Analysis Meets Data: Efficient Implementation and Optimized Time Integration Methods with Automatic Step Size Control for Compressible Computational Fluid Dynamics

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Modern entropy-dissipative numerical methods for computational fluid dynamics (CFD) increase the robustness compared to standard schemes significantly. At the same time, their implementation becomes more involved and it is more difficult to achieve good performance. We briefly mention techniques for the efficient implementation of these methods and focus on the analysis and development of adaptive time integration methods for high-order entropy-stable spatial discretizations. We develop error-control based time integration algorithms and show that they are efficient and robust in both the accuracy-limited and stability-limited regime for CFD applications using discontinuous spectral element discretizations. We demonstrate the importance of choosing adequate controller parameters and provide a means to obtain these in practice by combining analysis with a data-driven approach, which we apply to design new controllers for existing methods and for some new embedded Runge-Kutta pairs. We compare a wide range of error-control-based methods, along with the common approach in which step size control is based on the Courant-Friedrichs-Lewy (CFL) number. The new optimized methods give improved performance and naturally adopt a step size close to the maximum stable CFL number at loose tolerances, while additionally providing control of the temporal error at tighter tolerances. The numerical examples include challenging industrial CFD applications.