# SU2-NEMO: NonEquilibrium MOdels for Hypersonic Flows Using Mutation++

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# Outline

1. NEMO ambitions and roadmap *(M. Fossati)*
2. Some background equations and models *(M. Fossati)*
3. Recasting the TNE2 solver into NEMO *(W.T. Maier)*
4. Verification/validation *(W.T. Maier)*
5. Class hierarchy incorporating Mutation++ *(A.C. Gomes)*
6. Hypersonic flow over double wedges *(A.C. Gomes)*

SU2 The Open-Source CFD Code

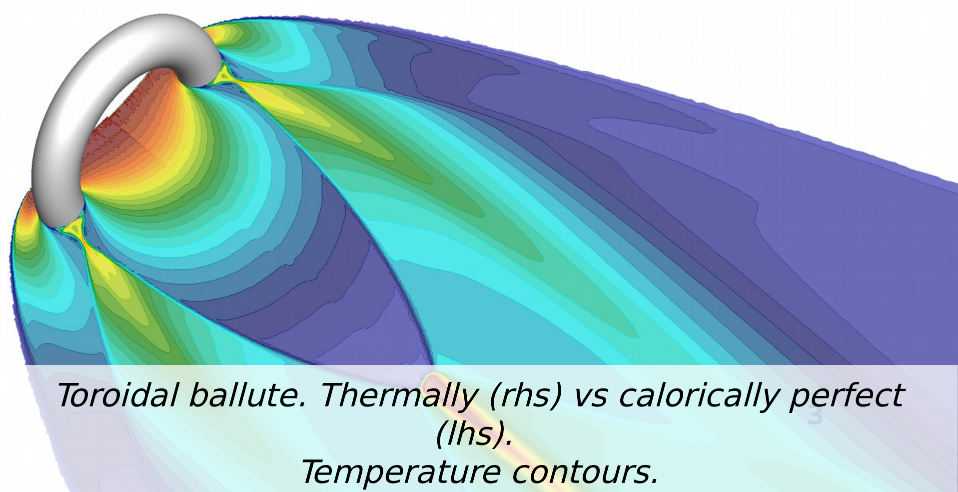
4th Annual Developers Meeting

# Ambition and objectives

*“Enhance the multi-physics capabilities of SU2 and extend the spectrum of applications, <u>with a focus on design</u>”*

- Reboot modelling of high-temperature effects using latest versions of SU2
- Define roadmap for coordinated development of thermochemistry and nonequilibrium models
- Incorporate advanced models for finite-rate chemistry and thermal nonequilibrium
- Consolidate implementation and use of advanced thermodynamic models

*X43 vehicle. Thermally (rhs) vs calorically perfect (lhs). Temperature contours.*



*Toroidal ballute. Thermally (rhs) vs calorically perfect (lhs). Temperature contours.*

# NEMO roadmap

- **Define and implement an efficient thermochemistry interface**
- **Augment library of schemes for improved robustness in high Mach**
- Extend BC formulations to account for radiative equilibrium and potentially slip flow (for high-Mach)
- **Formulate and implement models for finite-rate energy exchange (i.e. multiple temperature and energy modes)**
- **Ensure consistency with algorithmic differentiation for discrete adjoint formulation**
- Treatment of Jacobian matrix of source terms
- **Consolidate multi-species and finite-rate chemistry models with attention to the stiffness of the problem**
- Introduce compressibility effects for turbulence modeling
- Transition modeling in highly-compressible flows
- Coupling with conjugate heat transfer approach
- Coupling with Maxwell to account for MHD

# Some background equations and models

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \vec{u} - \rho_s \vec{u}_{d,1}) = \dot{w}_s$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot \left(\rho \vec{u} \otimes \vec{u} + P\bar{I} - \bar{\tau}\right) = 0$$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot \left(\rho e \vec{u} + P\bar{I} \cdot \vec{u} - \bar{\tau} \cdot \vec{u} + \vec{q}\right) = \nabla \cdot (-\textstyle\sum_s h_s \rho_s \vec{u}_{d,s}) - \nabla \cdot \vec{q}_v$$

$$\frac{\partial \rho e_v}{\partial t} + \nabla \cdot (\rho e_v \vec{u} + \vec{q}_v + \textstyle\sum_s e_{v,s}\, \rho_s \vec{u}_{d,s}) = \textstyle\sum_s Q_s^v + \sum_s Q_S^{t-v}$$

$$P = P(\rho_s, T)$$

$$e = e(X_s, T)$$

$$\rho e_v = \textstyle\sum_s \rho_s e_{v,s}$$

$$\vec{q}_v = -k_v \nabla T_v$$

$$e_{v,s} = \frac{R}{W_s} \frac{\theta_{v,s}}{\exp(\theta_{v,s}/T_v) - 1}$$

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu \delta_{ij} \nabla \cdot \vec{u}$$

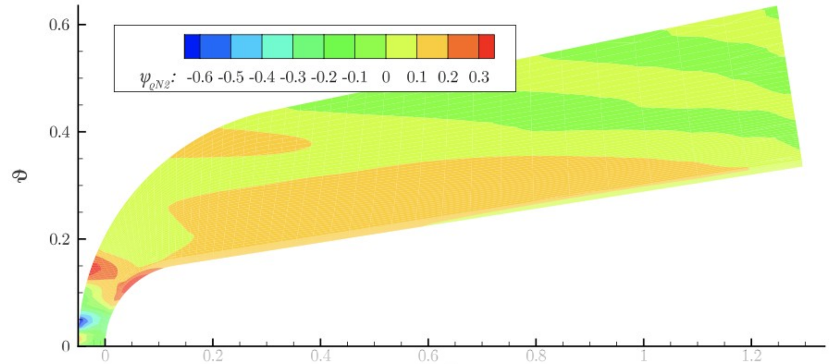
$$\vec{q} = -k \nabla T$$

$$\mu = \textstyle\sum_s \dfrac{\mu_s X_s}{\phi_s}, \quad k = \textstyle\sum_s \dfrac{k_s X_s}{\phi_s}$$

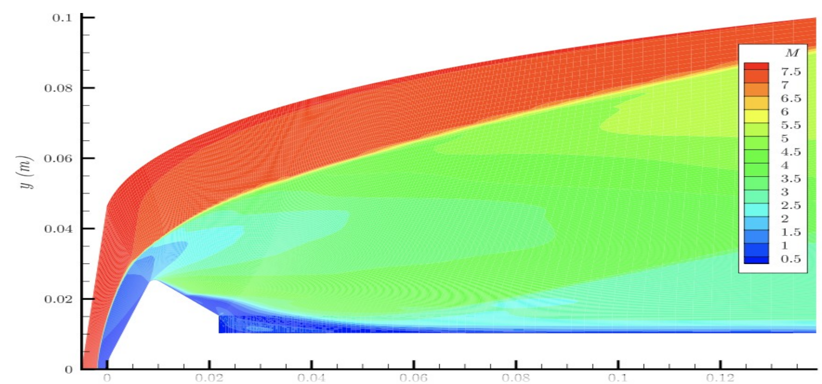
# Some background equations and models

**Initial efforts by Sean Copeland (PhD, 2015, Stanford University):** *"A Continuous Adjoint Formulation for Hypersonic Flows in Thermochemical Nonequilibrium"*

- continuum, steady, viscous, multi-component, gas mixture in thermochemical nonequilibrium
- Transport properties
  - Diffusion — Fick's Law w/ closure terms
  - Viscosity — Newtonian fluid w/ Stokes' Hypothesis
  - Thermal Cond. — Fourier's Law
- Transport coefficients: Blottner/Eucken + Wilke's semi- empirical mixing rule
- Landau-Teller vibrational relaxation with Park's limiting cross section
- Finite-rate chemistry (Arrhenius-type)
- Derivation of continuous adjoint system, boundary conditions & surface sensitivities




***RAM-C test article (Jones, 1972)***

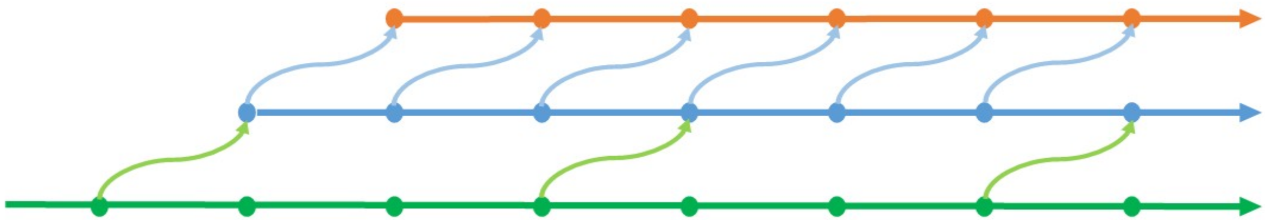



***Mars entry vehicle, M = 7.7***

… SU2 has continued to evolve … new and more general implementation needed!

# New TNE2 Solver - State of SU2-NEMO Branch

SU2
The Open-Source CFD Code




- **Code Structure**
  - Follows current SU2 structure (solver, numerics, variable structure)
  - Tracking additional equations: species continuity and vibrational energy
  - Independent from mean-flow solver (Solver_direct_mean.cpp -> solver_direct_tne2.cpp)

- **Config Structure**
  - Requires options for Gas Model and Gas Composition (N2 and AIR-5 supported and tested; options to add Argon, AIR-7, AIR-21 )
  - Requires CONV_NUM_SCHEME_TNE2, MUSCL_TNE2, etc.

- **Supported Numerical Methods**
  - Advection Upstream splitting Method (AUSM) and AUSM+-Up2 convective schemes

- **Boundary Conditions**
  - Implemented: Supersonic Inlet/Outlet, Euler Wall, Symmetry, simple convective flux far-field
  - In progress: Subsonic inlet/outlet, heat flux and isothermal walls (catalytic and non-catalytic)

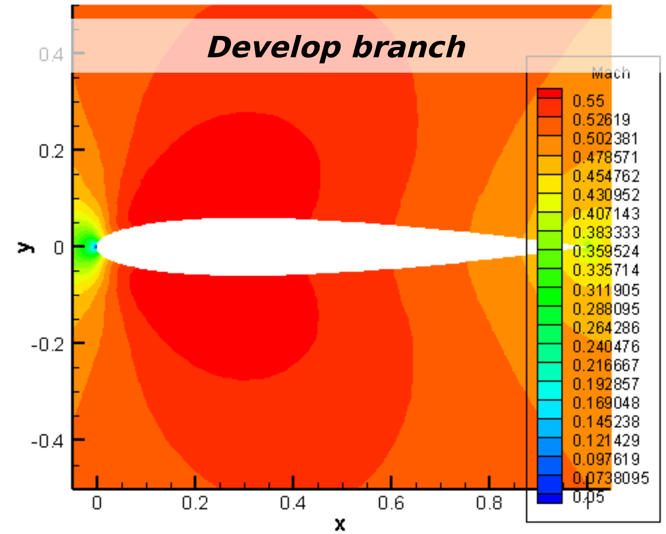
- **Discrete Adjoint Implemented and Running**
  - Some sensitivities being verified

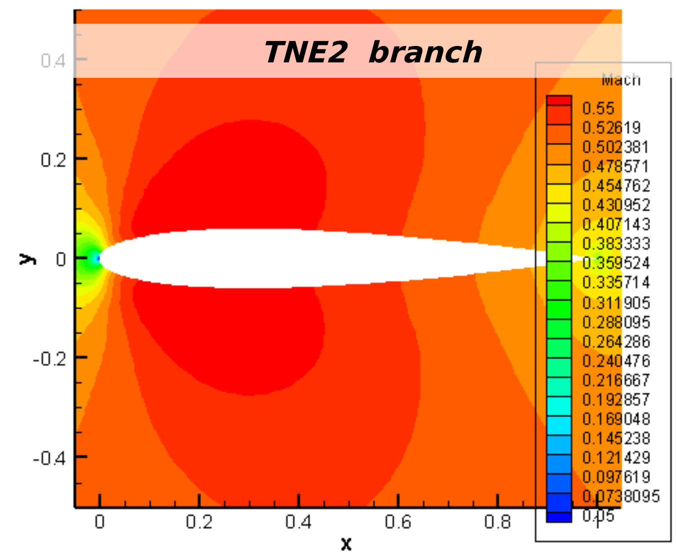
# Verification of TNE2 Euler Solver: NACA0012

| | |
|---|---|
| **Mach** | 0.5 |
| **Pressure [Pa]** | 100,000 |
| **Temperature [K]** | 300 |

- **Implicit AUSM Scheme**
  - Exact Jacobian derived by Copeland (TNE2 Case)
- **TNE2 Case Specifics**
  - AIR-5 Model used to simulate pure $N_2$ flow
    - Eliminate source terms, strange behavior at low

| | $C_L$ | $C_D$ |
|---|---|---|
| **Develop** | 0.001057 | 0.027511 |
| **TNE2** | 0.001068 | 0.027505 |

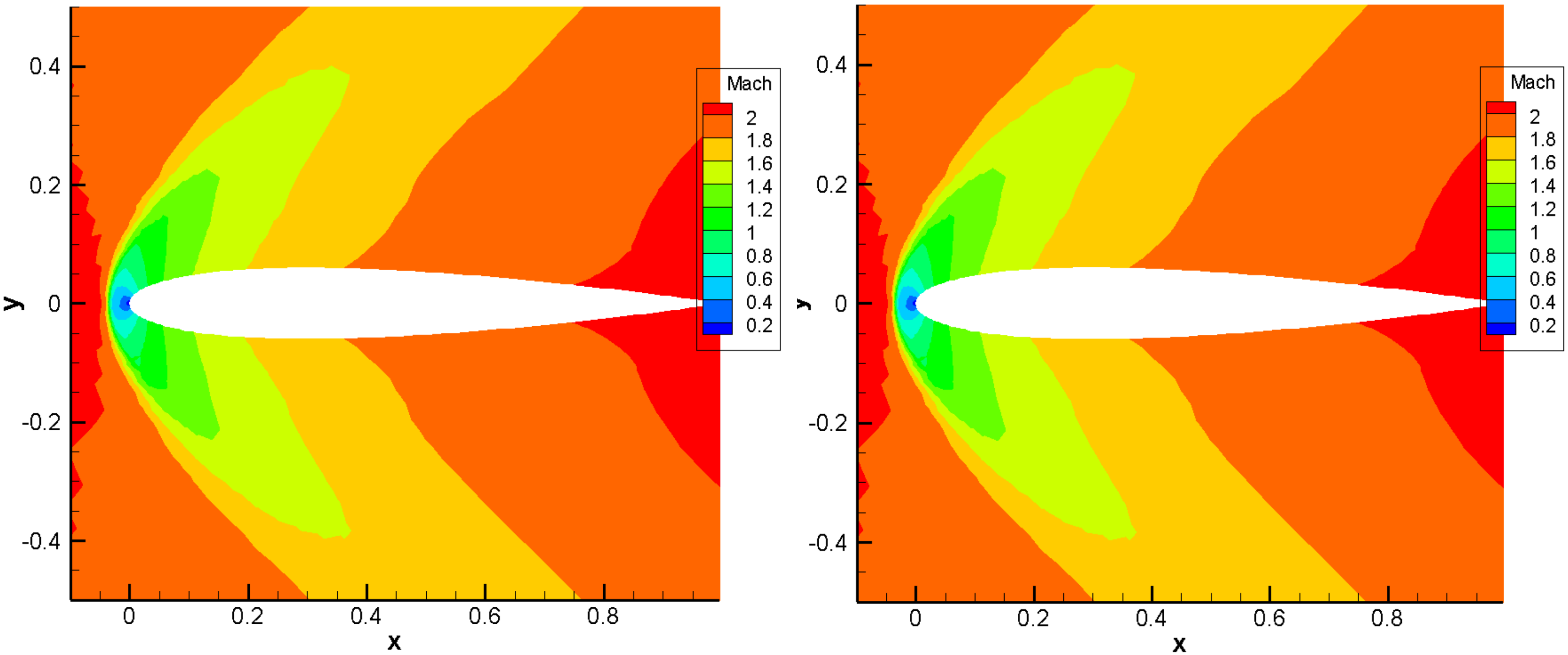


# Verification of TNE2 Euler Solver: NACA0012

| | |
|---|---|
| **Mach** | 2 |
| **Pressure [Pa]** | 100,000 |
| **Temperature [K]** | 300 |

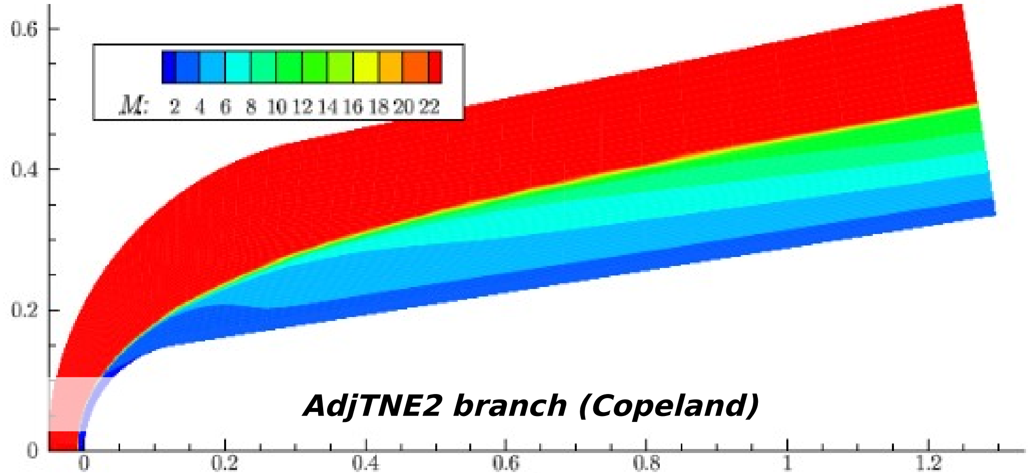
| | $C_L$ | $C_D$ |
|---|---|---|
| **Develop** | -0.000065 | 0.098630 |
| **TNE 2** | -0.000065 | 0.098630 |



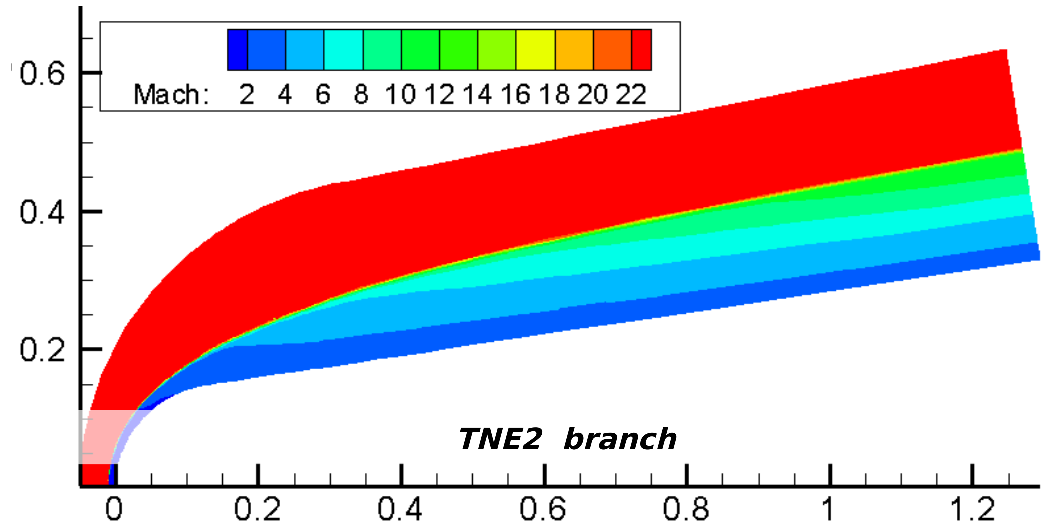

***Mach number contours. Develop branch (left), TNE2 branch (right)***

# Validation of TNE2 Euler Solver: RAM-C II case

| | |
|---|---|
| **Mach** | 23.9 |
| **Pressure [Pa]** | 19.7 |
| **Temperature [K]** | 254 |

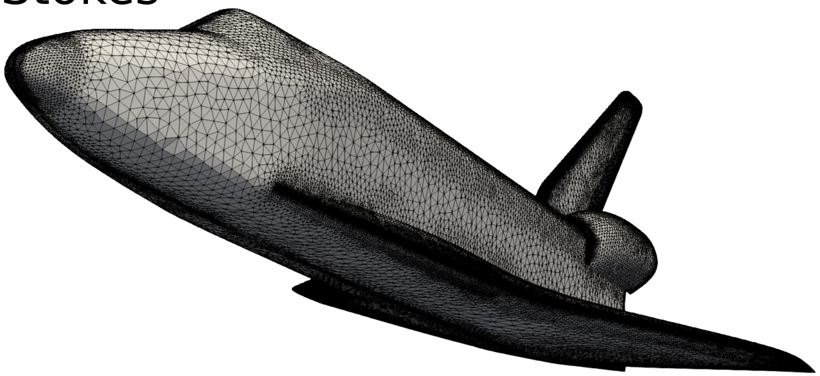



- **Implicit AUSM Scheme**
- **TNE2 Case Specifics**
    - AIR-5 Model (76% $N_2$, 23% $O_2$)
- Slight differences in shock structure
    - May be due to mesh differences



# Ongoing Developments

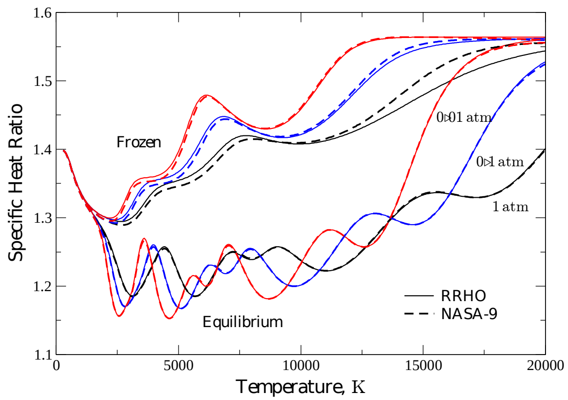
- Implementation of subsonic, characteristic-based outlet boundary
- Validation and verification of Navier-Stokes solver/boundary conditions
  *Space shuttle wing or Mars entry vehicle*

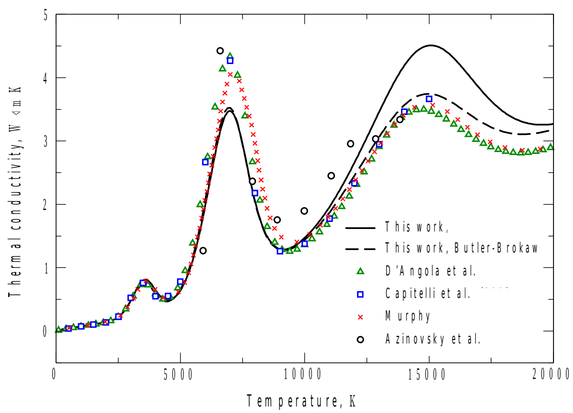


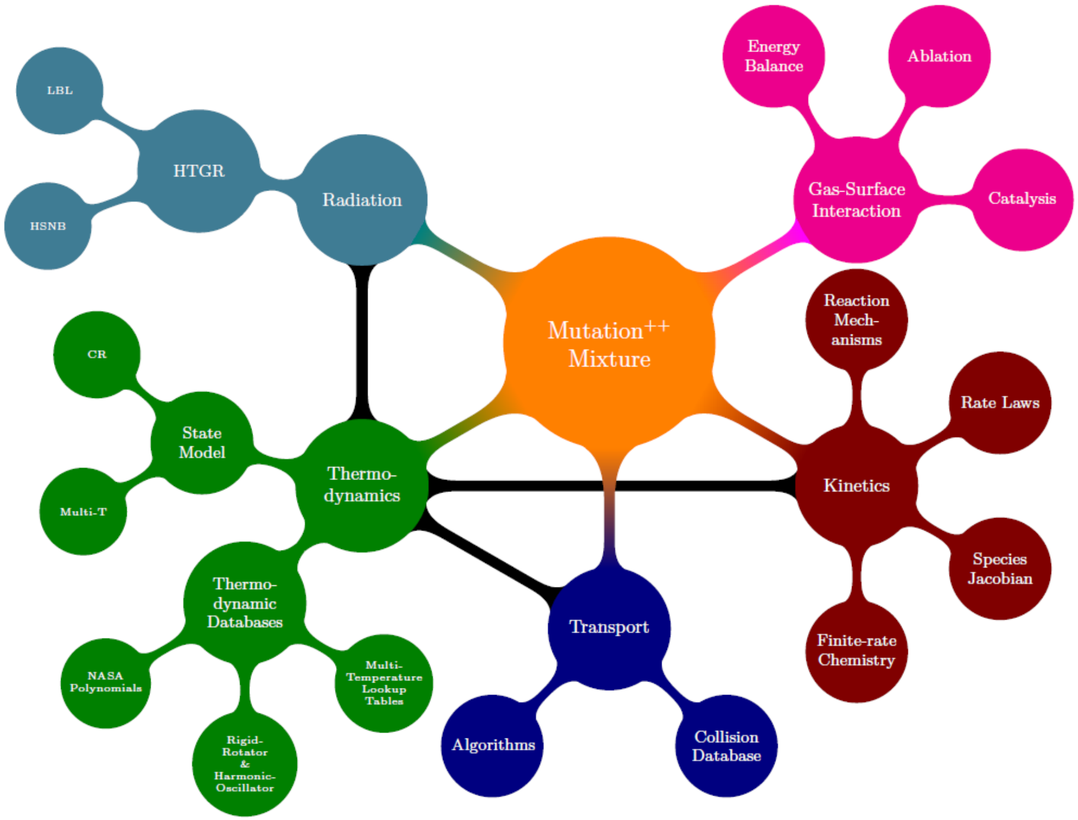
- Discrete adjoint sensitivity
  *Validate using RAM-C II case*
- Verify TNE2 source terms at low speed/temperature regimes
- Strong interest in transitional flow prediction using RANS-style modeling

# Consistency and flexibility through Mutation++

- Thermodynamic properties
- Multicomponent transport properties
- Finite rate chemistry in thermal nonequilibrium



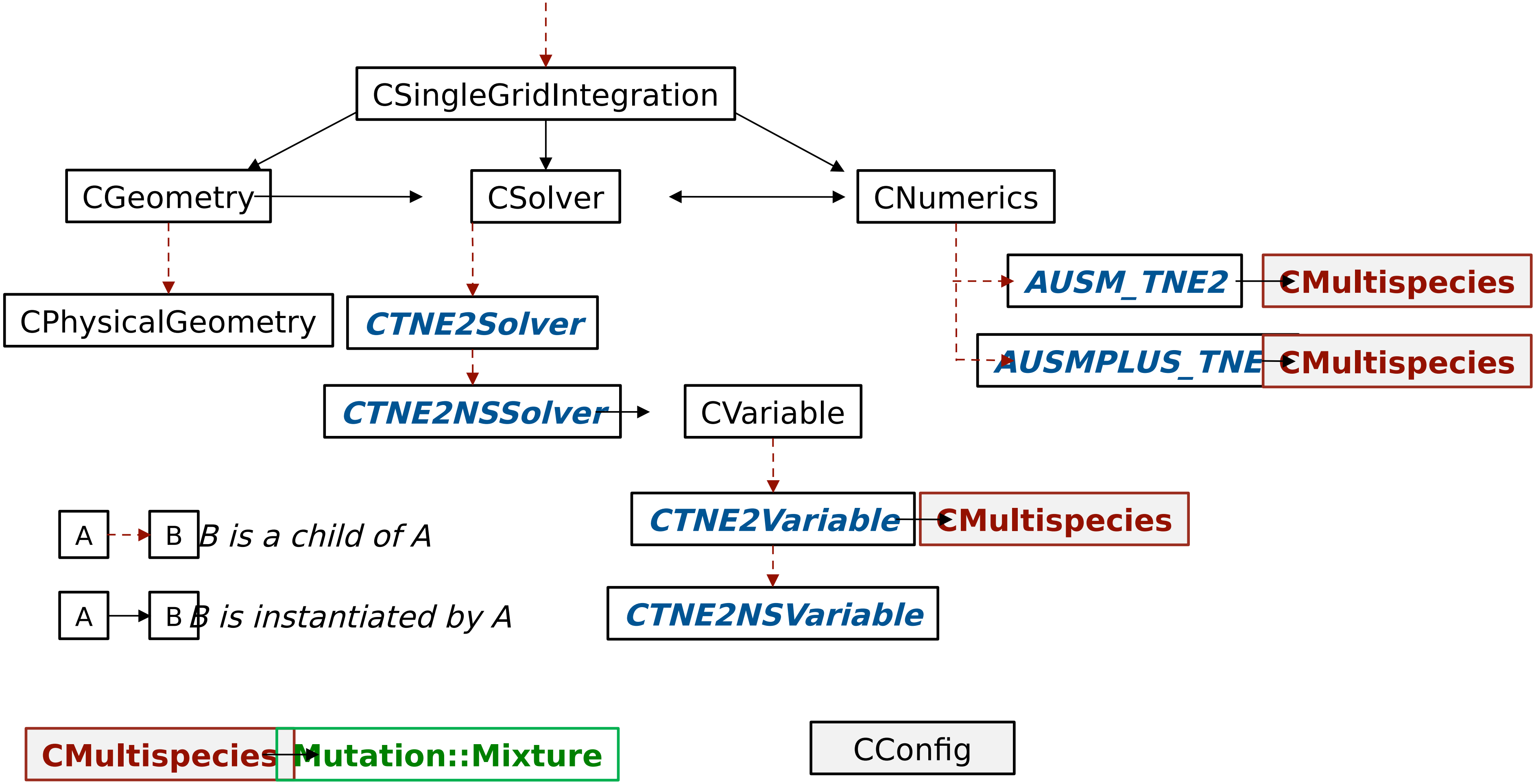

local state

physicochemical properties

**Mutation++**
- physicochemical models,
- algorithms, and
- data

https://sync.vki.ac.be/mpp/mutationpp

# Class hierarchy incorporating Mutation++




- CMultispecies = Class in SU2
- Mixture = Class in Mutation++

- GAS_MODEL = (USER_DEFINED, file_name.xml)
- GAS_COMPOSITION = (0.0, 0.0, 0.0, 0.79, 0.21)

# Mach 9 flow of air over a 15-35 double wedge

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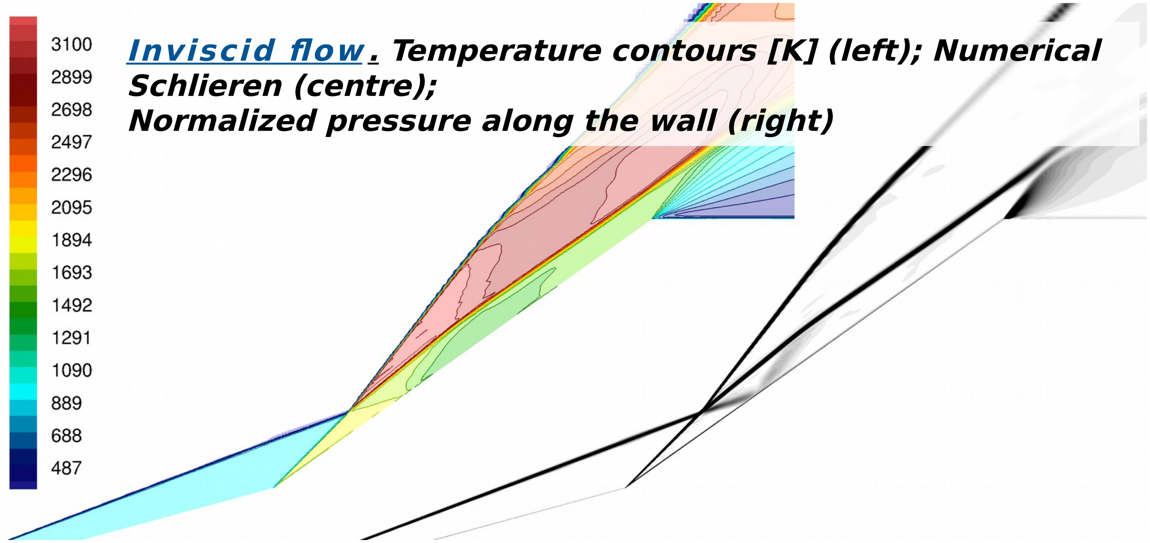
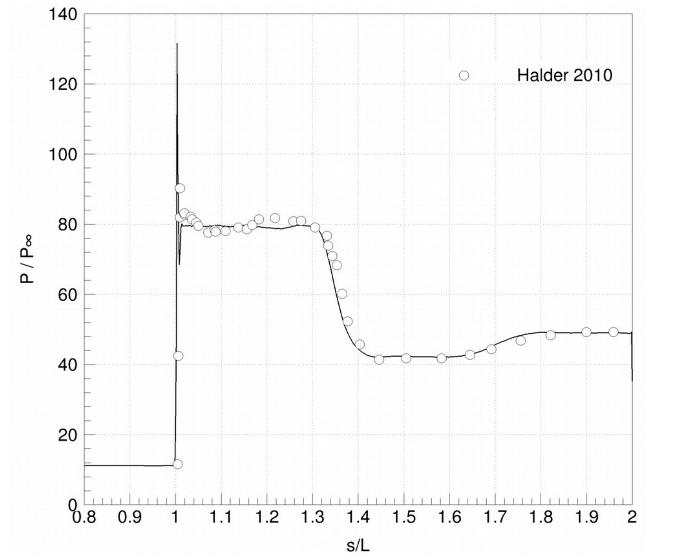
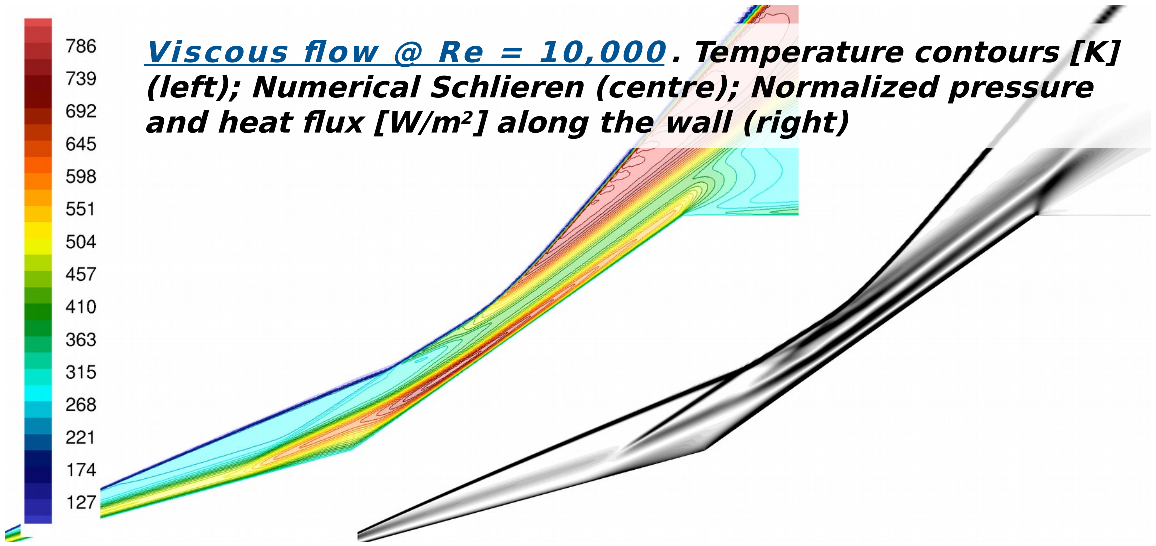
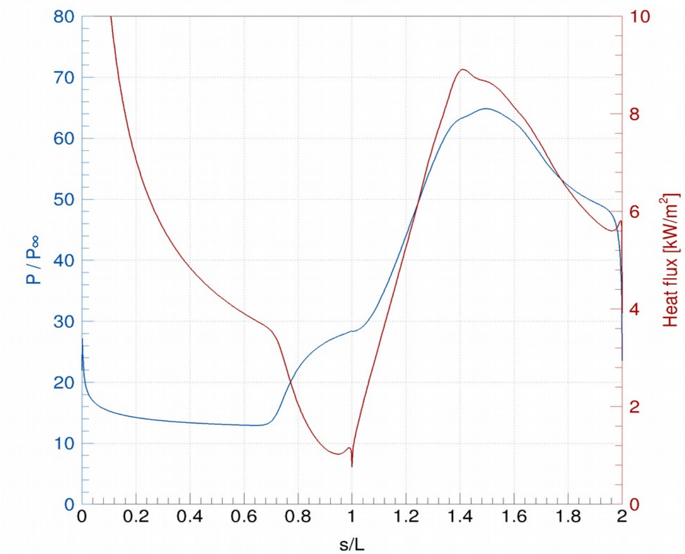
***Inviscid flow*. Temperature contours [K] (left); Numerical Schlieren (centre); Normalized pressure along the wall (right)**



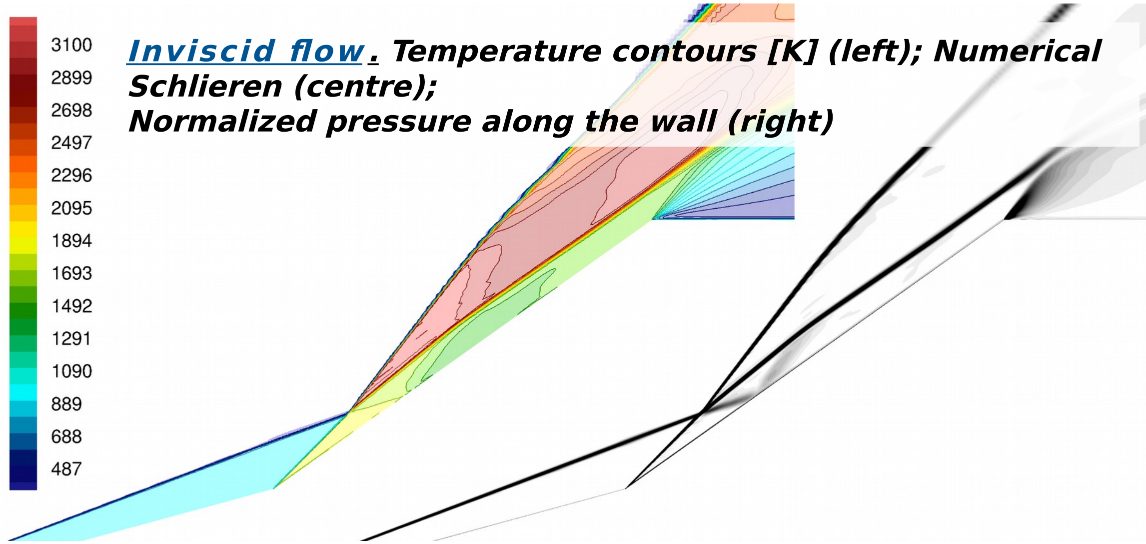

***Viscous flow @ Re = 10,000*. Temperature contours [K] (left); Numerical Schlieren (centre); Normalized pressure and heat flux [W/m²] along the wall (right)**

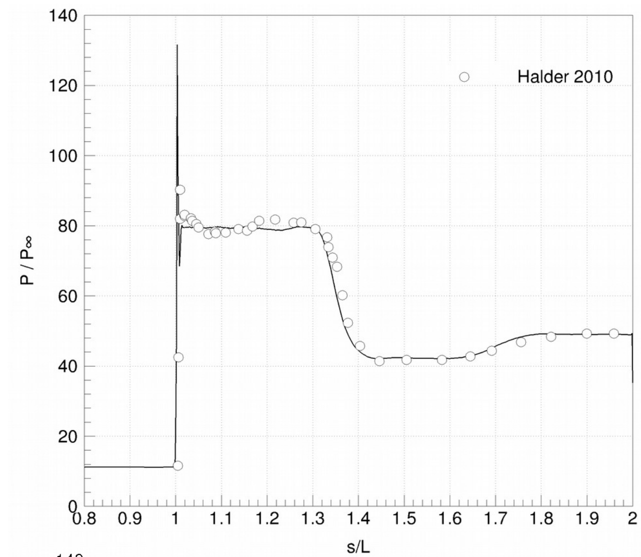


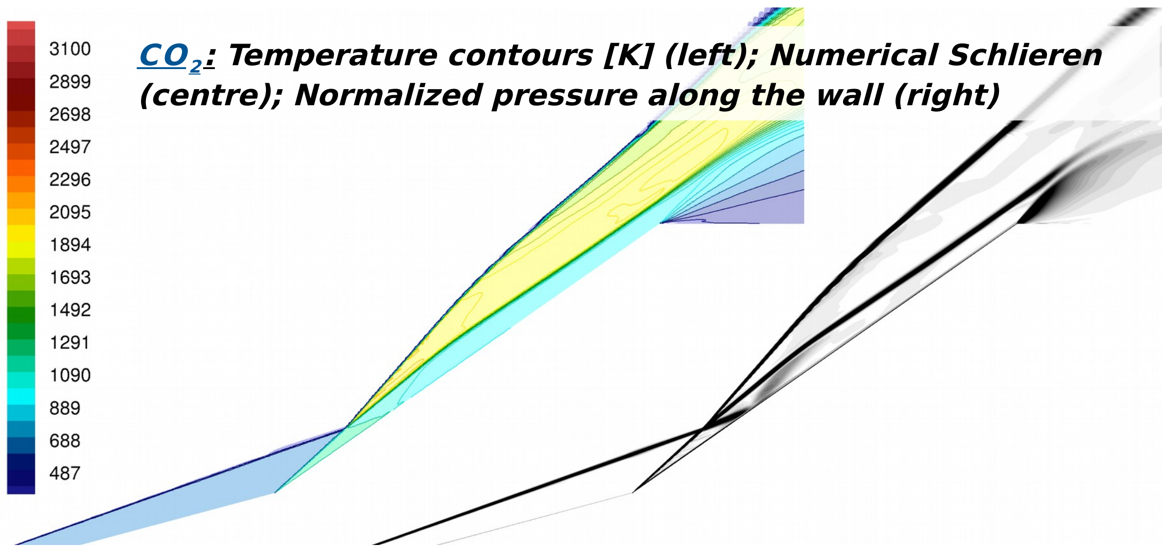
# Mach 9 flow of $CO_2$ over 15-35 double wedge

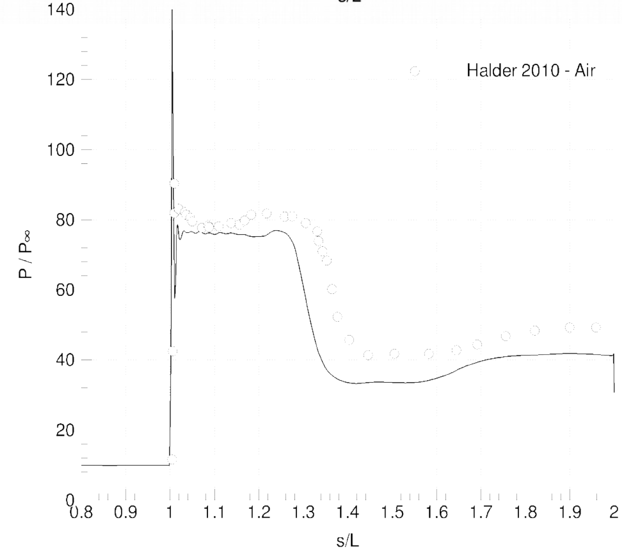
***Inviscid flow*. Temperature contours [K] (left); Numerical Schlieren (centre); Normalized pressure along the wall (right)**



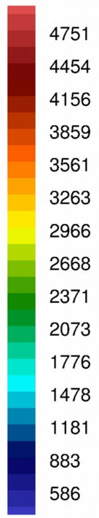

***$CO_2$*: Temperature contours [K] (left); Numerical Schlieren (centre); Normalized pressure along the wall (right)**

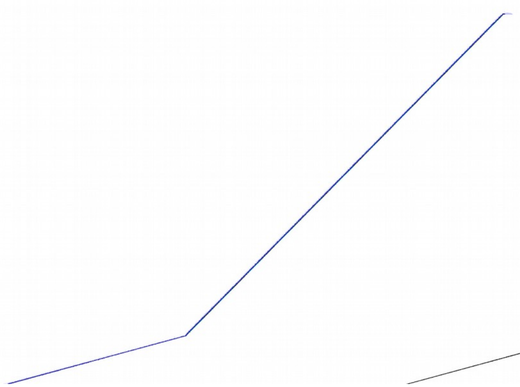


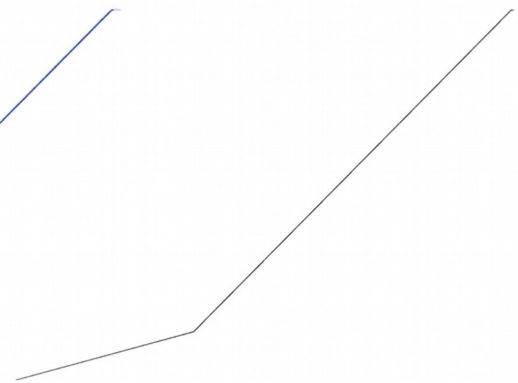



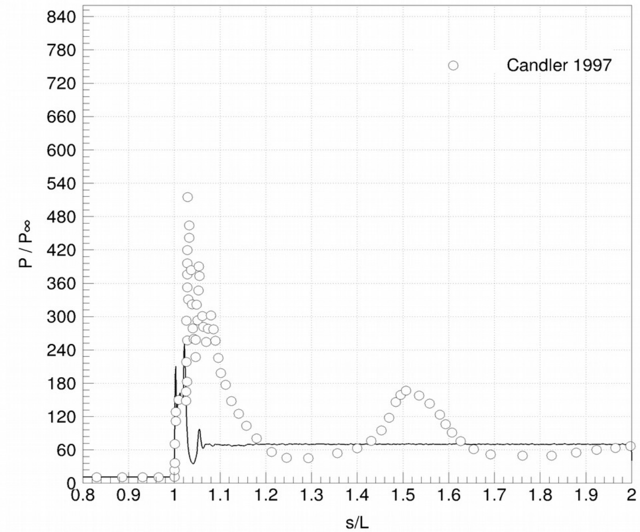
# Mach 9 flow of air over a 15-45 double wedge

***Inviscid flow*. Temperature contours [K] (left); Numerical Schlieren (centre);**
***Normalized pressure along the wall (right)***

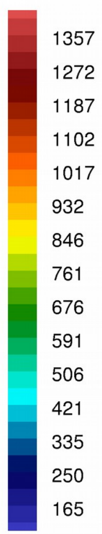


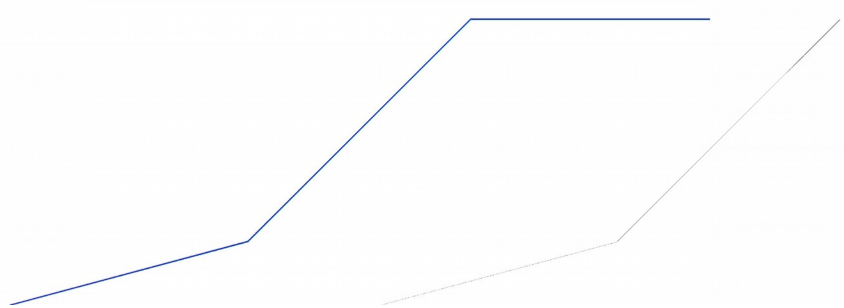



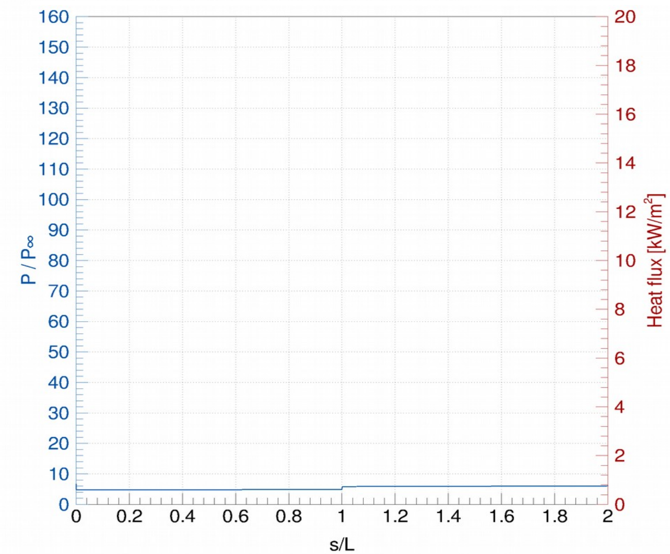





***Viscous flow @ Re = 10,000*. Temperature contours [K] (left); Numerical Schlieren (centre); Normalized pressure and heat flux [W/m²] along the wall (right)**





# Ongoing/near future developments

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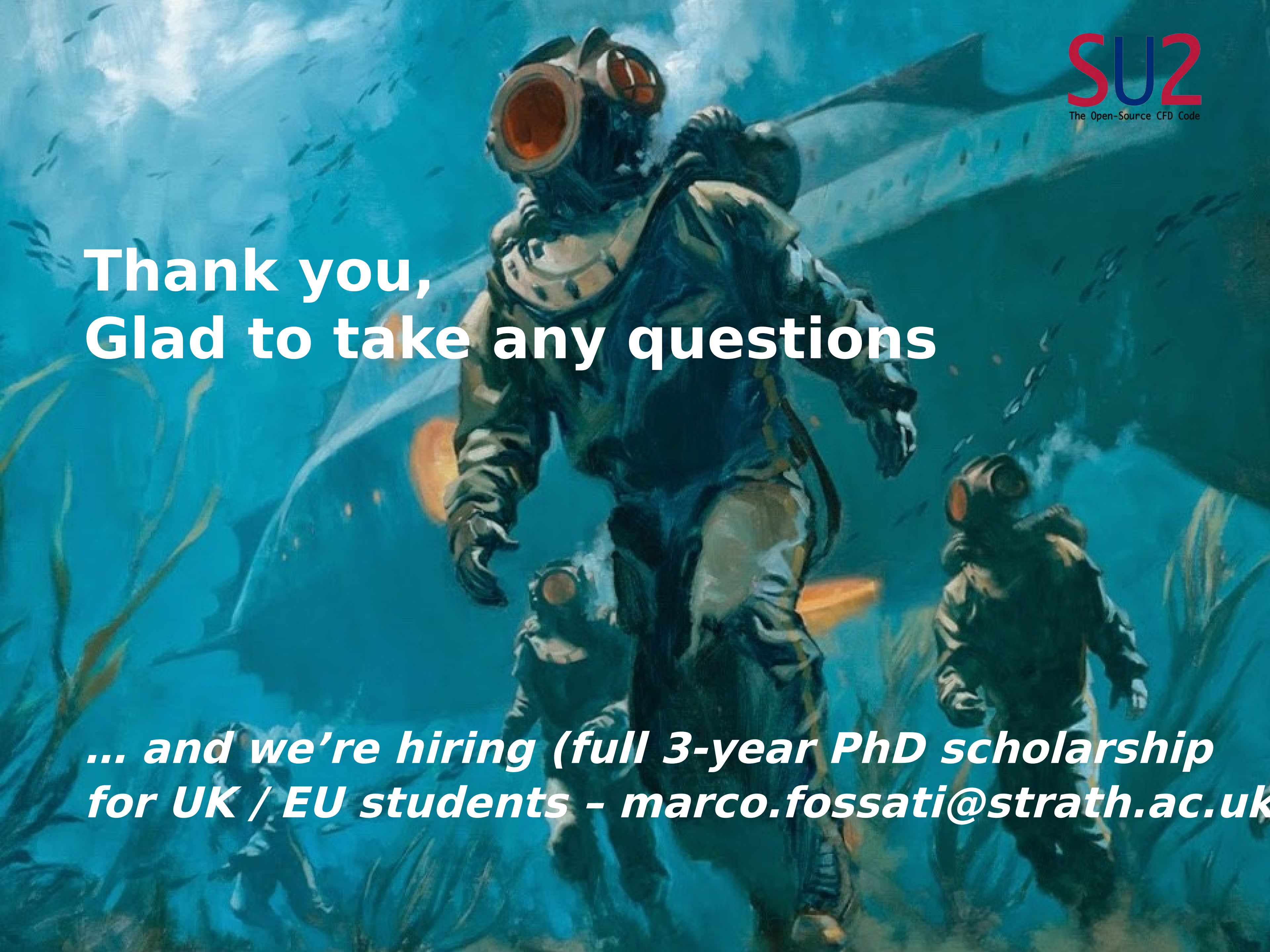
- Finalize the link with Mutation to incorporate diffusion properties, vibro-electronic modes and chemical kinetics (95% complete)
- Verify and validate NEMO with respect to the hard-coded TNE2 and existing literature model for AIR-5 and Nitrogen (N – $N_2$) flows (75% complete)
- Study the shock interference patterns with different-than-air mixtures (e.g. CO2-based mixtures) for the 15-35 and 15-45 double wedges (60% complete)
- Streamline the use of the AMG library (currently discussing with Adrien Loiseille from Gamma3 team at INRIA) inside NEMO (10% complete)
- Streamline the configuration and installation of Mutation with autotools (0% complete)

Presentation to the coming AIAA Aviation conference in Dallas: A.C. Gomes, M. Fossati, W.T. Mayer, J.J. Alonso, J.B. Scoggins, T. Magin, T. Economon, "*Numerical Study of Shock Interference Patterns for Nonequilibrium Gas Flows*"



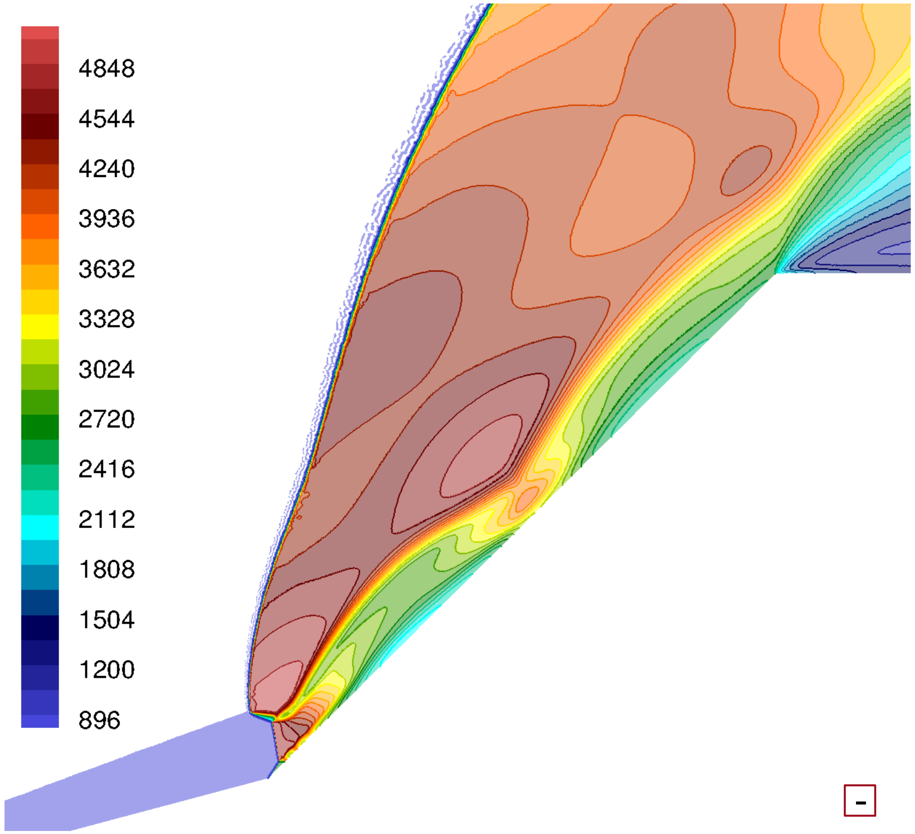
SU2

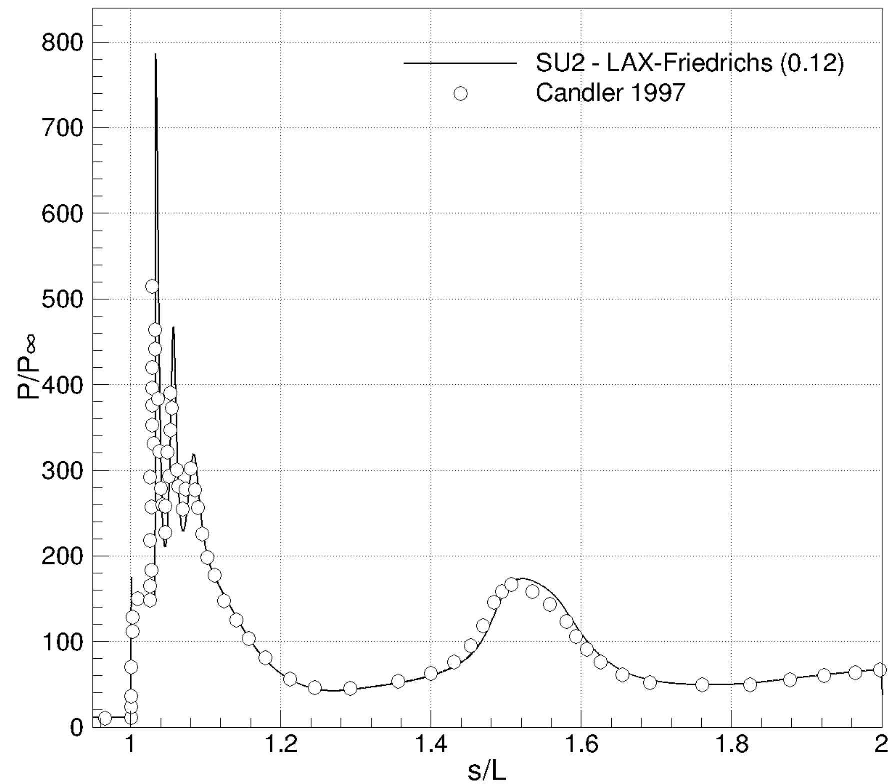
The Open-Source CFD Code

# Thank you,
# Glad to take any questions

***… and we’re hiring (full 3-year PhD scholarship for UK / EU students – marco.fossati@strath.ac.uk***

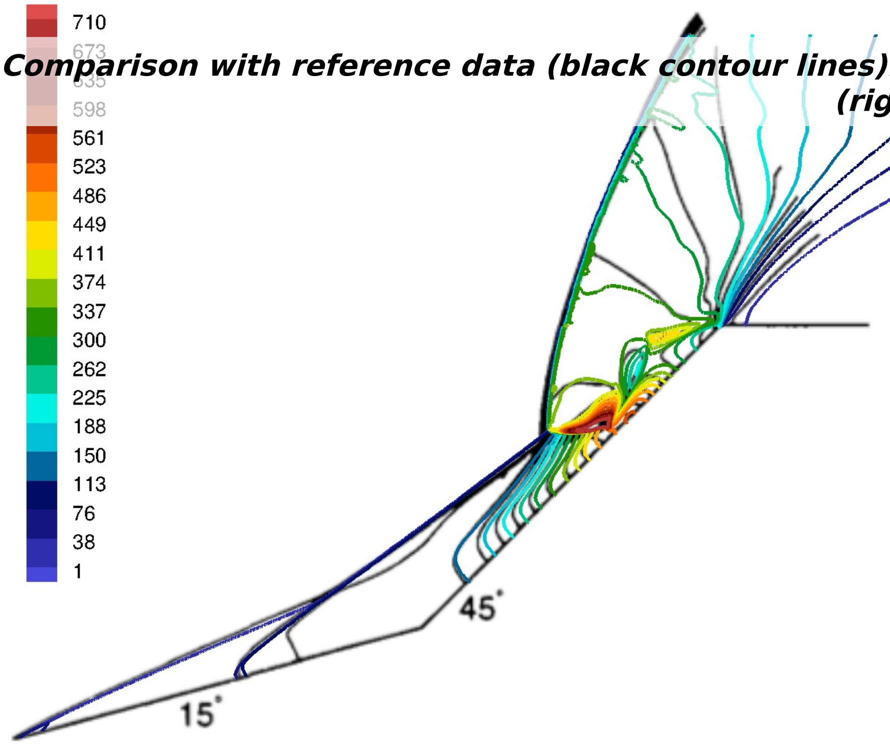
# Mach 9 inviscid flow over 15-45 double wedge

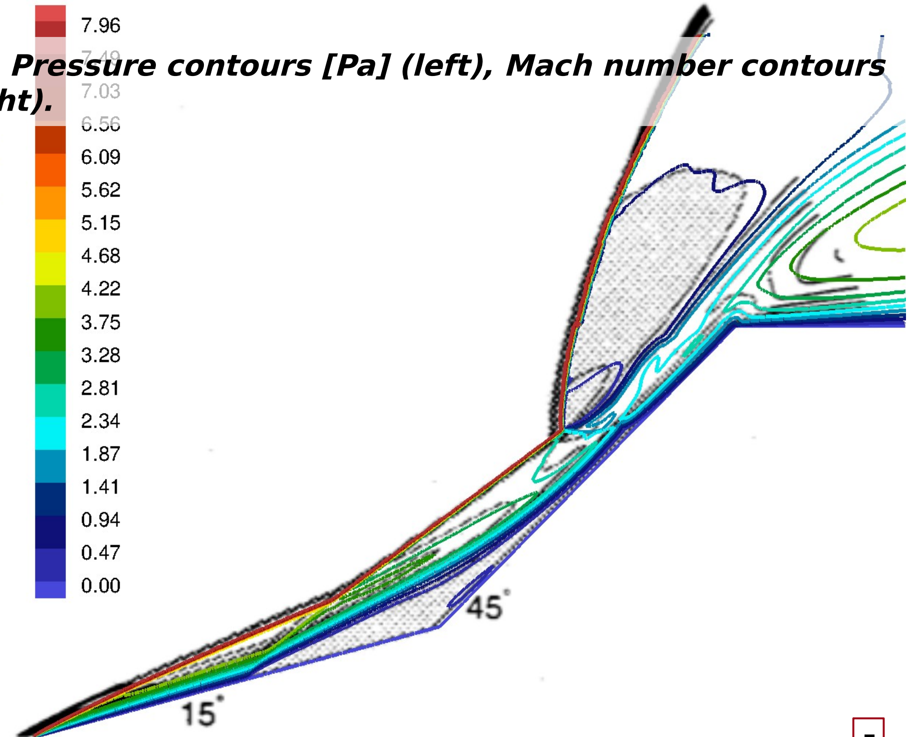



- A steady state solution is obtained by introducing a fair amount of artificial dissipation
- In this case, a fair matching with available numerical data [Candler and Olejniczak 1997] is obtained

# Mach 9, Re 10,000 flow over 15-45 double wedge



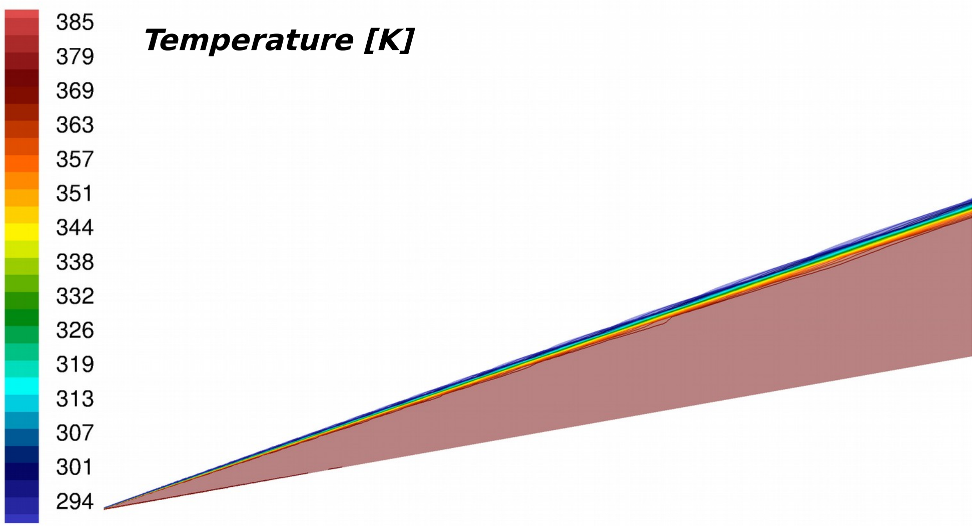



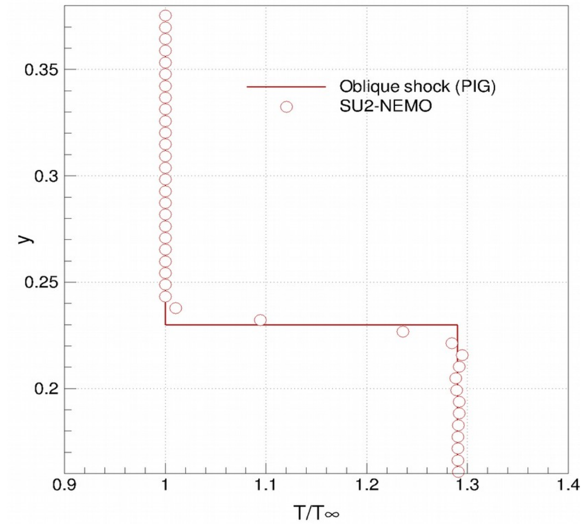

***Comparison with reference data (black contour lines). Pressure contours [Pa] (left), Mach number contours (right).***

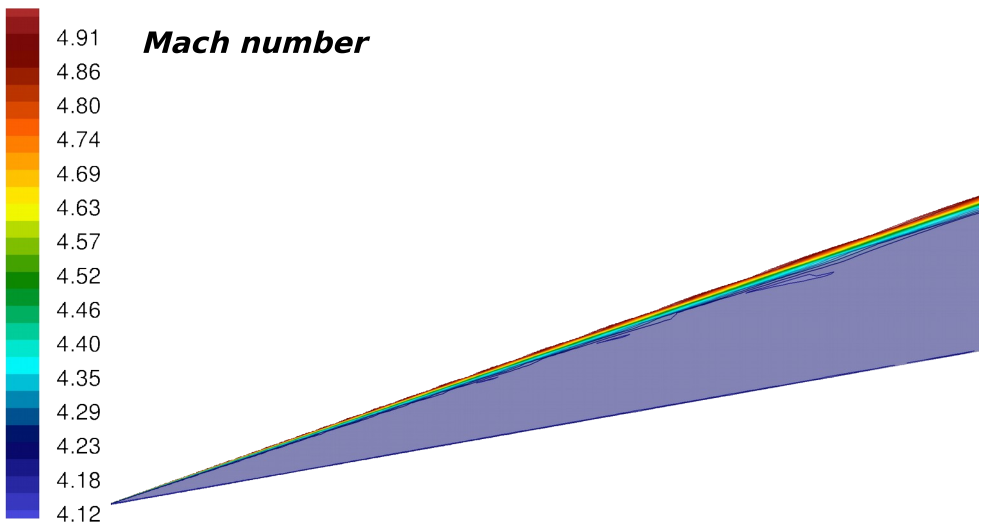
| | |
|---|---|
| $Mach_{FS}$ | 9 |
| Reynolds | 10,000 |
| $Temperature_{FS}$ [K] | 80 |
| $Pressure_{FS}$ [Pa] | 3.89 |
| $Temperature_{W}$ [K] | 300 |

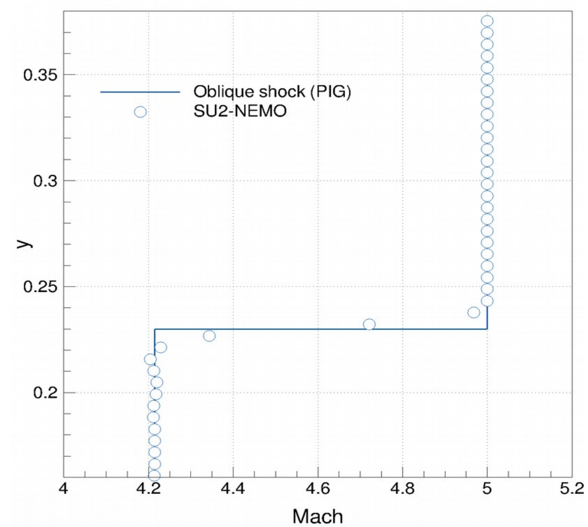
- A steady state solution is obtained by introducing a fair amount of artificial dissipation
- In this case, a fair (*granted the uncertainty on the levels*) matching with available numerical data [Candler and Olejniczak 1996] is obtained

# Mach 5 inviscid flow of $CO_2$ over 10° ramp

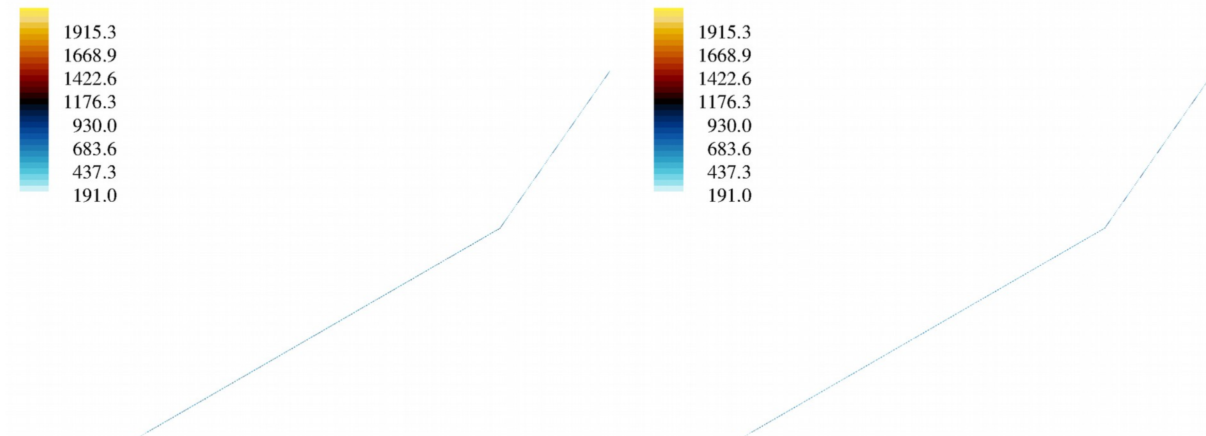


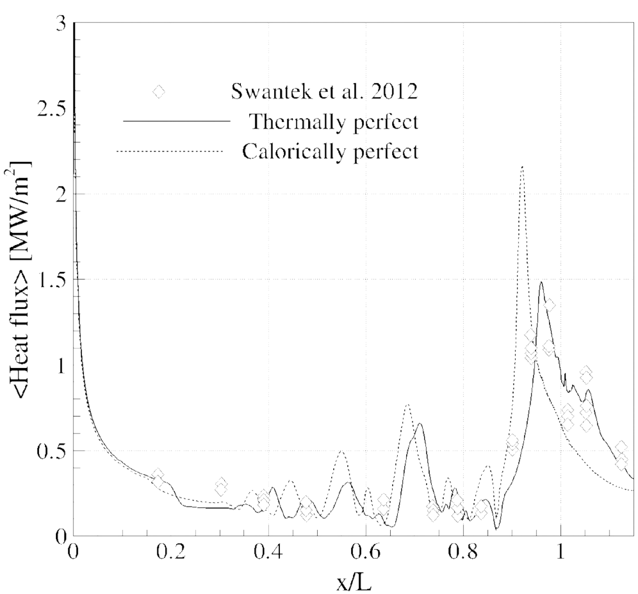



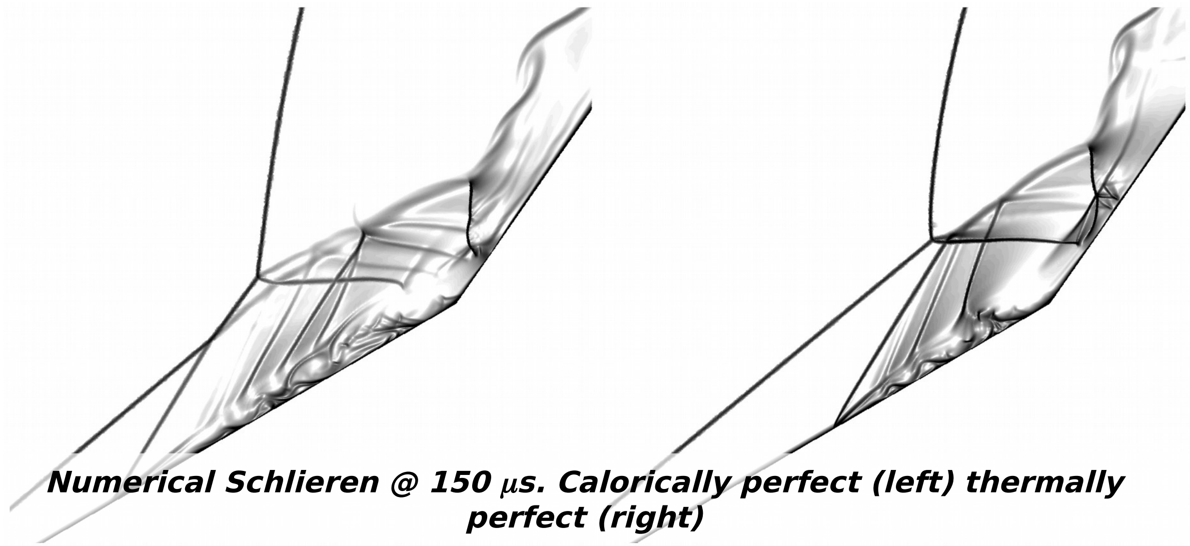



| | |
|---|---|
| $Mach_{FS}$ | 7.11 |
| Unit Reynolds [m⁻¹] | 55,880 |
| $Temperature_{FS}$ [K] | 191 |
| $Pressure_{FS}$ [Pa] | 391.735 |
| $Temperature_{W}$ [K] | 300 |




***Temperature contours [K]. Calorically perfect (left), thermally perfect (right)***



***Numerical Schlieren @ 150 μs. Calorically perfect (left) thermally perfect (right)***

# Mesh details

| Test case | Type of mesh | Elements | Nodes |
|---|---|---|---|
| NACA0012 subsonic | Unstructured | 10,216 | 5,233 |
| NACA0012 supersonic | Unstructured | 10,216 | 5,233 |
| RAMC II | Structured (quadrilaterals) | 7,936 | 12,285 |
| Wedge 15-35 Viscous | Structured (quadrilaterals) | 182,284 | 183,400 |
| Wedge 15-45 Inviscid | Unstructured hybrid | 766,988 | 385,853 |
| Wedge 15-45 Viscous | Unstructured hybrid | 827,977 | 621,762 |
| Wedge 10 | Structured (quadrilaterals) | 25,392 | 25,830 |
| Wedge 30-55 Viscous | Unstructured hybrid | 457,121 | 261,620 |