Fast preconditioned solution of Navier-Stokes equations for compressible flows with physics

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Jameson 80th Birthday

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Lecture outline

RK/Implicit smoother scheme
Turbulent models
Low Mach flows
Time dependent - Dual time step
Real gas equation of state
Chemical reactions source terms
Two-phase flow
Results
Conclusions

Why Accelerate

- Complicated multiple industrial applications
- Dual time step
- Multiple trial runs to improve accuracy

(partial) **History**

- JST
- Jameson multigrid
- Jameson Implicit Residual Smoothing
- Jameson & Caughey
- Rossow , Swanson & Turkel

- High order accurate schemes (?)

Navier-Stokes Equations

The Navier-Stokes equations for the conservative variables:

$$Q = \{\rho_1 \quad \rho_2 \quad \dots \quad \rho_n \quad \rho u \quad \rho v \quad \rho w \quad \rho e\}^T \quad ; \quad \rho = \sum_{i=1}^{n} \rho_i$$

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

$$F \cdot \vec{n} = \begin{pmatrix} \rho_1(\vec{V}\cdot\vec{n}) \\ \vdots \\ \rho_N(\vec{V}\cdot\vec{n}) \\ \rho u(\vec{V}\cdot\vec{n}) + n_x P \\ \rho v(\vec{V}\cdot\vec{n}) + n_y P \\ \rho w(\vec{V}\cdot\vec{n}) + n_z P \\ (E+P)(\vec{V}\cdot\vec{n}) \end{pmatrix} \qquad F_v \cdot \vec{n} = \begin{pmatrix} -\rho_1\vec{\upsilon}_1\cdot\vec{n} \\ \vdots \\ -\rho_N\vec{\upsilon}_N\cdot\vec{n} \\ \tau_x\cdot\vec{n} \\ \tau_x\cdot\vec{n} \\ \tau_x\cdot\vec{n} \\ (-q_x + \tau_x V - \sum_{k=1}^{N}\rho_k\vec{\upsilon}_k h_k)\cdot\vec{n} \end{pmatrix} \qquad S = \begin{pmatrix} \dot{\rho}_1 \\ \vdots \\ \dot{\rho}_n \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$E = \rho\left(\frac{P}{(\gamma-1)\rho} + \frac{1}{2}u^2\right)$$ **for ideal gas** $$E = \sum_{k=1}^{N}\rho_k e_k(T) + \rho\frac{1}{2}u^2$$ **for a real gas**

$\vec{\upsilon}_j$ are the diffusion velocities of the species j

h_j are the specific enthalpy per unit mass of the species j

τ_x is the stress tensor and q is the heat flux

P is the pressure and V is the velocity of the gas

RK/Implicit smoother with source terms

The equations set we solve in conservative form is:

$$\frac{\partial Q}{\partial t} + \nabla F = S(Q)$$

Applying the Gauss theorem for an arbitrary control volume and discretization in time yields the basic scheme:

$$\frac{\Delta Q}{\Delta \tau} = S - \frac{1}{V}\oint_S F \cdot \vec{n} ds = S - \frac{1}{V}\sum_{all\ faces} F \cdot \vec{n} ds$$

The Runge-Kutta time marching scheme is:

$$Q^{k+1} = Q^0 - \alpha_k \Delta t R^k$$

The residual of the k-th step is:

$$R^k = S^k - \frac{1}{V} \sum_{all\ faces} F^k \cdot \vec{n} ds$$

For accelerating the calculations using large CFL numbers the residual is replaced by a spatially smoothed residual $\tilde{R}^k$

Following Rossow 2006, Swanson et al. 2007,

we start with the spatially discretized equation:

$$\frac{\Delta Q}{\Delta t} + \frac{1}{V} \sum_{all\ faces} F \cdot \vec{n} ds - S = 0$$

Linearizing F and S in time we obtain:

$$\left(I + \frac{\Delta t}{V} \sum_{all\ faces} A \cdot \vec{n} ds - \Delta t \frac{\partial S}{\partial Q} \right) \Delta Q = R^k$$

$A \equiv \frac{\partial F}{\partial Q}$ - the flux Jacobian

$\frac{\partial S}{\partial Q}$ - the source Jacobian

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:

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

$$= R^{k} - \varepsilon\Delta\tau \sum_{all\ faces} A^{-}\Delta\tilde{Q}_{NB}\vec{n}dS$$

- k-ω SST model equations - nonconservative

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

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

- Spalart-Allmaras model equation - nonconservative

$$\frac{\partial \tilde{\nu}}{\partial t}+\vec{u}\cdot\nabla\tilde{\nu} = C_{b1}\left(1-f_{t2}\right)\tilde{S}\tilde{\nu} + \frac{1}{\sigma}\left\{\nabla\left[\left(\nu+\tilde{\nu}\right)\nabla\tilde{\nu}+C_{b2}\left|\nabla\tilde{\nu}\right|^2\right]\right\} -$$

$$\left[C_{w1}f_w - \frac{C_{b1}}{\kappa^2}f_{t2}\right]\left(\frac{\tilde{\nu}}{d}\right)^2$$

Low speed artificial flux:

$$f_{i+1/2} = \frac{1}{2} A \cdot \left(u_{i+1} + u_i \right) - \frac{1}{2} \left| A \right| \cdot \left(u_{i+1} - u_i \right)$$

where $\left| A \right| = \left| A \right| \left(c' \right)$

$$c' = \sqrt{\alpha^2 q^2 + M_r^2 c^2} \qquad \alpha = \tfrac{1}{2} \left(1 - M_r^2 \right)$$

$$M_r^2 = \min \left(\max \left(M^2, k M_\infty^2 \right), 1 \right)$$

and in the RK implicit smoother operator

$$R = R \left(c' \right)$$

Time dependent - Dual time step

- For steady state use pseudo time approach
- Dual time stepping used for time dependent flow to use acceleration methods developed for steady state flow
- Physical time derivative is source term in equations
- Approximate physical time derivative with a backward difference scheme:

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

Since we do not know Q^{n+1} we approximate by with Q^{k}. The residual is now

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

For dual time steps the smoothing operator is slightly modified:

$$\left(I + \varepsilon \frac{\Delta t}{Vol} \sum_{all\ faces} A^+ \vec{n} dS + c_t \alpha_k \frac{\Delta \tau}{\Delta t} I \right) \Delta \tilde{Q}_{local}$$

$$= R^k - \varepsilon \Delta t \sum_{all\ faces} A^- \Delta \tilde{Q}_{NB} \vec{n} dS$$

Real gas equation of state

The equation of state is: $$P = \frac{\rho RT}{W} = RT \sum_{i=1}^{n} \omega_i$$

ω_k, w_k - Molar concentration and molecular weight of the species

The mean molecular weight is: $$W^{-1} = \sum_{i=1}^{n} \frac{\rho_i}{\rho} \frac{1}{w_i}$$

The mean internal energy per unit mass is:

$$e(T) = \sum_{i=1}^{N} y_i e_i(T)$$

Chemical reactions source terms – Arrhenius model

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

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

- ω_k, w_k - Molar concentration and molecular weight of the species
- v_{ik} - Stochiometric coefficients of the species k in the reaction i
- q_i - 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:

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

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:

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

- 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

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

Two-phase flow

- Solution of reactive, turbulent two-phase flow
- Gaseous main phase
- Continuous dispersed phase includes mixture of liquid and solid particles
- Particles void fraction is negligible

Coupled Navier-Stokes and dispersed phase system

In N-S equations a source term due to the dispersal phase is added

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

The EDP equation model – “fluidized” equation for the dispersed phase

The variables we solve for are $\{\rho_p, \vec{v}_p, T_p, \chi_p\}^T$

$\rho_p, \vec{v}_p, T_p$ are the disperse phase density, velocity and temperature

χ_P is the solid fraction $0 \le \chi_p \le 1$

when $\chi_p = 1$ the particles are totally solid,

when it’s equal to zero, the particles are liquid.

Conservation of mass

$$\frac{\partial \rho_p}{\partial t} + \nabla\left(\rho_p \vec{v}_p\right) = 0$$

Momentum

$$\left(\frac{\partial v_{p,i}}{\partial t} + \vec{v}_p \cdot \nabla v_{p,i}\right) = \frac{f_D}{\tau_u} \cdot \left(v_{g,i} - v_{p,i}\right) \quad ; i = (x, y, z)$$

Temperature

$$\frac{\partial T_p}{\partial t} + \vec{v}_p \cdot \nabla T_p = \begin{cases} \dfrac{\dot{Q}}{m_p C_{p,p}} & T \neq T_{melt} \\ 0 & \text{otherwise} \end{cases}$$

where

$$\dot{Q} = m_p C_{p,p} \frac{f_N}{\tau_T}\left(T_f - T_p\right)$$

Solid fraction

$$\frac{\partial \chi_p}{\partial t} + \vec{v}_p \cdot \nabla \chi_p = \begin{cases} -\dfrac{\dot{Q}}{m_p L_m} & T = T_{melt} \\ 0 & \text{otherwise} \end{cases}$$

The source terms for the N-S EDP equations are

$$\vec{S}_f^{cons} = \begin{pmatrix} 0 \\ -\frac{f_D}{\tau_u}\rho_p\left(u_f - u_p\right) \\ -\rho_p\frac{f_D}{\tau_u}\left(v_f - v_p\right) \\ -\rho_p\frac{f_D}{\tau_u}\left(w_f - w_p\right) \\ -\rho_p C_{p,p}\frac{f_N}{\tau_T}\left(T_f - T_p\right) - \frac{f_D}{\tau_u}\rho_p\vec{u}_p\cdot\left(\vec{u}_f - \vec{u}_p\right) \end{pmatrix}$$

where

$$F_D = \begin{cases} 1 + 0.15\,\mathrm{Re}_p^{\,0.687} & \mathrm{Re}_p < 1000 \\ 0.01833\,\mathrm{Re}_p & else \end{cases}; \quad F_N = 1 + 0.3\,\mathrm{Re}_p^{\,0.5}\,P_r^{\,0.33}$$

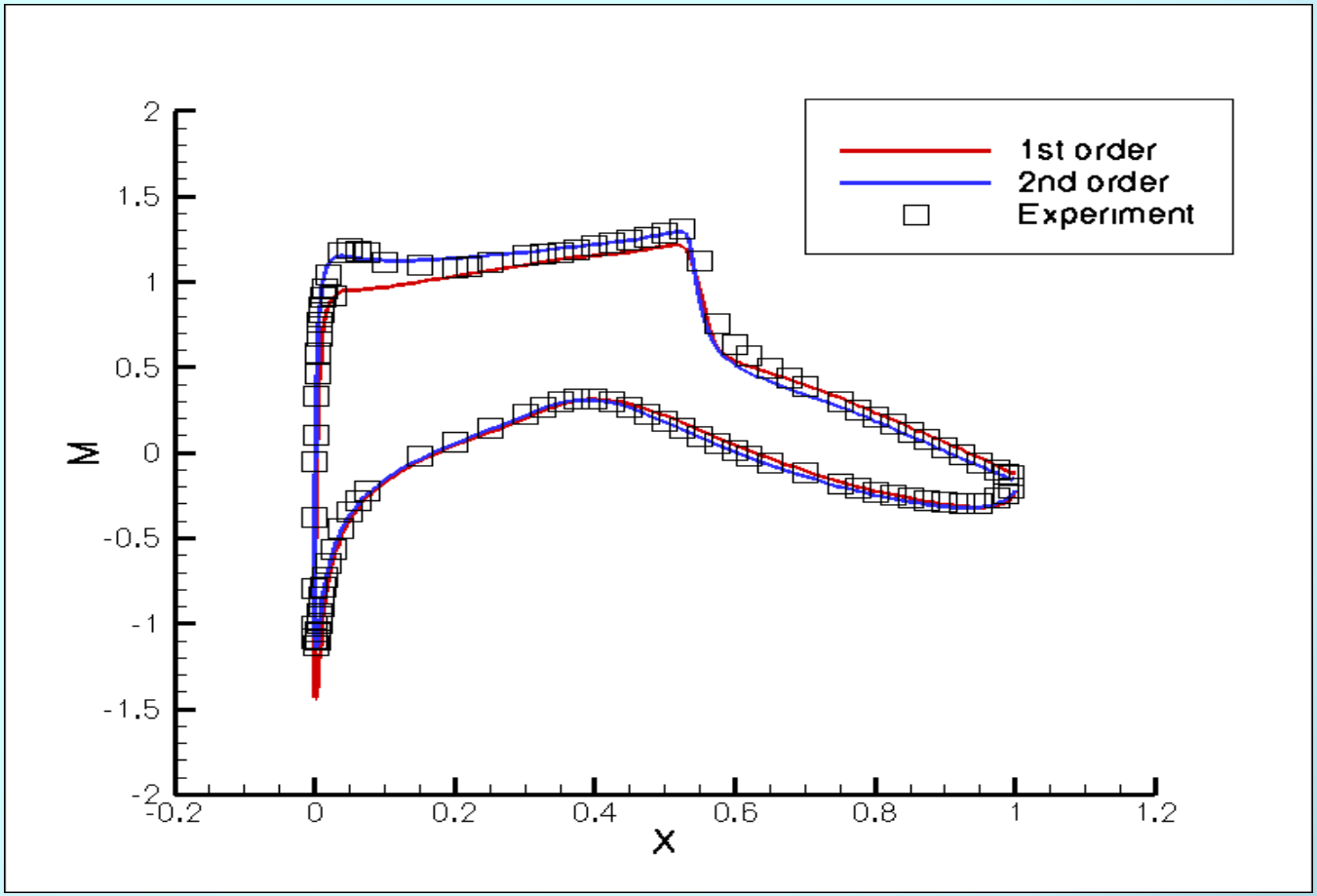
Results

- Turbulent flow – Transonic flow over RAE 2822 airfoil
- Turbulent reactive flow – rocket motor plume
- Time dependent - high angle of attack over NACA0012
- Low Mach Flow
- Two phase flow inside ballistic evaluation motor
- Conjugate heat transfer flow in converging-diverging nozzle

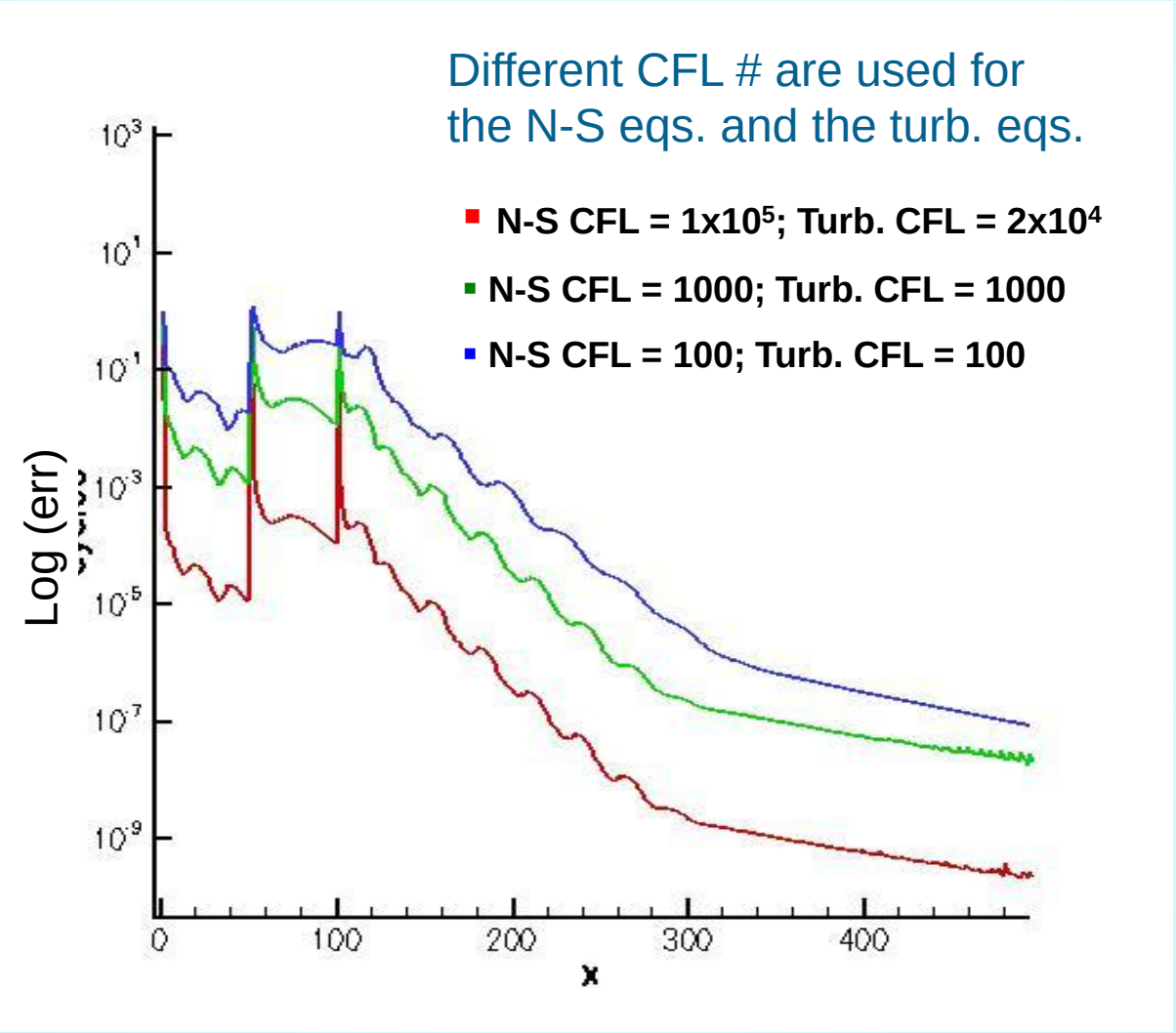
SST Turbulent flow – Transonic flow over RAE 2822 airfoil

$$M = 0.73 \quad \alpha = 2.79^{\circ} \quad \mathrm{Re} \sim 17x10^{6}$$

Comparison between experimental and computational pressure coefficient - C_p



Convergence History for Various CFL Numbers

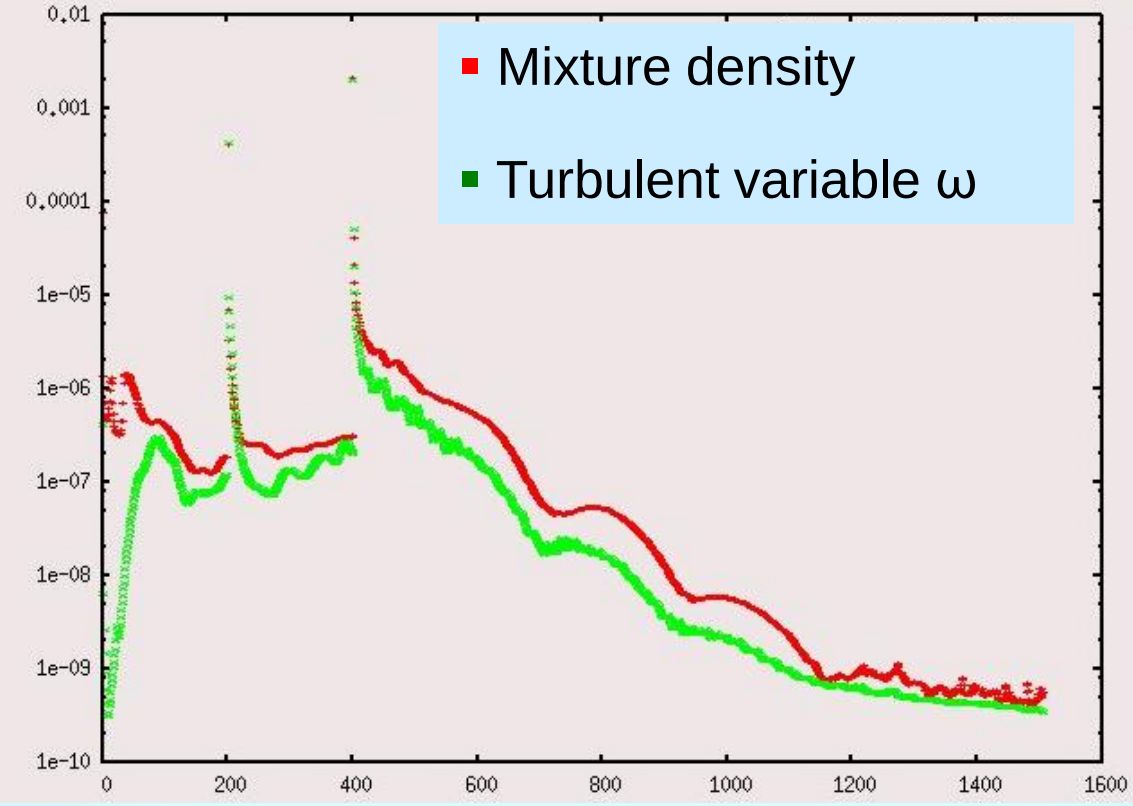


Turbulent reactive flow – rocket motor plume

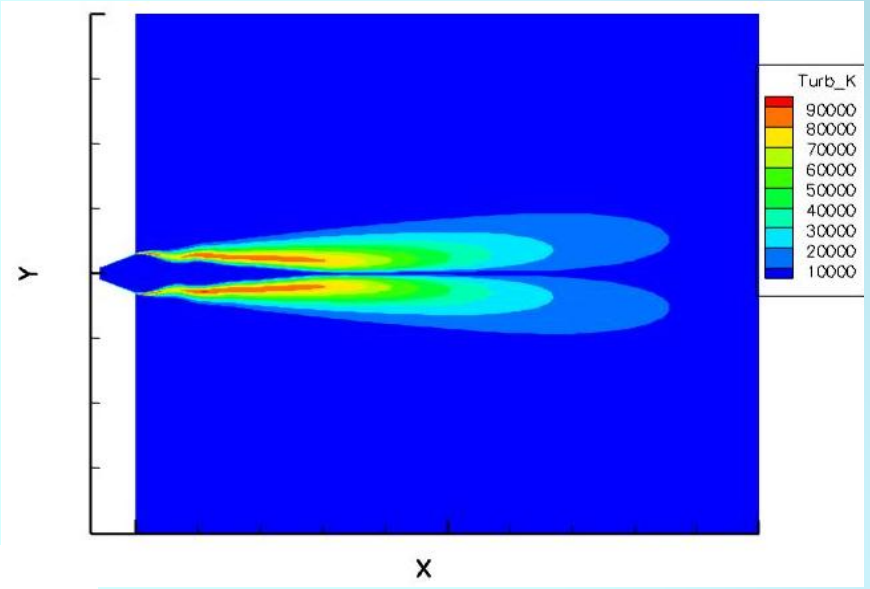
- A rocket motor plume exiting from the motor nozzle into a low Mach number free stream flow.
- The flow velocity on the nozzle throat is sonic and the species mass fractions are defined.
- The species used for this problem are: H, O, OH, H2, O2, CO, CO2, H2O, HCl and N2.
- About 50 chemical reactions were considered

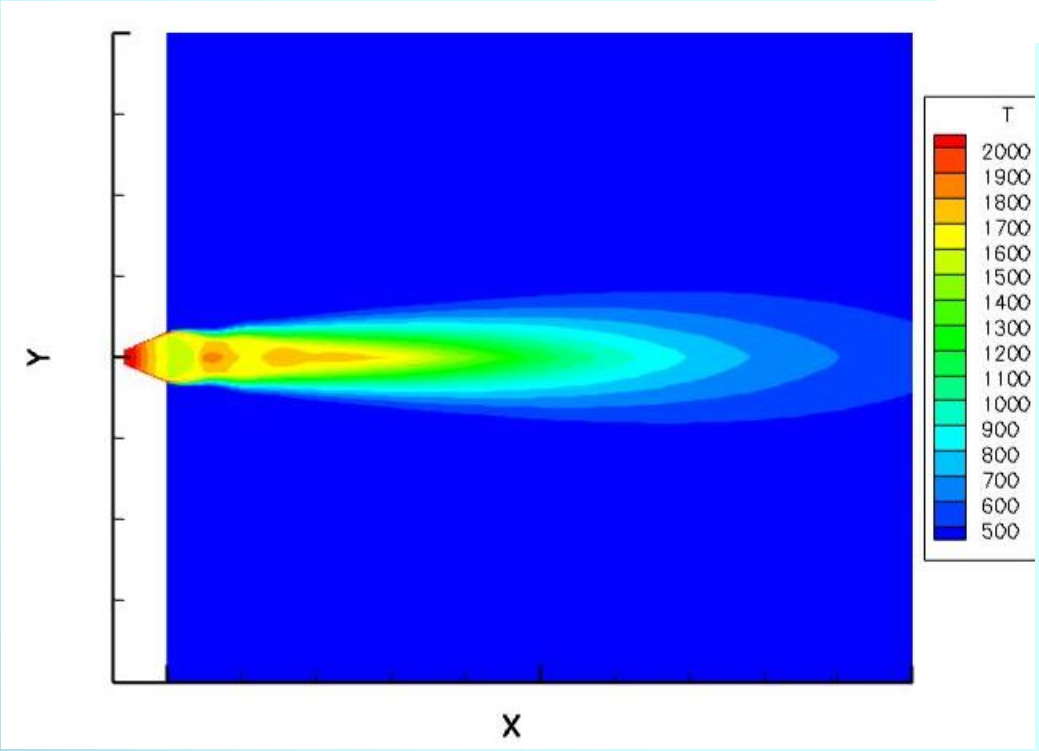
Convergence history

fluid CFL =100,000 and turbulent CFL =200



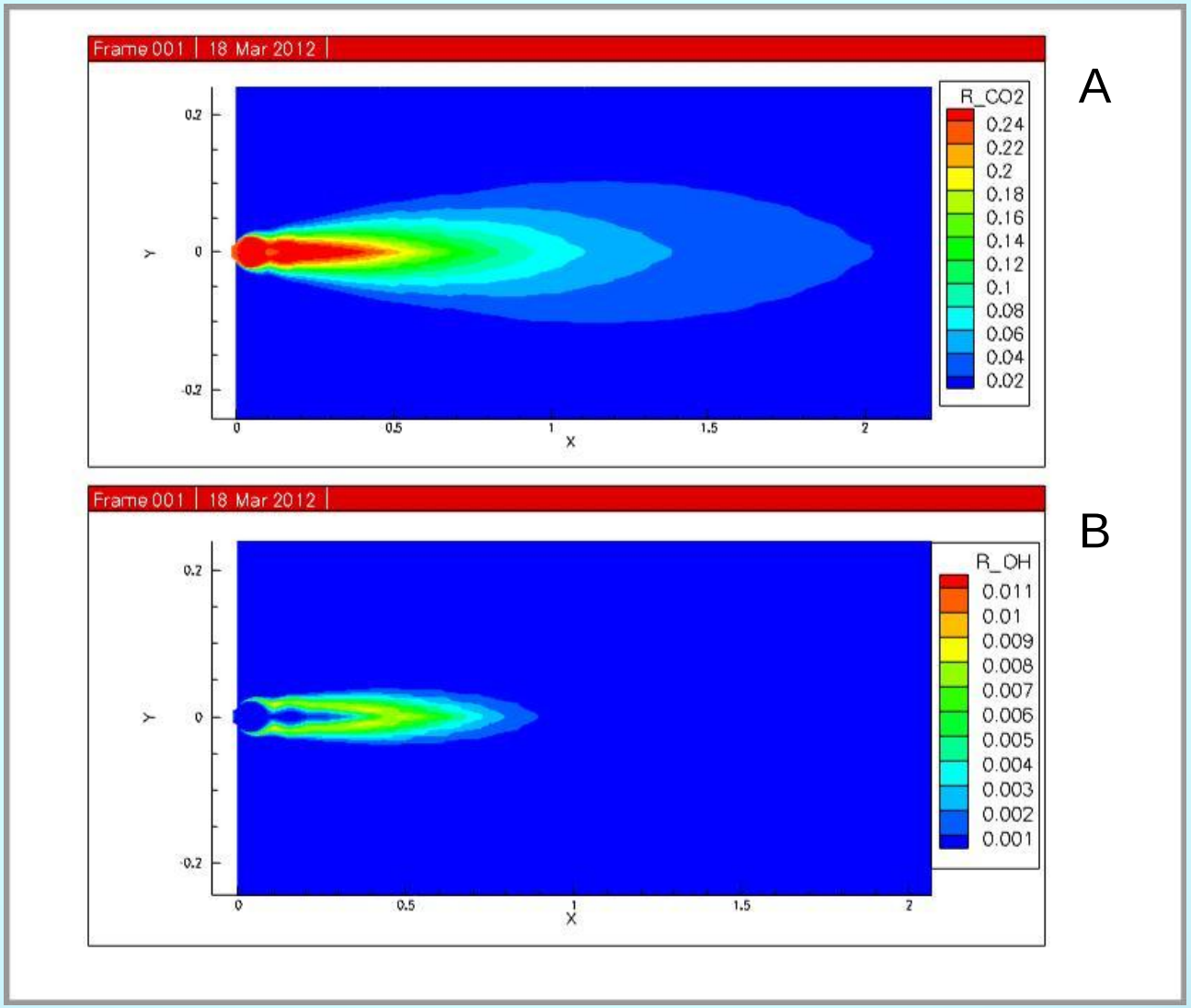
Turbulent kinetic energy





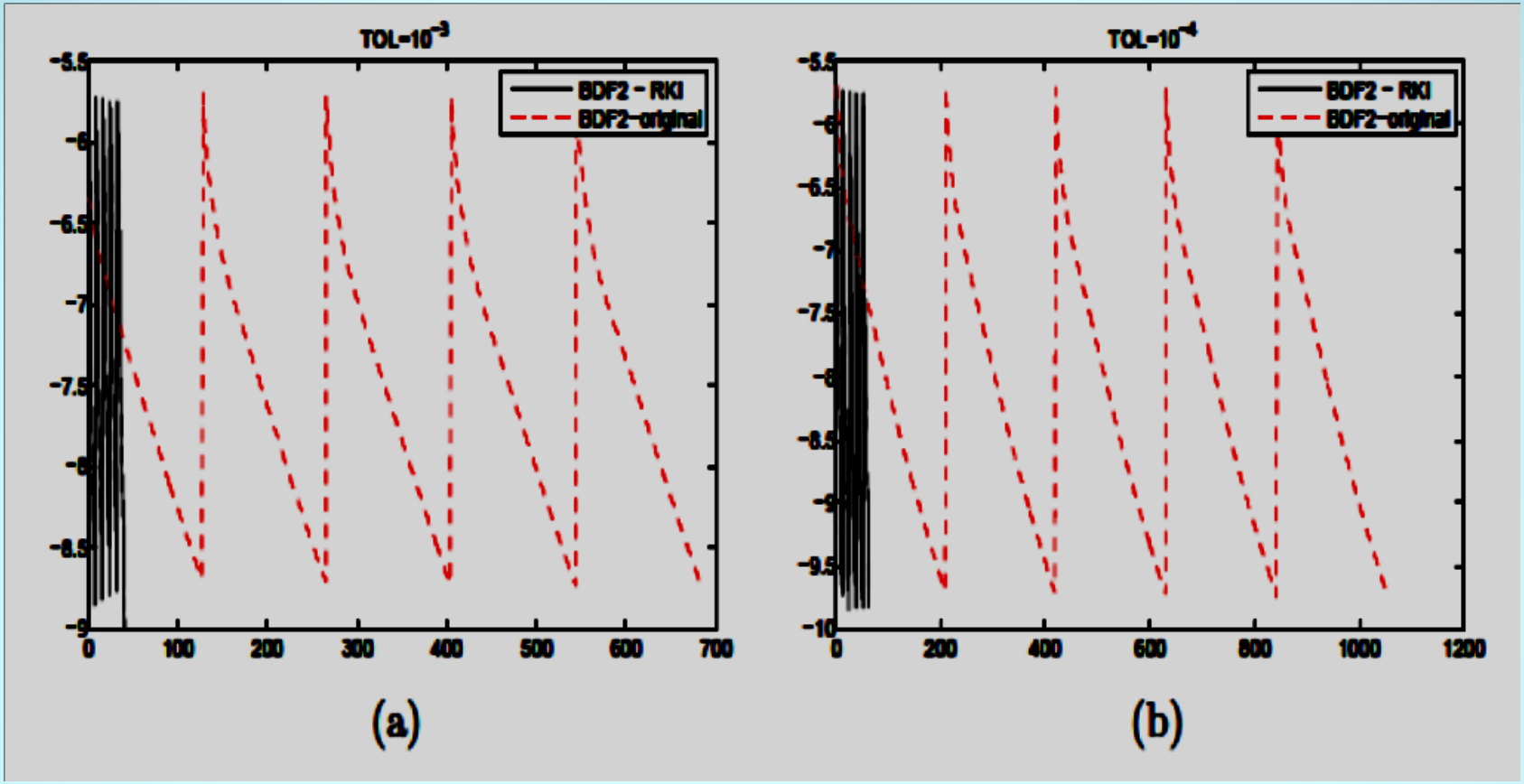
Temperature

CO_2 mass fraction (A) and OH radical (B)



Dual time step for flow over NACA0012

- M_∞=0.1, angle of attack = 30°, Re = $3x10^6$
- 150 physical time steps. $\Delta t_{physical}$ = 0.2 sec.
- CFL = 100, relaxation factor ε = 0.5



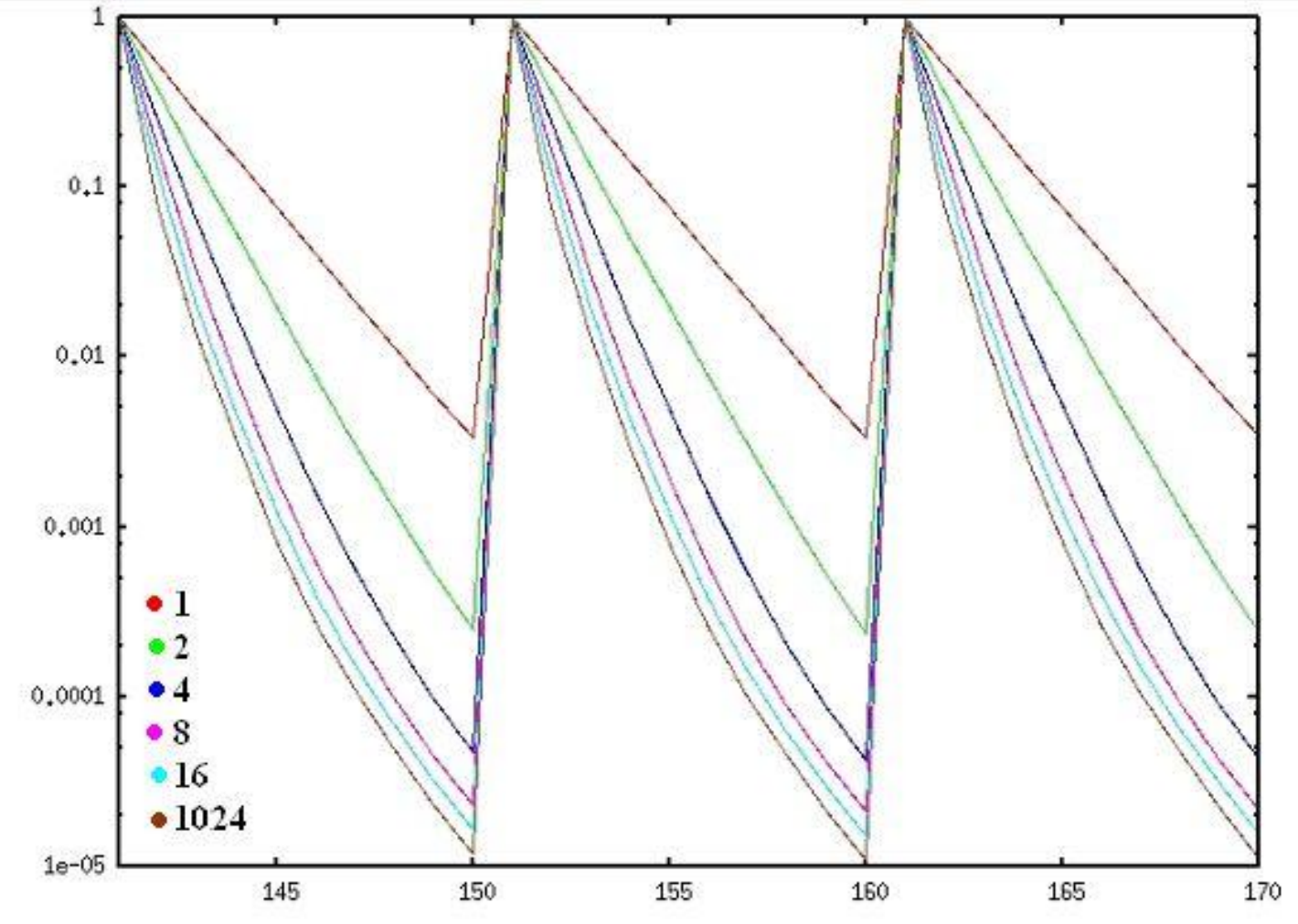
Residual reduced 3 orders

Residual reduced 4 orders

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

Convergence history for series of CFL numbers

Time Dependent Riemann problem

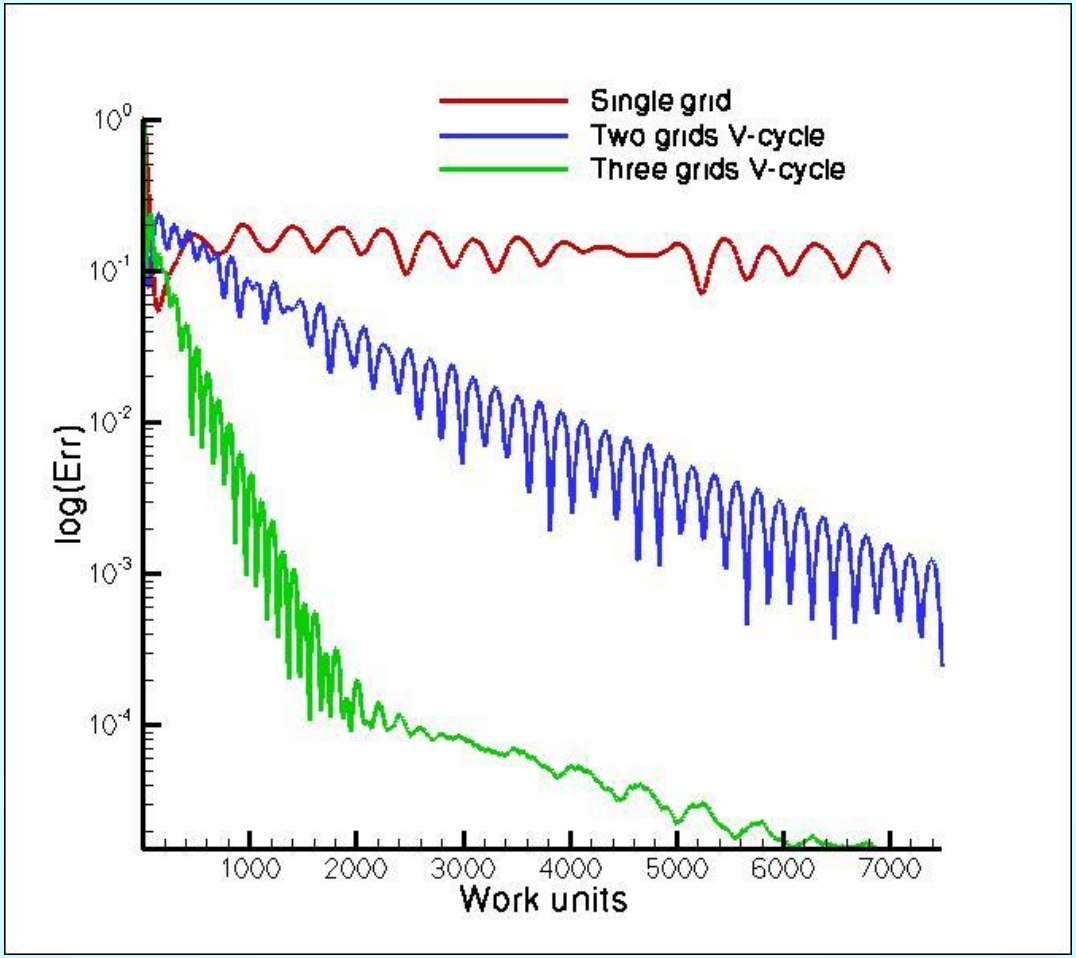


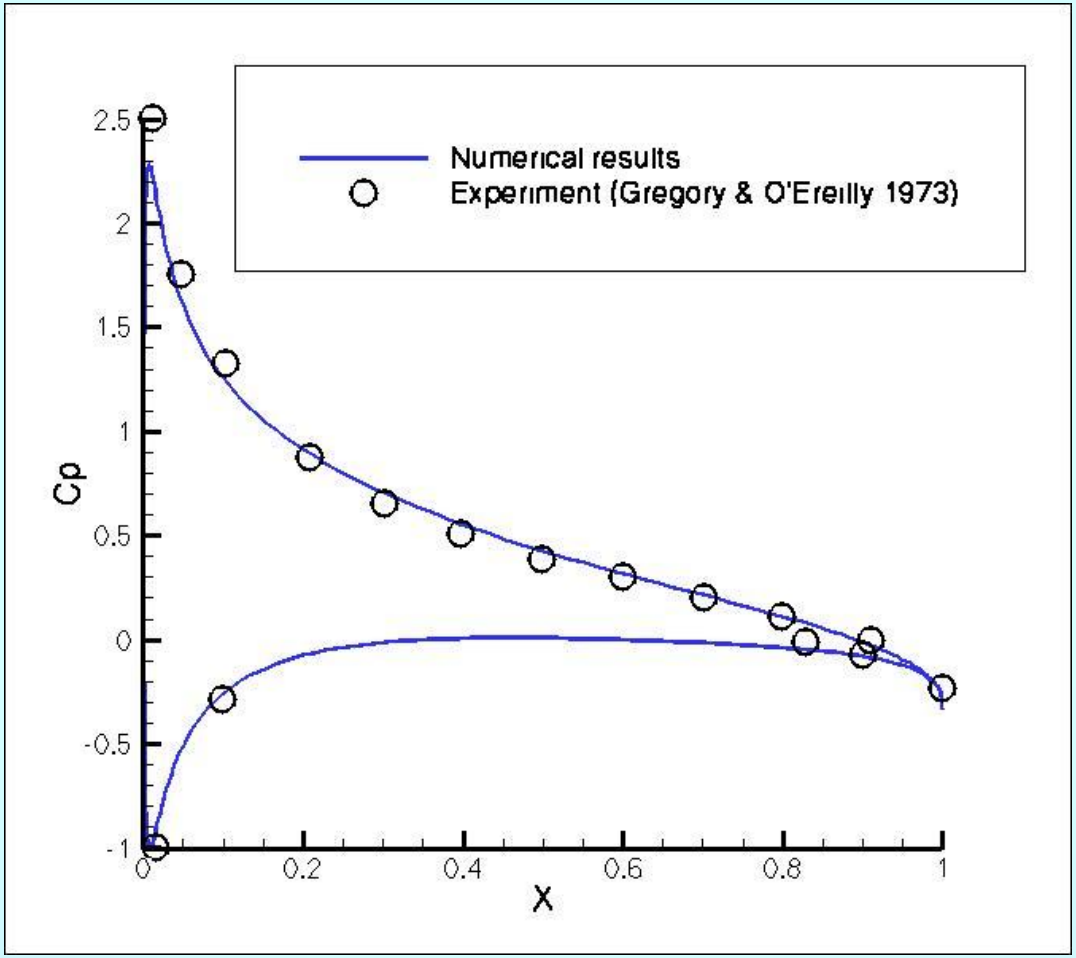
Efficiency of MG for dual time steps Depends on Δt

	TOL $=10^{-3}$		TOL $=10^{-4}$	
# MG levels	Avg # subiteration	CPU	Avg # subiteration	CPU
no MG	14.56	12 min 8 sec	Δt 23.93	19 min 58 sec
2	9.79	11min 51 sec	16.97	20 min 22 sec
3	9.22	11 min 3 sec	16.29	20 min 2 sec
4	8.98	12 min 17 sec	16.23	19 min 16 sec

Low Mach Flows

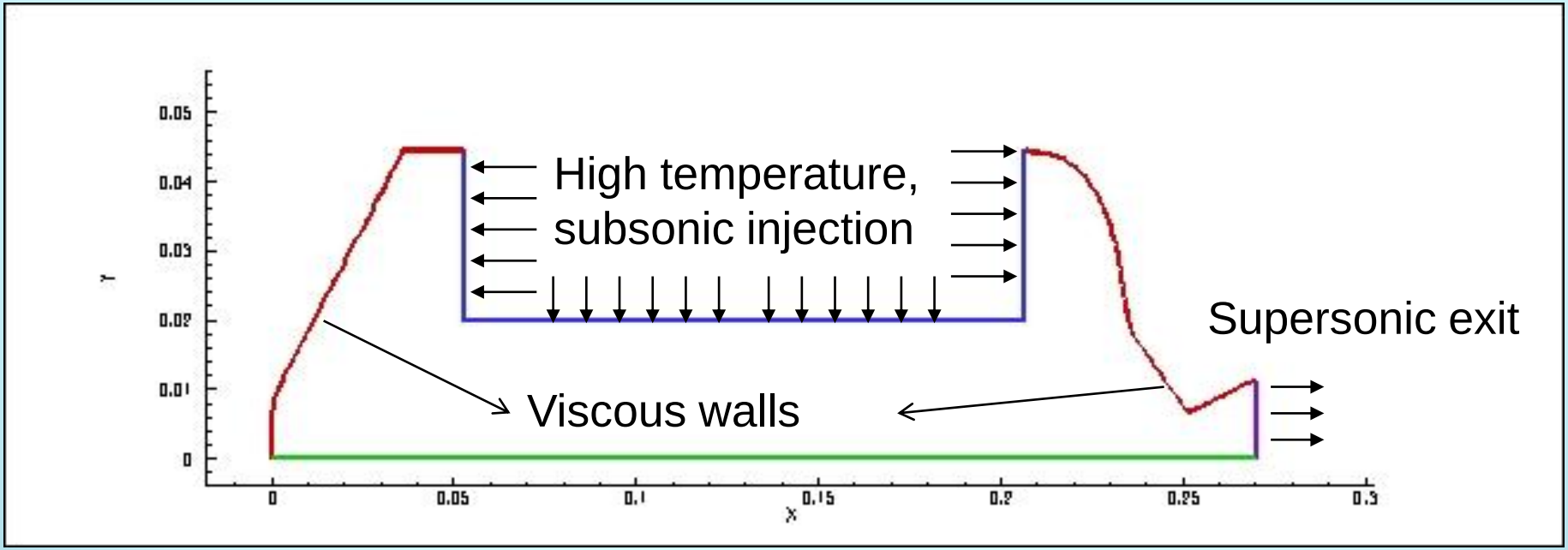
NACA0012 M=0.001



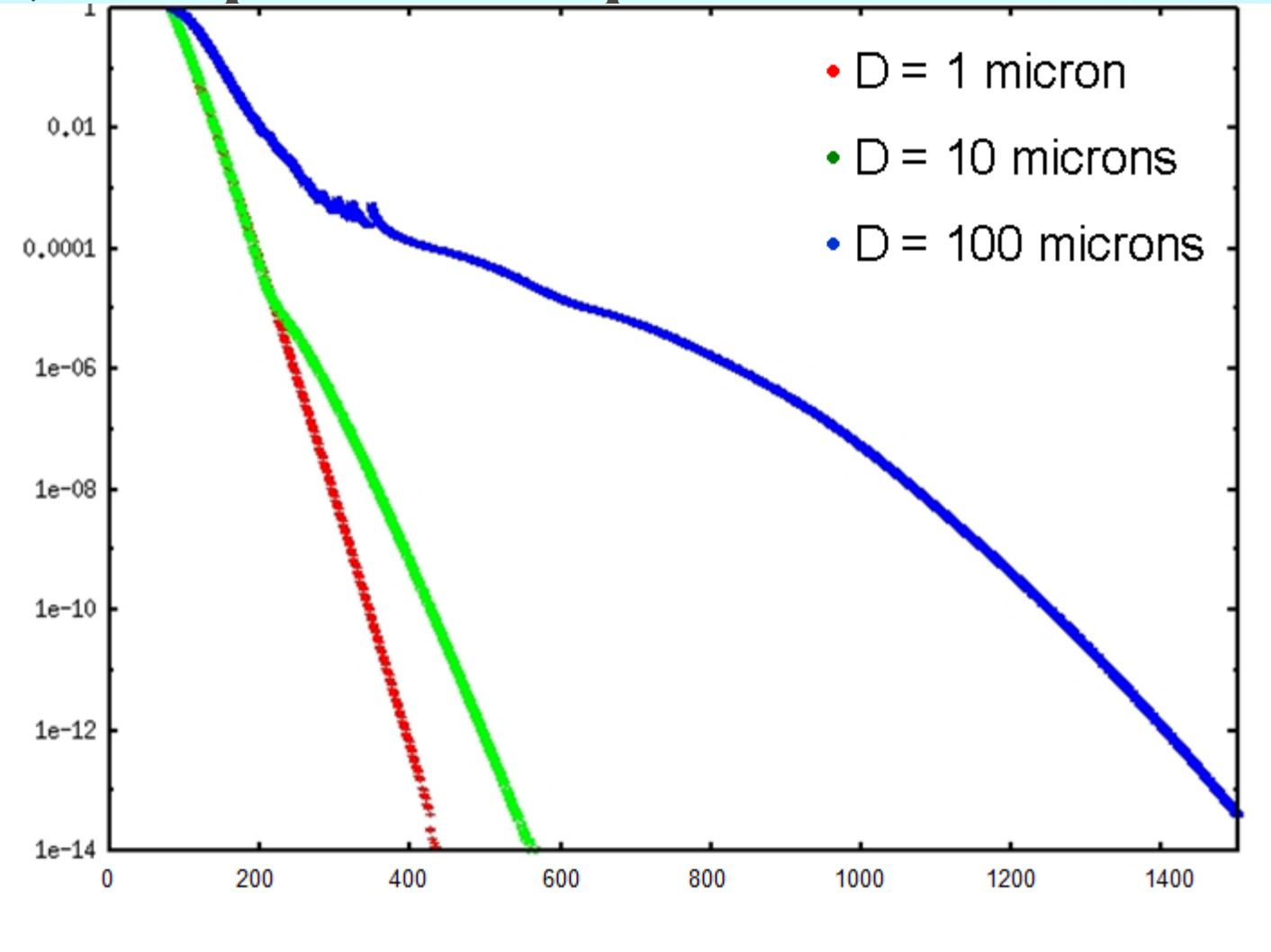

Numerical results
Experiment (Gregory & O'Ereilly 1973)
Cp
X
2.5
2
1.5
1
0.5
0
-0.5
-1
0
0.2
0.4
0.6
0.8
1

Two phase flow inside a Ballistic Evaluation Motor (BEM)- EDP

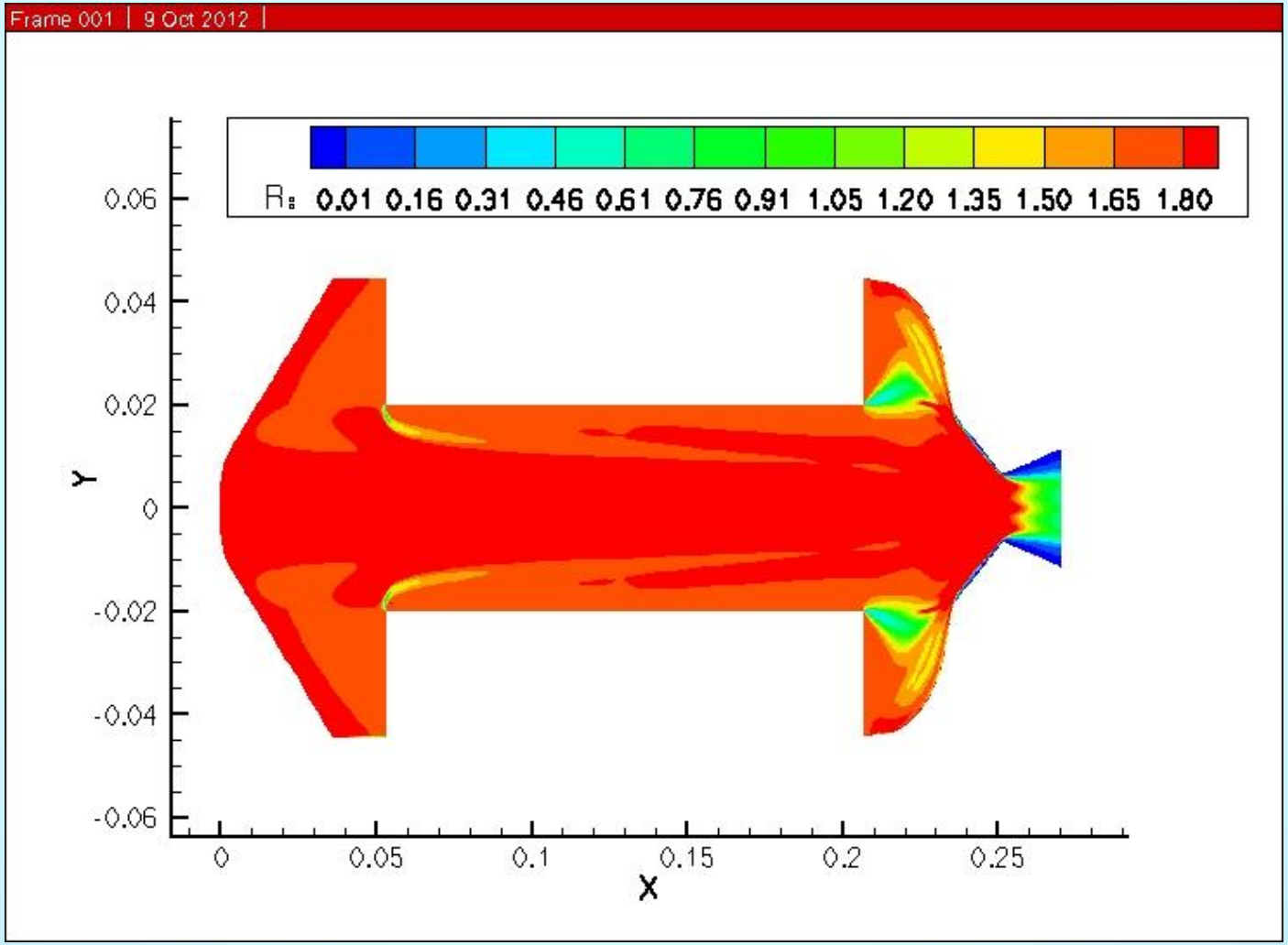
- The problem of flow inside a solid rocket motor is solved using:
- Finite volume, local time step, 3 levels sequencing and multigrid acceleration
- The schemes that were used are first order upwind for the EDP system and AUSM+UP for the gas phase system



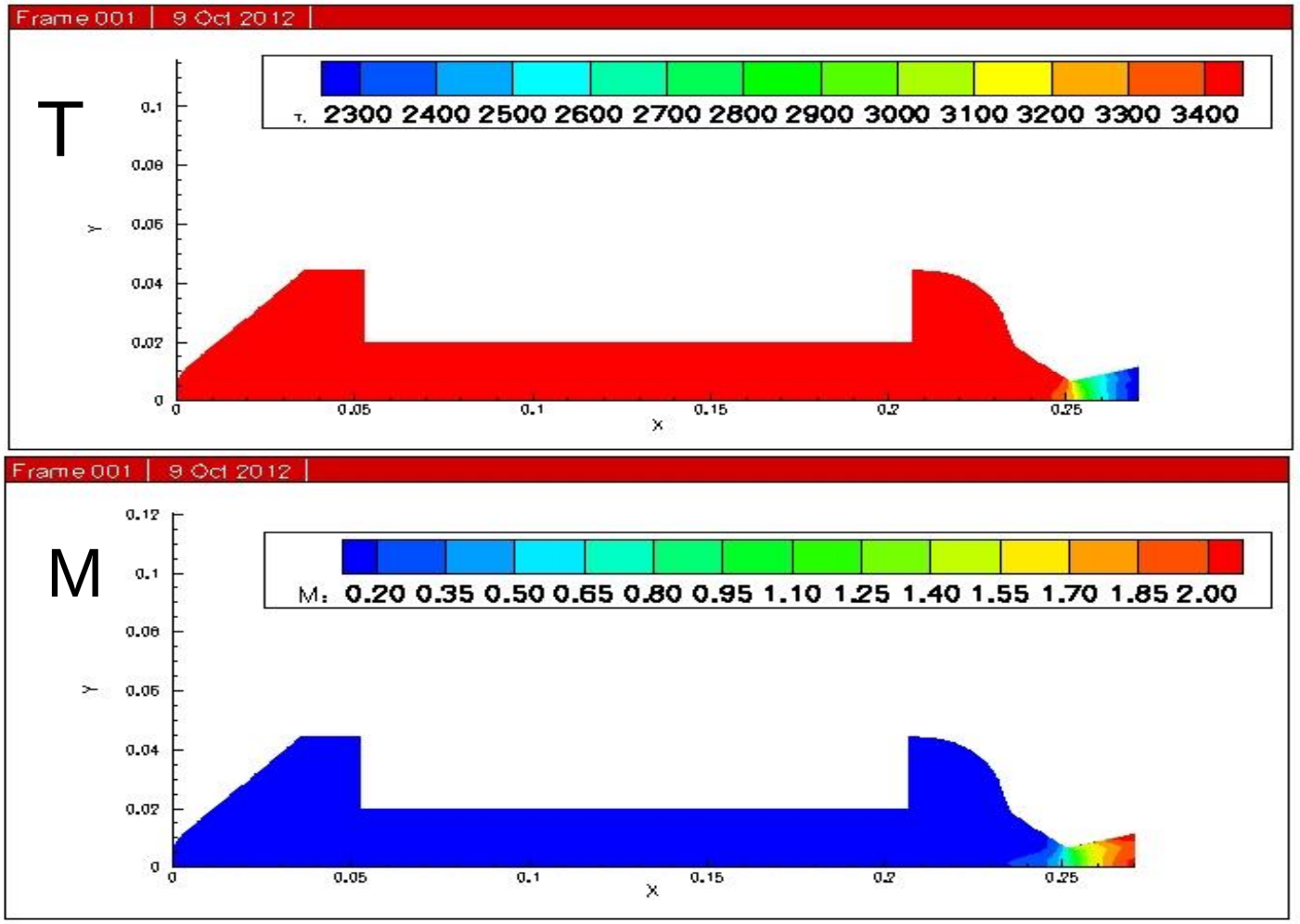
Typical convergence history (Dispersed phased density)



Global view of contour map for disperse phase density (5 microns)



Typical contour map for gas phase temperature and Mach number



Conclusions

- RK/implicit smoothing allows larger time step
- The smoother allows faster convergence of complex and stiff flow problems including turbulent reactive flow
- Reactive flow equations are solved without operator splitting
- Two Phase Flow
- Faster convergence in sub-iterations of dual time step
- Low Mach M=0.001 solved
- More robust solutions