Derivative Calculations for an Euler/Roe Dissipation Scheme

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We describe our efforts to compute exact derivatives for the finite-volume Euler equations with Roe dissipation in preparation to eventually perform shape optimization. Exact forward and adjoint Jacobian-vector products for the first- and second-order reconstructions are derived through the use of hybrid symbolic and automatic-differentiation (AD) methods where much of the Jacobian constructions are derived symbolically. The exception is the complex and expensive Roe dissipation term which was non-symbolic differentiated using finite differencing, complex step and forward AD methods. Efforts to derive and implement symbolic derivatives for the dissipation term were much slower in comparison to automatic differentiated derivatives and resulted in slower code. AD was also compared to symbolic differentiation for the second-order reconstruction and flux-limiter computations. Various schemes that trade storage for speed are investigated, including 1) matrix-free (i.e. no storage) methods using only edge-based loops, 2) edge-based loops using increasing levels of storage and 3) node-based sparse matrix assemblies requiring sophisticated linear algebra capabilities. Although these derivatives are intended for adjoint sensitivity calculations in shape optimization, they have proven to be also computationally advantages in a forward Newton-based equation solver. The use of AD and other exact approaches allow for solving the problem to near machine precision and thereby resulting in higher convergence rates compared to finite-difference methods. The impact on a production Sandia compressible fluid flow code is described.