

Open Source Thermodynamic Properties

Synopsis

There is a *massive* body of high quality models for the thermodynamic properties of substances, and their implementations are mostly in proprietary codes. What projects are available in the open-source domain?

Audience: Intermediate to advanced users. This talk is for people with at least some familiarity with the Python language with an interest in the dark arts of thermodynamics.

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Our Project: PYroMat :: pyromat.org :: [PYroMat Git](#)

What are we talking about?

- **The problem:** how do substances heat up, expand, contract, boil, condense, etc.? (5 min)
- Basic Properties are pressure, temperature, density, volume
- Less intuitive properties are internal energy, enthalpy, entropy, specific heat, and many more...
- Geek out about the **history of codes** (5min)
- Stanjan (Fortran)
- GRI Mech (Data Set)
- Chemkin (Proprietary)
- Cantera (Open Source)
- NIST Webbook (web)
- REFPROP (semi-proprietary)
- CoolProp (semi-proprietary)
- PYroMat (Open Source)
- MANY proprietary codes
- **What do these code do?** (5 min)
- Where do their data come from? JANAF, NIST, Journals
- What do the models look like?
- **Ten Minutes with PYroMat** (10min)
- Import: `import pyromat as pm`
- Search: `pm.search(name='water')`
- Info: `pm.info('mp.H2O')`
- Get: `h2o = pm.get('mp.H2O')`
- Have some fun ...
- Change our units: `pm.config['unit_temperature'] = 'F'`
- Find the docs! [PYroMat Docs](#)
- **Let the audience lead:** Time for questions, answers, and discussion (5min)