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Efficient goal-oriented global error estimators for BDF methods using discrete adjoints

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Abstract

In this paper we develop new goal-oriented global error estimators for variable multistep backward differentiation formulae (BDF) methods. These estimators use, for the first time in the context of multistep methods, discrete adjoints computed by adjoint differentiation of the nominal integration scheme. The derivation is based on the recently developed Petrov-Galerkin finite element formulation of BDF methods and their discrete adjoint schemes and makes use of the dual weighted residual methodology. Defect integrals or local truncation errors are used as local error quantities. We prove the asymptotic correctness and optimal convergence of the novel estimators for the one-step BDF method. For multistep BDF methods using a selfstarting procedure we show that the estimator with defect integrals converges but suboptimal and that its effectivity index converges to an offset value. On the other hand, the estimator with local truncation errors is again asymptotically correct and of optimal order. We confirm these results numerically. With a real-world example from chemical engineering, we give promising numerical results for the estimation accuracy in variable BDF-type methods with changing orders and stepsizes. Finally, we give a first use of the novel estimators for goal-oriented global error control of a challenging stiff test problem.

Keywords: BDF methods, discrete adjoints, Petrov-Galerkin discretization, global error estimation, dual weighted residual methodology.
2000 MSC: 65L05, 65L06, 65L60, 65L20, 65L70

1. Introduction

In this paper we numerically solve initial value problems (IVPs) in ordinary differential equations (ODEs) with sufficiently smooth right hand side $\boldsymbol{f}\colon [t_\mathrm{s}, t_\mathrm{f}] \times \mathbb{R}^d \to \mathbb{R}^d$

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