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Improved Chemical Kinetics and Algorithms for More Accurate, Faster Simulations

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I.9 Improved Chemical Kinetics and Algorithms for More Accurate, Faster Simulations (Lawrence Livermore National Laboratory)

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Project Introduction

Internal combustion engine design is increasingly driven by computational models used to predict change in performance due to change of design. The design process previously depended on limited intuition and expensive and time-consuming physical testing. Improved model capabilities shorten design cycles and enable the production of cleaner and more efficient engines. This project focuses on advancing the state of the art in internal combustion engine simulations. The overarching goal is to enable predictive models and reduced time to solution for simulations that impact combustion engine design.

Objectives

Overall Objectives

- Advance state of the art in engine simulation through the development of fast and accurate models.
- Work with industry partners to prove capability and impact of combustion software.

Fiscal Year 2021 Objectives

- Create new Zero-Order Reaction Kinetics (Zero-RK) applications for perfectly stirred reactors (PSR) and counterflow laminar flames.
- Apply Zero-RK solvers for reaction model reduction and tuning.
- Improve Zero-RK computational fluid dynamics (CFD) interface and link to DOE Exascale codes Nek5000 and Pele.

Approach

This project is part of the Partnership to Advance Combustion Engines (PACE) program. PACE's primary goals are to improve fundamental knowledge; create faster, more accurate design tools; and produce data for rigorous model development and validation to enable market-competitive powertrain solutions powered by combustion. This project leverages and extends previous DOE investment in the Zero-RK software for fast solution of detailed chemical kinetics problems. The focus of this project in fiscal year (FY) 2021 is on three areas: (1) apply core Zero-RK algorithms to new problem domains of counterflow laminar flames and PSR, (2) enable use of more accurate chemistry in CFD applications via mechanism reduction and tuning with Zero-RK and high-performance computing (HPC), and (3) improve the Zero-RK CFD plugin and create preliminary interfaces to Nek5000 and Pele reacting flow codes.

Results

Zero-RK for perfectly stirred reactors and counterflow flames

The core ideas that have enabled dramatic acceleration of detailed chemical kinetics simulations embodied in the Zero-RK suite of tools have been extended to two new application domains. The first domain, known as the PSR model, closely approximates experiments using an apparatus known as a jet-stirred reactor. Here, input streams of fuel and oxidizer are rapidly mixed with controlled initial temperature, pressure, composition, inflow rate, and residence time, and the outflow rate, composition, and temperature are measured or modelled. Comparisons between model and experiment can provide important insight into oxidation and pyrolysis processes for transportation fuels and can result in strong constraints on kinetic model performance. The available methods for solution of the PSR model equations were hindering kinetic model development due to the cost in computational time. By applying previously developed expertise in sparse, preconditioned methods and parallelization on HPC platforms, this bottleneck in the model development process has been substantially widened. Single reactor simulations are accelerated by more than 10 times for large (>1,000 species) kinetic models, and hundreds or thousands of simulations (e.g., to study sensitivity to the fixed conditions) can be run simultaneously across the available resources in an HPC cluster.

The second new application is for the one-dimensional laminar flame with counterflow geometry. This is a natural extension of methods reported previously for premixed and flamelet configurations of laminar flames. The counterflow flame is very similar to the flamelet model, with the difference that the counterflow equations are formulated in physical space as opposed to mixture fraction space. The flamelet solvers are very useful for generating lookup tables to be used in certain non-premixed CFD combustion models but do not allow for direct comparison to experimental measurements. The new Zero-RK solver for counterflow laminar flames scales linearly in solution time with respect to the number of species modeled, resulting in a solution time that is 100 times faster than that achieved by previously available methods for a reaction model containing ~3,000 species. Further acceleration is also possible in the Zero-RK solver by solving across multiple central processing unit cores. The new solver was applied to the computation of extinction strain rates of (1) the PACE-20 surrogate with a detailed model (>4,000 species) and (2) an ethanol–toluene–primary reference fuel (ETPRF) surrogate with two smaller models (98 and 246 species, respectively) (see Figure I.9.1), and the results were compared. Such comparisons were previously unattainable, as extinction strain rate calculations with the detailed model were infeasible with previous solvers. The comparison validates the use of the reduced models in direct numerical simulation of flame kernel growth by Chen and Soriano at Sandia National Laboratories as part of the PACE effort.

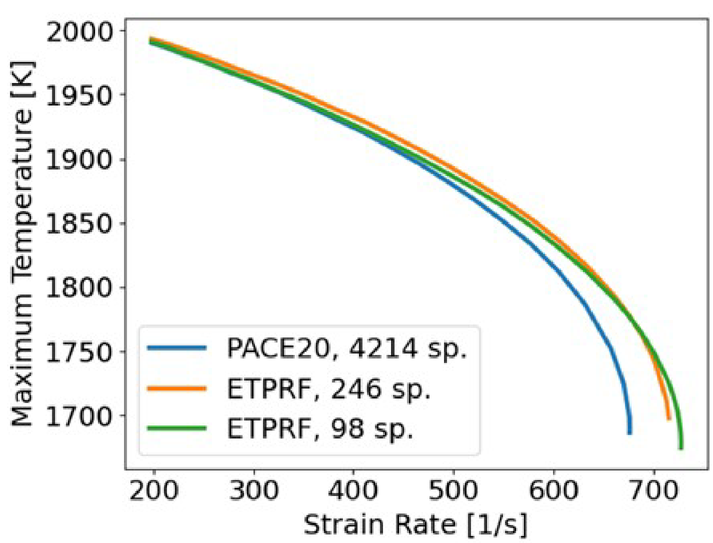

Figure I.9.1 Extinction strain rate calculations for three different models, computed with the new Zero-RK solver for counterflow laminar flames

Improved kinetic model performance in CFD via model reduction and tuning

Despite the continued acceleration of detailed kinetic model solutions through work in this project and elsewhere, reaction models containing thousands of species continue to be infeasible in most engine CFD simulations. In FY 2021, a new effort was made to improve chemical fidelity in practical engine simulations via the creation and tuning of compact reaction models that closely match the predictions of the full detailed models. Two development areas were the focus: (1) accelerating the Global Pathway Selection (GPS) methodology for reaction model reduction [1] using HPC clusters and faster model calculations with Zero-RK and (2) a new toolkit for reaction rate parameter tuning to reduce discrepancies between predictions of the full and reduced kinetic models. The GPS method for model reduction computes global fluxes of atoms from fuel to combustion products to identify hub species and dominant reaction pathways and thereby mark unimportant species and reactions, which can be eliminated with little impact on predictions for a given set of reacting conditions. Reduced models created with the GPS method have been shown to be more accurate with similar species counts than those generated with competing methods (including Path Flux Analysis and Direct Relation Graph with Error Propagation). These qualities make GPS attractive for reducing the fully detailed gasoline surrogate reaction model containing more than 4,000 species to more tractable size(s) given a specified surrogate and engine operating conditions. However, the implementation of the method made available by the original authors [2] was too slow to be practical for such large models, as it was estimated that performing the calculations necessary would take multiple weeks. In FY 2021, this project has accelerated the method by using Zero-RK solvers as the “back-end” for the ignition delay and PSR calculations that are used to generate the atomic flux graphs and make benchmark comparisons between the reduced and detailed models. In addition, the code was modified such that reactor calculations were computed in parallel across all available central processing unit cores in an HPC cluster node. Depending on the computer hardware used and the model being reduced, the results of these acceleration efforts can reduce the necessary wall time by a factor over 300, and the full gasoline surrogate reaction model can be reduced to multiple levels of fidelity in less than one hour.

The reaction model reduction process creates a tradeoff between model fidelity and cost, with smaller models trending cheaper and less accurate. Generally, the engine modeler is not fully satisfied with either fidelity or cost, and the selection of model is made by choosing the largest “affordable” model and accepting the associated (lack of) fidelity to the detailed model. This can lead to significant questions in terms of the resulting simulations, where any disagreement with experiment may be blamed on deficiencies in the kinetic model. To improve this situation, a new toolkit for reduced model tuning was created using Zero-RK as its core, and HPC clusters and existing optimization methods were leveraged to reduce discrepancies between the reduced and detailed models. An objective function that quantifies the deviation between the reduced and detailed models in terms of reaction rate parameters is defined, and then a search is conducted to minimize the objective function by varying reaction rate parameters within defined constraints. Key enablers of this process for the large parameter space involved are the fast model simulations of Zero-RK and the HPC clusters of the National Laboratories. Following the creation of these tools, many model-tuning campaigns were conducted in FY 2021, including multiple gasoline and diesel surrogate reaction models. Typically, the tuning involves the evaluation of tens of thousands of models at hundreds or thousands of conditions, resulting in tens of millions of individual reactor simulations. The resulting tuned models significantly decreased maximum and average reduced-model errors (with respect to the full model). In the case of a 315-species reduced model for the PACE-20 surrogate, maximum error was reduced from over 100% to less than 10% over a wide range of temperature, pressure, and equivalence ratio values (see Figure I.9.2).

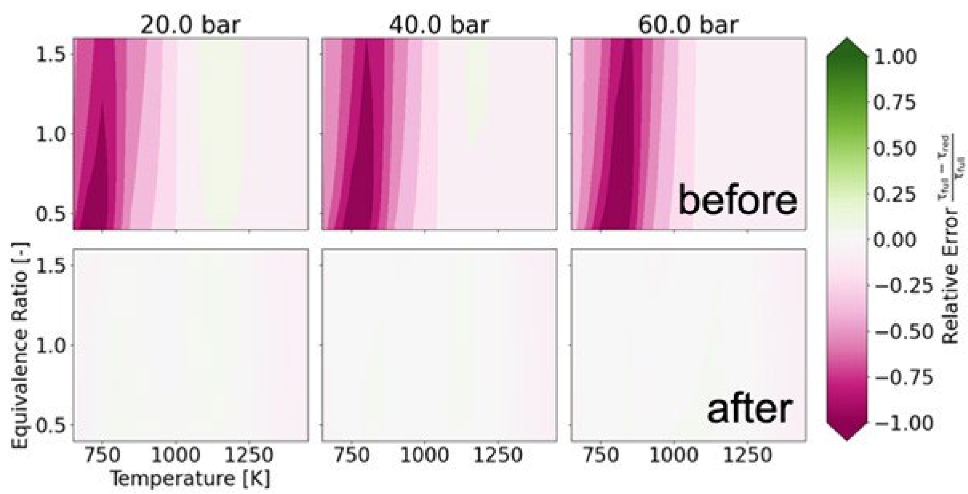

Figure I.9.2 Comparison of reduced PACE-20 surrogate reaction model predictions of ignition delay time to those of the detailed model. Top row is prior to reaction rate parameter tuning and bottom row is after tuning.

Zero-RK CFD interface improvements and linking to Nek5000 and Pele codes

Many reacting flow CFD codes implement species evolution by chemical reactions through operator splitting techniques. A CFD plugin in the Zero-RK software repository has been developed to enable easy incorporation of the kinetic solvers into many different CFD applications. In FY 2021, this interface has been improved, and new features have been added. The interface was made to be compatible with multi-threaded applications, and the method for setting options was made more convenient. In addition, prototype implementations for using Zero-RK as the kinetic engine in the Nek5000 [3] and Pele [4] codes have been developed. Both codes are part of DOE's Exascale Computing Project and have attractive properties for simulating reacting flows on future generations of world-leading computing platforms. The incorporation of Zero-RK into these codes can enable the highest impact in kinetic model fidelity to study combustion phenomena at highly resolved scales. For a closed reactor simulation in the Nek5000 code, the Zero-RK solver significantly reduces the chemistry time over the previously implemented solver, with approximately 5x reduction in time for the 315-species reaction model for the PACE-20 surrogate (see Figure I.9.3).

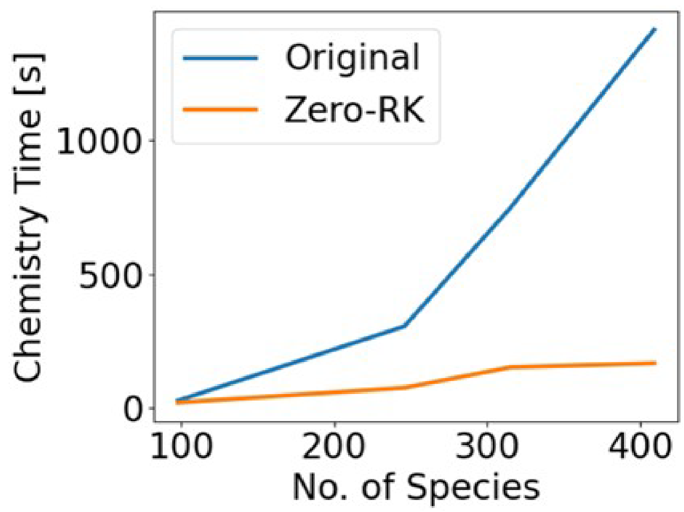

Figure I.9.3 Comparison of chemistry time for Nek5000 simulation of closed, homogeneous reactor using the original solver and Zero-RK. Shorter times are better.

Conclusions

- Development of chemical kinetic models has been accelerated by the development of new Zero-RK applications for PSR and counterflow laminar flames.
- Significant improvements in the compactness and accuracy of reaction models for CFD simulations have been made with new Zero-RK-based reduction and tuning methods. The wall-time cost for model reduction has been reduced by as much as a factor of 300.

- The Zero-RK CFD interface has been improved, and prototype connections to DOE Exascale codes Nek5000 and Pele have been created.

Key Publications

1. Pal, P., K. Kalvakala, Y. Wu, M. McNenly, S. Lapointe, R. Whitesides, T. Lu, S.K. Aggarwal, and S. Som. 2020. "Numerical Investigation of a Central Fuel Property Hypothesis Under Boosted Spark-Ignition Conditions." *Journal of Energy Resources Technology* 143. https://doi.org/10.1115/1.4048995.

2. Yue, Z., C. Xu, S. Som, C.S. Sluder, K.D. Edwards, R.A. Whitesides, and M.J. McNenly. 2021. "A Transported Livengood–Wu Integral Model for Knock Prediction in Computational Fluid Dynamics Simulation." *Journal of Engineering for Gas Turbines and Power* 143. https://doi.org/10.1115/1.4050583.

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1. Gao, X., S. Yang, and W. Sun. 2016. "A Global Pathway Selection Algorithm for the Reduction of Detailed Chemical Kinetic Mechanisms." *Combustion and Flame* 167: 238–247. https://doi.org/10.1016/j.combustflame.2016.02.007.

2. https://github.com/golsun/GPS

3. https://nek5000.mcs.anl.gov

4. https://amrex-combustion.github.io/PeleLM/overview.html

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