Motivation

- After 4000 centuries, combustion still accounts for about 75% of the total energy supplies, huge room for energy efficiency improvements.
- Advanced combustion strategies span broad combustion regimes and require detailed fuel chemistry modeling to capture both ignition development and pollutant formation.
- Detailed reaction mechanisms for combustion chemistry can involve thousands of species and reactions; their incorporation into CFD simulations requires extremely efficient and accurate numerics.

Chemical Kinetics in Engine CFD simulations

Incorporation of chemical kinetics in internal combustion engine simulations requires an efficient engineering approach to find the best compromise among:

1. Reaction mechanism dimensions
2. Computational complexity of the thermodynamic functions describing gas-phase equilibrium and kinetics
3. Computational cost for the integration of the ODE system arising from the mass and energy conservation equations
4. Number of integrations required by the size of the engine’s CFD mesh

The evolution of species due to chemical reactions in CFD codes such as KIVA is part of an operator-splitting procedure, where non-fluid-mechanics-related terms such as chemistry and spray/multiphase dynamics are computed separately from the fluid flow solution.

Proposed solution:

Development of an open-source computer code with state-of-the-art numerics for integrating chemical kinetics systems, “SpeedCHEM”

An analytical Jacobian formulation for chemical kinetics

- Kinetics of gas-phase mixtures are described by a reaction mechanism, i.e., a set of \( n_i \) arbitrary reactions involving \( n_{total} \) total species:
  \[
  \sum_i \nu_i M_i = \sum_j \sum_i \nu_{ij} M_j,
  \]
- Evolution of the species due to chemistry in every cell of the CFD mesh is described by mass and energy conservation for a constant-volume, adiabatic reacting system:
  \[
  \frac{dY_i}{dt} = \sum_j \nu_{ij} \frac{dY_j}{dt} - \sum_k \nu_{ki} \frac{dY_k}{dt} - \sum_l \nu_l Y_l + \sum_m \nu_m W_m,\]

Standard ODE solvers evaluate the system’s Jacobian matrix derivatives using finite differences, to integrate the ODEs using large integration time steps.

Chemistry Jacobian sparsity

- In reaction mechanisms, only basic species forming the O-H system typically interact with many other species; the Jacobian matrix can be very sparse:

While the finite difference method scales with \( O(n_i^3) \), the analytical formulation allows only the non-zero elements to be computed, using sparse matrix algebra to perform internal operation with maximum efficiency.

Optimal-degree interpolation

- Expensive thermodynamic functions and their derivative involve exponentials, powers, logarithms.
- Optimal-degree interpolation chooses the most adequate degree of interpolation among tabulated data points to guarantee the requested function accuracy (typically 10 digits).

Validation against engine simulations

- FIAT 1.3L HSD engine, KIVA, n-heptane mechanism:
  - Speed-up with \( n_i = 29 \) and \( n_{total} = 160 \)
  - Good agreement in local quantities
- Ford 0.83L single cylinder engine, KIVA-ERC, multiChem mechanism (128s, 503r):
  - Global agreement
- ERC n-heptane ignition, multiChem mechanism (128s, 503r):
  - Total CPU time reduction for chemistry of about 7 times

Conclusions and Future Work

- The developed code allows computational time savings of the order of one order of magnitude for chemical kinetics in practical engine simulations, allowing more detailed grids to be adopted.
- Real-world engine simulations yet involve much bigger CFD grids and thus require appropriate chemistry grouping techniques on the CFD domain.
- Solution of the linear system associated to the chemistry Jacobian is the most demanding task for most reaction mechanisms.
  - Study of ODE integration methods that require few Jacobian inversions
  - Study of analytical and numerical techniques to speed up the Jacobian inversion.

References


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