DS289 NSDE Project - ODE Module
Group - 01
Chemical kinetics of hydrogen combustion

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Governing Equations

- Detailed chemical kinetics by Li[1] with 9 species and 21 reactions
- Species: $H_2, H, O_2, O, OH, HO_2, H_2O, H_2O_2, N_2$

$$\frac{dX_k}{dt} = \frac{W}{\rho}\dot{\omega}_k$$

where $k = 1, \ldots, N_s$

$\dot{\omega}_k$: net production rate of species k

[1] J. Li et al., *An updated comprehensive kinetic model of hydrogen combustion*, IJCK, 2004

Objectives

Assigned Objectives:

- Use of adaptive time stepping (explicit schemes)
- Effect of precision on capturing physics

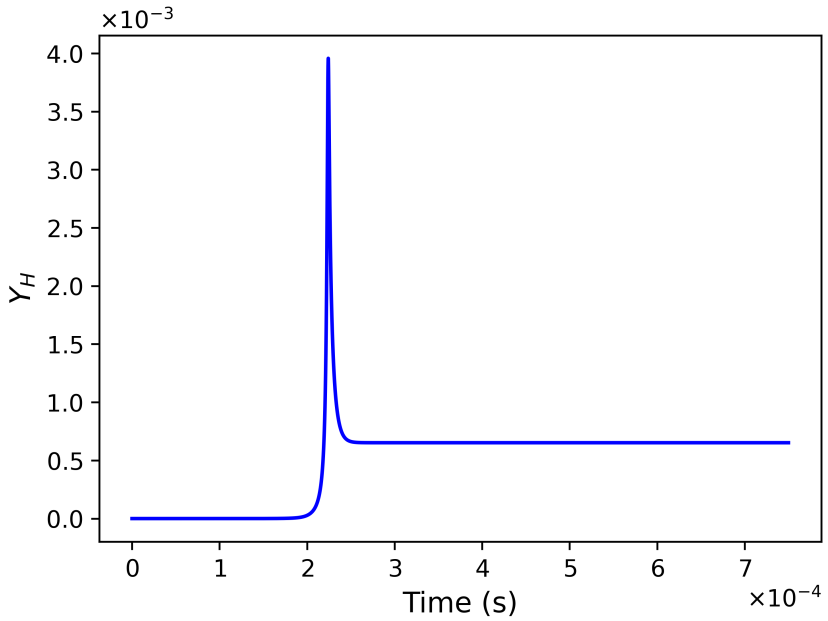
Exploratory Objectives:

- Studying effect of free parameters like tolerance
- Computational time vs Accuracy by varying the local error term using two different reference schemes
- Exploring implicit adaptive time stepping

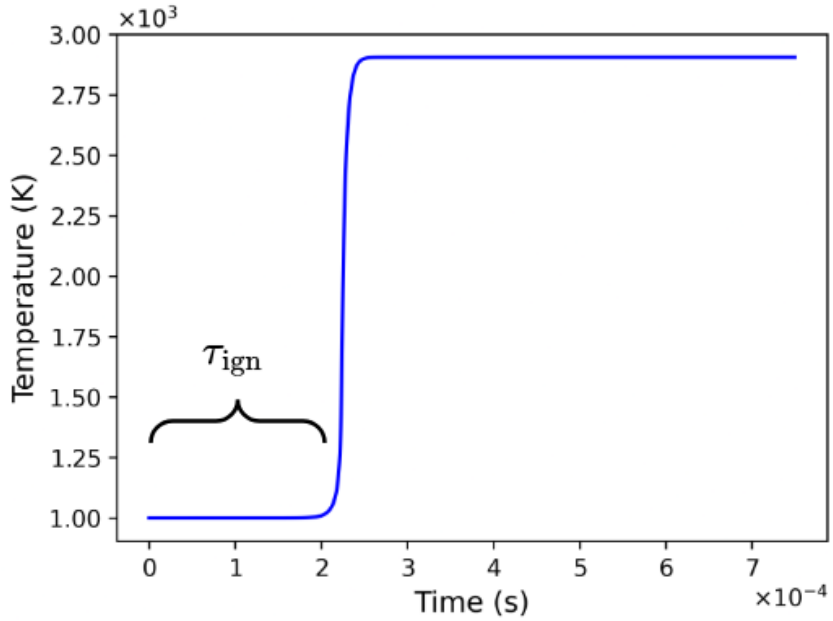
Methodology

- Determine Δt based on local error
- **Schemes**
  1. Main scheme: Lower order
  2. "Reference" scheme: Higher order
- **Performance / Analysis metrics**
  1. Δt_{min} for adaptive time stepping
  2. Use of Δt_{min} as constant time step (comparison metric)
  3. Effect of precision (double vs single vs half) on auto-ignition problem by comparing
     - 3.1 Ignition delay time
     - 3.2 Minor species evolution
- **Programming language**
  - Python (cantera library for chemical kinetics)
- **LLM tools**
  - ChatGPT, Copilot, Gemini, DeepSeek

Expected Outcomes



Sensitive quantities are expected to be affected by precision



Adaptive time stepping expected to be faster than traditional solver

Plots generated with cantera constant volume reactor