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An equation-based algorithmic differentiation technique for differential algebraic equations

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Abstract

This work presents a novel Algorithmic Differentiation (AD) approach for sensitivity analysis of Differential Algebraic Equation systems (DAEs). For the first time, the algorithmic specification of a computationally memory-efficient equation-based AD technique is presented. This approach is mainly targeting equation-based modeling and simulation tools capable of constructing high-level models using state of the art object-oriented modeling principles. The approach is based on fundamental tree algorithms that are (even manually) applicable on implicit equation systems of long formulas, the main building blocks of model components. By applying the presented forward differentiation scheme on a given DAE, efficient representation of Sensitivity Equation Systems (SESs) is computed. Parameter sensitivities are evaluated by direct integration of the derived SESs. To overcome the runtime performance drawback of direct numerical integration, a system decomposition approach is recommended. It is shown that the runtime performance using modern variable-step integration methods tends to achieve the expected theoretical complexity of the forward differentiation scheme under few realistic assumptions.

Keywords: algorithmic differentiation, differential algebraic equations, sensitivity analysis, tree algorithms, equation-based languages, Modelica

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