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

A.C. Garbacz-Gomes, W.T. Maier, J.B. Scoggins, T. Magin, T. Economon, M. Fossati, J.J. Alonso
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)*
Ambition and objectives

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

- 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
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

- 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

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

\[
\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u} + P \vec{I} - \vec{\tau}) = 0
\]

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

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

\[
P = P(\rho_s, T)
\]

\[
e = e(X_s, T)
\]

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

\[
\vec{q}_v = -k \nabla T
\]

\[
\vec{q}_v = -k_v \nabla T_v
\]

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

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

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

SU2 NonEquilibrium Models

SU2 has continued to evolve ... new and more general implementation needed!
**New TNE2 Solver - State of SU2-NEMO Branch**

- **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

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<table>
<thead>
<tr>
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<tbody>
<tr>
<td>Mach</td>
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</tr>
<tr>
<td>Pressure [Pa]</td>
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<tr>
<td>Temperature [K]</td>
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</table>

- **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

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<tbody>
<tr>
<td></td>
<td>$C_L$</td>
<td>$C_D$</td>
</tr>
<tr>
<td>Develop</td>
<td>0.001057</td>
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<tr>
<td>TNE2</td>
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Verification of TNE2 Euler Solver: NACA0012

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<tr>
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<tr>
<td>Pressure [Pa]</td>
<td>100,000</td>
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<tr>
<td>Temperature [K]</td>
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</table>

<table>
<thead>
<tr>
<th></th>
<th>(C_L)</th>
<th>(C_D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Develop</td>
<td>-0.000065</td>
<td>0.098630</td>
</tr>
<tr>
<td>TNE 2</td>
<td>-0.000065</td>
<td>0.098630</td>
</tr>
</tbody>
</table>

Mach number contours. Develop branch (left), TNE2 branch (right)
Validation of TNE2 Euler Solver: RAM-C II case

- Implicit AUSM Scheme

- **TNE2 Case Specifics**
  - AIR-5 Model (76% N₂, 23% O₂)

- Slight differences in shock structure
  - May be due to mesh differences

### Table

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<tr>
<th>Parameter</th>
<th>Value</th>
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<tr>
<td>Mach</td>
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<tr>
<td>Pressure [Pa]</td>
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<tr>
<td>Temperature [K]</td>
<td>254</td>
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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
**Class hierarchy incorporating Mutation++**

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

**SU2 NonEquilibrium Models**

- **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

**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

• 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\textsubscript{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)

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
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

**Temperature [K]**

**Mach number**
M7.11 flow of air over a 30-55 double wedge

Mach_{FS} \quad 7.11

Unit Reynolds [m^{-1}] \quad 55,880

Temperature_{FS} [K] \quad 191

Pressure_{FS} [Pa] \quad 391.735

Temperature_{W} [K] \quad 300

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

Numerical Schlieren @ 150 \mu s. Calorically perfect (left) thermally perfect (right)
## Mesh details

<table>
<thead>
<tr>
<th>Test case</th>
<th>Type of mesh</th>
<th>Elements</th>
<th>Nodes</th>
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<tbody>
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<td>NACA0012 subsonic</td>
<td>Unstructured</td>
<td>10,216</td>
<td>5,233</td>
</tr>
<tr>
<td>NACA0012 supersonic</td>
<td>Unstructured</td>
<td>10,216</td>
<td>5,233</td>
</tr>
<tr>
<td>RAMC II</td>
<td>Structured (quadrilaterals)</td>
<td>7,936</td>
<td>12,285</td>
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<tr>
<td>Wedge 15-35 Viscous</td>
<td>Structured (quadrilaterals)</td>
<td>182,284</td>
<td>183,400</td>
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<td>Wedge 15-45 Inviscid</td>
<td>Unstructured hybrid</td>
<td>766,988</td>
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<td>Wedge 15-45 Viscous</td>
<td>Unstructured hybrid</td>
<td>827,977</td>
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<td>Wedge 10</td>
<td>Structured (quadrilaterals)</td>
<td>25,392</td>
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<tr>
<td>Wedge 30-55 Viscous</td>
<td>Unstructured hybrid</td>
<td>457,121</td>
<td>261,620</td>
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