Comments on

CVODES: An ODE solver with sensitivity analysis capabilities

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1 Summary of the contents

The paper describes the software tool CVODES as a multistep ODE solver with comprehensive capabilities for sensitivity analysis. The ODE integration itself is performed by a BDF method for stiff systems or an Adams-Moulton formula for non-stiff systems. Arising linear systems can be solved by either a dense direct method, a banded direct method or an iterative Krylov subspace method.

The sensitivity analysis features of CVODES comprise forward sensitivity analysis by the simultaneous corrector method as described in [5], or two versions of the staggered corrector method as introduced in [1]. The right-hand sides of the arising sensitivity systems can be currently obtained through analytical user input, finite differences or directional derivatives, and an automatic differentiation option is envisaged in the conclusion section.

Furthermore, CVODES also allows to compute sensitivities via adjoint sensitivity analysis by implementing a check-pointing strategy.

In Section 3, the paper describes details of the software setup and code organization, as part of a larger family of solvers, the SUNDIALS package. Section 4 of the paper is concerned with giving a detailed overview about the usage of the tool.

2 Comments on the contents and assessment of relevance for a publication in TOMS

The features of the tool mentioned in this paper are apparently not new. A BDF solver for DAE systems with dense direct, banded direct or Krylov subspace based linear solvers is available as the well-established code DDASPK

[2]. DDASPK also contains the three common methods for forward sensitivity analysis, i.e. the staggered direct, the simultaneous corrector and the staggered corrector method. The code DSL48S [1] contains a BDF solver for DAE systems with the staggered corrector sensitivity method using the sparse direct linear algebra solver MA48. The statement in Section 2.2.1 of the paper, that the staggered direct method is always unattractive, is not correct. As shown in [4], it can outperform the other methods in case that $N_s \gg N$. In contrast to CVODES, DDASPK already contains automatic differentiation capabilities according to [2].

Regarding the adjoint approach, the concepts and implementation in this paper appear to be close to what has been reported in [3]. The checkpointing has already been described in that reference. DDASPKADJOINT additionally contains optional automatic differentiation facilities for obtaining the required derivative information.

According to the paper, the key benefit of CVODES appears to be the modular software implementation, which collects all subelements for ODE integration and sensitivity evaluation under one common roof. The modular approach allows an easy exchange of low-level tools such as linear solvers etc.

The editorial charter of TOMS states that "the purpose of a TOMS communication is the presentation of the results of novel research and development efforts in support of significant mathematical computer application". Taking the findings above into account, it is rarely possible to accept the paper as "novel research". An acceptable paper should also contain "a demonstration of superiority compared to alternative approaches", typically carried out by an experimental evaluation of computer implementations. The paper at hand is completely lacking this issue. Basically it is a description of a new software implementation of well-known numerical concepts.

3 Recommendation

In line with the argumentation above we would recommend to reject the paper in the current form.

References

[1] W. Feehery, J. Tolsma, and P.I. Barton. Efficient sensitivity analysis of large–scale differential–algebraic systems. *Appl. Numer. Math.*, 25:41–54, 1997.

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[3] S. Li and L. Petzold. Description of DASPKADJOINT: An Adjoint Sensitivity Solver for Differential-Algebraic Equations. Technical report, Department of Computer Science, University of California Santa Barbara, USA, 2002.

[4] S. Li, L. Petzold, and W. Zhu. Sensitivity analysis of differential-algebraic equations: A comparison of methods on a special problem. *Appl. Numer. Math.*, 32:161–174, 2000.

[5] T. Maly and L. Petzold. Numerical methods and software for sensitivity analysis of differential-algebraic systems. *Appl. Numer. Math.*, 20, 1996.