SU2-NEMO: NonEquilibrium MOdels for Hypersonic Flows

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Outline

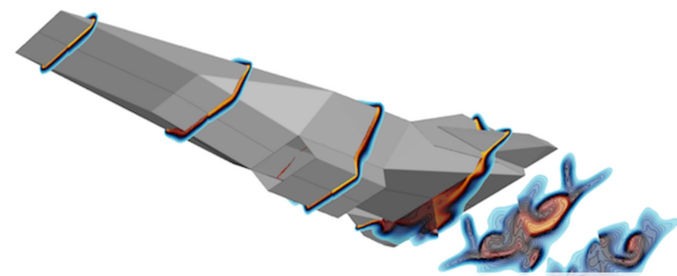
SU2

1. Multi-species multi-temperature solver
2. Update to "develop" and regression tests (C. Garbacz)
3. Turbulence modeling (W. Maier)
4. Ionization modeling (J. Needels)
5. Adaptive solutions (A. Loseille, B. Munguía)

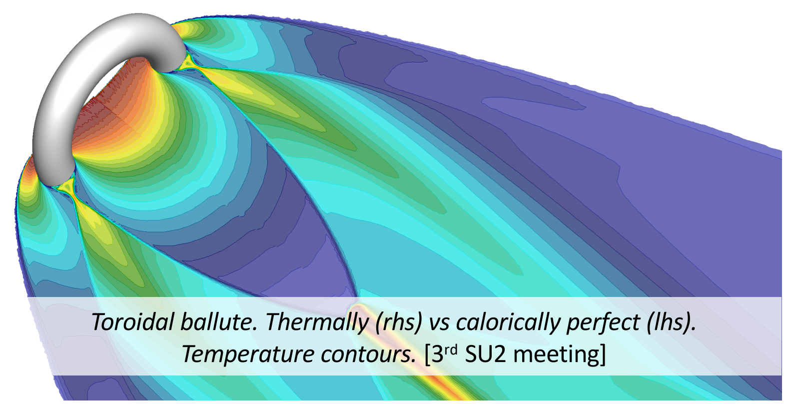
Ambition and objectives

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

- Reboot modeling 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. [2nd SU2 meeting]



Toroidal ballute. Thermally (rhs) vs calorically perfect (lhs). Temperature contours. [3rd SU2 meeting]

Some background equations and models

SU2

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

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

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

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

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

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

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

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

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

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

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

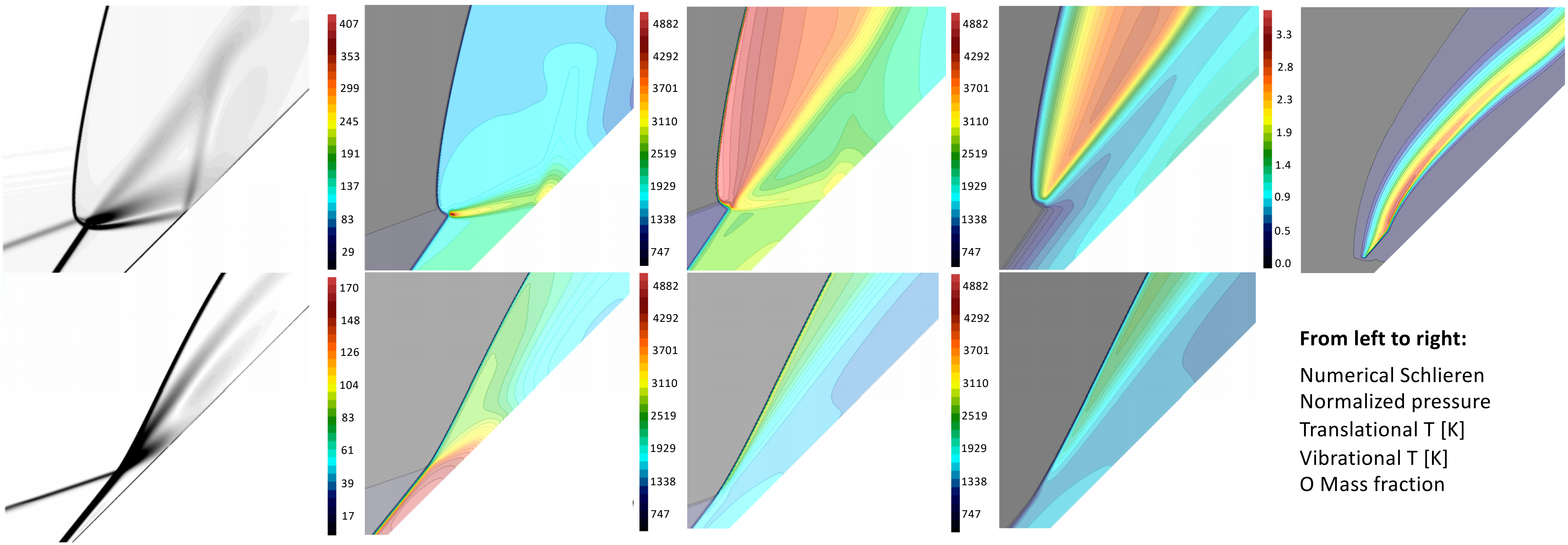
$$\vec{q} = -k\nabla T$$

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

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

Shock interference patterns on double wedges (C. Garbacz)

SU2-NEMO with Mutation++

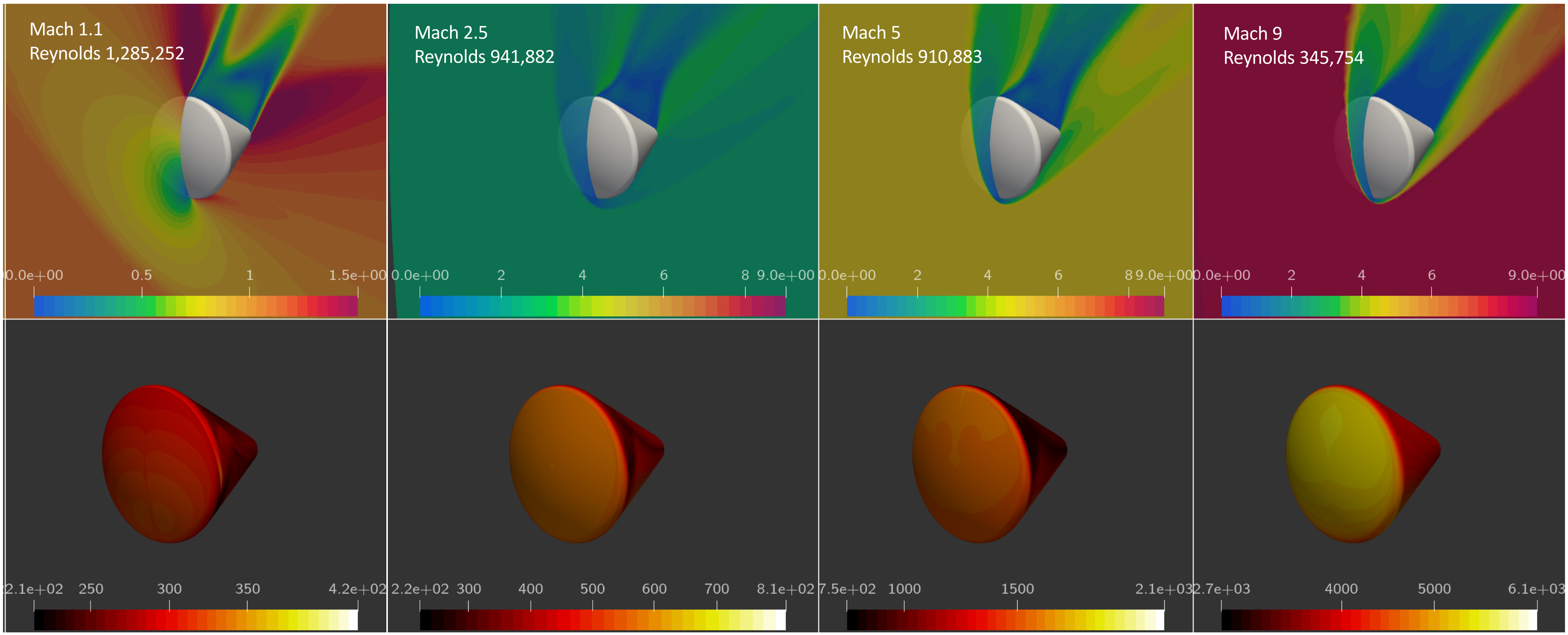


From left to right:

Numerical Schlieren
Normalized pressure
Translational T [K]
Vibrational T [K]
O Mass fraction

Simulation of a hypersonic Mach 9 flow over a double wedge. Shock interaction patterns with thermal nonequilibrium and finite-rate chemistry. Air-5 top, CO_2*-*N_2 *bottom*

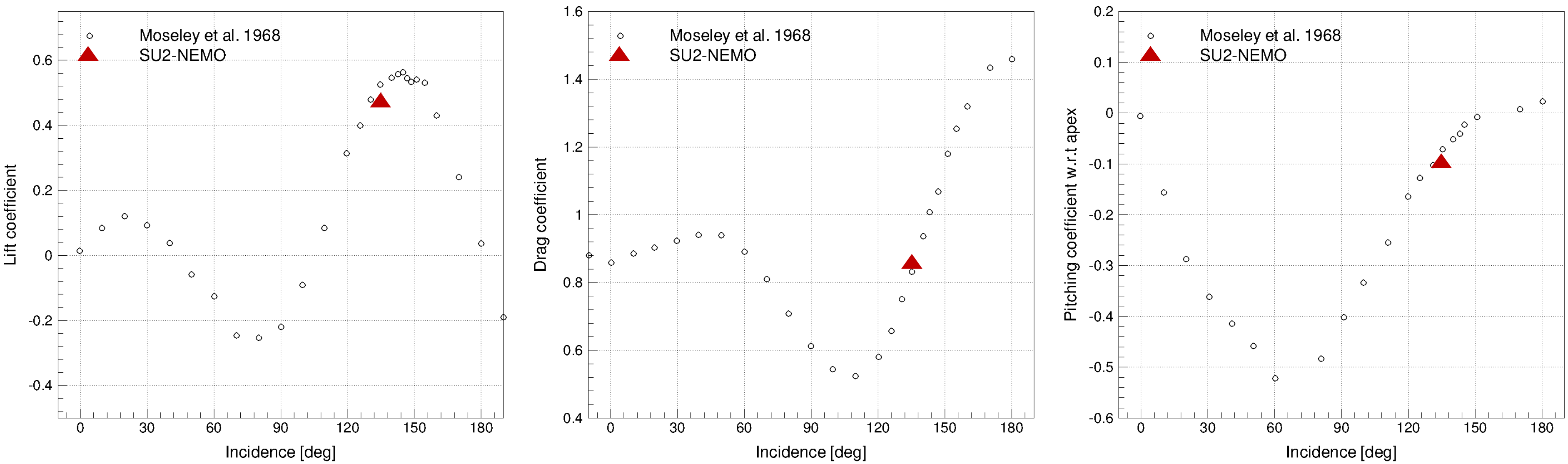
Apollo command module at 45deg (C. Garbacz, W. Maier)



Mach number contours (top row), Temperature [K] (bottom row)

Apollo command module at 45deg (C. Garbacz, W. Maier)

SU2

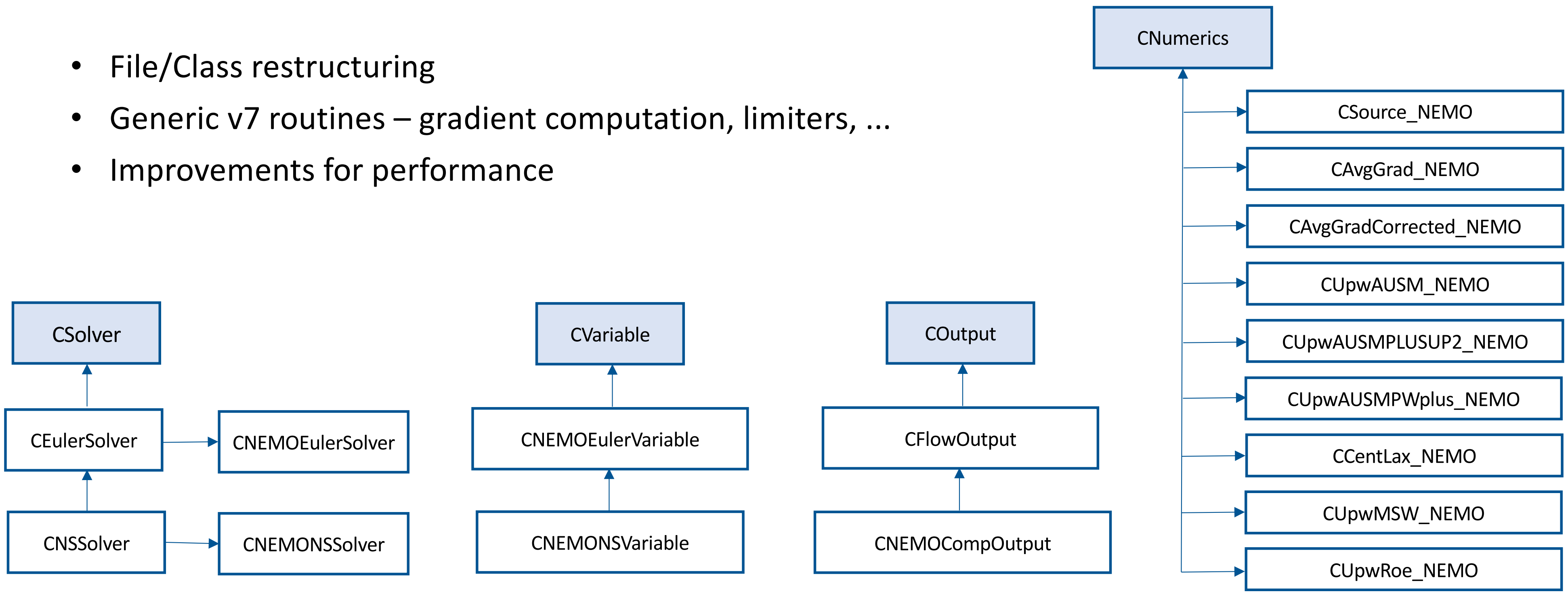


Aerodynamic coefficients for Mach 2.5 case

Update to "develop" (C. Garbacz)

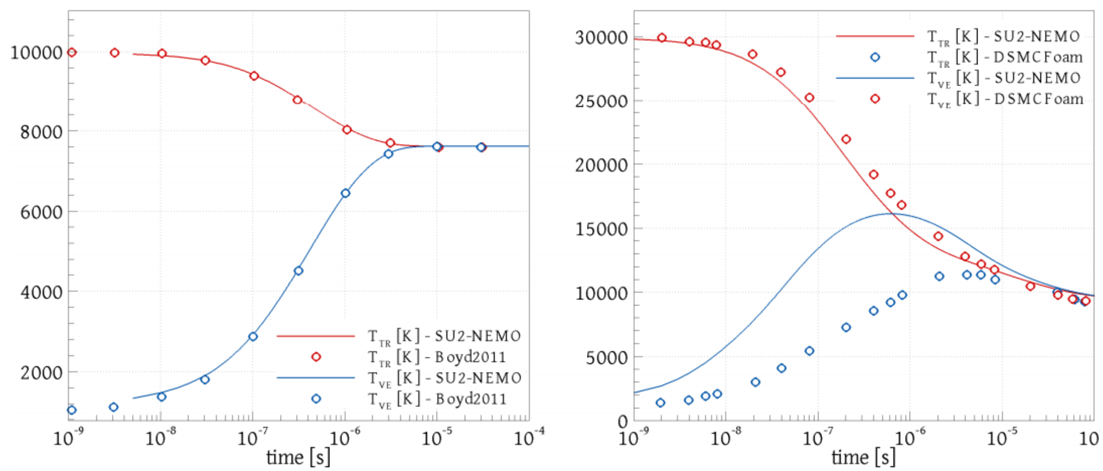
SU2-NEMO

- File/Class restructuring
- Generic v7 routines – gradient computation, limiters, ...
- Improvements for performance



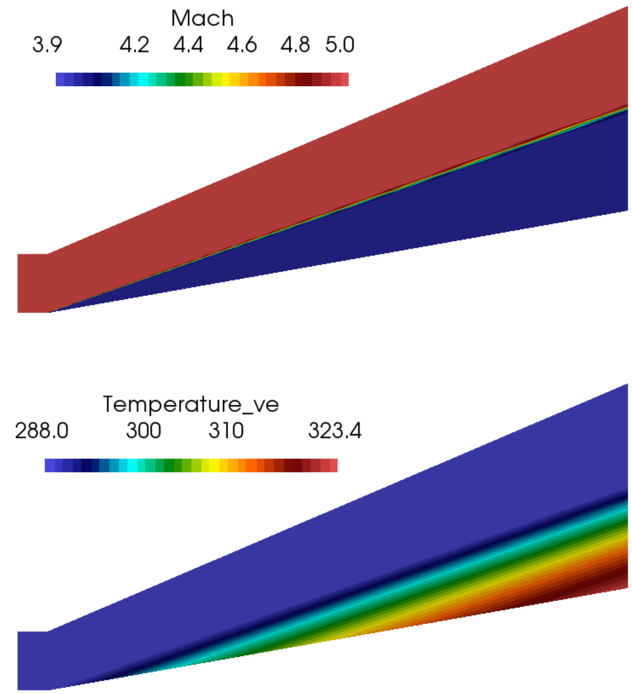
Update to “develop” (C. Garbacz)

Regression test cases



0D adiabatic heat bath with relaxation and finite-rate chemistry (N_2-N)

Reaction Mechanism	Frozen	$N_2 + N_2 \rightarrow 2N + N_2$
T_{tr} [K]	10,000	30,000
T_{ve} [K]	1,000	1,000

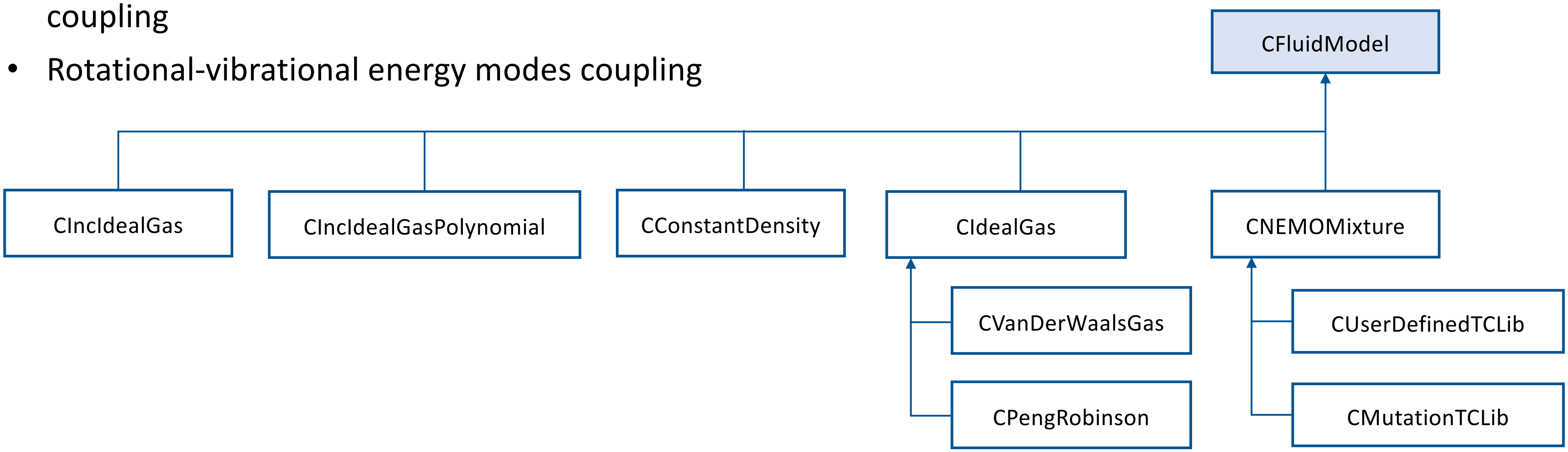


2D Mach 5 inviscid flow over a 10° wedge

Update to “develop” (C. Garbacz)

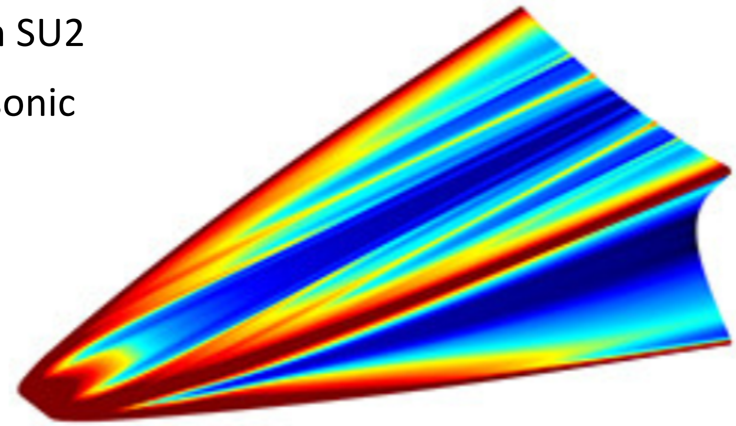
Roadmap

- Incorporate ***CFluidModel*** class to handle all mixture-related computations (thermodynamics, chemistry, transport)
- Merge link ***SU2-NEMO*** — ***Mutation++***
- Preferential vs. non-preferential modeling of vibration-chemistry coupling
- Rotational-vibrational energy modes coupling



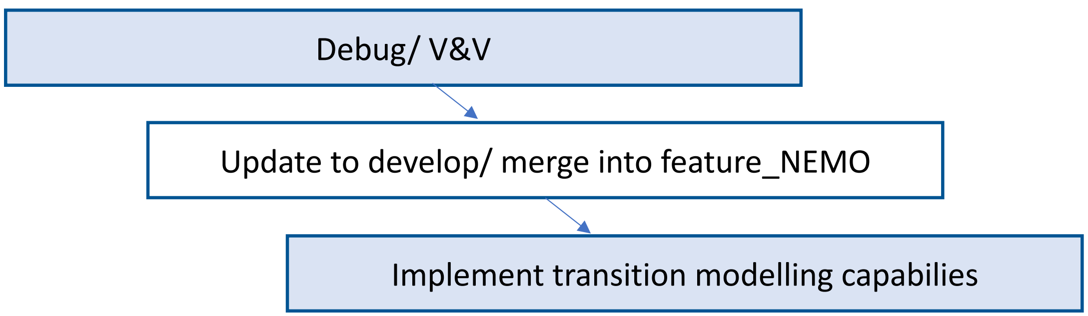
Turbulence modeling (W. Maier)

- Make use of the existing turbulence model structure within SU2
- SA-Catris, SA-Neg, and SST-V models are standard in hypersonic flows (e.g., US3D)
- Currently in debugging phase.



Bolt Surface Heat Transfer Rate
https://cse.umn.edu/aem/computational-hypersonics-research-lab

Steps forward:

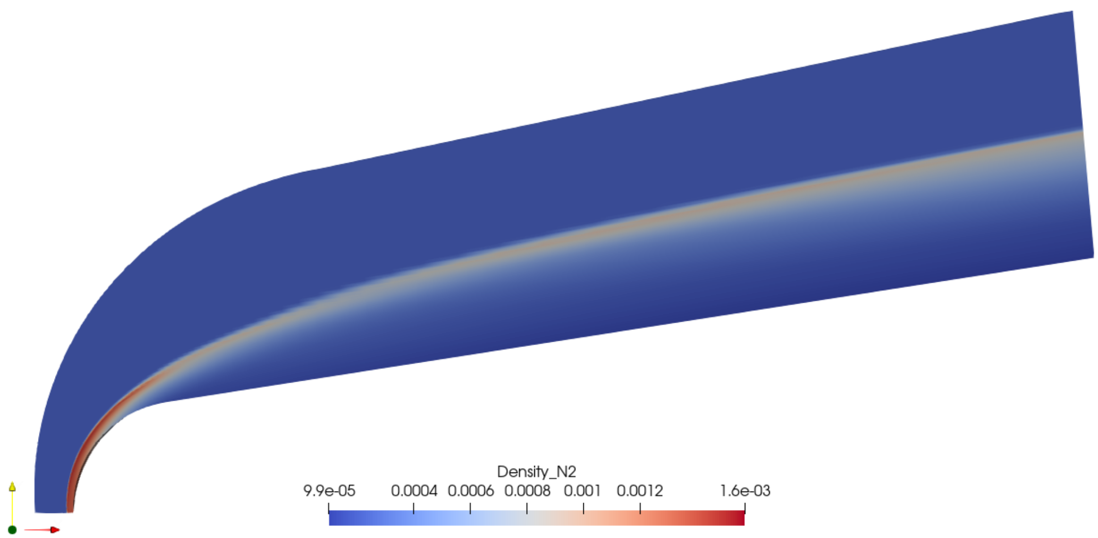


Ionization modeling (J. Needels)

- Implementation of 7-species air chemistry model to capture ionization effects during hypersonic re-entry
- Validation against experimental data (RAM-C II flight experiment)
- Air-11 model implemented, validation in progress

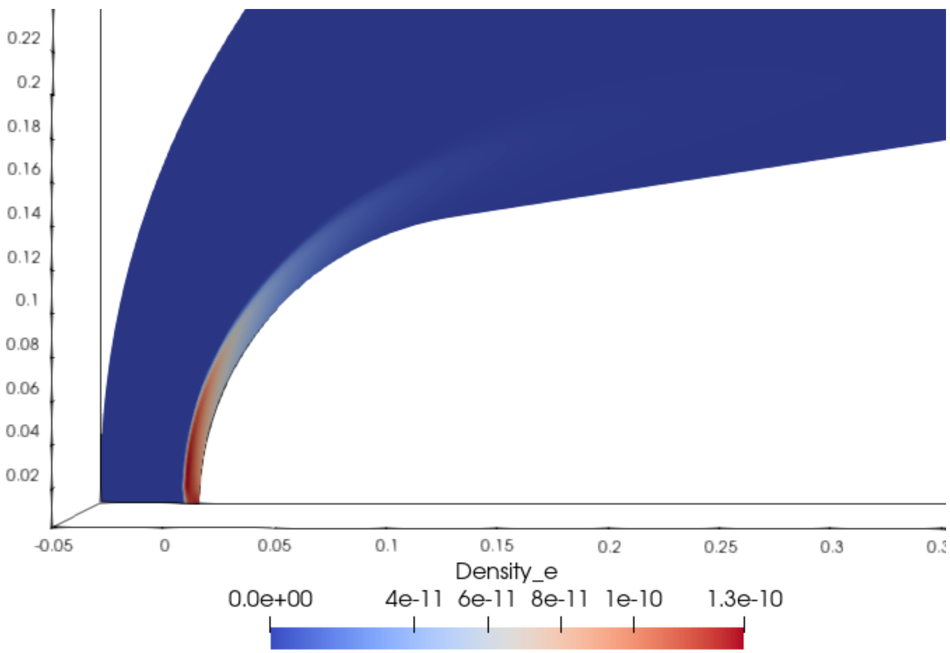
Free-stream Parameter	Value
Altitude [km]	61
M	23.9
T [K]	254
P [Pa]	19.8
Kn	0.0012

7-Species Air Chemistry Model:
S : {N2, O2, N, O, NO, NO+, e-}

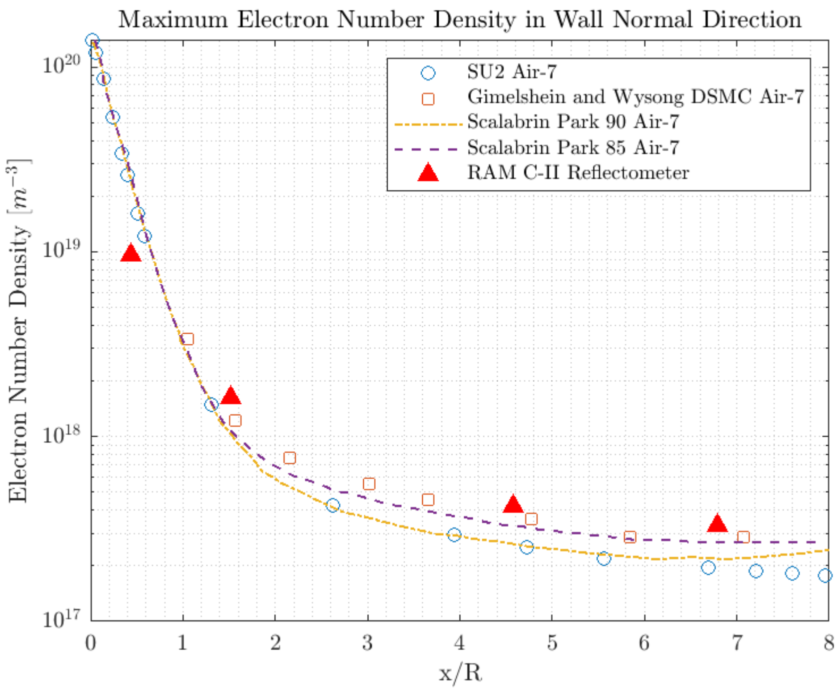


Test Case: RAM-C II 7,936 Element 3D Hexahedral Mesh

Ionization modeling (J. Needels)



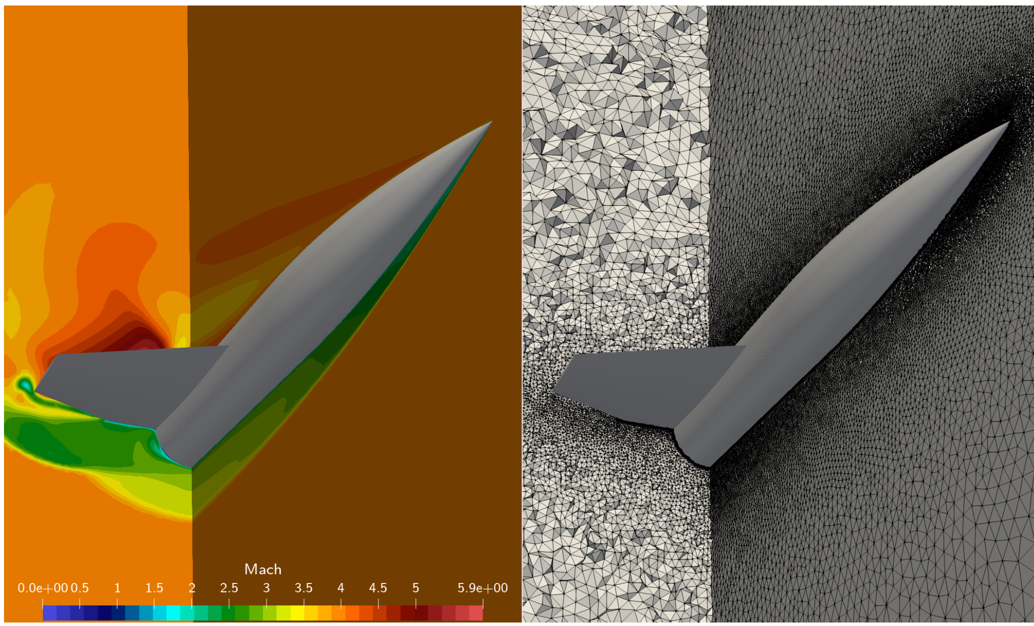
Electron Density over 3D RAM-C II Forebody M = 23.9

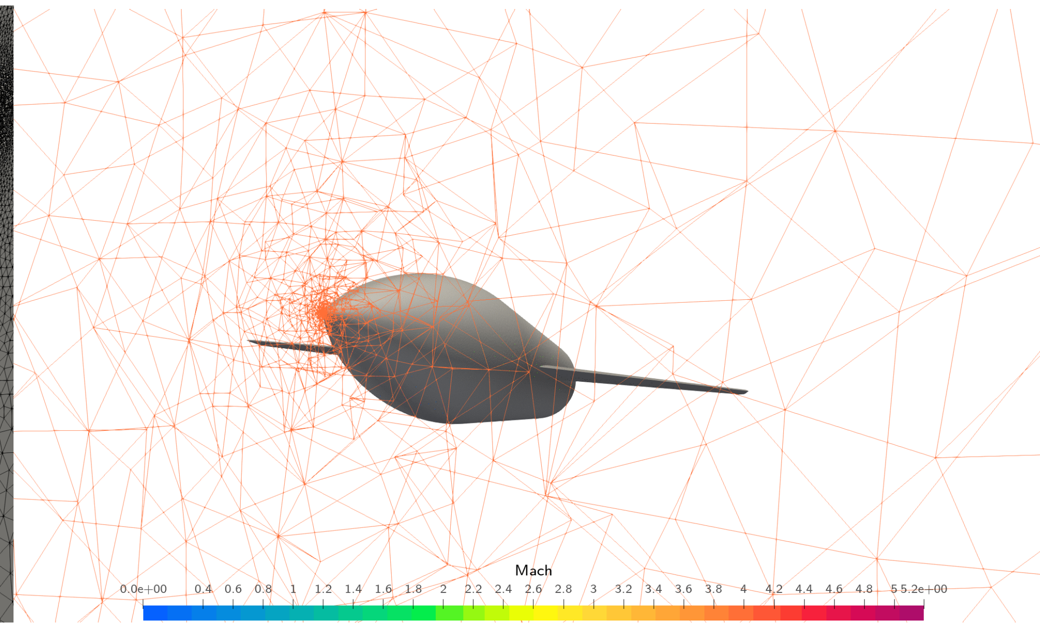


Comparison with Numerical Results and Flight Data

SU2-NEMO + AMG library for viscous flows (A. Loseille, B. Munguía)

Mach 4 flow over a wing-body configuration (Bedford vehicle) at 20deg incidence

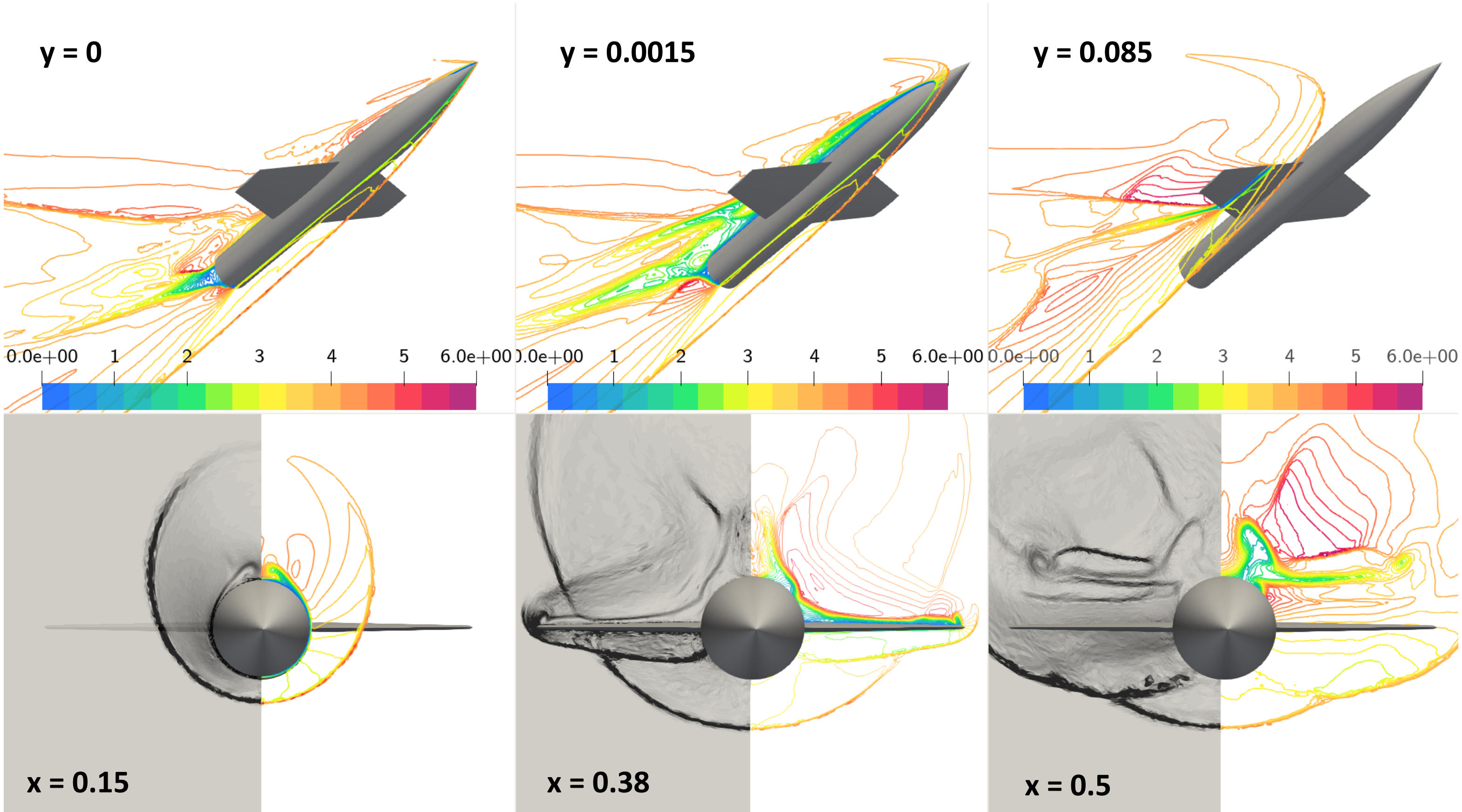




Original mesh/solution
Nodes: 3,109,217
Elements: 11,473,410 (prisms, pyramids, tets)

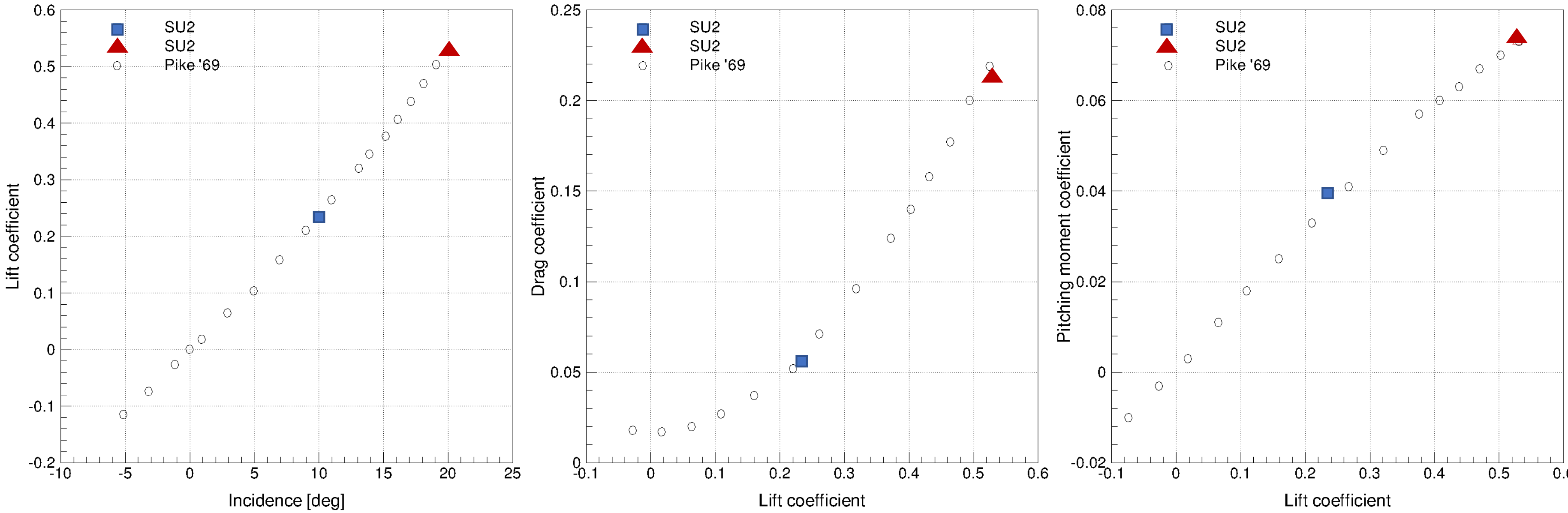
Adapted mesh/solution
Nodes: 2,111,391
Elements: 10,699,929 (prisms, pyramids, tets)

SU2-NEMO + AMG library for viscous flows (A. Loseille, B. Munguía)



Mach number contours and Numerical Schlieren

SU2-NEMO + AMG library for viscous flows (A. Loseille, B. Munguía)



Reference area 0.04021 m^2 (/2)
Reference length 0.15207 m (MAC)
Point for C_{My} 0.318 m

	C_L	C_D	C_{My}
10º	0.23438	0.06242	0.04013
20º	0.52490	0.21944	0.074768

Pike, J., Wind Tunnel Tests on Six Wing-Body Models at M = 4, Ministry of Technology, Aeronautical Research Council, 1969

A little ways down the road …

- Vibration-dissociation modeling
- Advanced turbulence modeling
- Ionization and magneto-gasdynamics effects
- Advanced thermal boundary conditions (e.g. equilibrium radiation)
- Coupling with 6-DOF model and fragmentation for re-entry problems

1. Gomes, A.C., Fossati, M., Maier, T., Alonso, J.J., Scoggins, J.B., Magin, T., Economon, T. (2020). **Numerical Study of Shock Interference Patterns for Nonequilibrium Gas Flows**. AIAA 2020 Scitech Forum and Exposition. Orlando (FL), US. January. https://doi.org/10.2514/6.2020-1805
2. Gomes A.C., Maier, T., Alonso, J.J., Scoggins, J.B., Magin, T., Economon, T., G. Barrenechea and Fossati, M. **Shock Interactions in Inviscid Air and CO_2-N_2 Flows in Thermochemical Nonequilibrium**. Shock waves. *Under review*
3. Gomes A.C., Maier, T., Alonso, J.J., Scoggins, J.B., Magin, T., Economon, T., B. Munguia, A. Loseille, G. Barrenechea and Fossati, M. **Nonequilibrium Shock Interference Patterns over Hypersonic Vehicles.** *In preparation*
4. Gomes A.C., Maier, T., Alonso, J.J., Scoggins, J.B., Magin, T., Economon, T., G. Barrenechea and Fossati, M. **Characterization of shock wave interaction for Viscous Air and CO_2 Flows in Thermochemical Nonequilibrium**. *In preparation*