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Improving the efficiency of sensitivity analysis algorithms for combustion problems through reformulation and adjoint methods

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Assessing the influence of input parameters on the prediction of a certain set of quantities of interest (QoIs) is a task of key relevance for both the development and optimization of chemical kinetic models. To this end, sensitivity analysis has been widely used for the identification of critical parameters that require further investigation and refinement [1]. Extinction strain rates and ignition delay times are among the fundamental combustion properties frequently used as validation targets in the development of chemical kinetic models. Ignition delay times and extinction strain rates are computed from the solutions of systems of differential equations that approximate the experimental apparatus as closed adiabatic homogeneous systems and quasi-one-dimensional counterflow flames, respectively. Even for such simple, idealized configurations, the disparity between the often large number of input parameters and the limited number of QoIs makes adjoint methods a useful approach for enhancing the efficiency of sensitivity analysis algorithms. However, the application of adjoint methods to these QoIs is not straightforward. This study demonstrates how they can be applied effectively. For both quantities, the application of adjoint sensitivity analysis builds upon existing solutions and analysis methods that exhibit a crucial feature: Through a coordinate transformation [2, 3], the set of equations describing the idealized configurations can be reformulated to explicitly express the QoI as a function of the system output. For large systems, the proposed combination of methods offers improved time complexity compared to conventional sensitivity analysis approaches, and computational costs are analyzed for our implementation. The proposed methods are validated through comparisons with results from conventional sensitivity analysis techniques, demonstrating good agreement between the different methods. From a practical perspective, the measurements of the execution time demonstrate the method's ability to greatly reduce computational costs, making it a valuable tool for developing chemical kinetic models, especially for large mechanisms where traditional sensitivity analyses may become computationally prohibitive.

References

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