

Improving Dynamical Core Scalability, Accuracy, and Limiting Flexibility with Differential Transforms (DTs) and the ADER-DT Time Discretization

Matthew R. Norman
Oak Ridge National Laboratory

In the current explosion of on-node and off-node parallelism, the cost of data transfer is only increasing relative to the cost of computation. We need to explore new algorithms that better exploit new machines without sacrificing accuracy, robustness, and time-to-solution. The Arbitrary DERivatives using Differential Transforms (ADERDT) time discretization appears to balance the many constraints of effective scientific computing well, while providing distinct advantages for large parallel computers. Multi-stage time integrators require many stages of communication within a time step, and they become difficult to formulate for non-linear PDEs past fourth-order accuracy. ADERDT provides non-linear, arbitrarily high-order-accurate time integration in a single stage, using the linear maximum stable CFL limit of $1/D$ where D is the number of spatial dimensions. This reduces the frequency of parallel communication and eases the path forward to very high-order-accurate solvers in space and time. ADER methods maintain the non-oscillatory properties of underlying spatial reconstructions, further simplifying the path to *limited* very high-order-accurate solvers. Using WENO reconstruction, in fact, no additional parallel transfers are required to maintain stability or even essential shape preservation in the presence of shocks and discontinuities. This is in contrast to hyperdiffusive and Flux Corrected Transport (FCT) approaches to stability and shape preservation, which do require additional parallel data transfers for limiting, and often many additional transfers. Note that using FCT only for positivity preservation does not incur additional parallel data transfers, and this approach is utilized here to maintain strict positivity. ADERDT is also economical because we only evolve a half-tensor of space-time derivatives and all space-time quadrature is removed in lieu of analytical space-time integration.

The Finite-Volume (FV) and Multi-Moment Finite-Volume (MMFV) frameworks are also advantageous in conjunction with ADER-DT because the time step does not change, no matter how high-order-accurate the method is. In contrast, most Galerkin time steps decrease nearly quadratically with increasing order. This rewards very high-order-accuracy, particularly because data is reused well on-node and because the time step remains large. The MMFV framework can utilize Hermite WENO (HWENO) limiting, which uses derivatives as well as values of the fluid state. A big advantage of using MMFV schemes is that the effective grid spacing of the reconstruction is reduced, greatly improving accuracy compared to traditional FV methods. A sixth-order-accurate genuinely multi-dimensional HWENO+MMFV+ADERDT method will demonstrate this capability.

Often, WENO and HWENO limiting are considered too expensive for practical use. However, we demonstrate that with ADERDT at even fifth-order and seventh-order accuracies with genuine multi-dimensionality, the cost of WENO can be as little as 40% overhead or less. The overhead becomes even smaller at higher-order accuracies and with more spatial dimensions. This is cheaper than the overhead of many hyperdiffusive limiters, it doesn't require additional data transfers, and it can be made shape preserving to magnitudes of 10^{-3} or less relative to the size of the discontinuity in question. This is because we only need to limit once per time step with ADERDT, and weights can be reused in 1-D sweeps for genuinely multi-dimensional reconstruction. The WENO and HWENO approaches also come with two continuous and tunable parameters that allow a very wide range of flexibility in how accurate or how limited the user wants the solution to be for their application. This flexibility comes at minimal additional computational overhead (less than 5%).

These ADERDT methods, WENO and HWENO limiting, and approaches to genuine multi-dimensionality will be described in detail. Then, these approaches will be evaluated in terms of accuracy, runtime, parallel transfers, and limiting with respect to Cartesian, 2-D transport and Cartesian, 3-D, non-linear, compressible Euler simulation.