

A Multi-Resolution Sparse Hash Table Strategy for Efficient Numerical Integration of Stiff Combustion Systems using the G-Scheme

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The G-Scheme [1] is an explicit integration method designed to address the multi-scale stiffness challenges inherent in systems of ordinary and partial differential equations, particularly those encountered in combustion modeling. Its efficiency hinges on minimizing the computational cost of evaluating the eigensystem of the Jacobian matrix of the vector field that defines the system dynamics. Inspired by the recent work of S. Rao et al. [2], which introduced a dynamic tabulation technique for Jacobian matrices in implicit stiff solvers, this work introduces a novel multi-resolution hash table strategy to accelerate the G-Scheme by reusing precomputed eigensystems. The hash table enables efficient storage and retrieval of the eigensystem, either from a predefined training dataset or dynamically during integration. Key features of this approach include: (i) the look-up table remains one-dimensional, regardless of the system's state dimension; (ii) the retrieval cost of the kernel set (eigensystem of the Jacobian matrix) is independent of the state dimension, ensuring high computational efficiency; (iii) the multi-resolution hash function enables a coarse-to-fine granularity for retrieval, effectively minimizing the table size while maximizing the likelihood of successful retrieval.

The sensitivity of this method's performance to the system dimension, quantified by the number of species in the kinetic mechanism, was evaluated using a series of skeletal mechanisms for n-heptane/air, generated with PyCSP [3], ranging from 88 to 376 species.

This approach demonstrates a ten- to twenty-fold speedup for systems with varying dimensionalities and maintains robustness by ensuring accuracy even when retrieving approximate eigensystems. The methodology is validated through simulations of autoignition processes using skeletal mechanisms of varying complexity, showcasing its potential for large-scale turbulent reacting flow simulations. By combining the G-Scheme with the proposed hash table and skeletal mechanism simplification, computational efficiency is enhanced, promising a paradigm shift in handling stiff reactive systems.

References

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