Non-Ideal Compressible-Fluid Dynamics in the SU2 Framework

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Outline

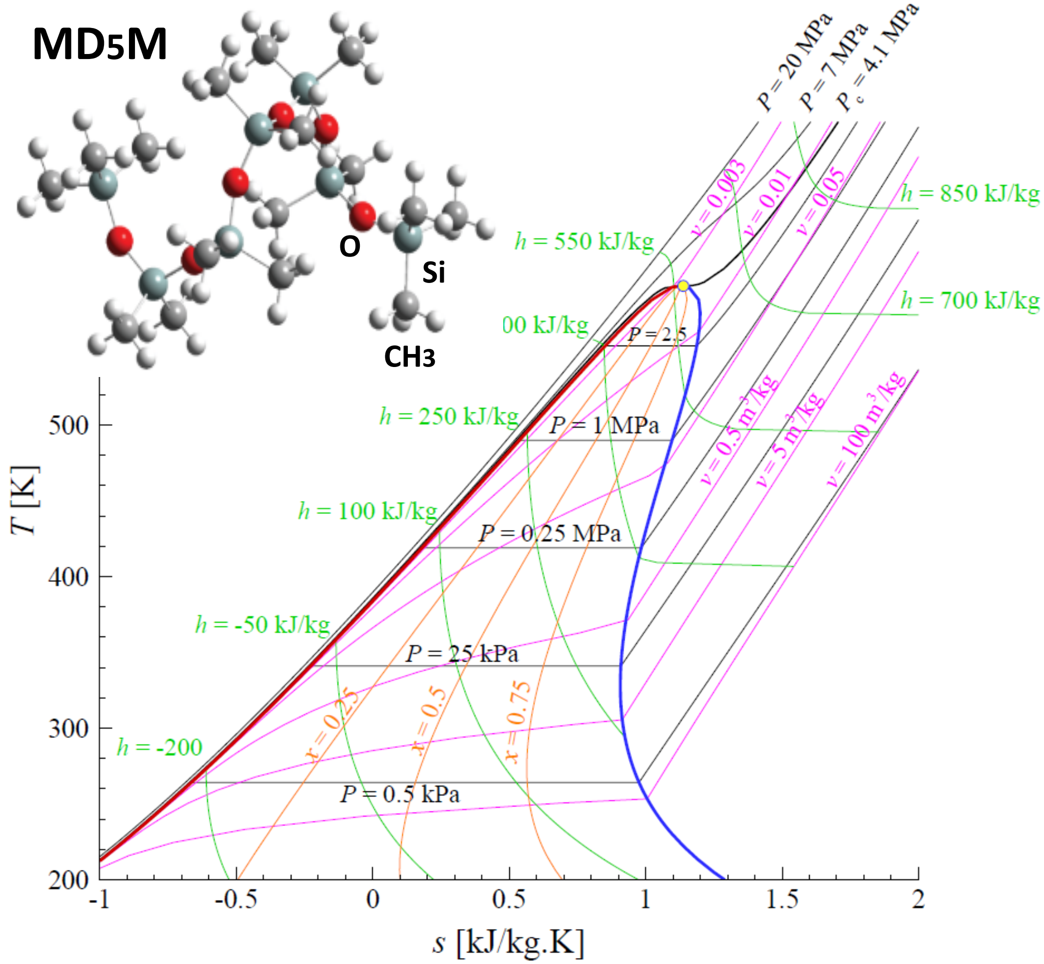
- What is NICFD?
- Applications
- Making SU2 a NICFD solver
- Where are we now?
- What's next

NICFD: what is that?

Non-Ideal Compressible-Fluid Dynamics

NICFD: PV ≠ RT

- Dense vapor flows
- High-compressibility
- Non-ideal speed-of-sound behavior
- Critical point effects
- Phase transition
- Super-critical flows



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NICFD of molecularly complex fluids ($\Gamma < 1$)

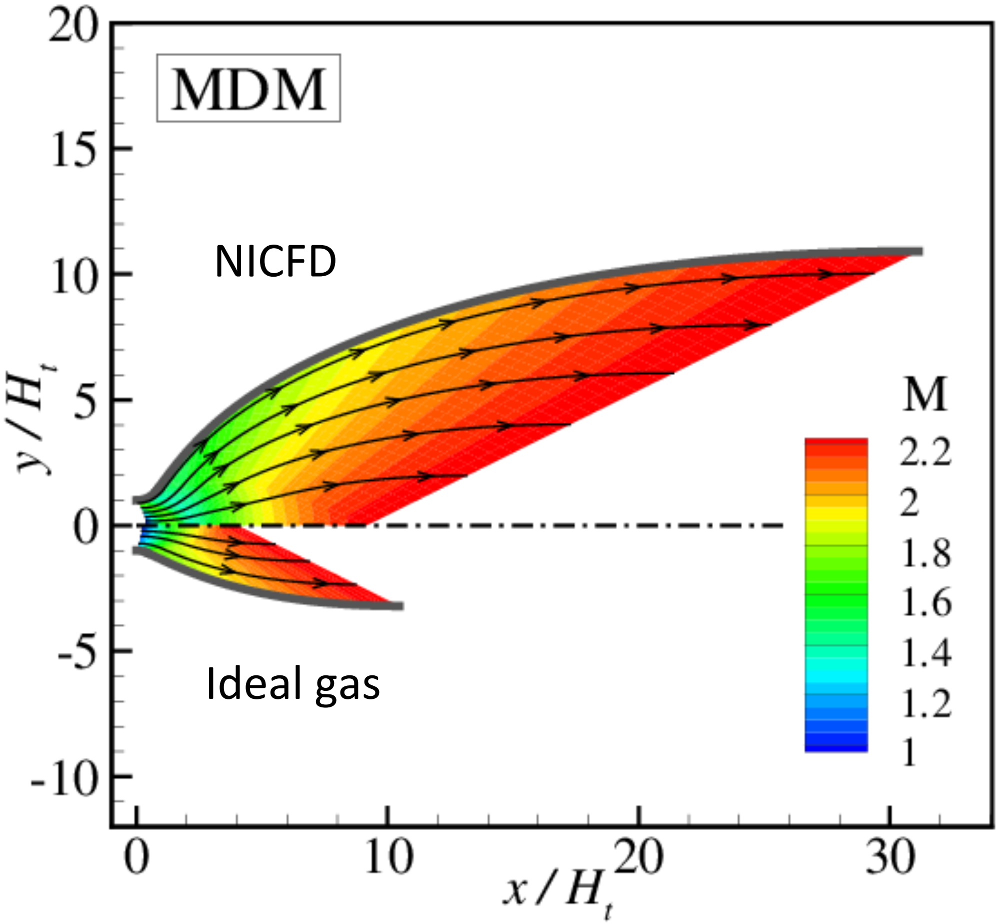
<u>Nozzle design for uniform outflow</u>

Exit Mach = 2.25

P0 = 25 bar, T0 = 310.3

Exp. Ratio b = 25

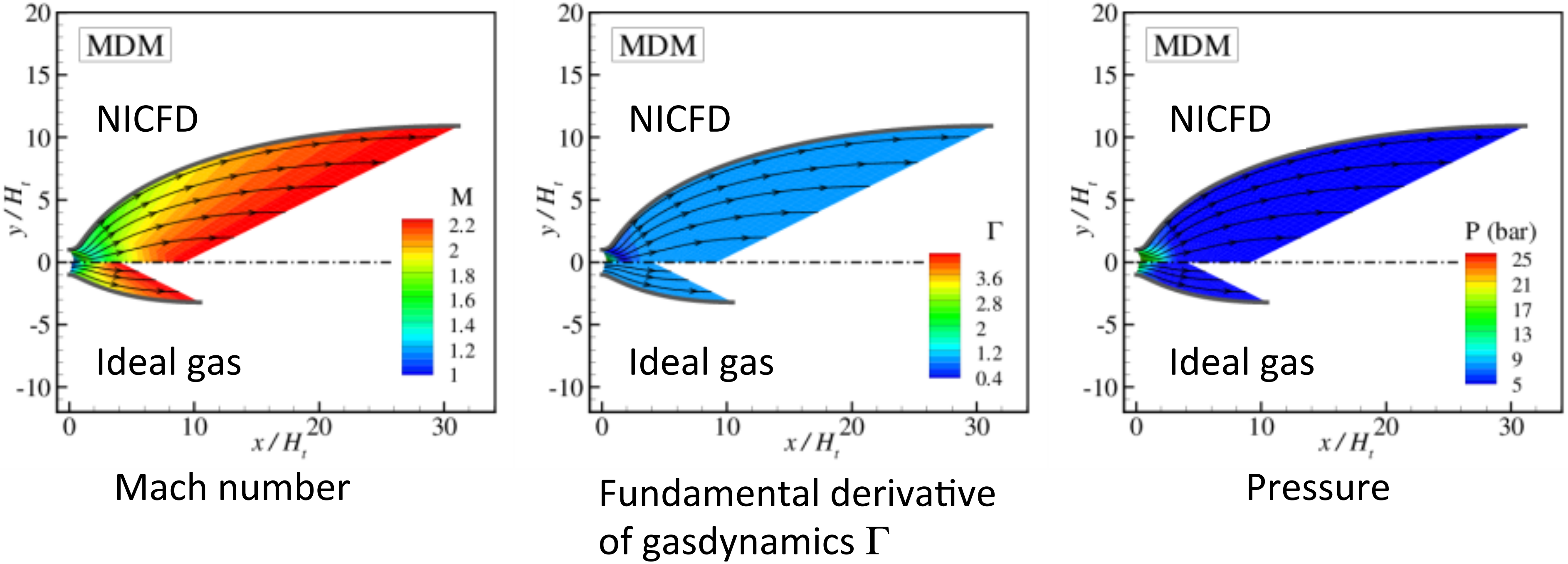
Fluid siloxane: MDM



Non-ideal vs ideal:

- nozzle length is x 3!
- exit section x 3!

NICFD of molecularly complex fluids ($\Gamma < 1$)

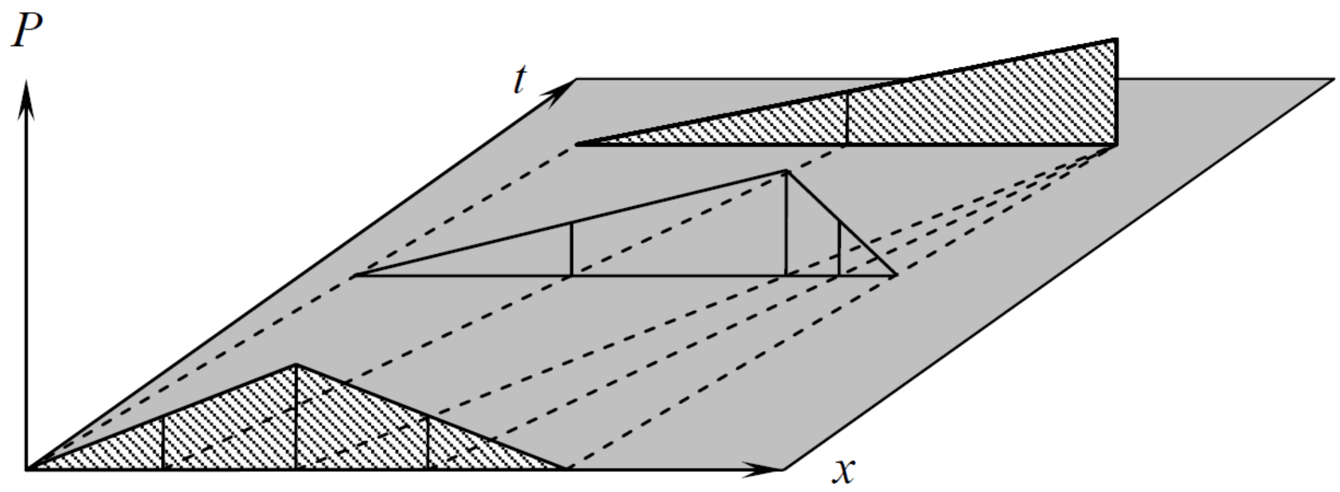


The Mach number variation along an isentropic expansion is NON-MONOTONE if $\Gamma < 1$!

Shock formation in a non-ideal fluid

Fundamental derivative of gasdynamics

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



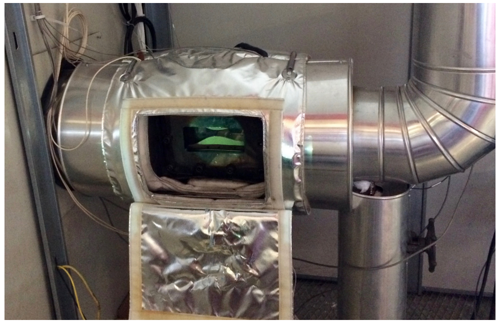
Speed of sound $c^2 \equiv -v^2 \left(\frac{\partial P}{\partial v}\right)_s$

Acoustic wave speed $w = u + c$

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

Applications

- Fundamentals of fluid mechanics
- ORC power systems
- $scCO_2$ 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
- …

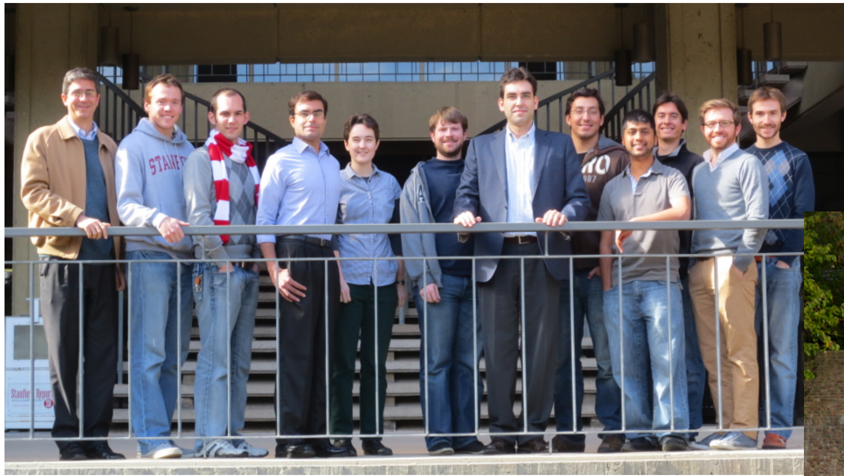


Making SU2 a NICFD solver

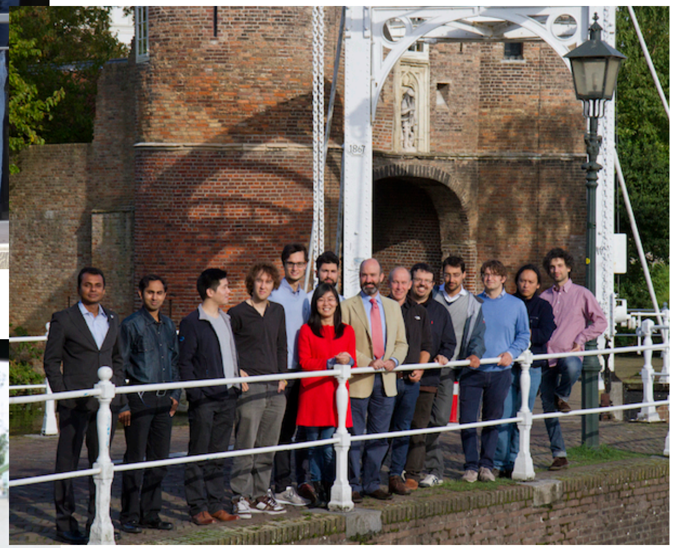
Making SU2 a NICFD solver

SU2

The Open-Source CFD Code



Stanford University



First: get the smart people!

TUDelft

POLITECNICO DI MILANO

Rules of the game: governing equations

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

$$\begin{cases} \partial_t \rho + \nabla\cdot(\rho \boldsymbol{u}) = 0, \\ \partial_t(\rho \boldsymbol{u}) + \nabla\cdot(\rho \boldsymbol{u}\otimes \boldsymbol{u} + P) = 0, \\ \partial_t E^{\mathrm{t}} + \nabla\cdot[(E^{\mathrm{t}} + P)\,\boldsymbol{u}] = 0, \quad \text{with } E^{\mathrm{t}} = \rho e + \frac{1}{2}\rho\,|\boldsymbol{u}|^2 \end{cases}$$

Thermodynamic closure is needed!

Perfect gas: $P = P(E,\rho) = (\gamma\text{-}1)\rho e = (\gamma\text{-}1)E$

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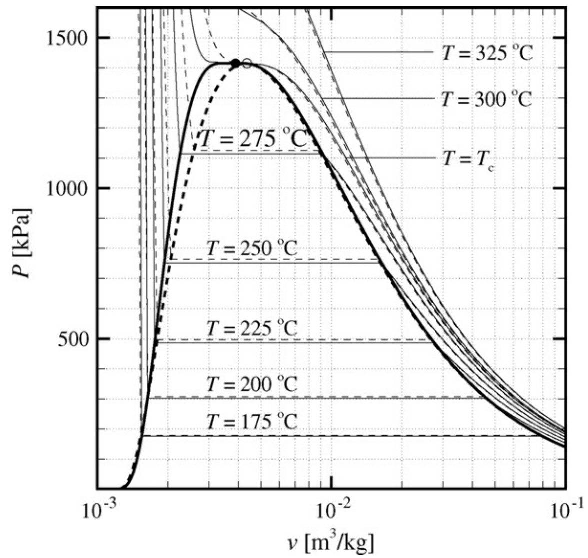
Thermodynamics models… PV ≠ RT!

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

Span-Wagner 12-parameter EoS (2003)

$$\psi^0(\tau,\delta) = \frac{h_0^0 \tau}{RT_{\mathrm{c}}} - \frac{s_0^0}{R} - 1 + \ln\left(\frac{\tau_0 \delta}{\delta_0 \tau}\right) - \frac{\tau}{R}\int_{\tau_0}^{\tau} \frac{C_P^0}{\tau^2} d\tau + \frac{1}{R}\int_{\tau_0}^{\tau} \frac{C_P^0}{\tau} d\tau$$

$$\begin{aligned}\psi^{\mathrm{r}}(\tau,\delta) = {} & n_1\delta\tau^{0.250} + n_2\delta\tau^{1.125} + n_3\delta\tau^{1.500} + n_4\delta^2\tau^{1.375} \\ & + n_5\delta^3\tau^{0.250} + n_6\delta^7\tau^{0.875} + n_7\delta^2\tau^{0.625}\mathrm{e}^{-\delta} \\ & + n_8\delta^5\tau^{1.750}\mathrm{e}^{-\delta} + n_9\delta\tau^{3.625}\mathrm{e}^{-\delta^2} + n_{10}\delta^4\tau^{3.625}\mathrm{e}^{-\delta^2} \\ & + n_{11}\delta^3\tau^{14.5}\mathrm{e}^{-\delta^3} + n_{12}\delta^4\tau^{12.0}\mathrm{e}^{-\delta^3}\end{aligned}$$



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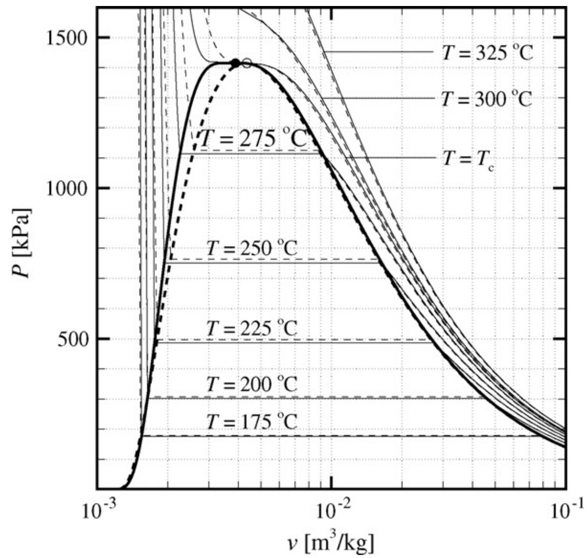
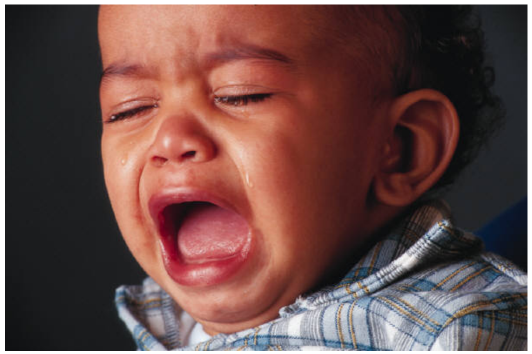


$P = P(E,\rho)$



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?

<u>Thermodynamic modeling</u>

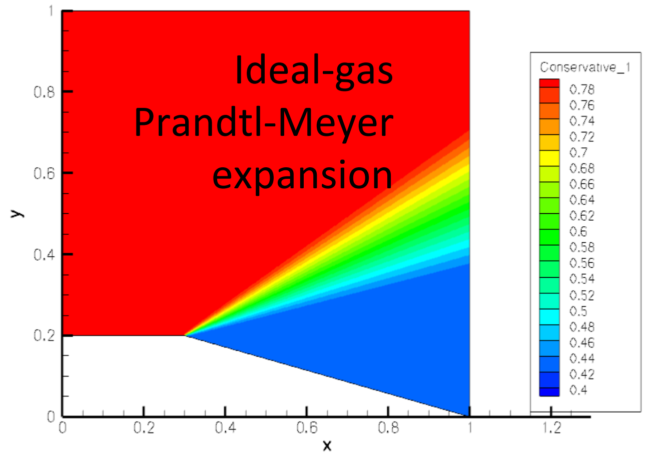
- Constant-specific-heat ideal gas
- van der Waals fluid
- Peng-Robinson Stryjek-Vera
- Coupling to FluidProp

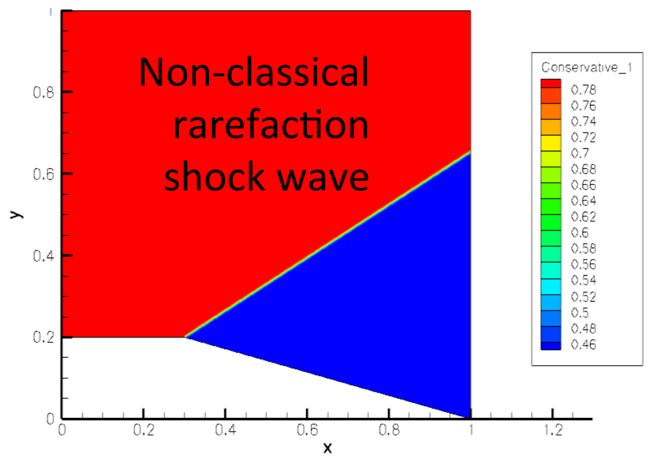
<u>Numerical schemes</u>

- Roe scheme
- HLLC scheme
- AUSM+

<u>Boundary conditions</u>

- Riemann boundary conditions
- Diverse input data: *P*, *(ρ,u)*, *(h,s)*, …

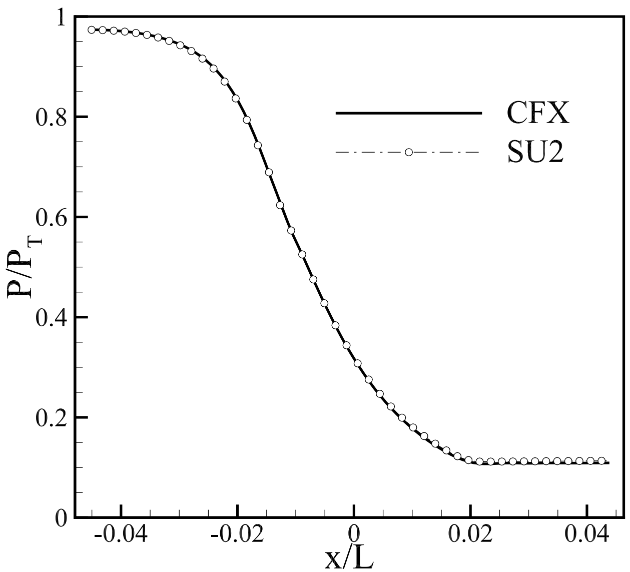


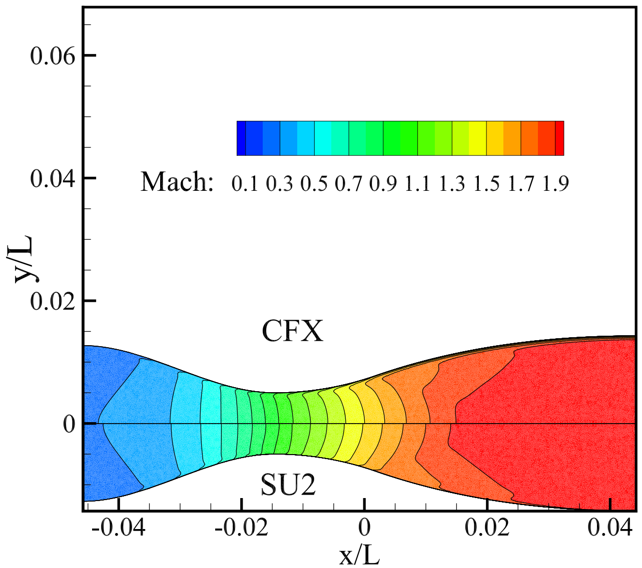


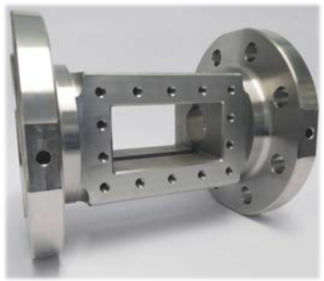
Density

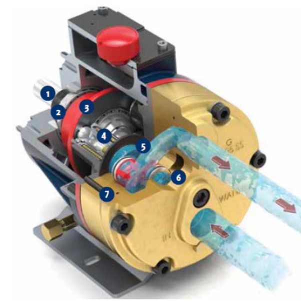
ORCHID: ORC Hybrid Integrated Device @TUDelft

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









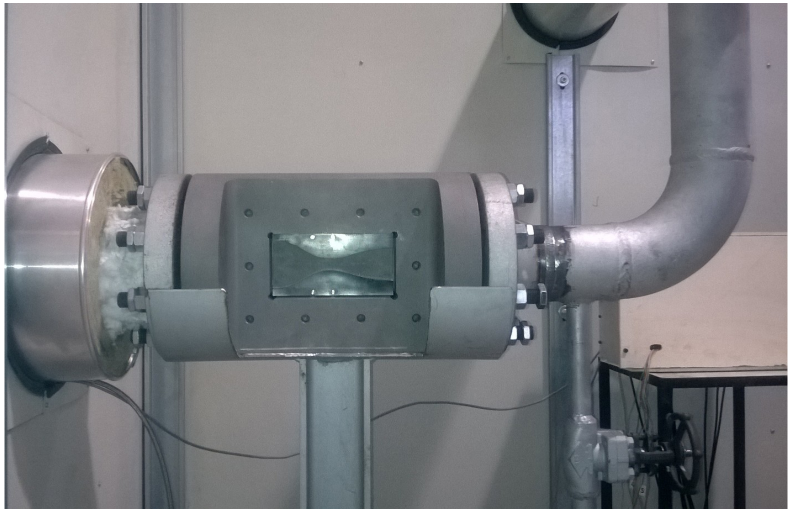
TROVA: Test-Rig for Organic Vapours @Politecnico di Milano

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

European Research Council

Established by the European Commission



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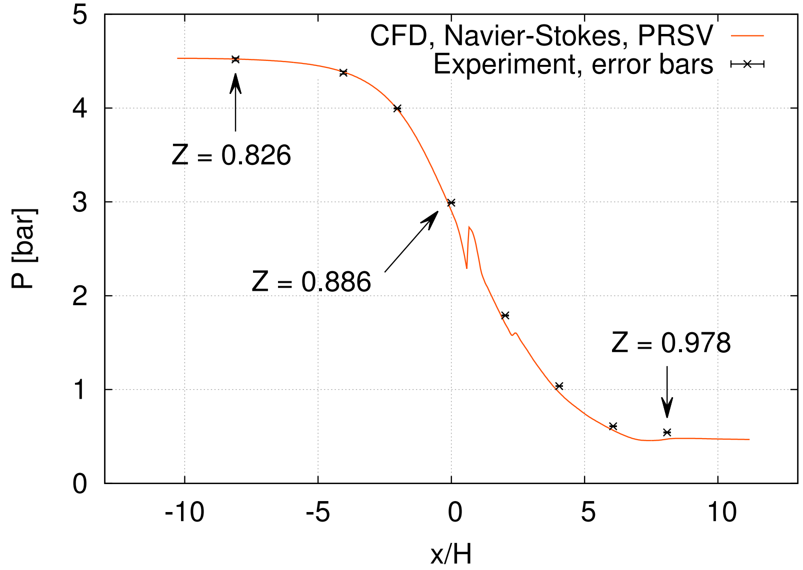
TROVA: Test-Rig for Organic Vapours @Politecnico di Milano

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

Numerical schlieren from SU2

Pressure measurements vs numerical simulations with SU2



Test conditions P^t = 4.68 bar (meas.)

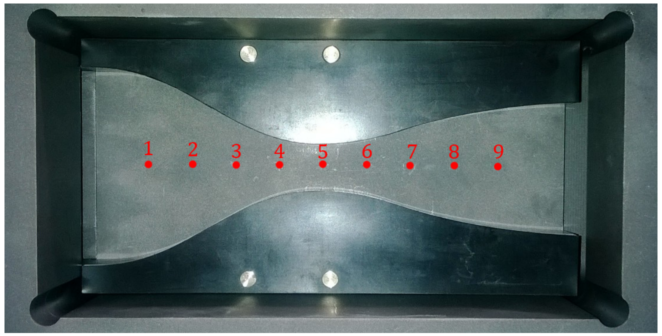
T^t = 246.9 °C (meas.)

Z^t = 0.826 (model)

European Research Council
Established by the European Commission

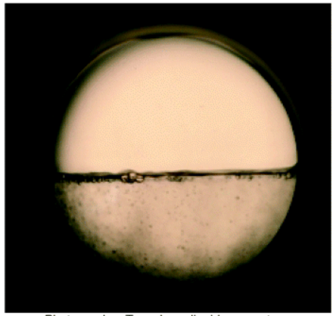
Compressibility factor

$Z = P/(RT\rho)$

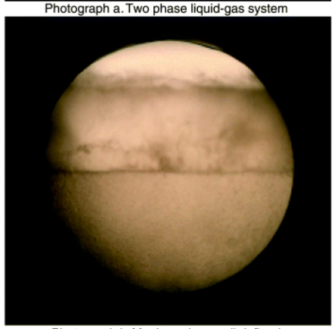


What's next?

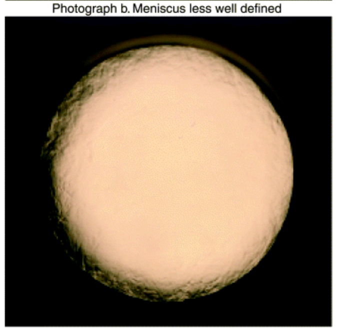
What's next: modeling



Photograph a. Two phase liquid-gas system



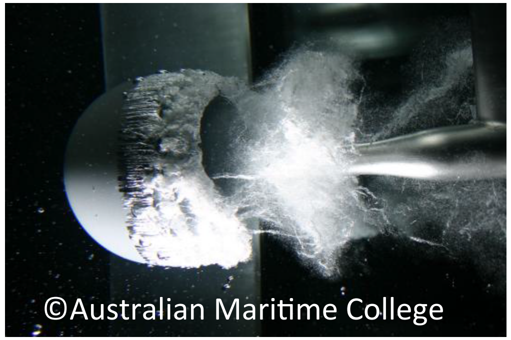
Photograph b. Meniscus less well defined

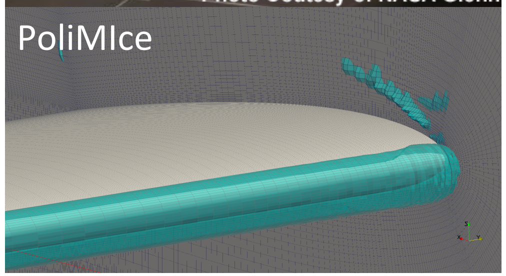


Photograph c. Homogeneous supercritical fluid

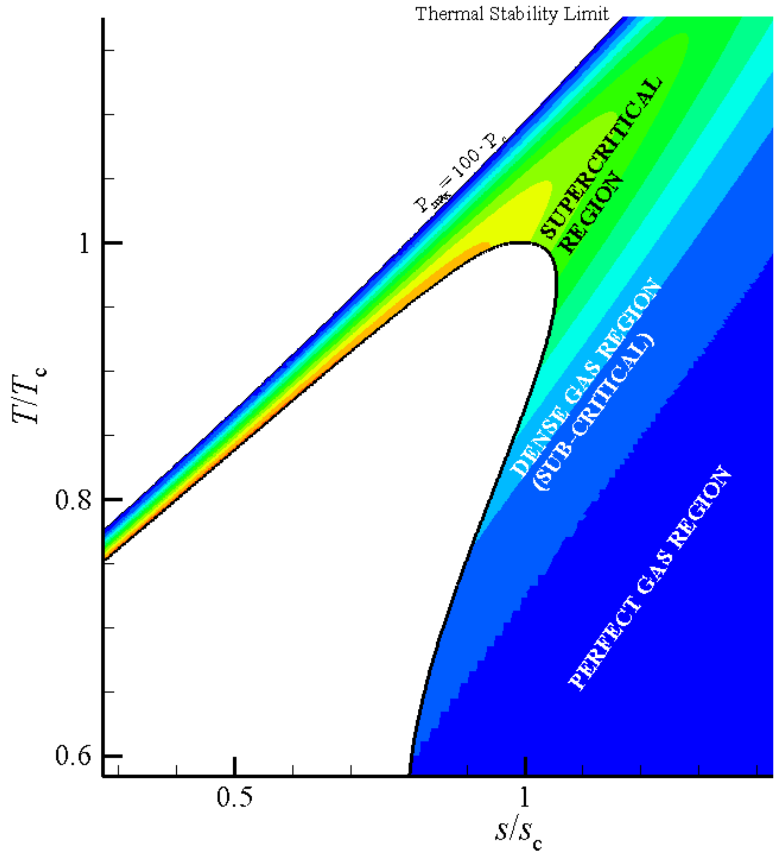
Oaks et al. (2001)

- 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

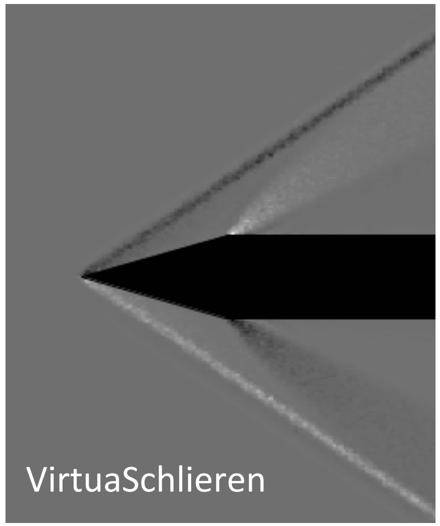




What's next: algorithms



- 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

Conclusions

Thank you for you attention!

Question?

CREA Lab @PoliMI: crealab.polimi.it
Propulsion & Power Group @TUDelft: www.lr.tudelft.nl
Download SU2 from GitHub: https://github.com/su2code/SU2