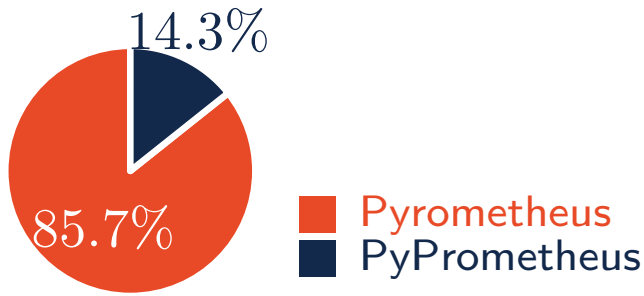
Pyrometheus

- Need code to compute chemical source terms
- Libraries (e.g., Cantera) can provide, but slow down computation
- *Pyrometheus*: Automated thermochemistry-code generation
  - Name selected by CEESD vote



- Code generation: established approach[1,2], but *Pyrometheus* has two advantages
  - Based on a code template, reflecting equations of chemical kinetics
  - Compatible with automatic differentiation (AD) for Jacobians
    $\Rightarrow$ only need to implement source terms, no derivatives
- **ACT II simulations**: faster with generated code than Cantera by factor of 1.7

[1] Bisetti, *Combust. Theory & Model.* (2012)
[2] Neimeyer et al., *Comput. Phys. Commun* (2017)

Chemical Kinetics

Reaction Mechanism:

$$\sum_{\ell=1}^{N} \nu'_{\ell j} \mathcal{S}_\ell \rightleftharpoons \sum_{k=1}^{N} \nu''_{kj} \mathcal{S}_k, \qquad j = 1, \ldots, M,$$

ν'_{ij}, ν''_{ij}: Stoichiometric coefficient of species $\mathcal{S}_i$ in j^{th} reaction
T, $\{C_i\}_{i=1}^{N}$, $\mathscr{R}$: temperature, and species concentrations, univ. gas constant

Source term:

$$\dot{\omega}_i = \sum_{j=1}^{M} (\nu''_{ij} - \nu'_{ij}) R_j, \; i = 1, \ldots, N$$

Reaction rates:

$$R_j = k_j(T) \left[\prod_{m=1}^{N} C_m^{\nu'_{mj}} - \frac{1}{K_j(T)} \prod_{n=1}^{N} C_n^{\nu''_{nj}} \right]$$

Rate coefficients e.g., Arrhenius:

$$k_j(T) = A_j T^{b_j} \exp\left(-\frac{E_{a,j}}{RT} \right)$$

Equilibrium constants:

$$K_j(T) = \exp\left[-\sum_{i=1}^{N} \frac{(\nu''_{ij} - \nu'_{ij}) \hat{g}_i^0(T)}{\mathscr{R} T} \right]$$

Gibbs functions:

$$\hat{g}_i^0 = \hat{h}_i(T) - T\, \hat{s}_i^0(T)$$

Species enthalpies & entropies (NASA Poly):

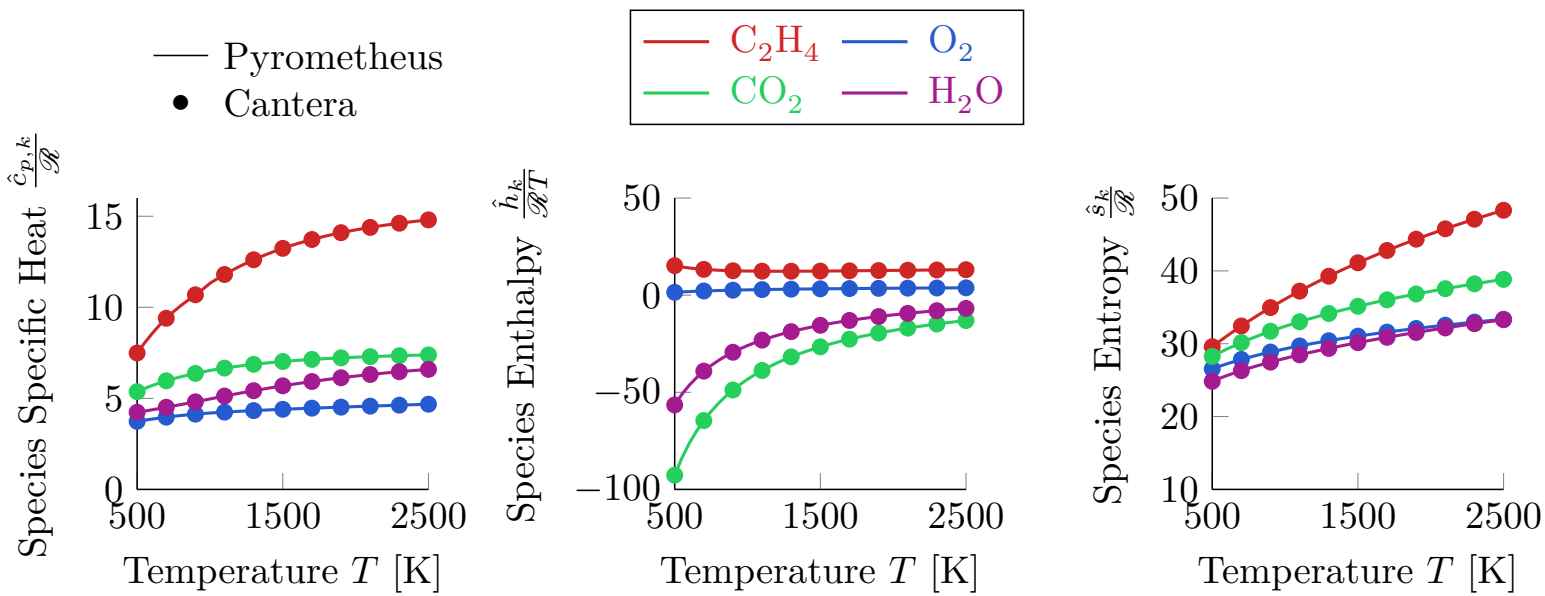
$$\frac{\hat{h}_i}{\mathscr{R} T} = \frac{\alpha_h}{T} + \sum_{m=1}^{5} \frac{\alpha_m}{m} T^{m-1}$$

$$\frac{\hat{s}_i^0}{\mathscr{R}} = \alpha_s + \alpha_h \log T + \sum_{m=2}^{5} \frac{\alpha_m}{m-1} T^m$$

Verification

- Verify against Cantera (itself tested upon installation)
- Illustration: 32-species ethylene mechanism Luo et al., *Combust. Flame* (2012)
- Full verification suite provided with distribution

Species Thermo:



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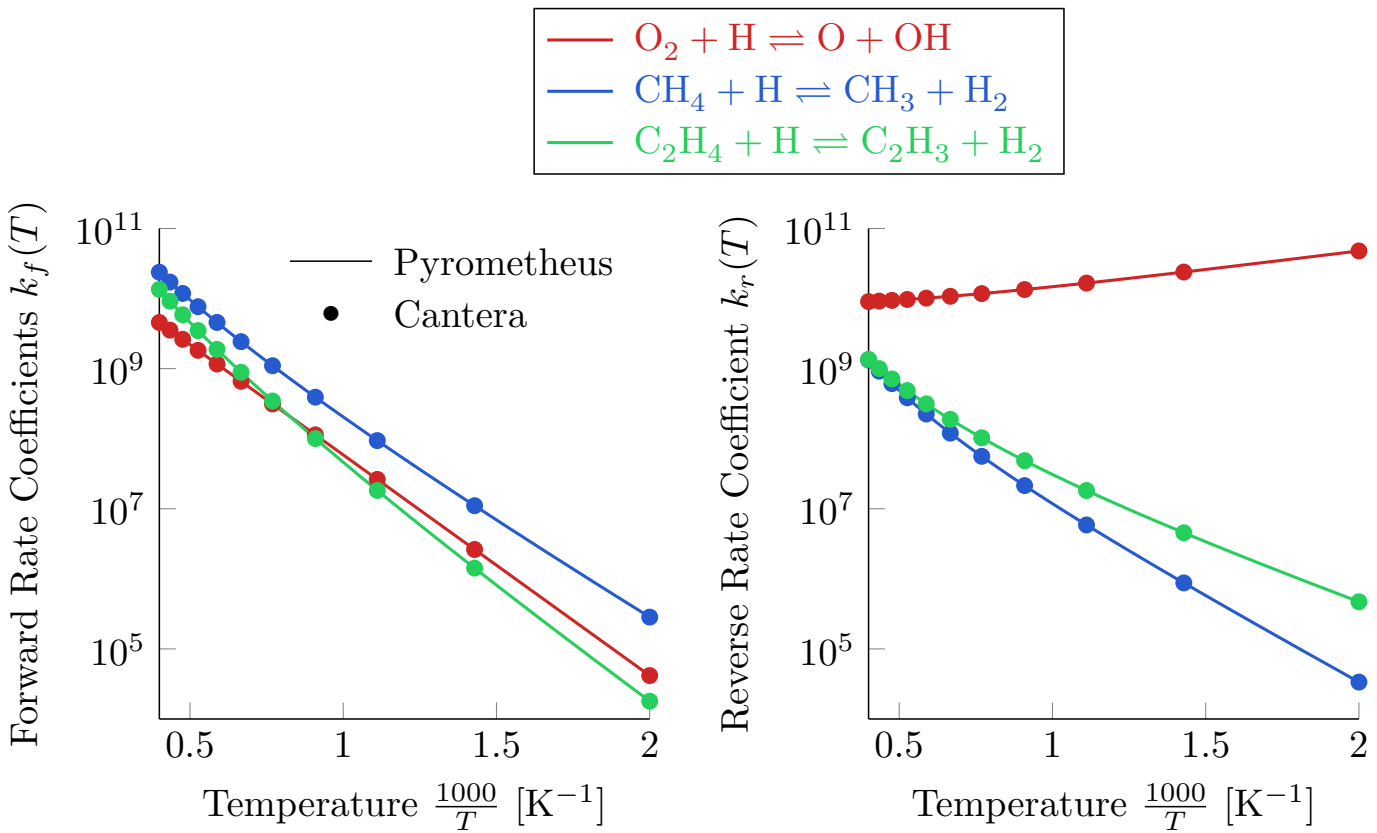
Kinetics:



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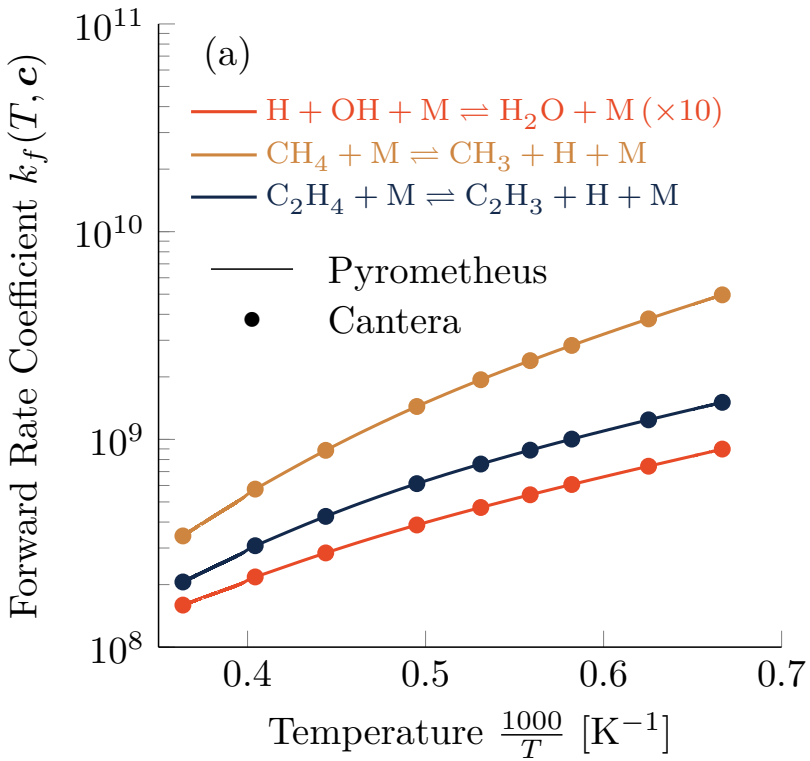

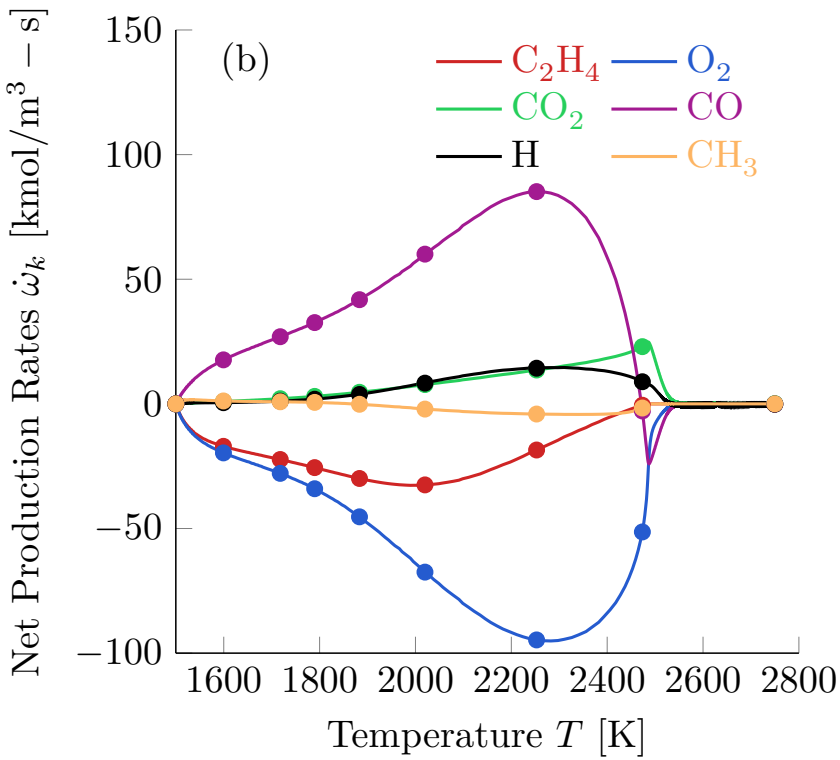

Summary & Discussion

- Package for thermochemistry-code generation
  - Uses Cantera to handle mechanism parameterization, and for verification
  - Based on **code template**, **automatic diff.** $\rightarrow$ facilitate extensions
- Freely-available: `https://github.com/ecisneros8/pyrometheus`
- Applications:
  - Reacting-flow simulations: *PlasCom2*, *MirgeCOM*
  - Mechanism design
  - Chemical model reduction and uncertainty quantification
    Cisneros–Garibay, Pantano & Freund, *Combust. Flame* (2019)
- **ACT II simulations**: faster with generated code than Cantera by factor of 1.7