Positivity preserving simulation of Differential-Algebraic Equations

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Positive dynamical systems arise in every application in which the considered variables represent a material quantity that does not take negative values, like e.g. the concentration of chemical and biological species or the amount of goods and individuals in economic and social sciences. Beside positivity, the dynamics are often subject to constraints resulting from limitation of resources, conservation or balance laws, which extend the differential system by additional algebraic equations. In order to obtain a physically meaningful simulation of such processes, both properties, the positivity and the constraints, should be reflected in the numerical solution. In this talk, we discuss these issues for linear time-varying systems, as they arise for example in the linearization of non-linear systems in chemical reaction kinetics or process engineering.
As for linear time-invariant systems [1], we pursue a projection approach based on generalized inverses that admits to separate the differential and algebraic components without changing coordinates.
We first consider index-1 problems, in which the differential and algebraic equations are explicitly given and explain under which conditions we can expect a positive numerical approximation that meets the algebraic constraints.
We then extend these results to higher index problems, i.e., problems in which some of the algebraic equations are hidden in the system, using derivative arrays and the index reduction developed by Kunkel and Mehrmann [2].

References

[1] Numerical Integration of Positive Linear Differential-Algebraic Systems. A.K. Baum and V. Mehrmann, Preprint TU Berlin, 2012. www3.math.tu-berlin.de/multiphysics/Publications/Articles/BauM12_pp

[2] Differential-Algebraic Equations. Analysis and Numerical Solution, P. Kunkel and V. Mehrmann, EMS Publishing House, Zürich, CH, 2006.