Rapid Convergence using Implicit Smoothing with Runge-Kutta Schemes for Navier-Stokes

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Eli Turkel

Introduction

- Efficiency is a challenge with increasing
  - Problem Size
  - Flow Complexities
- Improvements in computational efficiency
  - Multigrid
  - Local Time Stepping
  - Implicit Residual Smoothing
- Explicit time marching Runge-Kutta scheme
- Space centered or upwind schemes

RK/implicit smoother scheme

- RK/Implicit smoother scheme finite volume + source terms
- Extension to turbulent flow
- Extension to chemical reactions
- Time dependent - dual time step

Navier-Stokes Equations

The Navier-Stokes (N-S) equations for the conservative variables:

$$Q = \{\rho_1 \quad \rho_2 \quad \ldots \quad \rho_n \quad \rho u \quad \rho v \quad \rho w \quad \rho e\}^T$$

N-S equations in conservative form:

$$\frac{\partial Q}{\partial t} + \frac{\partial (F - F_V)}{\partial x} + \frac{\partial (G - G_V)}{\partial y} + \frac{\partial (H - H_V)}{\partial z} = S$$

- *F , G and H* are the inviscid fluxes
- F_v , G_v *and* H_v are the viscous fluxes

k-ω SST Turbulent model

- In turbulent flow, the viscosity is the sum of the laminar and the turbulent viscosity

- In addition to N-S equation we solve the k-ω SST turbulence model equations -

$$\frac{\partial k}{\partial t} + \vec{u} \cdot \nabla k = P_k - \beta^* k\omega + \frac{\partial}{\partial x_j}\left[\left(\nu + \sigma_k \nu_T \right) \frac{\partial k}{\partial x_j} \right]$$

$$\frac{\partial \omega}{\partial t} + \vec{u} \cdot \nabla \omega = \alpha S^2 - \beta \omega^2 + \frac{\partial}{\partial x_j}\left[\left(\nu + \sigma_\omega \nu_T \right) \frac{\partial \omega}{\partial x_j} \right] + 2\left(1 - F_1\right)\sigma_{\omega 2} \frac{1}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}$$

The turbulent viscosity μ_t is given by

$$\mu_t = \rho \nu_T = \frac{\rho a_1 k}{\max\left(a_1 \omega, SF_2\right)}$$

- k and ω are the model variables,
- S is the magnitude of the vorticity,
- $F_{1,2}$ are dump functions,
- v, v_T are the laminar and turbulent viscosity parameters

Real gas equation of state

The equation of state is

$$P = \frac{\rho RT}{W} = RT \sum_{i=1}^{n} \omega_i$$

with the mean molecular weight

$$W^{-1} = \sum_{i=1}^{n} \frac{\rho_i}{\rho} \frac{1}{w_i}$$

Chemical reactions source terms

The source term vector, S, describes the rate of change of species k:

$$\dot{\rho}_k = \frac{\mathrm{d}\rho_k}{\mathrm{dt}} = w_k \dot{\omega}_k \qquad \dot{\omega}_k = \sum_{i \in \text{all reactions}} \nu_{ik} q_i \qquad \mathrm{k} = 1,2,\ldots,\mathrm{N}$$

where ω_k and w_k are the molar concentration and molecular weight of the species. v_{ik} are the stochiometric coefficients of the species k in the reaction i. q_i are the rate of progress variables given by -

$$q_i = q_{f,i} - q_{r,i}$$

$q_{f,i}$ and $q_{r,i}$ are defined by:

$$q_{f,i} \equiv k_{f,i} \prod_{k\, spieces} \omega_k^{\nu' ki} \; ; \qquad q_{r,i} \equiv k_{r,i} \prod_{k\, spieces} \omega_k^{\nu'' ki}$$

$$A + B \underset{k_{1,r}}{\overset{k_{1,f}}{\Leftrightarrow}} C$$

$$2C \underset{k_{2,r}}{\overset{k_{2,f}}{\Leftrightarrow}} E$$

The forward reaction rate k_f and the reverse rate k_r are empirically known functions of the temperature.

The forward constant is given by an Arrhenius expression of the type:

$$k_{f,i} = A_i T^{\beta_i} e^{-E_i / RT} \quad k_{r,i} = K_p \left(\frac{P_{atm}}{RT} \right)^{\sum_{k \in K_i} \upsilon_{ik}} \quad K_p = \exp\left(\frac{\Delta S}{R} - \frac{\Delta H}{RT} \right)$$

- A_i, β_i and E_i are the Arrhenius constants:
- A_i is the rate constant
- β_i is the temperature exponent
- E_i is the activation energy.

The source term for the temperature is

$$\dot{T} = -\frac{1}{\rho c_v} \sum_k h_k \dot{\rho}_k$$

RK/Standard Scheme: Three Components

- The 3 components are: RK scheme, implicit residual smoothing, multigrid
- The qth stage of the RK component can be written as

$$\mathbf{W}^{(q)} = \mathbf{W}^{(0)} - \alpha_1 \Delta t \, \mathbf{R}(\mathbf{W}^{(q-1)})$$

where $\mathbf{R}$ is the vector residual function, Δt is the time step, and the RK coefficients α_q are $[0.25,\ 0.1667,\ 0.375,\ 0.5,\ 1.0]$.

The residual function $\mathbf{R}$ is given by

$$\mathbf{R} = \mathbf{R}(\mathbf{W}^{(q)}) = \frac{1}{\mathcal{V}} \left[\mathcal{L}_c \mathbf{W}^{(q)} + \sum_{r=0}^{q} \gamma_{qr} \, \mathcal{L}_v \mathbf{W}^{(r)} + \sum_{r=0}^{q} \gamma_{qr} \, \mathcal{L}_d \mathbf{W}^{(r)} \right],$$

with the operators $\mathcal{L}_c$, $\mathcal{L}_v$, and $\mathcal{L}_d$ for convection, viscous diffusion and numerical dissipation.

RK/Implicit Scheme

- The change in the solution on the qth stage

$$\delta \mathbf{W}^{(q)} = \mathbf{W}^{(q)} - \mathbf{W}^{(0)} = -\alpha_q \frac{\Delta t}{\mathcal{V}} \mathcal{L}\, \mathbf{W}^{(q-1)} = \widehat{\mathbf{R}}(\mathbf{W}^{(q-1)}),$$

$\mathcal{L}$ is the complete difference operator.

- If we apply implicit residual smoothing, then

$$\mathcal{L}_i\, \overline{\delta \mathbf{W}} = \delta \mathbf{W}^{(q)},$$

where $\mathcal{L}_i$ is an implicit operator.

- Approximately inverting the implicit operator $\mathcal{L}_i$

$$\overline{\delta \mathbf{W}} = -\alpha_q \frac{\Delta t}{\mathcal{V}} \mathcal{P}\, \mathcal{L}\, \mathbf{W}^{(q-1)},$$

$\mathcal{P}$ is a preconditioner defined by the approximate inverse $\widetilde{\mathcal{L}}_i^{-1}$.

Transforming the equations to primitive variables, the flux Jacobian is written as:

$$A = A^{+} + A^{-}$$

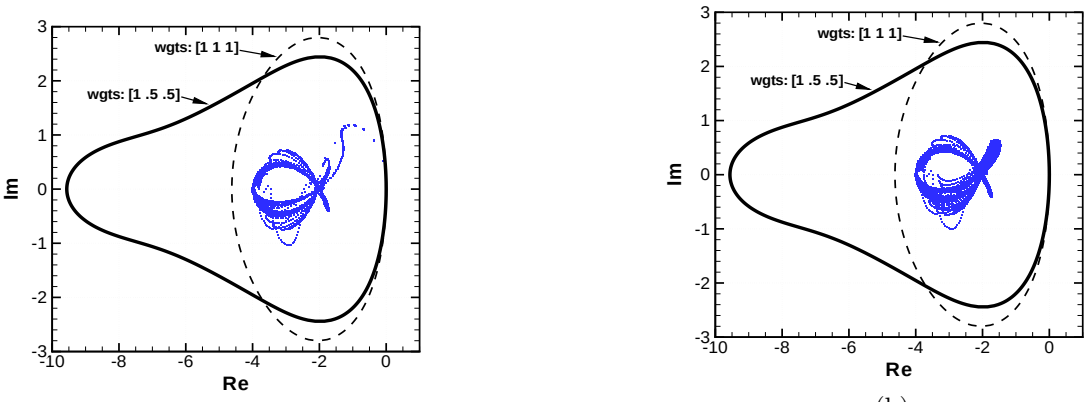
where

$$A^{\pm} = \frac{1}{2}\left(A \pm |A|\right)$$

Finally, the implicit smoothing scheme is given by:

$$\left(I + \varepsilon \frac{\Delta t}{V} \sum_{all\ \ faces} A^{+} \cdot \vec{n} dS - \Delta t \frac{\partial S}{\partial Q} \right) \Delta \tilde{Q}_{local} =$$

$$\Delta Q - \varepsilon \frac{\Delta t}{V} \sum_{all\ \ faces} A^{-} \Delta \tilde{Q}_{NB} \cdot \vec{n} dS$$



(a) (b)

Figure 1: Fourier footprints of RK(3,3) scheme with two preconditioners for all modes with high-frequency components (64×64, $M = 0.5$, $\alpha = 0°$, $CFL = 10^3$, $AR = 5$, $Re = \infty$). (a) Without entropy fix, (b) with entropy fix.

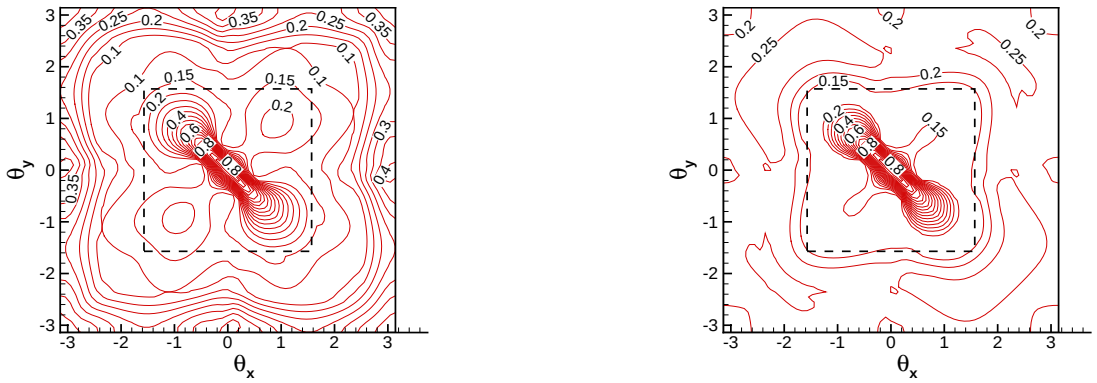


Figure 2: Effect of dissipation weights on damping behavior of RKI$(3,3)$ scheme (64×64, $M=0.5$, $\alpha=45°$, $CFL=10^3$, $AR=1$, $Re=\infty$, 2 SGS). (a) wgts: [1, 1, 1], (b) wgts: [1, 0.5, 0.5].

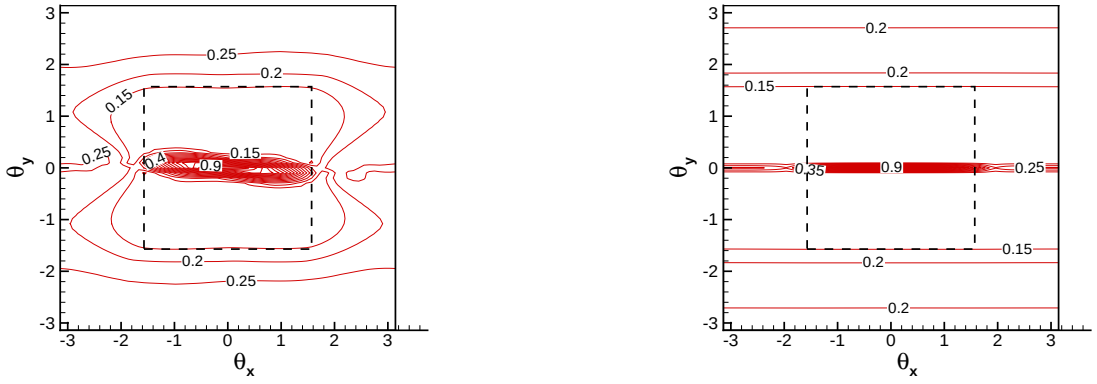


Figure 3: Damping behavior of RKI$(3,3)$ scheme with variation in Re and AR (64×64, $M=0.5$, $\alpha=45°$, 2 SGS). (a) $Re=10^2$, $AR=10$, $CFL=10^3$, (b) $Re=10^6$, $AR=10^3$, $CFL=10^4$.

Extension to turbulent flow

We solve two sets of equations for the smoothed residuals independently:

a) For the Eulerian primitive variables

b) For the turbulent model variables – k and ω

$$\Delta\tilde{Q} = \begin{pmatrix} \Delta\tilde{k} \\ \Delta\tilde{\omega} \end{pmatrix}$$

In the k- ω set we use the Jacobian of the source term:

$$\frac{\partial S}{\partial Q} = -\begin{pmatrix} \beta^{*}\omega & \beta^{*}k \\ 0 & 2\beta\omega \end{pmatrix}$$

Extension to chemical reactions

For a real gas, we insert part of the entries of the Jacobian source terms into the system for the Eulerian variables' residuals. For the $\{\omega, T, u\}$ primitive variables, the Jacobian matrix we use is

$$R_J\{\omega,T,u\} = \begin{pmatrix} \frac{\partial \dot{\omega}_1}{\partial \omega_1} & 0 & 0 & 0 & \frac{\partial \dot{\omega}_1}{\partial T} \\ 0 & \frac{\partial \dot{\omega}_2}{\partial \omega_2} & 0 & 0 & \frac{\partial \dot{\omega}_2}{\partial T} \\ 0 & 0 & \frac{\partial \dot{\omega}_3}{\partial \omega_3} & 0 & \frac{\partial \dot{\omega}_3}{\partial T} \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\partial \dot{T}}{\partial T} \end{pmatrix}$$

For {ρ, P, u} variables this matrix becomes

$$R_J\{\rho,P,u\}=\begin{pmatrix}
\frac{\partial\dot{\omega}_1}{\partial\omega_1}-\frac{\partial\dot{\omega}_1}{\partial T}\frac{TW}{\rho} & -\frac{w_1}{w_2}\frac{\partial\dot{\omega}_1}{\partial T}\frac{TW}{\rho} & -\frac{w_1}{w_3}\frac{\partial\dot{\omega}_1}{\partial T}\frac{TW}{\rho} & 0 & \frac{w_1W}{\rho R}\frac{\partial\dot{\omega}_1}{\partial T} \\
-\frac{w_2}{w_1}\frac{\partial\dot{\omega}_2}{\partial T}\frac{TW}{\rho} & \frac{\partial\dot{\omega}_2}{\partial\omega_2}-\frac{\partial\dot{\omega}_2}{\partial T}\frac{TW}{\rho} & -\frac{w_2}{w_3}\frac{\partial\dot{\omega}_2}{\partial T}\frac{TW}{\rho} & 0 & \frac{w_2W}{\rho R}\frac{\partial\dot{\omega}_2}{\partial T} \\
-\frac{w_3}{w_1}\frac{\partial\dot{\omega}_3}{\partial T}\frac{TW}{\rho} & -\frac{w_3}{w_2}\frac{\partial\dot{\omega}_3}{\partial T}\frac{TW}{\rho} & \frac{\partial\dot{\omega}_3}{\partial\omega_3}-\frac{\partial\dot{\omega}_3}{\partial T}\frac{TW}{\rho} & 0 & \frac{w_3W}{\rho R}\frac{\partial\dot{\omega}_3}{\partial T} \\
0 & 0 & 0 & 0 & 0 \\
\frac{RT}{w_1}\left(\frac{\partial\dot{\omega}_1}{\partial\omega_1}-\frac{T}{P}\frac{\partial\dot{P}}{\partial T}\right) & \frac{RT}{w_2}\left(\frac{\partial\dot{\omega}_2}{\partial\omega_2}-\frac{T}{P}\frac{\partial\dot{P}}{\partial T}\right) & \frac{RT}{w_3}\left(\frac{\partial\dot{\omega}_3}{\partial\omega_3}-\frac{T}{P}\frac{\partial\dot{P}}{\partial T}\right) & 0 & \frac{T}{P}\frac{\partial\dot{P}}{\partial T}
\end{pmatrix}$$

where

$$\frac{\partial\dot{P}}{\partial T}=RT\sum\frac{\partial\dot{\omega}_i}{\partial T}+\frac{\partial\dot{T}}{\partial T}\frac{P}{T}$$

Determination of temperature from internal energy

For a given internal energy e_0, we want to determine the temperature.

We solve the equation $f(T) = e(T) - e_0 = 0$ iteratively using the Newton-Rapson method

$$T_{n+1} = T_n - \frac{f(T_n)}{f'(T_n)}$$

$$\frac{de(T)}{dT} = c_v \quad \Rightarrow \quad T_{n+1} = \frac{c_v(T_n)T_n - e(T_n) + e_0}{c_v(T_n)}$$

Time dependent - Dual time step

For steady state calculations we use pseudo time approach. For time dependent calculations, in order to be able to use all of the acceleration methods we use a dual time step. An approximation to the physical time derivative now appears as a source term in the right hand side of the N-S equations.

$$\frac{\partial Q}{\partial \tau} + \frac{\partial Q}{\partial t} + \nabla F = 0$$

$$\frac{\partial Q}{\partial t} \approx \frac{3Q^{n+1} - 4Q^{n} + Q^{n-1}}{2\Delta t}$$

t is the physical time and τ is the pseudo time. We approximate the physical time derivative using a backward difference scheme.

Since we do not know Q^{n+1} we approximate it with Q^{k+1}

After some rearrangement of the above equation we have

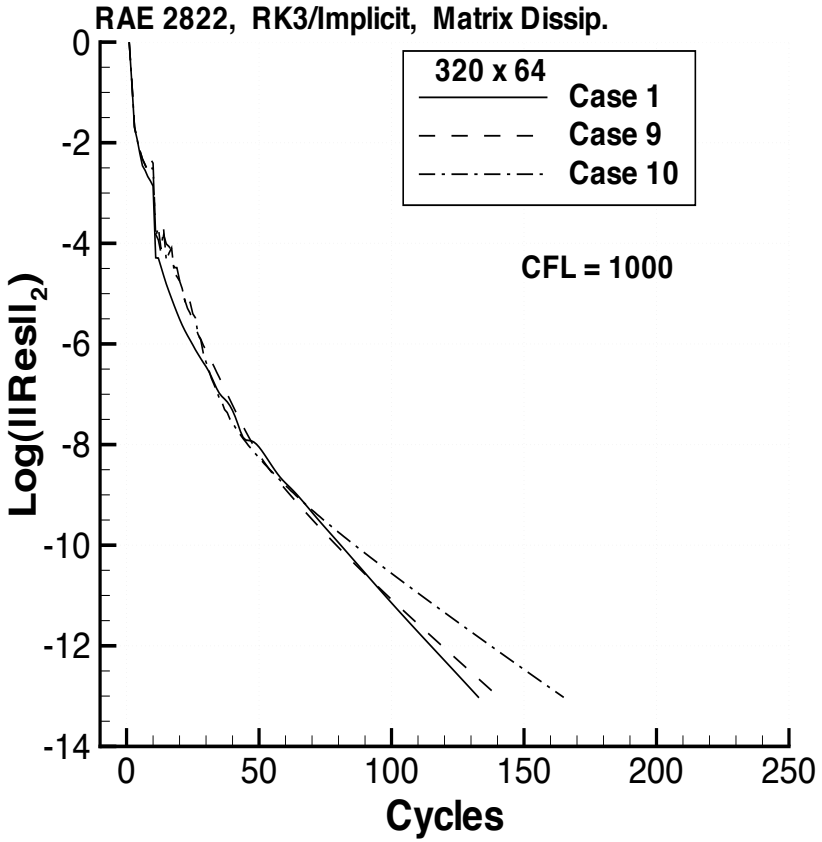
$$Q^{k+1} = \frac{Q^0 - \alpha_k \Delta\tau \tilde{R}^k + \frac{3}{2}\alpha_k \frac{\Delta\tau}{\Delta t} Q^k}{1 + \frac{3}{2}\alpha_k \frac{\Delta\tau}{\Delta t}}$$

$\tilde{R}^k$ is the smoothed residual and R^k is

$$R^k = \nabla F + \frac{3Q^k - 4Q^n + Q^{n-1}}{2\Delta t}$$

Preliminary results

Convergence Histories for Three-Stage Schemes



RAE 2822: Cases 1, 9, 10

Hobson Cascade transonic - Euler

Standard

FMG – 4 levels

RK – 4 stages, central differences

CFL=3

Zhu Implicit residual Smoothing

CPU = 16.6 seconds

MIRS

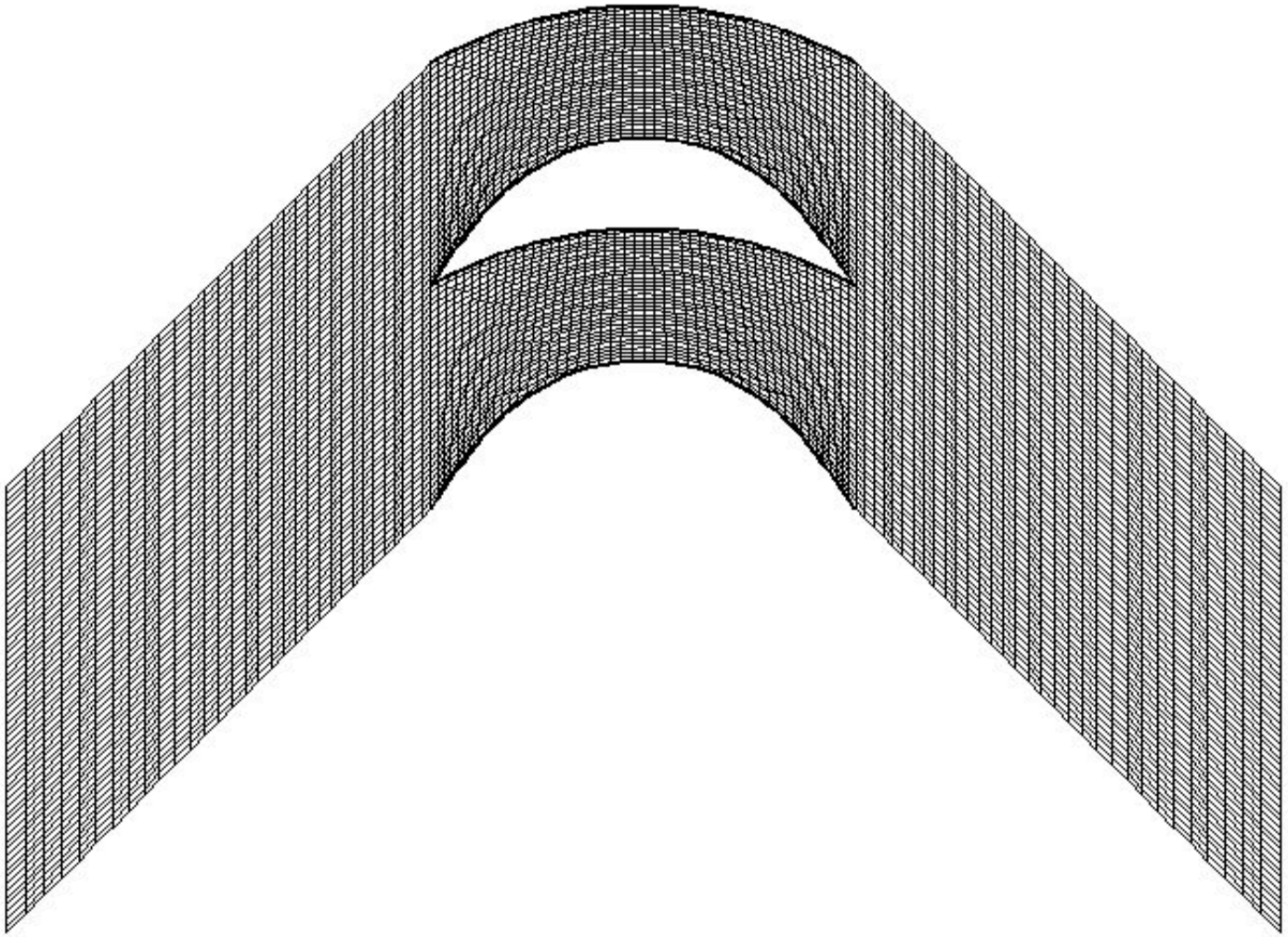
FMG – 4 levels

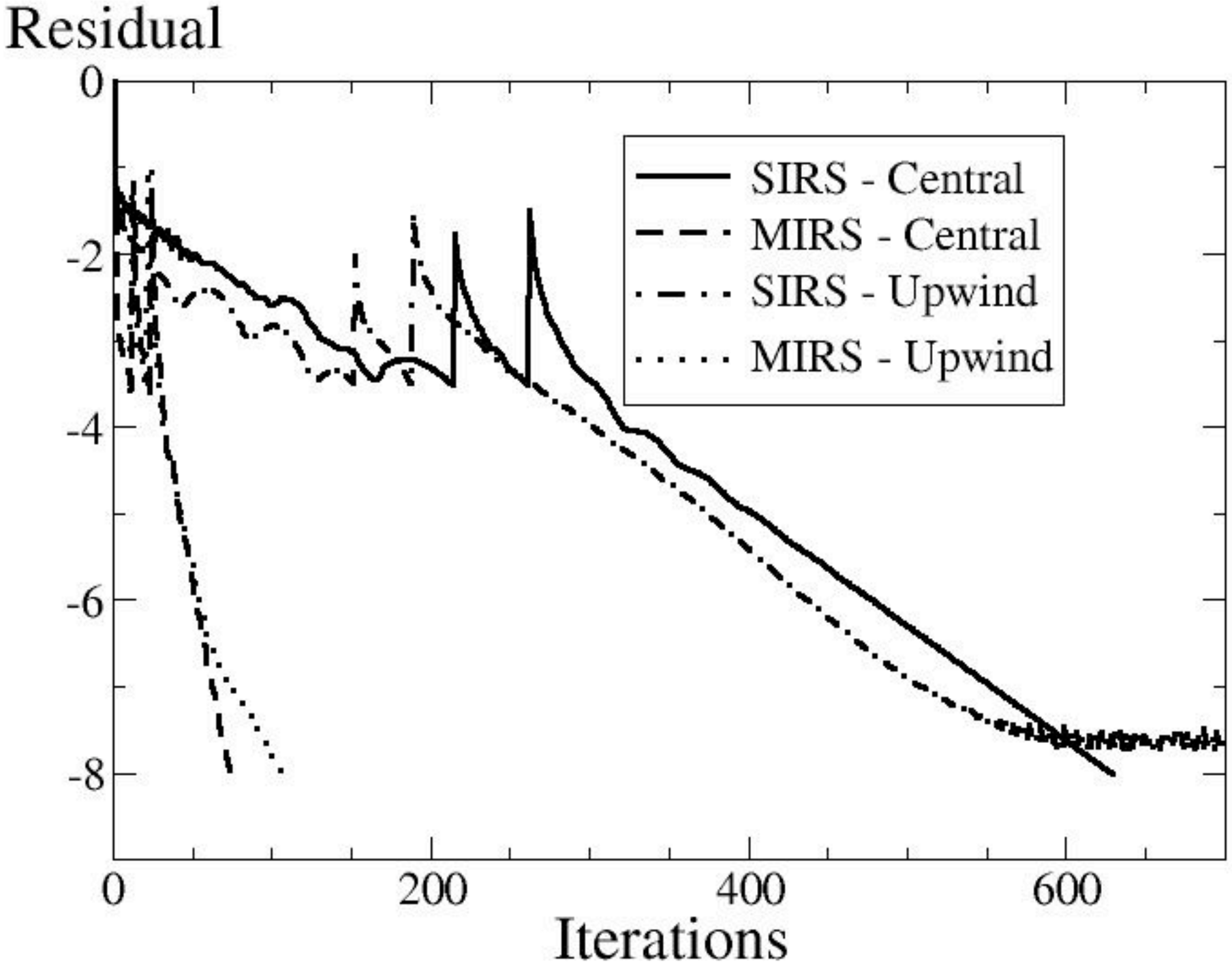
RK – 3 stages, central differences

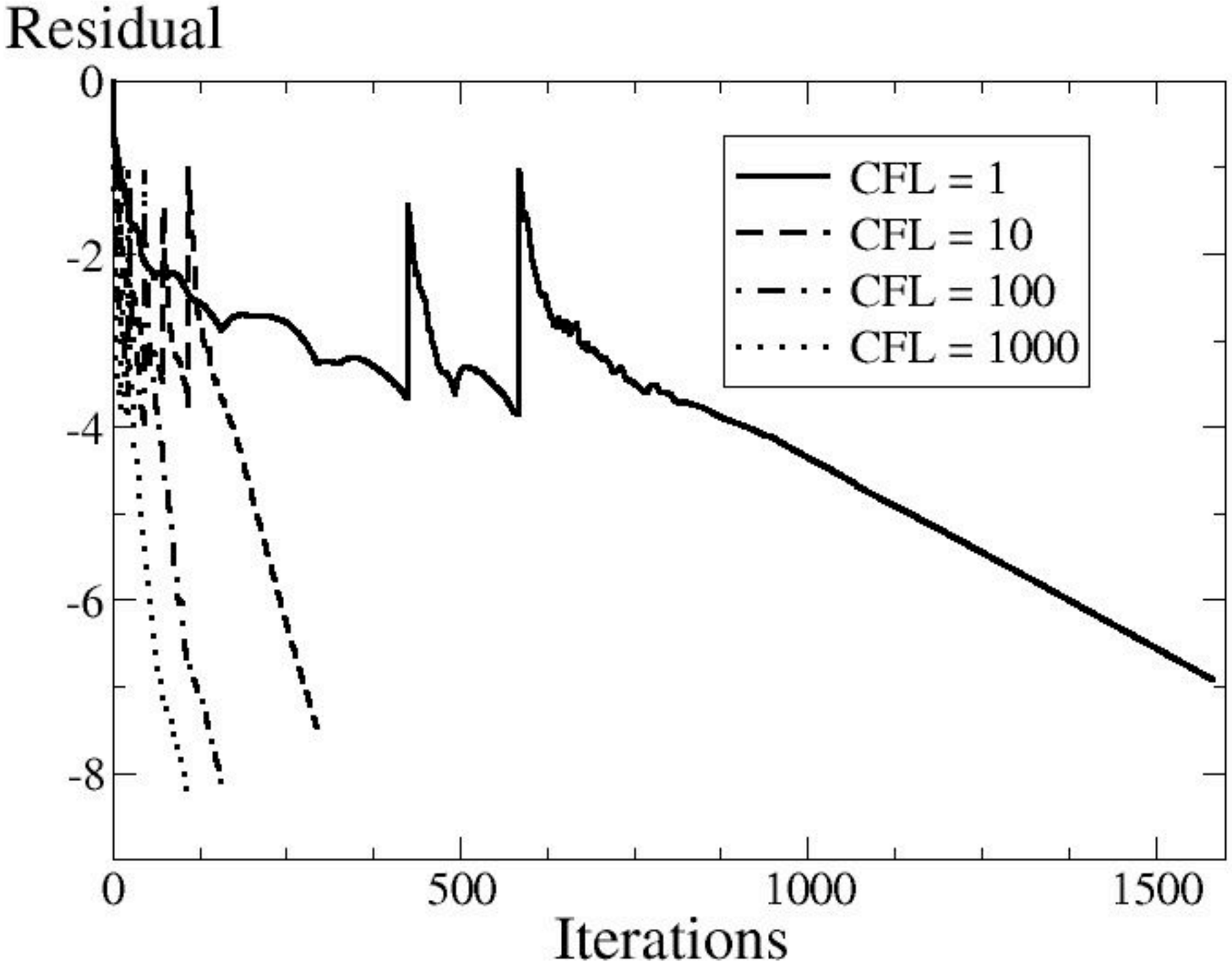
CFL=1000

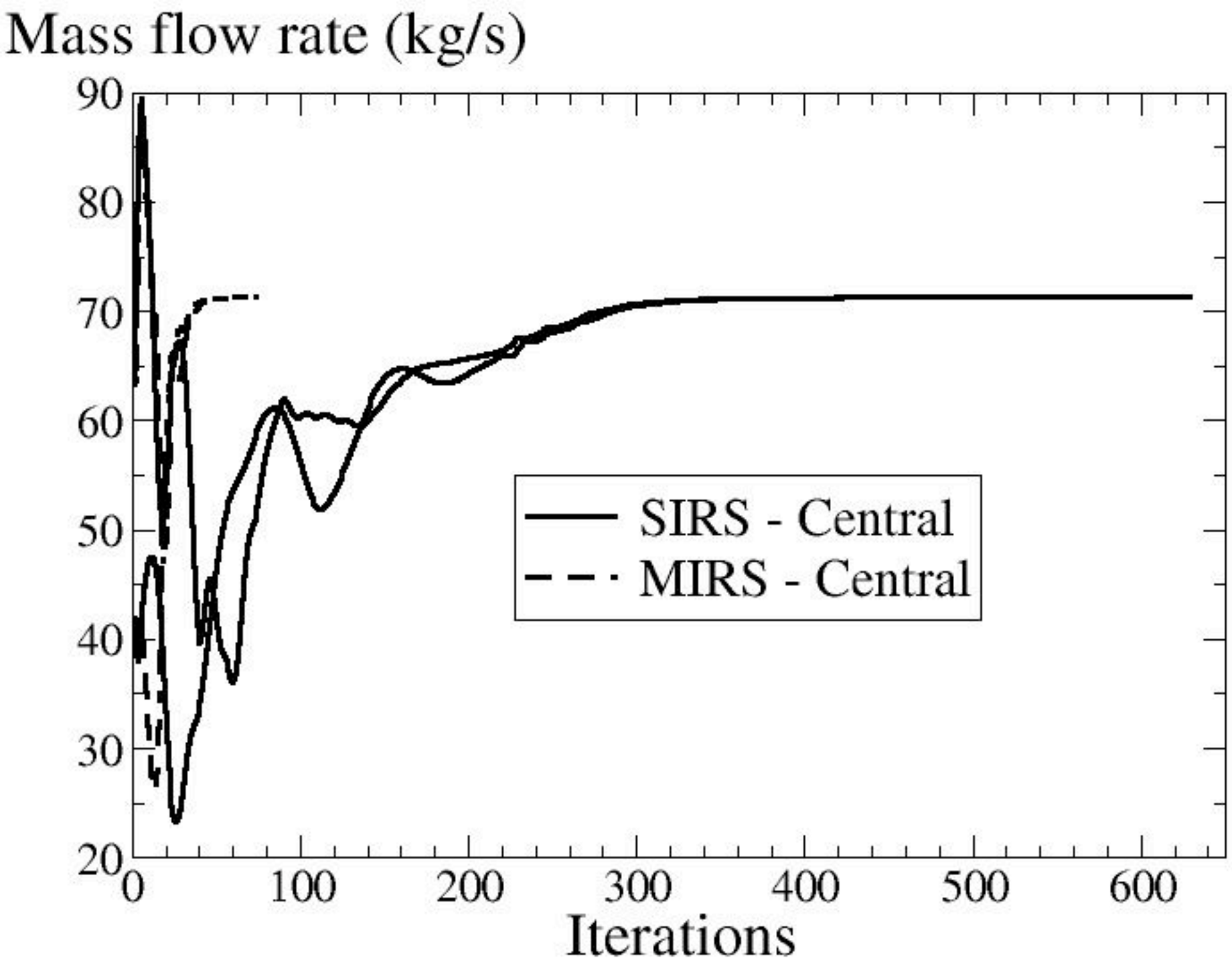
2 SGS sweeps ε=0.75

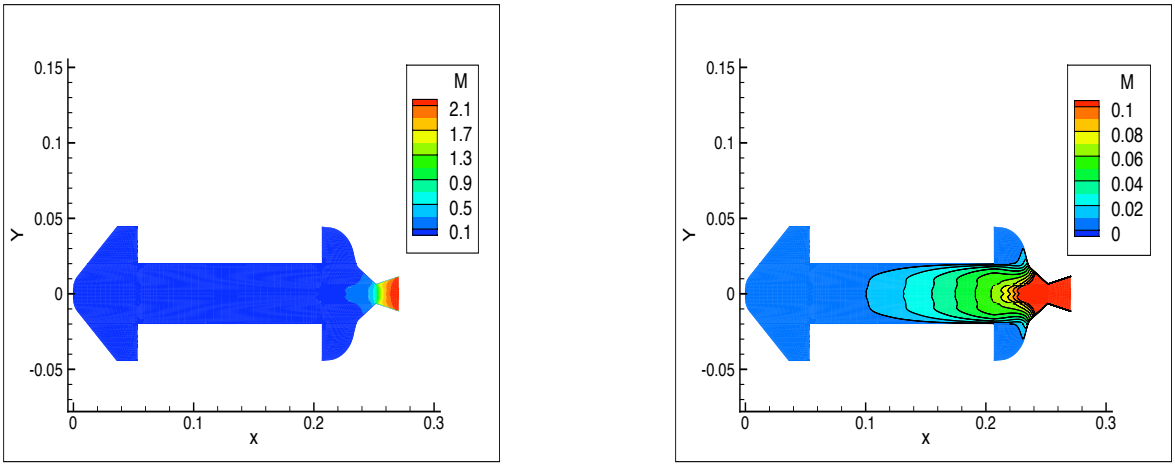
CPU = 4.5 seconds




Residual
0
-2
-4
-6
-8
0
200
400
600
Iterations
SIRS - Central
MIRS - Central
SIRS - Upwind
MIRS - Upwind


Residual
0
-2
-4
-6
-8
0
500
1000
1500
Iterations
CFL = 1
CFL = 10
CFL = 100
CFL = 1000


Mass flow rate (kg/s)
90
80
70
60
50
40
30
20
0
100
200
300
400
500
600
Iterations
SIRS - Central
MIRS - Central



(a) (b)

Figure 4: Rocket Motor (a) full range of Mach contours in the chamber and nozzle (b) zoom on the Mach values inside the motor where the sound speed is around 1000 m/s and the Mach values are low.

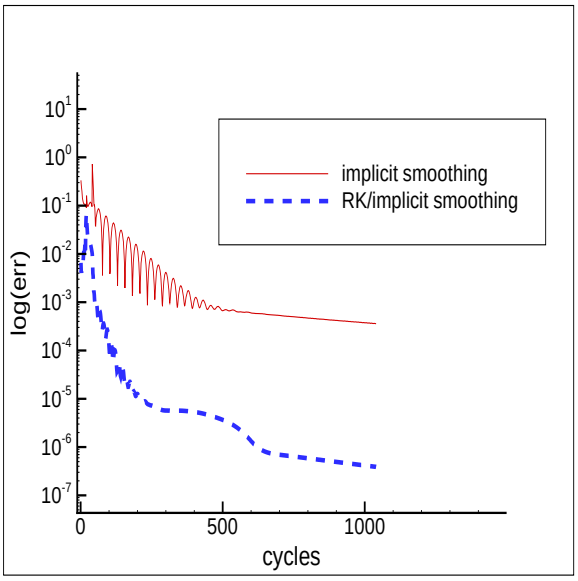
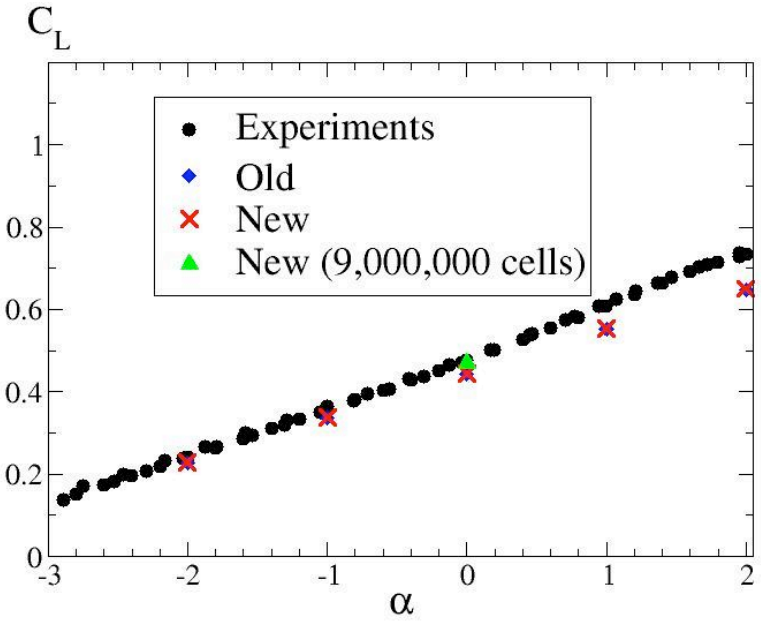


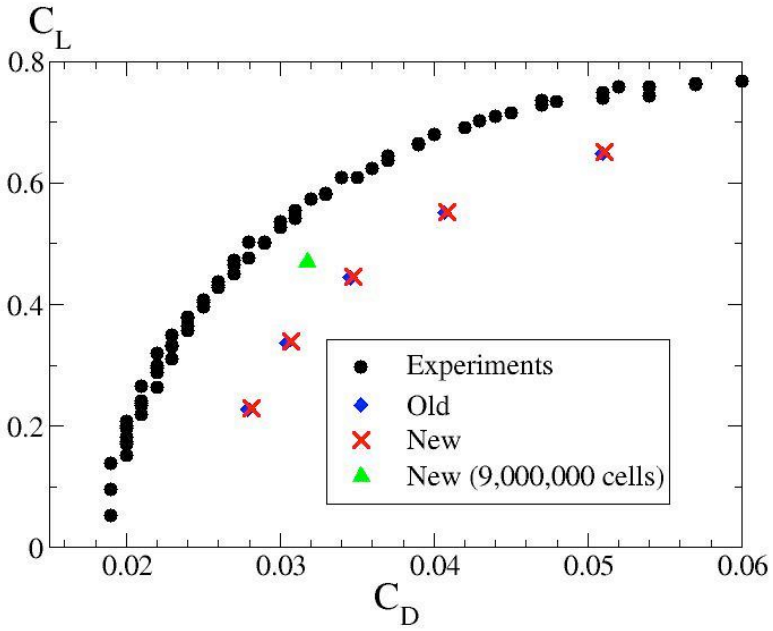
Figure 5: Convergence rate for rocket motor for original and improved schemes

Results: Unstructured Solver

DLR-F4 – SA Turbulence model

Re = 3.000.000 - M = 0.75

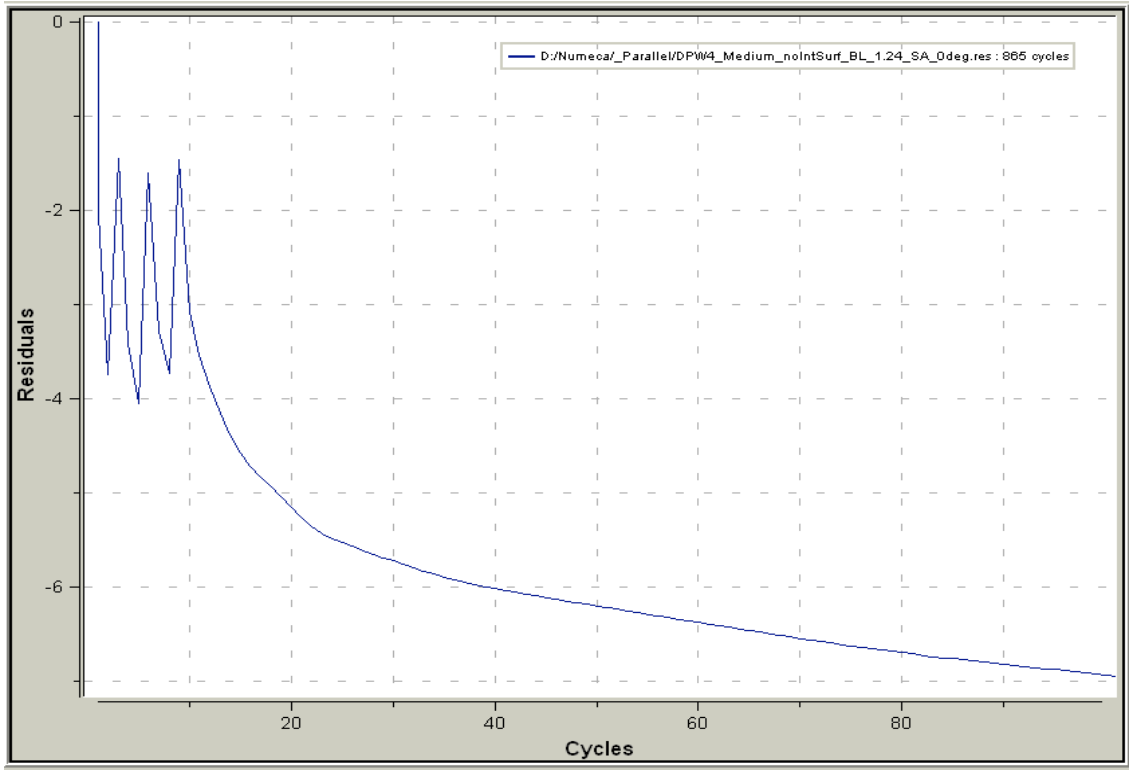


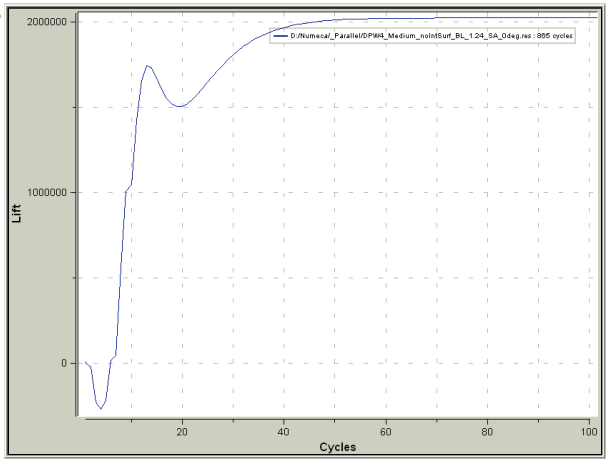


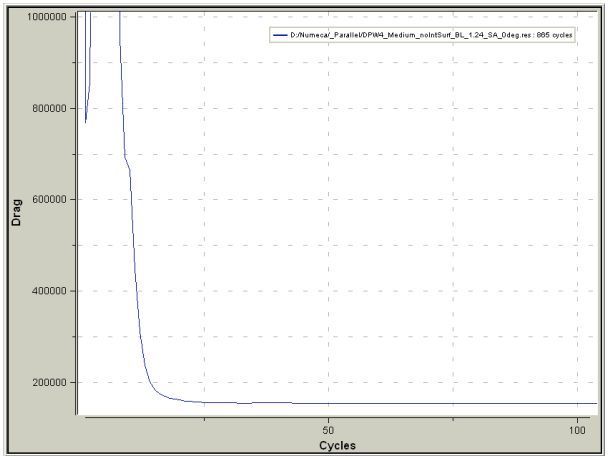
DPW-4: ~16.000.000 cells / SA / Double precision /4MG

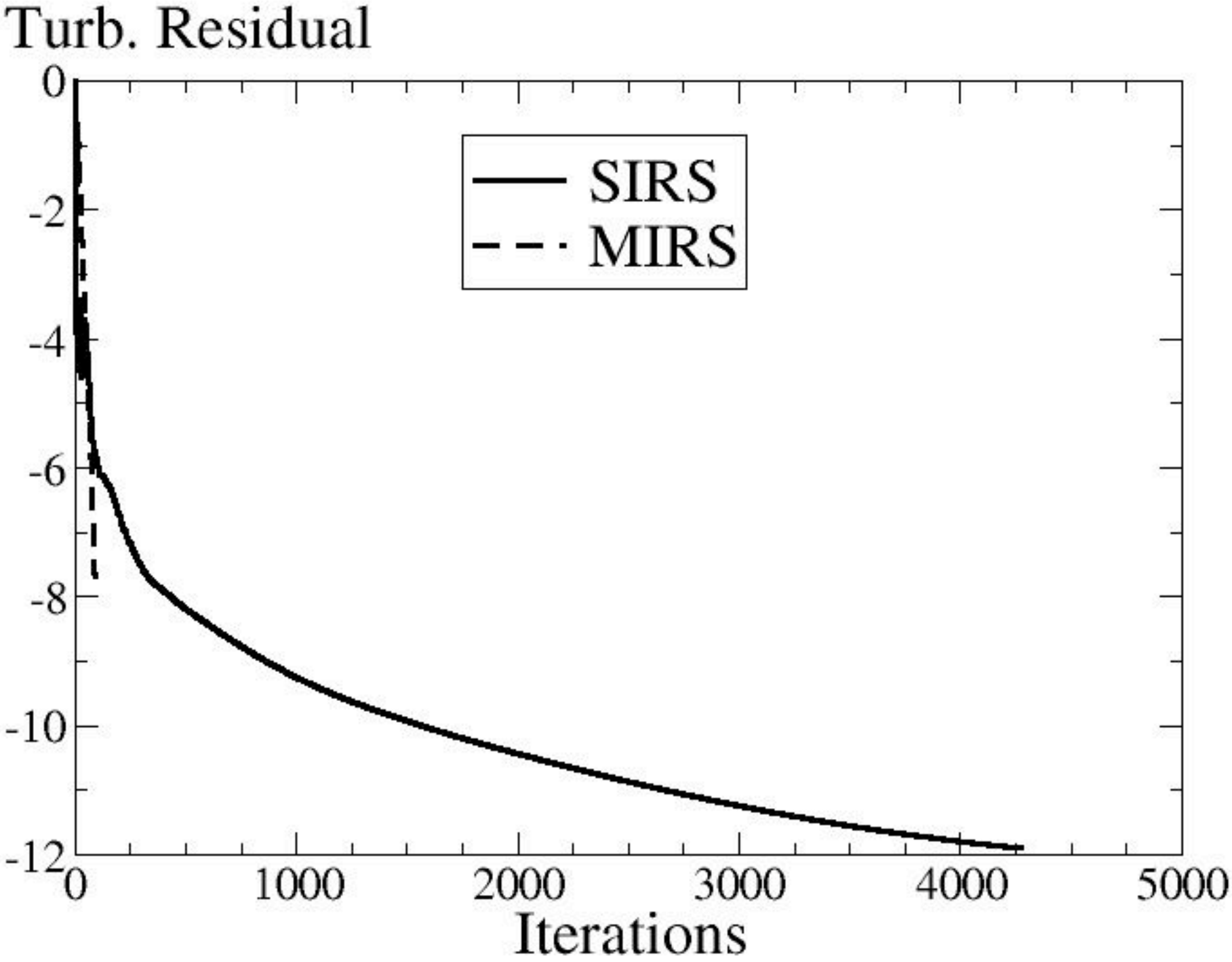
16 64bit-procs

CPU time: ~75 min for 6 orders convergence (50 cycles).







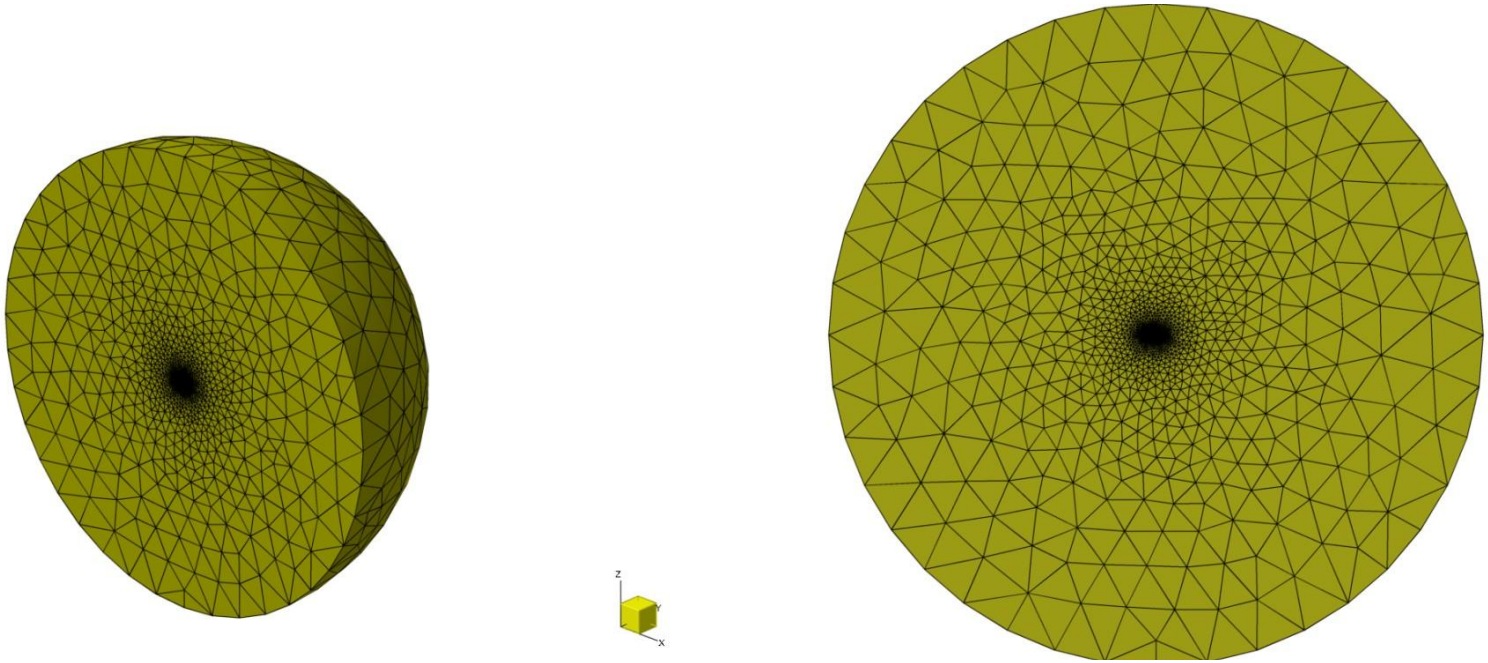

Turb. Residual
0
-2
-4
-6
-8
-10
-12
0
1000
2000
3000
4000
5000
Iterations
SIRS
MIRS

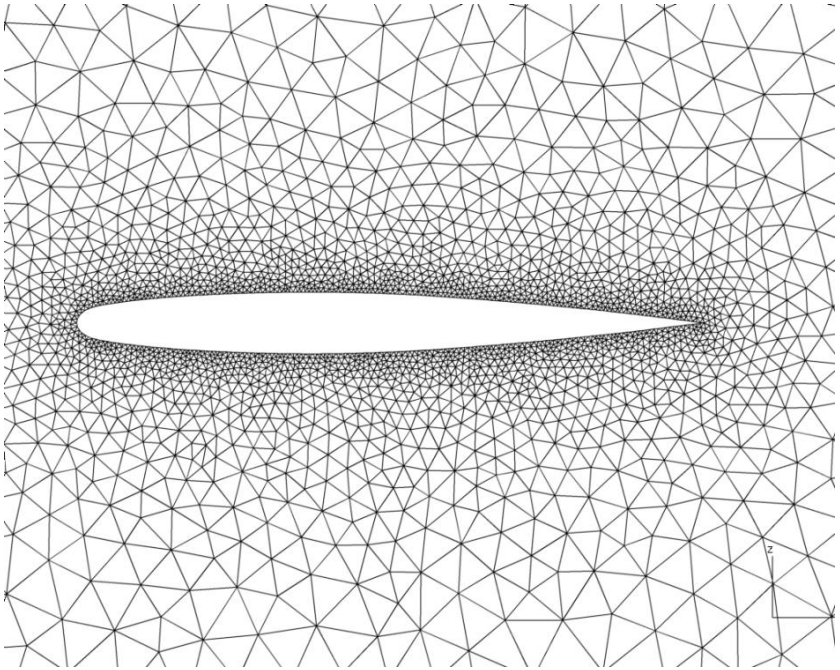
Inviscid computations on a ONERA M6 with a tetrahedral mesh

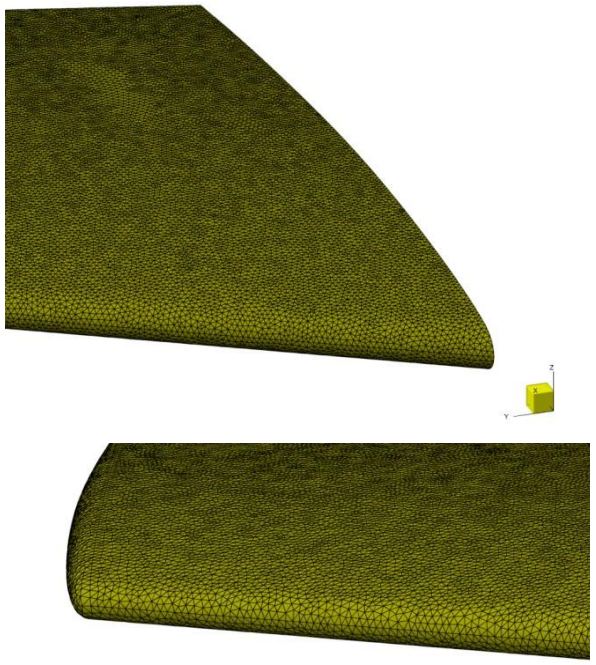
Geometry: ONERA M6

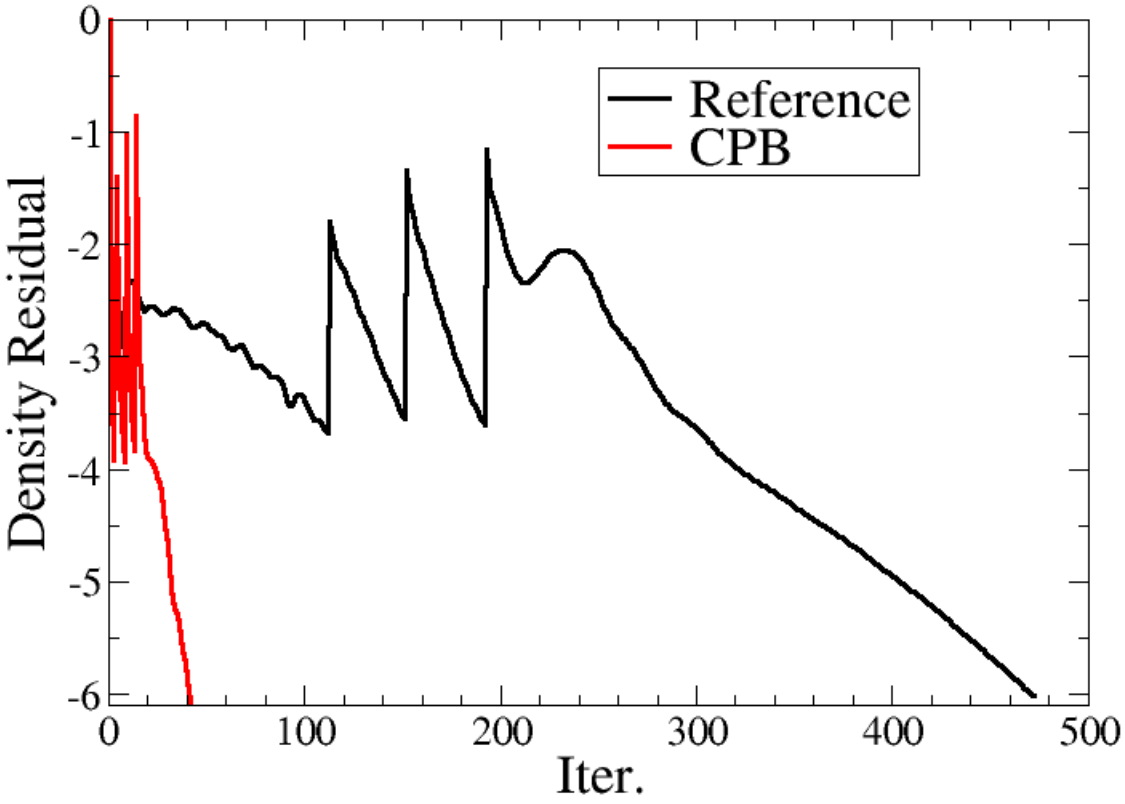
- Flow conditions:
  - M = 0.8395
  - Re = 11,720,000
  - α = 3.06°
- **inviscid**

- Euler mesh
- Made of 611,856 tetrahedral cells
- Generated using Gmsh

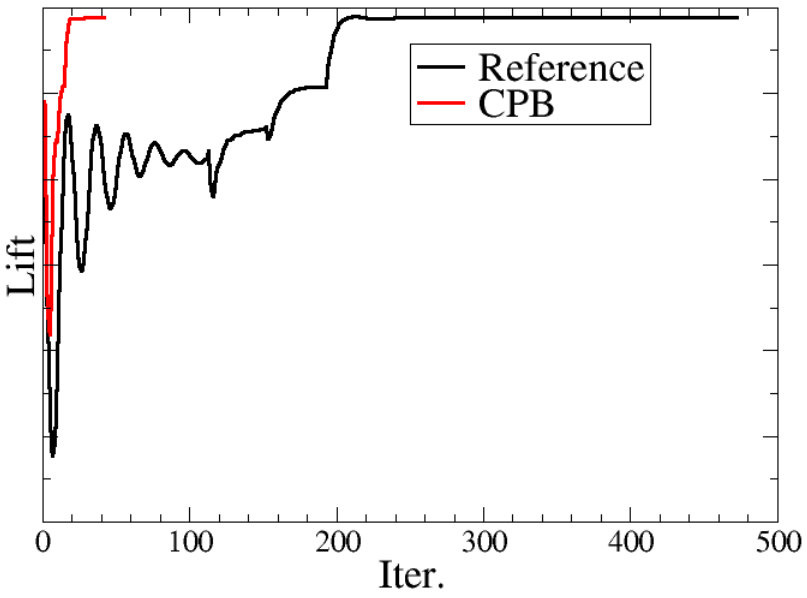


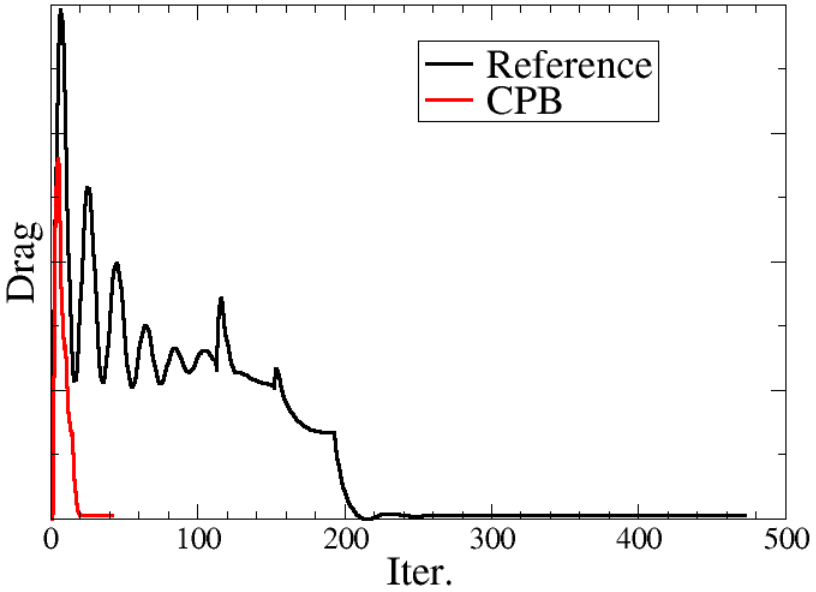




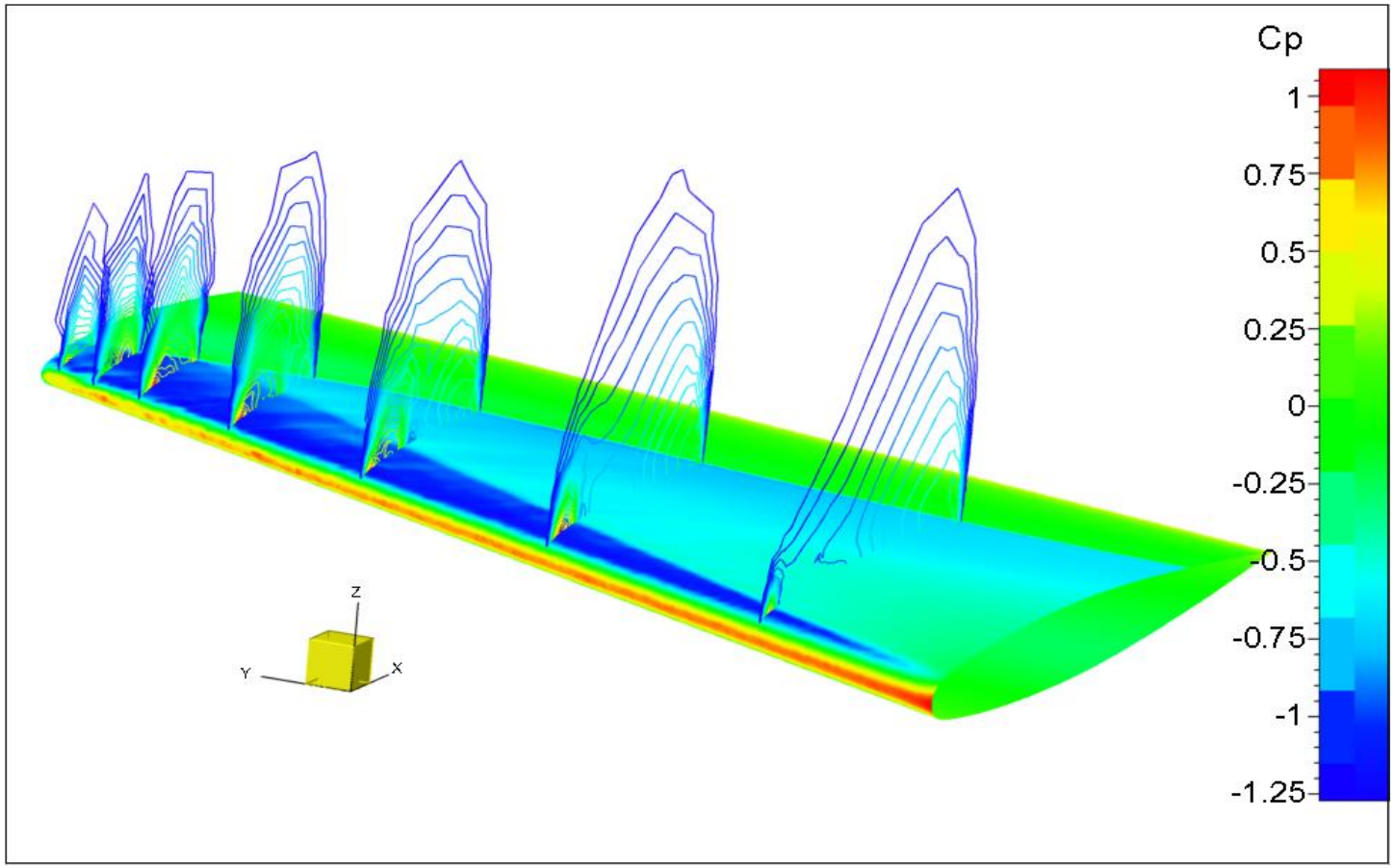


Decay of density residual for solvers with/without convergence acceleration





Evolution of lift and drag

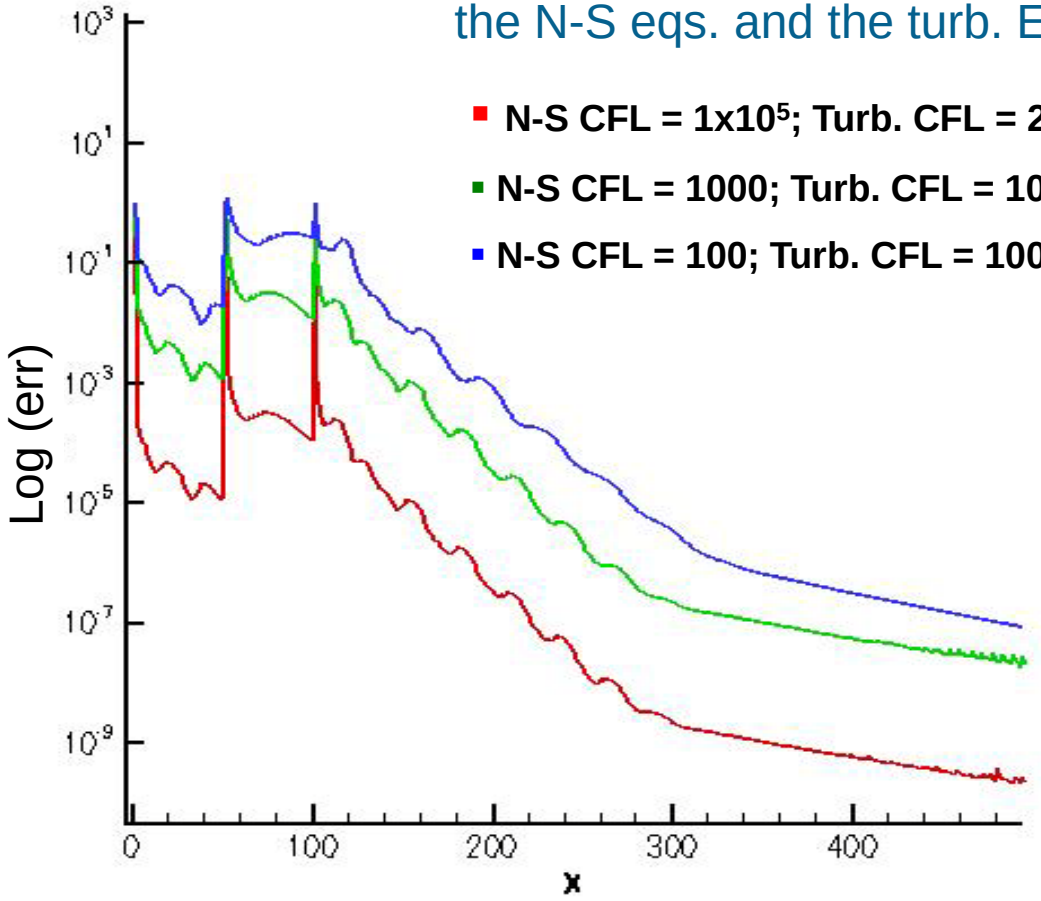


Distribution of pressure coefficient on the wing surface, with Mach iso-countours at different spanwise locations

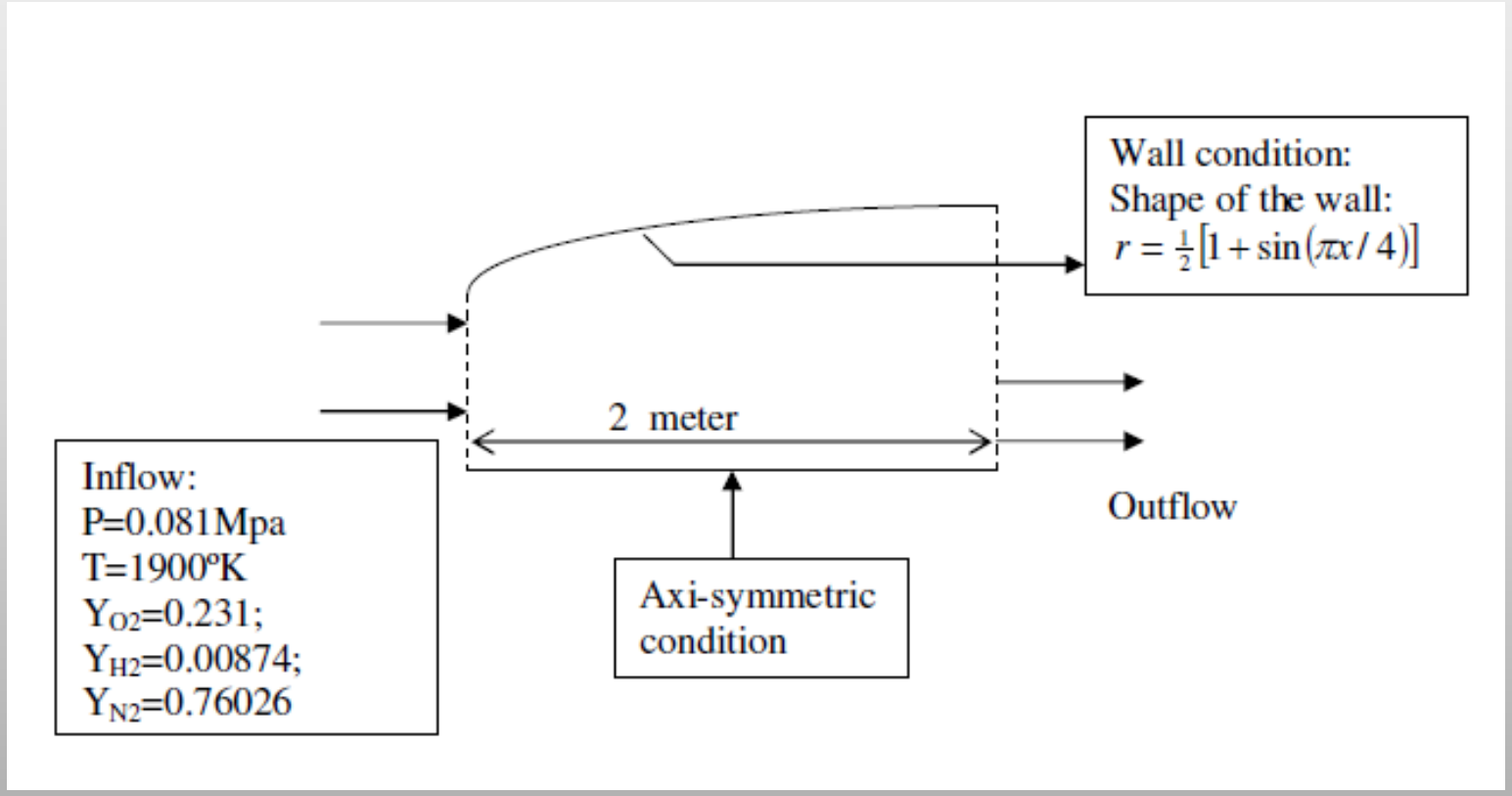
Convergence History for Various CFL Numbers

Different CFL # are used for the N-S eqs. and the turb. Eqs.

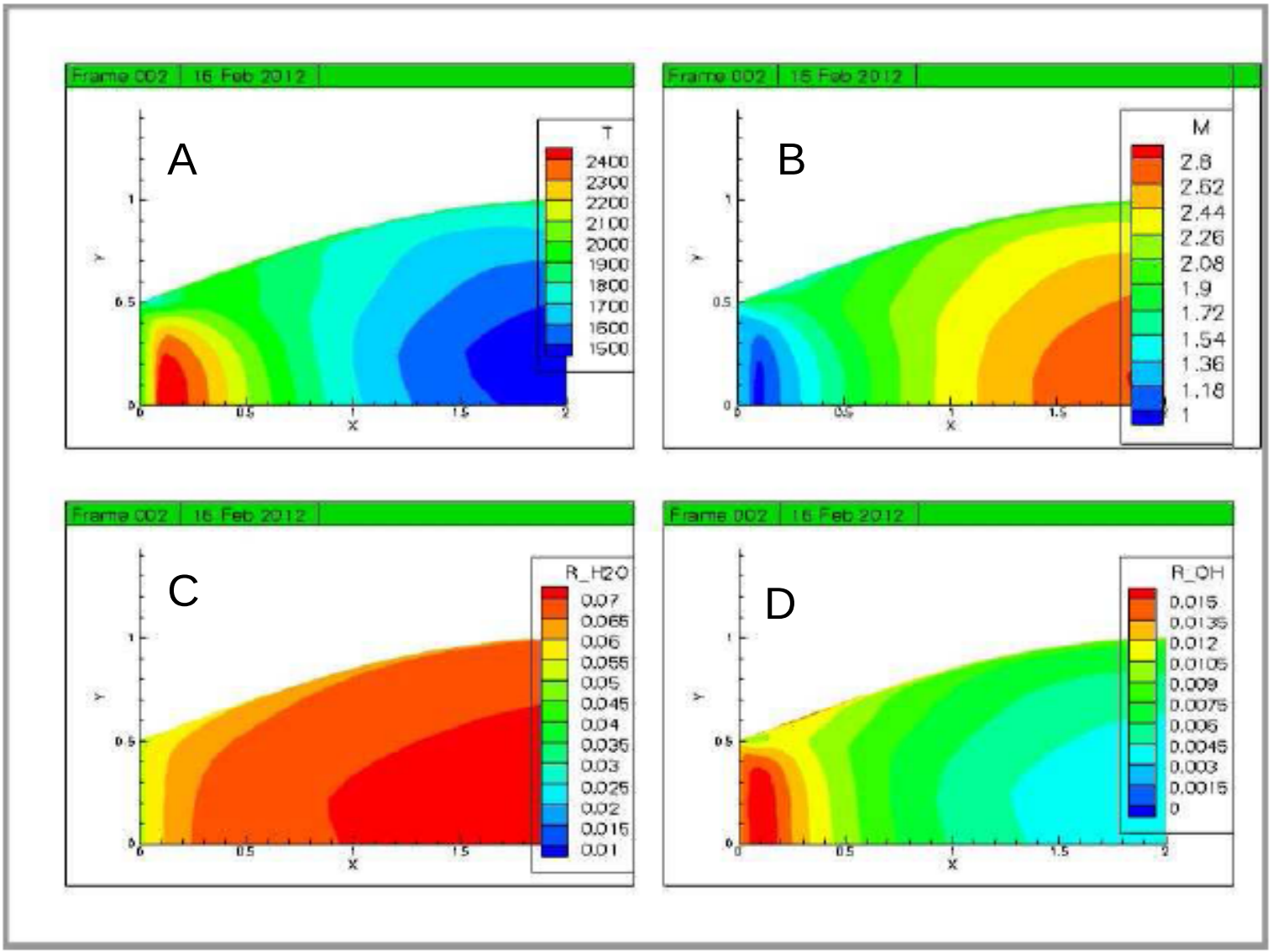
- **N-S CFL = $1x10^5$; Turb. CFL = $2x10^4$**
- **N-S CFL = 1000; Turb. CFL = 1000**
- **N-S CFL = 100; Turb. CFL = 100**



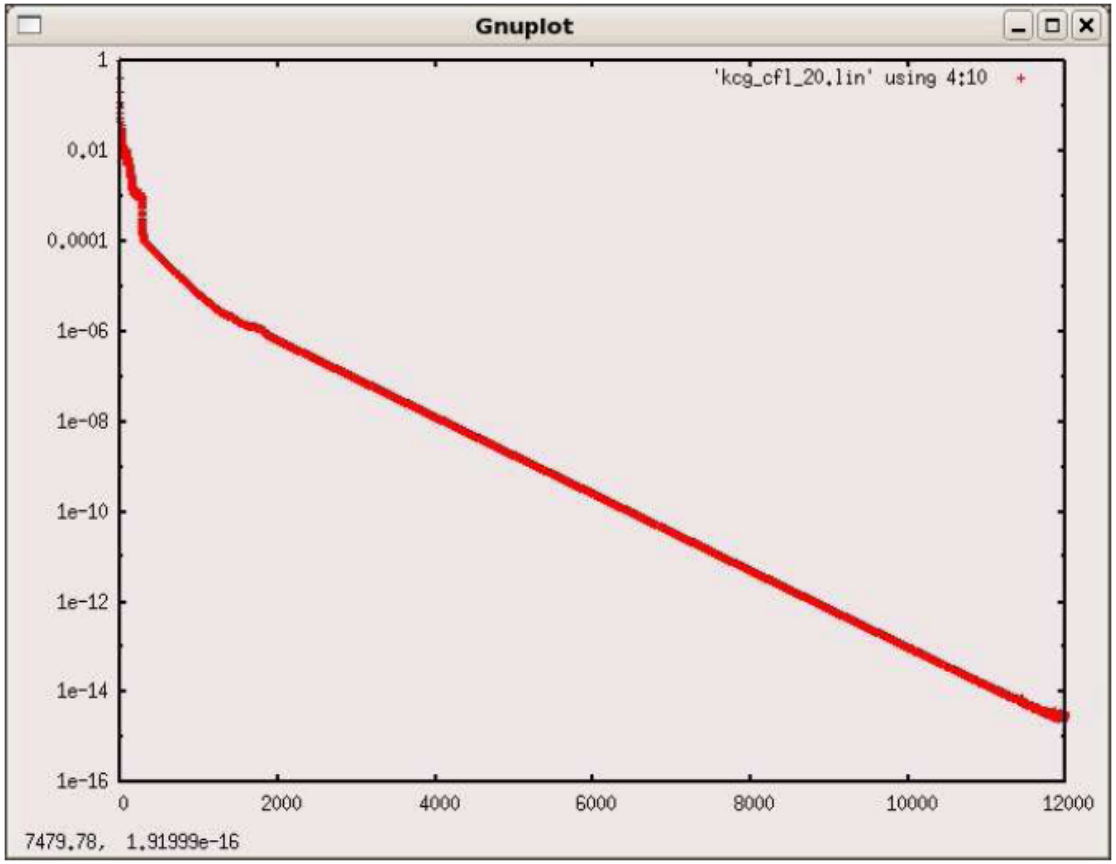
Laminar reactive flow – Rapid expansion diffuser



Contours maps for the temperature (A), Mach number (B), H2O mass fraction (C) and OH radical (D)



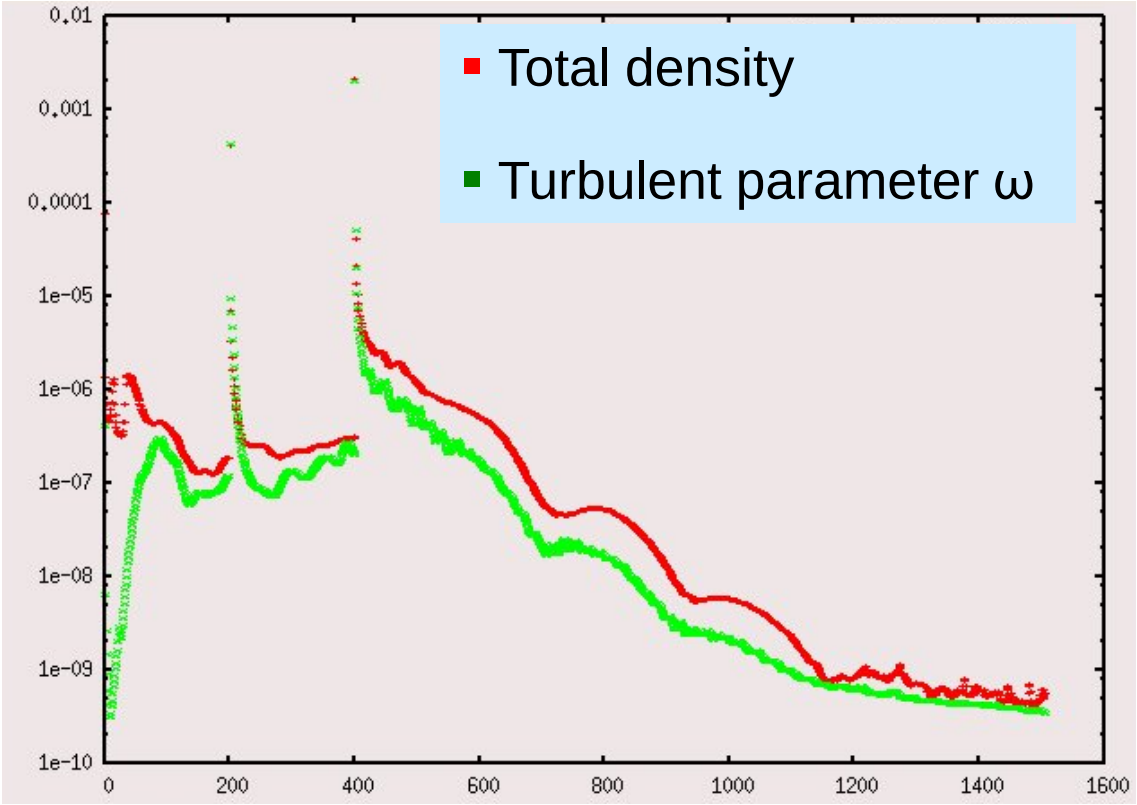
Convergence history for CFL 20 without multigrid acceleration



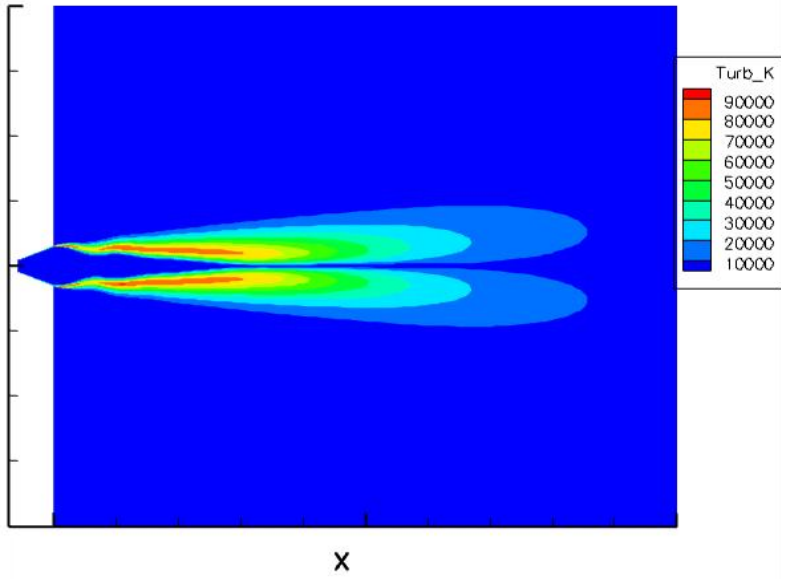
Turbulent reactive flow – rocket motor plume

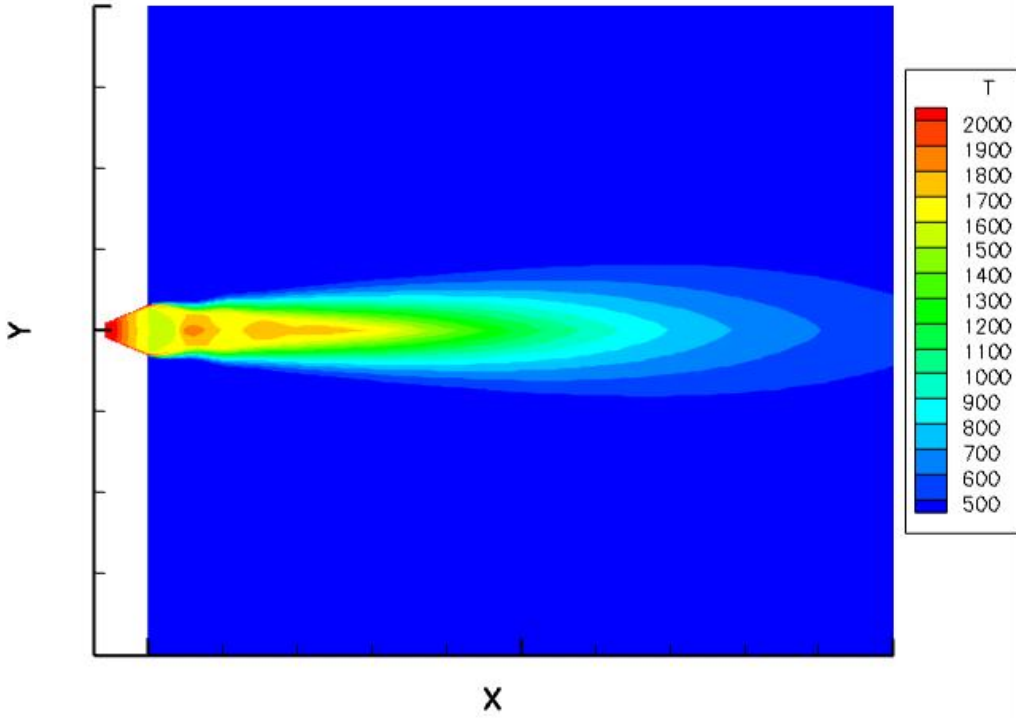
A rocket motor plume exiting from the motor nozzle into a low Mach number free stream flow is calculated. The plume boundary conditions are defined on the nozzle throat where the flow velocity is sonic and the species mass fractions are defined. The species used for this problem are: H, O, OH, H2, O2, CO, CO2, H2O, HCL and N2.

Convergence history: The fluid CFL is 100,000 and turbulent CFL is 200



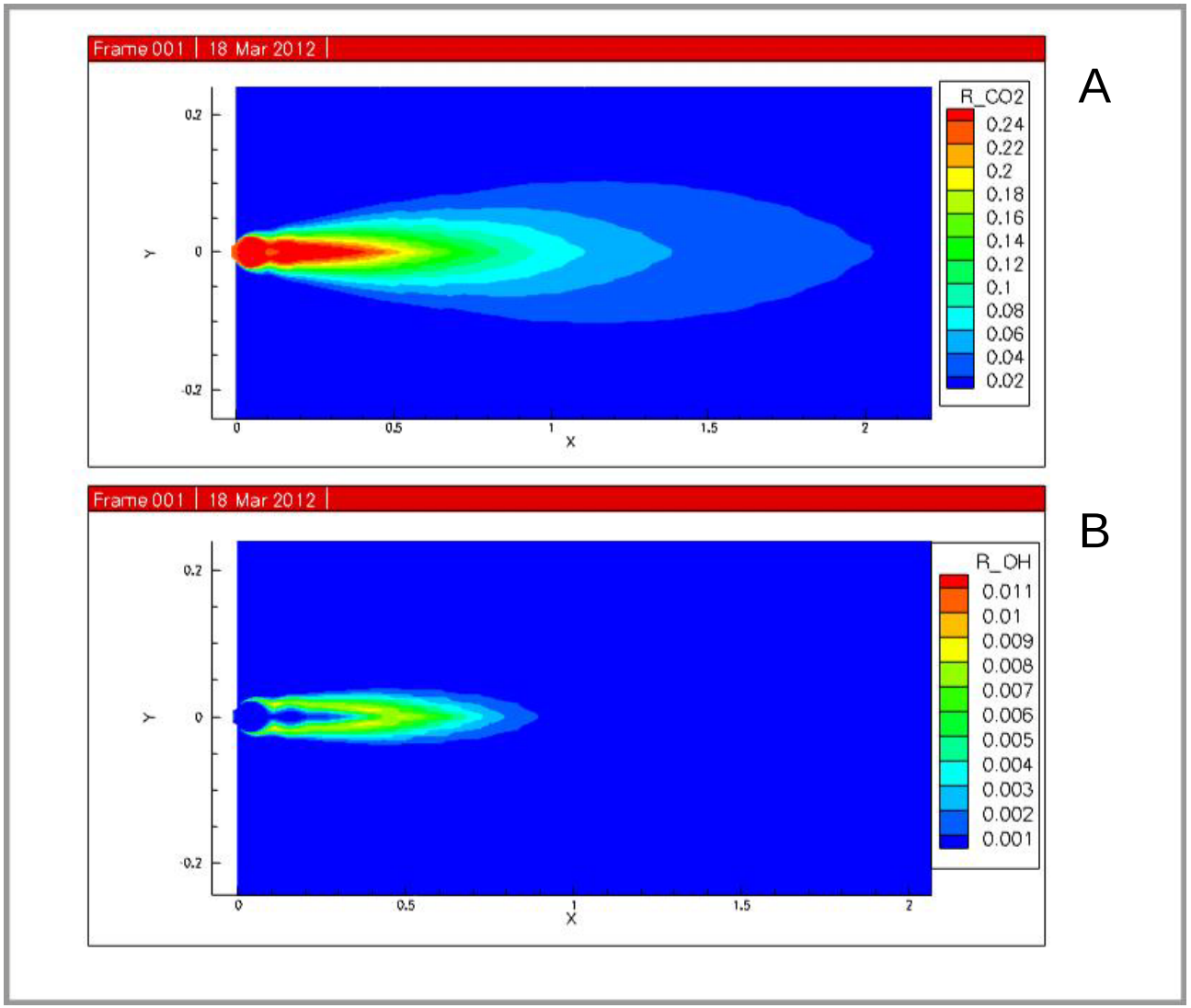
Turbulent kinetic energy





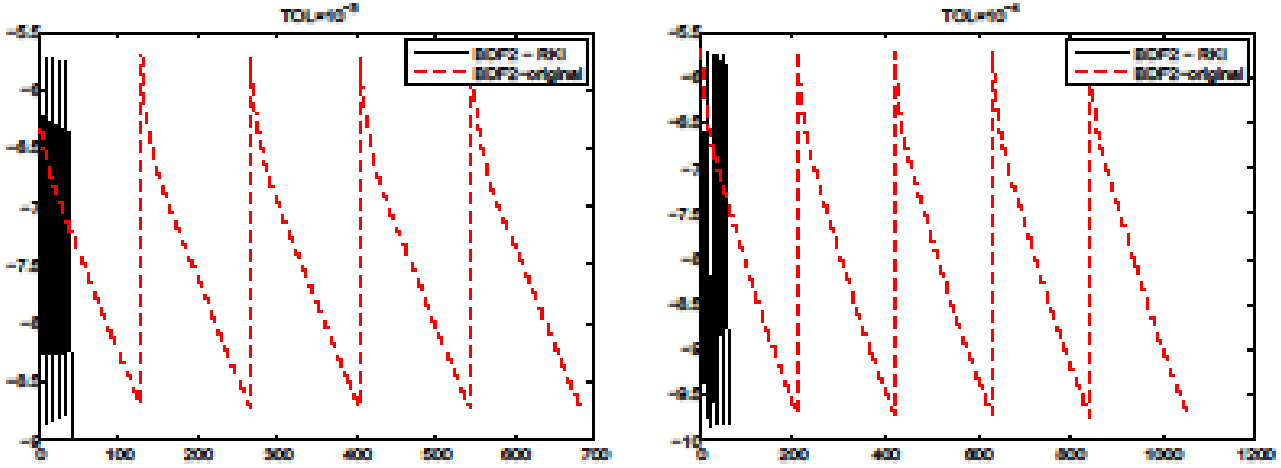
Temperature

CO2 mass fraction (A) and OH radical (B)



Dual time step for flow about NACA0012

$M_\infty = 0.10$, angle=30°, Re=3,000,000.
T=150 physical time steps, $\Delta t_{\text{physical}} = 0.20$. CFL=100, VIS0=3.5,
hfl1,2 =0.06, $\epsilon = 0.5$, niter=2



(a) (b)

Comparison of subiterative convergence for original and RKI schemes of the dual time-stepping algorithm.
(a) residual reduced 3 orders, (b) residual reduced 4 orders.

For CFL=100, $TOL = 10^{-3}$ we need on the average 5-10 subiterations per physical time step. For CFL=1000 this rises to 6-11 subiterations per physical time step with a total CPU increase of about 20-30%.
For CFL=100, $TOL = 10^{-4}$ we typically need 7-15 subiterations while for CFL=1000 we need 8-17 subiterations.

In summary: the preconditioned dual time step code needs only about 10% of the CPU of the original code.

Conclusions

- centered, upwind schemes
- structured, unstructured grids
- large time step for 2 equation turbulence model
- faster convergence chemical reactions
- faster convergence in subiterations of dual time step
- more robust solutions

Future Work

- Other turbulence models
- Multigrid in turbulence equations
- LES
- Higher Order accurate schemes (DGS, Spectral Volume/Difference, WENO)
- Non RK algorithms (ADI,GS,Krylov)