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Language and Library Agnostic Computational Representations of Combustion Thermochemistry for Automatic Differentiation and GPU Execution

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To conduct simulations of reacting flows, a computational representation of the thermochemistry is needed. Typically, the representation is designed to satisfy an application (e.g., sensitivity analysis) and target specific computing hardware such as accelerators, but these considerations constrain its properties in conflicting ways: from different data layouts to compile-time order. To address this challenge, we abstract the thermochemistry to a symbolic level, where conflicts across applications and hardware vanish. The representation is transformed through code generation to enable automatic differentiation and performant GPU execution. Crucially, our design is language and library agnostic. As such, it is compatible with existing high-performance flow solvers and it can represent multiple kinetics, such as plasma-coupled combustion, with mechanistic data taken from various sources. The Pyrometheus suite implements our proposed approach. We demonstrate its capabilities, quantify performance for various domain kinetics, and demonstrate how it enables simulations at scale with the state-of-the-art flow solver MFC.