Non-Ideal Compressible-Fluid Dynamics in the SU2 Framework

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Outline

• What is NICFD?
• Applications
• Making SU2 a NICFD solver
• Where are we now?
• What’s next
NICFD: what is that?
Non-Ideal Compressible-Fluid Dynamics

NICFD: $PV \neq RT$
- Dense vapor flows
- High-compressibility
- Non-ideal speed-of-sound behavior
- Critical point effects
- Phase transition
- Super-critical flows
NICFD of molecularly complex fluids ($\Gamma < 1$)

Nozzle design for uniform outflow
Exit Mach = 2.25
P0 = 25 bar, T0 = 310.3
Exp. Ratio b = 25
Fluid siloxane: MDM

Non-ideal vs ideal:
- nozzle length is x 3!
- exit section x 3!
NICFD of molecularly complex fluids ($\Gamma < 1$)

The Mach number variation along an isentropic expansion is NON-MONOTONE if $\Gamma < 1$!
Shock formation in a non-ideal fluid

Fundamental derivative of gasdynamics

\[ \Gamma \equiv 1 - \frac{\nu}{c} \left( \frac{\partial c}{\partial v} \right)_s \]

Speed of sound \( c^2 \equiv -\nu^2 \left( \frac{\partial P}{\partial v} \right)_s \)

Acoustic wave speed \( w = u + c \)

\[
dw = \left[ \frac{\nu}{c} - \frac{\nu^2}{c^2} \left( \frac{\partial c}{\partial v} \right)_s \right] dP \Rightarrow dw = \frac{\nu}{c} \Gamma dP
\]
Applications

- Fundamentals of fluid mechanics
- ORC power systems
- scCO₂ power systems
- Trans-critical heat exchangers
- Oil and Gas compressors/expanders
- Super / transcritical injection (I.C.E., gas turbines)
- Cryogenic processes
- Rocket engines (turbopumps)
- Refrigeration / HVAC
- Chemical processes
- ...
Making SU2 a NICFD solver
Making SU2 a NICFD solver

First: get the smart people!
Rules of the game: governing equations

Euler equation for mono-component fluid at chemical & thermodynamic equilibrium

\[
\begin{align*}
\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + P) &= 0, \\
\partial_t E^t + \nabla \cdot [(E^t + P) \mathbf{u}] &= 0, \quad \text{with} \quad E^t = \rho e + \frac{1}{2} \rho |\mathbf{u}|^2
\end{align*}
\]

Thermodynamic closure is needed!

Perfect gas: \( P = P(E, \rho) = (\gamma-1)\rho e = (\gamma-1)E \)
Thermodynamics models... PV ≠ RT!

\[
\frac{\Psi(T, \rho)}{RT} = \psi^0(\tau, \delta) + \psi^r(\tau, \delta)
\]


\[
\psi^0(\tau, \delta) = \frac{h^0_0}{RT} - \frac{s^0_0}{R} - 1 + \ln\left(\frac{\tau_0\delta}{\delta_0\tau}\right)
- \frac{\tau}{R} \int_{\tau_0}^{\tau} \frac{C^0_P}{\tau^2} d\tau + \frac{1}{R} \int_{\tau_0}^{\tau} \frac{C^0_P}{\tau} d\tau
\]

\[
\psi^r(\tau, \delta) = n_1\delta^0\tau^{0.250} + n_2\delta^1\tau^{1.125} + n_3\delta^2\tau^{1.500} + n_4\delta^2\tau^{1.375}
+ n_5\delta^3\tau^{0.250} + n_6\delta^4\tau^{0.875} + n_7\delta^2\tau^{0.625} e^{-\delta}
+ n_8\delta^5\tau^{1.750} e^{-\delta} + n_9\delta^3\tau^{3.625} e^{-\delta^2} + n_{10}\delta^4\tau^{3.625} e^{-\delta^2}
+ n_{11}\delta^3\tau^{14.5} e^{-\delta^3} + n_{12}\delta^4\tau^{12.0} e^{-\delta^3}
\]
Thermodynamics models... PV ≠ RT!

\[
\frac{\Psi(T, \rho)}{RT} = \psi^0(\tau, \delta) + \psi^r(\tau, \delta)
\]


\[
\psi^0(\tau, \delta) = \frac{h_0^0 \tau}{RT_c} - \frac{s_0^0}{R} - 1 + \ln \left( \frac{\tau_0 \delta}{\delta_0 \tau} \right)
\]

\[
- \frac{\tau}{R} \int_{\tau_0}^{\tau} \frac{C_P^0}{\tau^2} d\tau + \frac{1}{R} \int_{\tau_0}^{\tau} \frac{C_P^0}{\tau} d\tau
\]

\[
\psi^r(\tau, \delta) = n_1 \delta \tau^{0.250} + n_2 \delta \tau^{1.125} + n_3 \delta \tau^{1.500} + n_4 \delta^2 \tau^{1.375}
\]

\[
+ n_5 \delta^3 \tau^{0.250} + n_6 \delta^7 \tau^{0.875} + n_7 \delta^2 \tau^{0.625} e^{-\delta}
\]

\[
+ n_8 \delta^5 \tau^{1.750} e^{-\delta} + n_9 \delta^3 \tau^{3.625} e^{-\delta^2} + n_{10} \delta^4 \tau^{3.625} e^{-\delta^2}
\]

\[
+ n_{11} \delta^3 \tau^{14.5} e^{-\delta^3} + n_{12} \delta^4 \tau^{12.0} e^{-\delta^3}
\]

\[
P = P(E, \rho)
\]
There may be trouble ahead…

Structure of the code changes deeply:

- Flux Jacobian is possibly NOT an homogeneous function of degree one w.r.t. conservative variables (Roe scheme?)
- More complex eigenstructure w.r.t. ideal gas.
- Thermodynamics:
  - Computationally expensive
  - Possibly numerically unstable
  - Non-unique solutions (VLE)
  - Look-Up Table must be consistent
  - $e \neq e(T)$, $h \neq h(T)$, $c \neq c(T)$
- Boundary conditions

...let’s face the music and dance!
Where are we now?
Where are we now?

Thermodynamic modeling
• Constant-specific-heat ideal gas
• van der Waals fluid
• Peng-Robinson Stryjek-Vera
• Coupling to FluidProp

Numerical schemes
• Roe scheme
• HLLC scheme
• AUSM+

Boundary conditions
• Riemann boundary conditions
• Diverse input data: $P$, $(\rho,u)$, $(h,s)$, ...

Ideal-gas Prandtl-Meyer expansion

Non-classical rarefaction shock wave

Density
ORCHID: ORC Hybrid Integrated Device @TUDelft

- Single regenerated BoP, closed loop configuration, dual TS operation (at one time)
- Continuous, steady-state, flexible in operation (multiple WF and op. conditions)
ERC NSHOCK Project

- Goal: first-time observation of Rarefaction Shock Waves in nozzle flows!
- Mixture thermodynamics & gasdynamics
- New measurement techniques for non-ideal compressible-fluid dynamics
TROVA: Test-Rig for Organic Vapours @Politecnico di Milano

Schlieren visualisation of non-ideal nozzle flow of siloxane fluid MDM

Test conditions
- \( P^t = 4.68 \text{ bar (meas.)} \)
- \( T^t = 246.9 \degree C \text{ (meas.)} \)
- \( Z^t = 0.826 \text{ (model)} \)

Pressure measurements vs numerical simulations with SU2

\[ Z = \frac{P}{RT\rho} \]
What’s next?
What’s next: modeling

- Viscosity/thermal conductivity
- Critical point flows
- Two-phase equilibrium flows
  - Cavitation/condensation
- Single and two-phase mixtures
- Non-equilibrium two-phase:
  - Particle nucleation
  - Super/sub-cooled TMD state
- Three-phase TMD:
  - In-flight ice formation
  - Deposition processes

Oaks et al. (2001)
What’s next: algorithms

- Two-phase flow solver
- Robust schemes for CP flows
- Lagrangian particle tracking
- Multi-species solver
- Virtual Schlieren for non-ideal fluids
- Speed-up TMD
  - Look-Up Table
  - Inversion of $\psi(T,v)$
  - Hybrid LUT
Conclusions

• SU2 is now a fully capable NICFD solver for three-dimensional complex geometry
• It embeds state-of-the-art thermodynamic models for pure fluids and mixtures, which are relevant to diverse applications, ranging for ORC and scCO2 power systems to refrigeration
• NICFD development within SU2 is supported by a strong team and funded via numerous projects on fundamental science (ERC, Marie-Curie, NWO) and strong industrial partnership
• Preliminary validation against experimental data from the TROVA test-rig confirms the accuracy of the NICFD tool set
Thank you for your attention!

Question?

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Download SU2 from GitHub: https://github.com/su2code/SU2