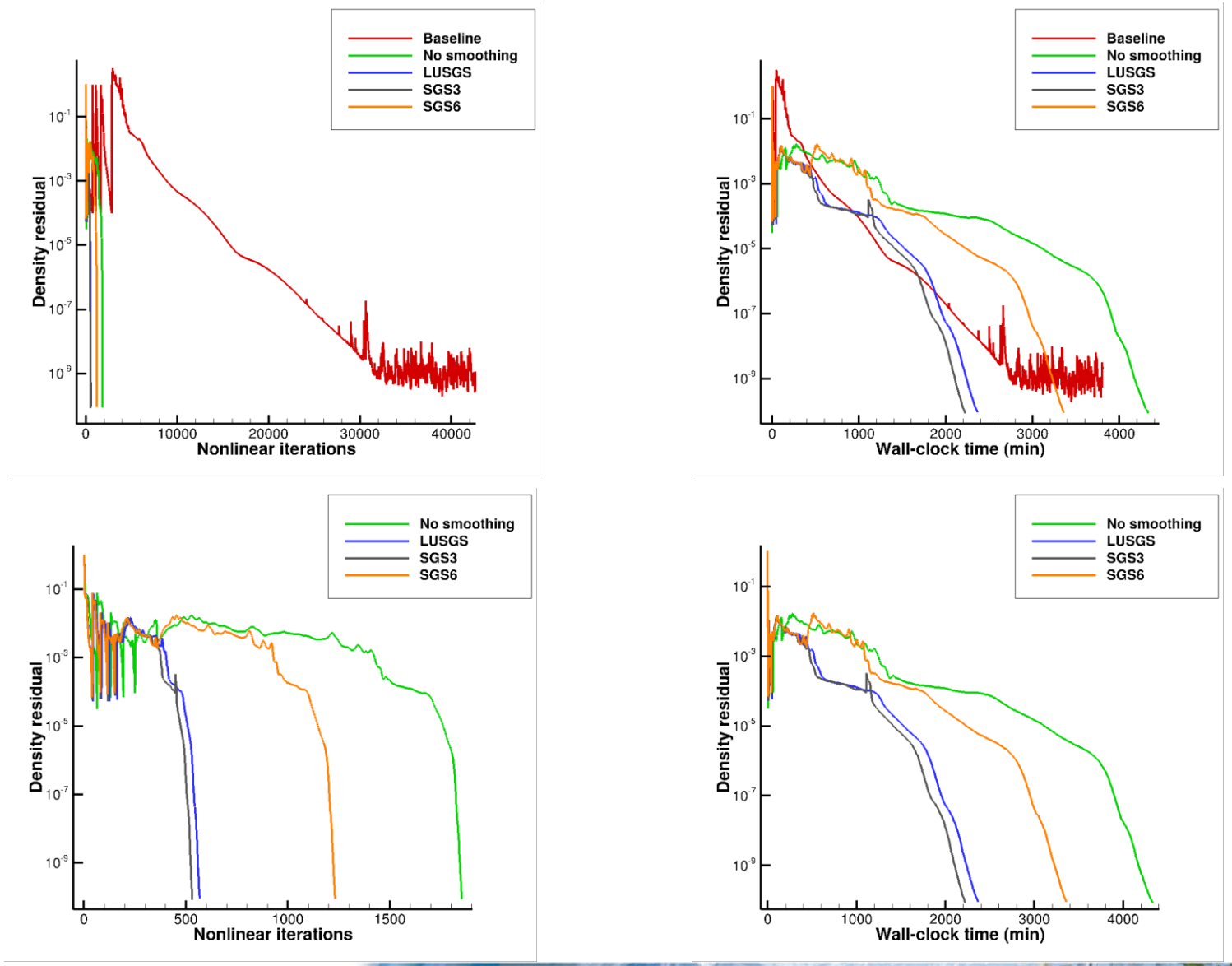




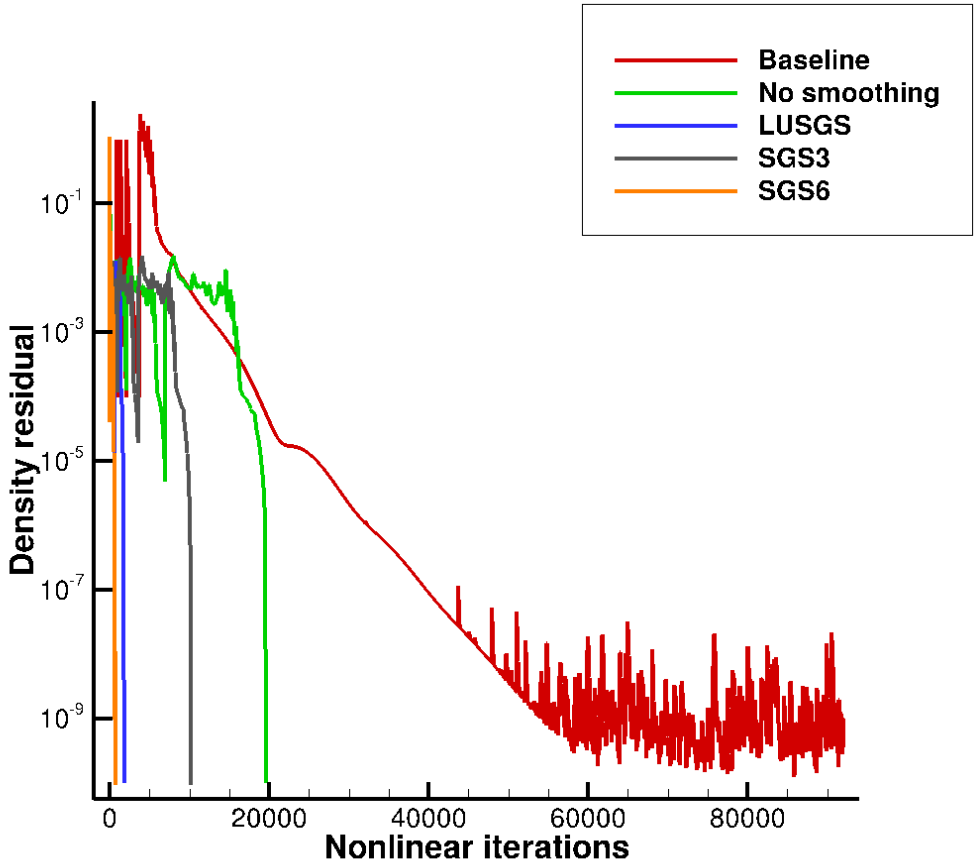


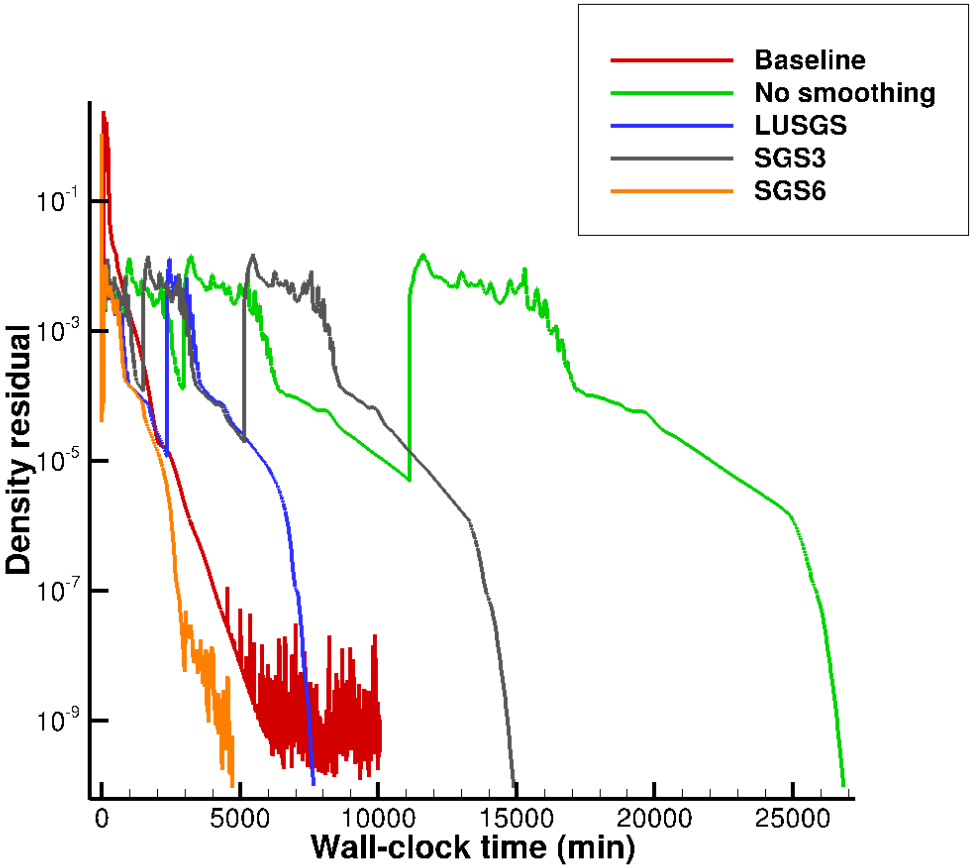


VFE-2, SA-neg: Grid 3 (~4.6e6 points): Residual smoothing

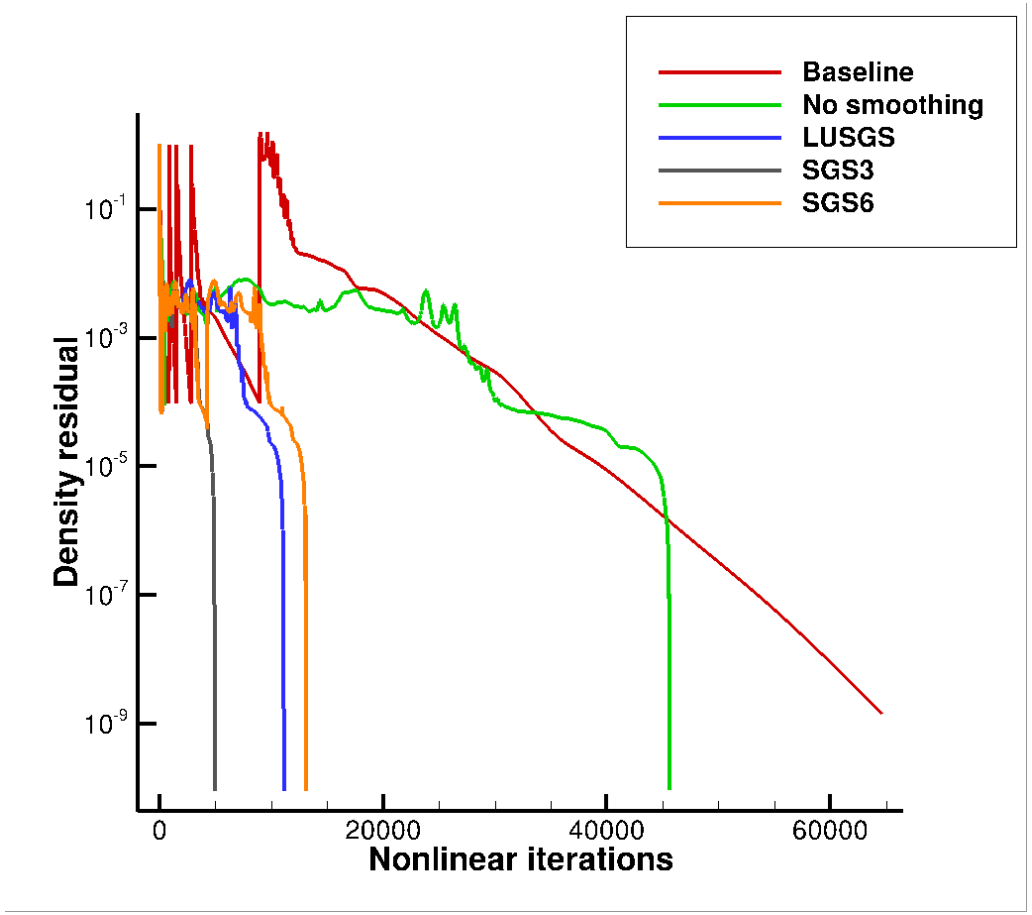


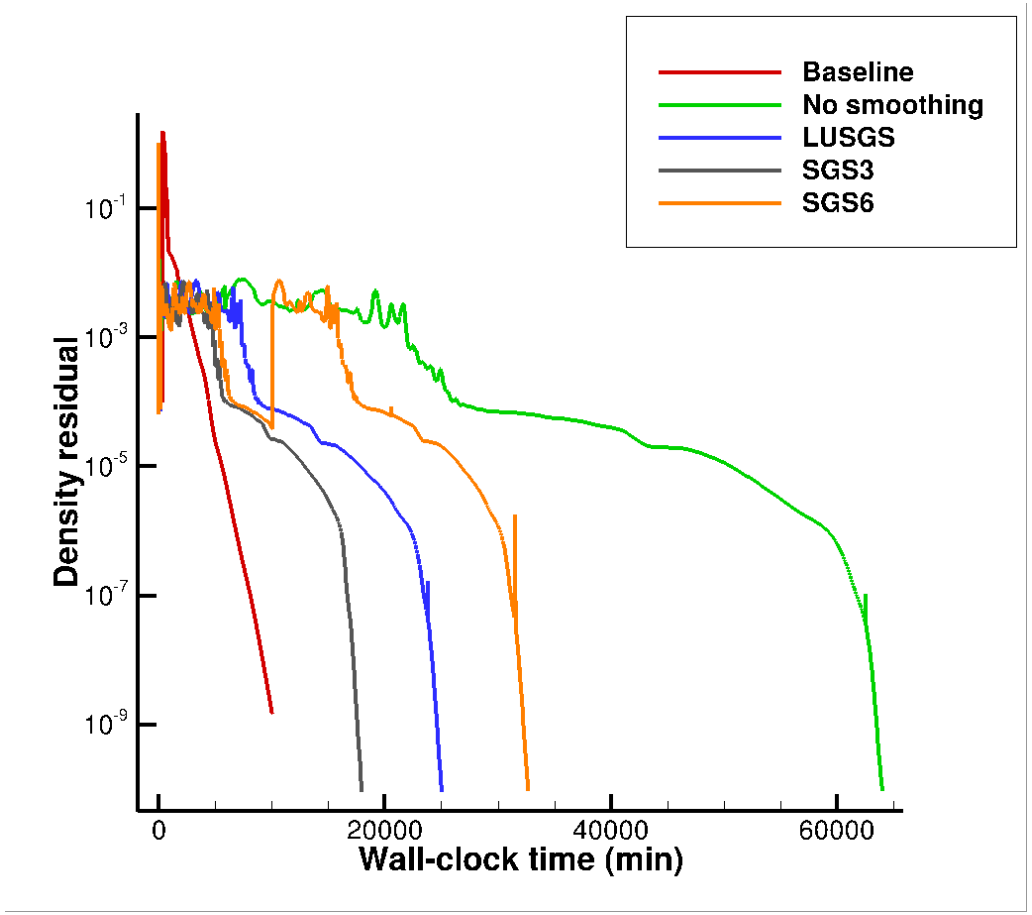
VFE-2, SA-neg: Grid 4 (~10e6 points): Residual smoothing





VFE-2, SA-neg: Grid 5 (~30.9e6 points): Residual smoothing





Outlook

- Integration into the TAU central version.
- Application to further test cases.
- Extension to the $k - \omega$ and RSM turbulence models.

Thank You
Questions ?