An Adaptive Chemistry Reduction Method for Detailed Modeling of Advanced Combustion Systems

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Combustion of hydrocarbon fuels provides 85% of energy in the modern United States [1]; the current energy crisis is in reality a fuel crisis. While renewable forms of energy are being pursued to supplement combustion-based sources, hydrocarbon fuels will remain the major component for the next few decades. Currently, there is high demand to improve the efficiency of combustion technology to decrease the amount of fuel consumed and to reduce the emissions in an effort to lessen the environmental impacts; in addition, fuel-flexible designs that can run on both conventional and alternative fuels are desired.

Computational modeling drives the design of new combustors and engines for aerospace, transportation, and energy applications, but accurate prediction of fuel consumption and pollutant emissions requires detailed chemical reaction mechanisms. Detailed mechanisms for liquid hydrocarbons of interest contain large numbers of species and reactions; for example, the reaction mechanisms for n-heptane (C_7H_{16}) and iso-octane (C_8H_{18}), important molecules for gasoline modeling, contain almost 1000 species and 8000 reactions [1]. Despite rapid advancements in computing power, it is generally formidable to integrate such detailed reaction mechanisms into large-scale computational simulations, in terms of CPU time and memory requirements. In addition, the wide range of time scales (from nanosecond to second) and the nonlinear coupling between species and reactions induces stiffness when governing equations are solved. Due to these computational demands, practical simulations using detailed chemistry are impossible with modern computational tools.

Mechanism reduction schemes are used to allow quantitative modeling while keeping realistic chemistry effects. Non-adaptive reduction methods perform reduction based on a predicted range of conditions typically by removing unimportant species and reactions and identifying the species with fast time scales for further reduction, providing a single global mechanism. Most adaptive reduction methods, on the other hand, operate by storing chemical kinetics information and retrieving necessary data during the simulation to avoid direct integration of the differential equations; newer techniques use multiple mechanisms reduced prior to the simulation at various points in the flow. I propose the development of a novel adaptive and computationally friendly reduction method that will remove unimportant species and reactions and eliminate stiffness on the fly. I aim to explore and develop new algorithms while using existing reduction methods as a basis.

Non-adaptive reduction methods attempt to provide a valid reduced mechanism by predicting the range of conditions (pressure, temperature, mixture composition) of interest in a simulation. However, the size of the reduced mechanism is limited by the locations in the computational domain that require more detailed chemistry due to high reaction activity. Many methods have been developed to reduce mechanisms in this manner, but the application of directed relation graph (DRG) theory [2] to describe reacting systems is particularly useful. In this method, nodes of the DRG represent species and directed edges represent dependences between species defined by normalized contributions to production rates. Important target species are defined (e.g. fuel, oxidizer, pollutants) and a graph-searching algorithm finds the dependent set of species needed to accurately predict the production rate of targets. Species with contributions below a certain error threshold are removed from the dependent set, and the final reduced mechanism contains the union of all dependent sets. The algorithm then eliminates reactions containing the unimportant species. For further elimination of stiffness in reaction

systems, the quasi steady state (QSS) and partial equilibrium (PE) assumptions are applied [3]. QSS species and PE reactions have very short time scales, causing stiffness, and the approximations seek to replace differential equations with algebraic relations to solve for species' concentrations. Computational singular perturbation (CSP) and intrinsic low dimensional manifold (ILDM) [3] are traditional methods for finding QSS species and PE reactions by separating fast and slow processes.

Adaptive reduction methods rely on different approaches to increase computational efficiency during simulations. Approaches such as *in situ* adaptive tabulation (ISAT) and artificial neural networks (ANN) [4] perform storage and retrieval of chemical kinetics information to save processing time. Newer adaptive methods such as genetic algorithms (GA) [5] and optimization-based approaches [6] use various techniques to provide multiple reduced mechanisms for use during the simulation at different points in the flow. Highly detailed chemistry needs to be considered at locations where reactions are actively occurring, while regions with little reactive activity can use extremely reduced mechanisms. However, all of the methods currently rely on predictive reduction, which will not provide the highest level of accuracy or reduction.

I propose the investigation of a new adaptive reduction methodology that will perform on the fly removal of species and reactions and elimination of stiffness. Identification and removal of unimportant species and reactions based on local conditions allows for the highest level of reduction and therefore the least computational demand, while keeping high accuracy. I will explore a novel algorithm for species and reaction removal using the DRG concept as a starting point; previous studies [2] based on DRG have shown it to be fast and reliable, suitable characteristics for on the fly application. Traditional methods for identifying QSS species and PE reactions such as CSP and ILDM are time-intensive [3] and therefore not well suited for on the fly stiffness removal; as such, I will also investigate efficient methods for identifying these fast processes.

The adaptive reduction method I have proposed can be directly applied to the simulation of combustion processes for aeropropulsion, transportation, and energy applications. The incorporation of detailed chemistry while providing speedy simulation will allow accurate modeling of fuel consumption and emissions and help drive the design of next-generation engines and combustors. A method based on graph theory could be also be applied to the modeling of other complex systems; broader applications consist of food web/ecosystem modeling, disease spreading modeling, climate modeling, and biological systems modeling. Also, a new methodology developed to perform mechanism reduction could also be used to mine important information about complex systems. For example, a CSP-based method was used to gather information about explosive processes in a simulation of a hydrogen/air turbulent lifted jet flame [7]- the new method I propose could be used similarly for data mining.

References

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