Efficient goal-oriented global error estimation for BDF-type methods

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The backward differentiation formulae (BDF) method is a state-of-the-art method to solve large-scale, highly nonlinear and stiff initial value problems (IVPs) in ordinary differential equations, as they may arise from solving instationary partial differential equations by the method of lines. So far, efficient realizations control only local error quantities, but in fact the global error of the numerical approximation should be controlled. To this end, the global error has to be estimated, which requires adjoint information. This information can be obtained either by solving the adjoint IVP or from adjoint internal numerical differentiation (IND) of the integration scheme. The latter discrete approach is highly desirable in terms of computational complexity and discrete consistency. However, for multistep BDF methods there is no apparent relation between the values from adjoint IND and the solution of the adjoint IVP. This contribution sheds light on this relation and shows how the global error is efficiently and accurately estimated with the help of discrete IND adjoints.

First, we present our recently developed functional-analytic framework based on the duality pairing of continuous functions and normalized functions of bounded variation. We show the equivalence of BDF schemes and their adjoint IND schemes to Petrov-Galerkin finite element (FE) discretizations.

With this FE formulation, we derive a novel goal-oriented global error estimator for BDF methods which uses, for the first time in the context of multistep methods, discrete IND adjoints. Our derivation makes use of the dual weighted residual methodology. We prove asymptotic correctness of the novel error estimator for constant BDF methods and confirm this numerically. Moreover, we give promising numerical results for the estimation accuracy in variable BDF-type methods with changing orders and stepsizes as used in practice. Finally, we give strong evidence that our estimator outperforms another estimator based on the solution of the adjoint IVP in terms of both efficiency and accuracy. The presented error estimation approach opens the way for the development of variable BDF-type methods with goal-oriented global error control.