CoolProp: An Open-Source Reference-Quality Thermophysical Property Library

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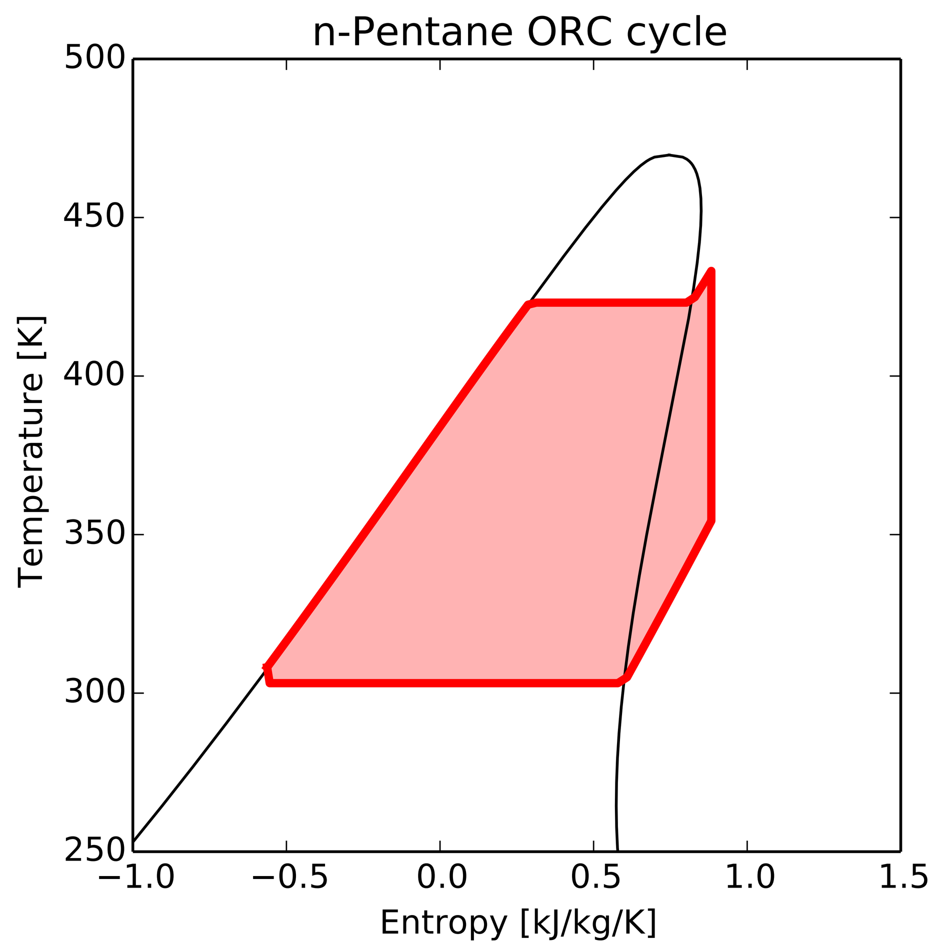


Motivation

- No mature open-source thermophysical property libraries currently exist
- Make state-of-the-art tools available to a wide audience
- Computationally efficient methods for the lookup of thermophysical properties
  - Properties consume most of the computational time in thermal systems simulation (dynamics, CFD, etc.)

Fluids Included

110 pure and pseudo-pure fluids. Fluids of particular interest to the ORC community include:

- Pure Refrigerants (R245fa, R134a, etc.)
- HFOs (R1234yf, R1234ze(Z), etc.)
- Other Organics (Ethanol, n-Pentane, etc.)
- Pseudo-pure Mixtures (Solkatherm SES36, R410A, etc.)
- Natural working fluids (CO_2, Ammonia, etc.)

Wrappers

Wrappers of CoolProp are available for a wide range of programming languages and environments:

- Python
- Modelica
- EES
- MATLAB
- Labview
- Octave
- Microsoft Excel
- C#
- Visual Basic
- Java

Code compiles on Windows, Linux, OSX

Other Features

- Properties for incompressible fluids and brines
- Properties for humid air
- Plotting functionalities in Python
- Development of mixture properties for blends of working fluids

Equations of State

Equations of state implemented in the state-of-the-art literature are based on Helmholtz-Energy-Explicit formulations. Helmholtz energy given by

$$\alpha = \underbrace{\alpha^r(T,\rho)}_{residual} + \underbrace{\alpha^0(T,\rho)}_{ideal}$$

Other properties obtained by analytic differentiation. For instance,

$$\frac{p}{\rho RT} = 1 + \delta\left(\frac{\partial \alpha^r}{\partial \delta}\right)_\tau \quad \text{or} \quad \frac{h}{RT} = \tau\left[\left(\frac{\partial \alpha^0}{\partial \tau}\right)_\delta + \left(\frac{\partial \alpha^r}{\partial \tau}\right)_\delta\right] + \frac{p}{\rho RT}$$

where $\delta = \rho/\rho_c$, $\tau = T_c/T$, and ρ_c is the critical density and T_c is the critical temperature

Tabular Taylor Series Expansion (TTSE)

Motivation

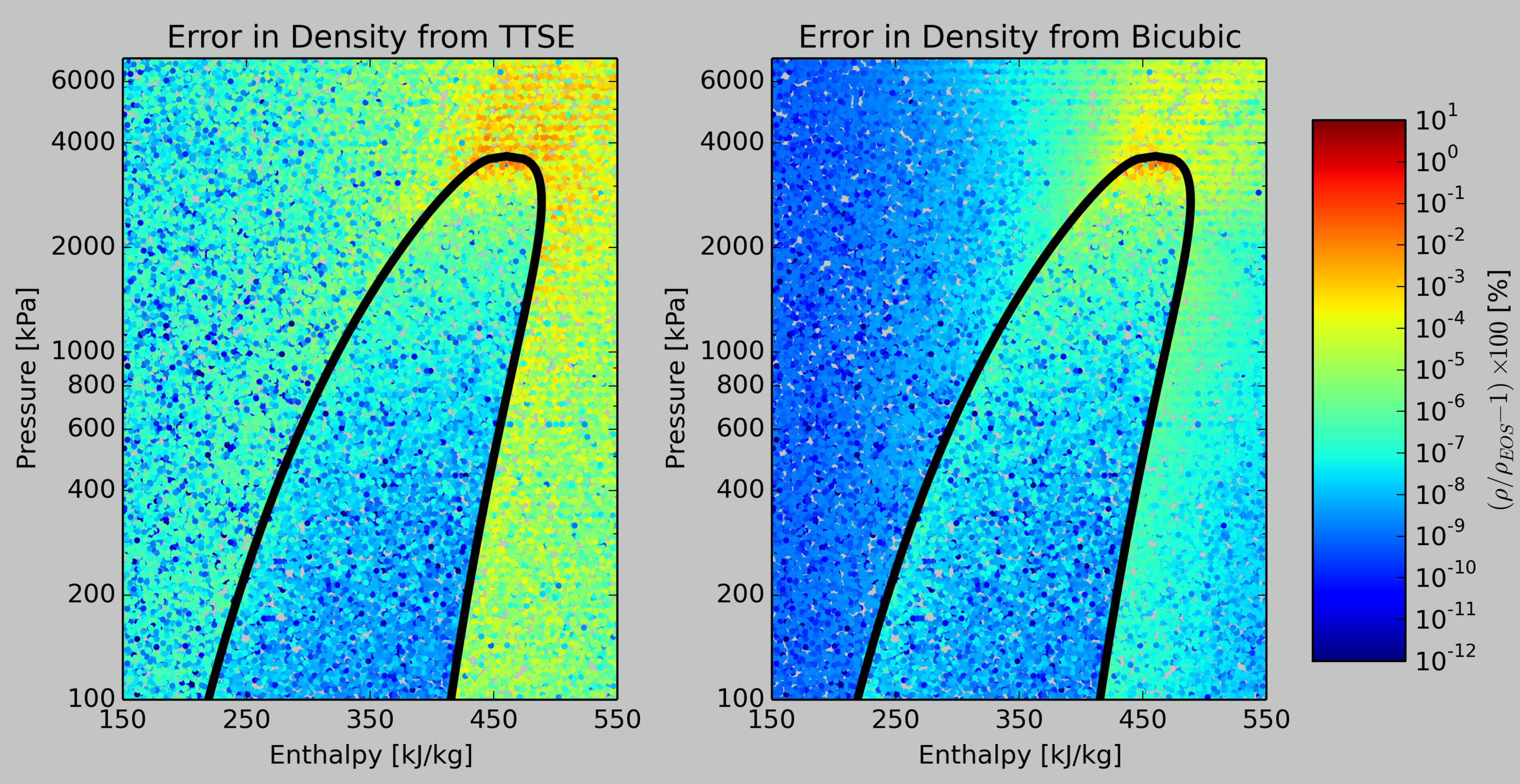
- Pressure-enthalpy are common inputs, especially in dynamic modeling in Modelica
- Equations of State use T,ρ as state variables - Need to solve $p,h \rightarrow T,\rho$
- This solver is very slow, requiring many calls to the equation of state

Implementation

$$T = T_{i,j} + \Delta h\left(\frac{\partial T}{\partial h}\right)_p + \Delta p\left(\frac{\partial T}{\partial p}\right)_h + \frac{\Delta h^2}{2}\left(\frac{\partial^2 T}{\partial h^2}\right)_p + \frac{\Delta p^2}{2}\left(\frac{\partial^2 T}{\partial p^2}\right)_h + \Delta h \Delta p\left(\frac{\partial^2 T}{\partial p \partial h}\right)$$

where all derivatives are evaluated at the grid point i,j

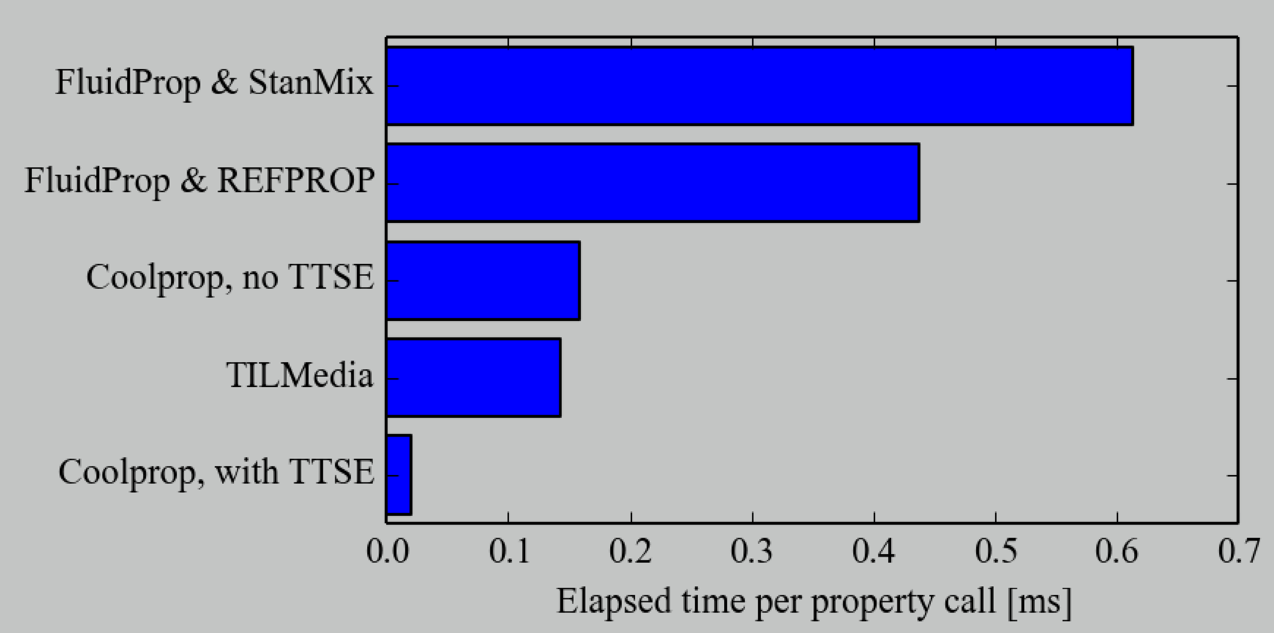
- Derivatives are pre-calculated at grid points once (slow)
- Derivatives used to extrapolate from grid point and evaluate $T(p,h)$ for instance (very fast)
- Also possible to use these derivatives with bicubic interpolation for higher accuracy than TTSE



R245fa, 200 x 200 grid

TTSE Example

Property retrieval in Modelica – CoolProp + TTSE is by far the fastest option



Acknowledgements

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