3rd Annual SU2 Developers Meeting
September 16th-18th, 2018
University of Strathclyde, Scottish Universities Insight Institute (SUII)
Glasgow, Scotland, UK

Meeting Agenda for Sunday September 16th

0900 – 0915: Welcome & Agenda
0915 – 1045: Introduction to developing in SU2: Covering high level class design, how to modify the code, working with GitHub (branching, PRs, regressions), etc.
1045 – 1615: Hack session: Separate groups working on various problems (lunch and snacks/coffee offered in the room while working)
1615 – 1700: Wrap-up Presentations: Two-slide presentations on major progress for the day, including discussion
1730 – open: Social at "The Counting House", 2 St Vincent Place, G1 2DH

Meeting Agenda for Monday September 17th

0800 – 0830: Welcome & Year in review, T. Economon (Bosch), J.J. Alonso (Stanford)
0900 – 0930: Toward optimization for reactive flows in SU2, N. Beishuijen (Bosch), D. Mayer, T. Economon
0930 – 1000: Conjugate heat transfer problems and computing coupled discrete adjoints using AD, O. Burghardt (TU Kaiserslautern), T. Albring, N. Gauger
1000 – 1030: Coffee break
1200 – 1300: Lunch
1300 – 1330: Unsteady optimization with SU2: application to turbomachinery design, A. Rubino (TU Delft), M. Pini, N. Anand, P. Colonna
1330 – 1400: Preliminary results on rotor-fuselage aerodynamics using SU2: status and challenges, M. Morelli (Politecnico di Milano), G. Gori, A. Guardone
1400 – 1430: Anisotropic mesh adaptation with the INRIA AMG library, A. Loseille (INRIA), V. Menier, B. Munguia, J.J. Alonso
1430 – 1500: Coffee break
1500 – 1530: Simulation and adjoint-based design for variable density incompressible flows with heat transfer, T. Economon (Bosch)
1530 – 1600: Implementation of pressure-based Navier-Stokes for wind energy applications, A. Ravishankara (ECN part of TNO), H. Ozdemir, E. van der Weide
1630 – 1700: Wrap up, J.J. Alonso (Stanford)

In order to participate (in-person or virtually), please register for the meeting by following the link on the SU2 home page (https://su2code.github.io).

*Please note that all stated times are British Summer Time (BST). **The presenter author is underlined.
1. Driver structure
2. Input/Output structure reformatting
3. Heterogeneous restart (e.g. RANS from an Euler and mesh mapping/interpolation)
4. Incompressible solver
5. Multiple config files and meshes multi-point optimization
6. General definitions for objective functions
7. SU2-NEMO thermochemistry structure and libraries interfaces
SU2-NEMO (Non-Equilibrium MOdelS): Thermochemistry and high-Mach flows

Ambition and objectives

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

• Define the roadmap for a coordinated development of thermochemistry and nonequilibrium models
• Incorporate advanced models for finite-rate chemistry and thermal nonequilibrium
• Consolidate the implementation and use of advanced thermodynamic models
• Reboot under a new perspective the modelling of high-temperature effects
People and selected applications, to date

- High-Mach and high-enthalpy external aerothermodynamics
- Laminar to turbulent transition in highly-compressible regimes
- Non-ideal gas dynamics of complex fluids departing from ideal gas laws
- Laminar premixed combustion for domestic heating
- Combustion in industrial processes
- From atmospheric entry and meteor to biomass pyrolysis
Outline

1. Some background equations and models
2. Mutation++, Cantera and FluidProp
3. Internal gasdynamics: SU2 and FluidProp
4. External aerodynamics: SU2 and Mutation++
5. The road ahead
Some background equations and models

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

\[
P = \rho RT
\]
\[
e = c_v T
\]
\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \nabla \cdot \vec{u}
\]
\[
\vec{q} = -k \nabla T
\]
Some background equations and models

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

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

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

\[
\begin{align*}
P &= P(\rho_s, T) \\
e &= e(X_s, T)
\end{align*}
\]

\[
\begin{align*}
\tau_{ij} &= \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \nabla \cdot \vec{u} \\
\vec{q} &= -k \nabla T \\
\mu &= \sum_s \frac{\mu_s X_s}{\phi_s}, \quad k = \sum_s \frac{k_s X_s}{\phi_s}
\end{align*}
\]
Some background equations and models

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\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \bar{u} - \rho_s \bar{u}_{d,1}) = \dot{w}_s
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\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho e \bar{u} + P \bar{I} \cdot \bar{u} - \bar{\tau} \cdot \bar{u} + \bar{q}) = \nabla \cdot (-\sum_s h_s \rho_s \bar{u}_{d,s}) - \nabla \cdot \bar{q}_v
\]

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

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

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

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

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

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

\[
\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \nabla \cdot \bar{u}
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\]
Some background equations and models: where were we?

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

• Fast coupling assumptions

• Rigid-Rotator-Harmonic-Oscillator (RRHO) thermodynamics

• Transport properties
  • Diffusion — Fick’s Law w/ closure terms (Sutton, 1998)
  • 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)
Some background equations and models: where were we?

- Derivation of continuous adjoint system, boundary conditions & surface sensitivities for steady, viscous, NE flow environments
- Implementation (in SU2) of flow and adjoint equations
- Adjoint equations formulated in a general way to support substitution of other thermochemical models
- All contributions in feature_TNE2 and feature_AdjTNE2,

... but SU2 has continued to evolve...new and more general implementation needed!
Some background equations and models: where we are heading

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

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\]
• Thermodynamic properties
• Multicomponent transport properties
• Finite rate chemistry in thermal nonequilibrium
• A robust multiphase equilibrium solver
Cantera is an open-source suite of object-oriented software tools for problems involving chemical kinetics, thermodynamics, and/or transport processes. The software automates the chemical kinetic, thermodynamic, and transport calculations so that the users can efficiently incorporate detailed chemical thermo-kinetics and transport models into their calculations.

• It is widely used in the combustion industry
• Low mach incompressible equilibrium chemistry

Some background equations and models: where we are

\[
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\]

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\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_v^s + \sum_s Q_{S-v}^s
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\rho e_v = \sum_s \rho_s e_v,s
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\]

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\vec{q} = -k \nabla T
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\[
\mu = \sum_s \frac{\mu_s X_s}{\phi_s}, \quad k = \sum_s \frac{k_s X_s}{\phi_s}
\]
FluidProp

Thermophysical property calculator for arbitrary fluids:

- entire thermodynamic plane liquid and gas phase
- easily switching between all equations of state
- accurate properties also close to critical point
- multicomponent mixtures
- computes “real” critical points of mixtures
- advanced methods for phase equilibria
- Look-up tables (under development)

http://www.asimptote.nl/software/fluidprop
Shock-induced flow with complex fluids

- Fluid: siloxane MM
- Fully turbulent, Roe scheme
- FluidProp-SW
Flow Past Supersonic ORC Turbine Cascade

- Fluid: siloxane MM
- Fully turbulent, Roe scheme
- Comparison FluidProp-SW vs FluidProp-LuT

Density Deviations

Numerical Schlieren
Thermodynamic Models: Computational Cost

The chart compares the computational cost of different models for various simulations. The x-axis represents different types of simulations: 2D Nozzle, 2D Cascade, and 3D Cascade. The y-axis shows CPU time in seconds.

- IGsim
- ug-LUTsim
- SWsim

The CPU time for each simulation type is as follows:

- 2D Nozzle: IGsim > ug-LUTsim > SWsim
- 2D Cascade: IGsim > ug-LUTsim > SWsim
- 3D Cascade: IGsim > ug-LUTsim > SWsim
External aerodynamics: Double wedge at M7.11

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mach_{FS}</td>
<td>7.11</td>
</tr>
<tr>
<td>Unit Reynolds [m^{-3}]</td>
<td>55,880</td>
</tr>
<tr>
<td>Temperature_{FS} [K]</td>
<td>191</td>
</tr>
<tr>
<td>Pressure_{FS} [Pa]</td>
<td>391.735</td>
</tr>
<tr>
<td>Temperature_{w} [K]</td>
<td>300</td>
</tr>
<tr>
<td>Fluid</td>
<td>N_2O_2</td>
</tr>
<tr>
<td>θ_1 / θ_2</td>
<td>30° / 55°</td>
</tr>
</tbody>
</table>

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

Numerical Schlieren @ 150 µs. Calorically perfect (left) thermally perfect (right)
# External aerodynamics: Edney IV interaction

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mach</td>
<td>8.03 / 5.25</td>
</tr>
<tr>
<td>Unit Reynolds [m⁻¹]</td>
<td>6.75 10⁶</td>
</tr>
<tr>
<td>Temperature [K]</td>
<td>111.56 / 238.04</td>
</tr>
<tr>
<td>Pressure [Pa]</td>
<td>985.01 / 6,996</td>
</tr>
<tr>
<td>Temperature₂ [K]</td>
<td>294.44</td>
</tr>
<tr>
<td>Fluid</td>
<td>N₂O₂</td>
</tr>
<tr>
<td>Impinging shock [deg]</td>
<td>18.1114</td>
</tr>
</tbody>
</table>

**Thermally perfect gas. Temperature (left), pressure (right)**

**Numerical Schlieren**
External aerodynamics: Proximal bodies

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mach</td>
<td>10</td>
</tr>
<tr>
<td>Temperature [K]</td>
<td>111.56</td>
</tr>
<tr>
<td>Pressure [Pa]</td>
<td>985.01</td>
</tr>
<tr>
<td>Fluid</td>
<td>N$_2$O$_2$</td>
</tr>
<tr>
<td>$D_p/D_s$</td>
<td>18.1114</td>
</tr>
<tr>
<td>$y/D_p$</td>
<td>1.088</td>
</tr>
<tr>
<td>$x/D_p$</td>
<td>4</td>
</tr>
</tbody>
</table>

Mach number contours. Inviscid flow BGK scheme
The road ahead ...

- Define and implement a smart thermochemistry interface
- Augment the library of schemes for improved robustness with high Mach (including MUSCL)
- Extend the BC formulations to account for radiative equilibrium and potentially slip flow (for high-Mach)
- Formulate and implement models for the finite-rate energy exchange (i.e. multiple temperatures and energy modes)
- Ensure consistency with the algorithm differentiation for adjoint formulation
- Treatment of the Jacobian matrix of source terms
- Consolidate the multispecies 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

... and counting
Thank you,
Happy to take any questions
**Hackathon topic(s)**

**Q:** What would be a “smart” interface for the thermodynamics and chemistry libraries (e.g. look-up tables, more integrated connection)?

**Q:** What is smart and what level of flexibility (i.e. plug-and-play) do we want to ensure/consider?

**Q:** What would be the impact on the config. file wrt to the thermodynamic models?

<table>
<thead>
<tr>
<th>FLUID_MODEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>STANDARD_AIR</td>
</tr>
<tr>
<td>USER_DEFINED</td>
</tr>
</tbody>
</table>

```java
if (FLUID_MODEL == USER_DEFINED){ more options might be needed
  THERMAL_EOS (Ideal_gas, Van_der_Waals, Peng_robinson, etc.)
  CALORIC_EOS (Perfect_gas, NASA_fit, etc.)
  COMPOSITION (Mass/Molar fractions of species)
}
```

**CHEMISTRY (Frozen, Equilibrium, Finite-rate)**

```java
if (CHEMISTRY == Equilibrium){ even more options might be needed}
if (CHEMISTRY == Finite_rate){ a lot of options might be needed}
```