Calculating Consistent Initial Values for Structurally Singular Differential–Algebraic Equation Systems

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Abstract: Solving partial differential equations (PDE) by using the *method of lines* can lead to differential-algebraic equations (DAE). When the number of differential equations in the system is less than number of differential variables, the DAE system is structurally singular as defined in Feehery 1998. For example, the equation for combustion ignition of a single component non-reacting gas in a closed cylindrical vessel in Lagrangian coordinates, or boundary layer equations describing fluid flow in a pipe, in particular, modeling of fluid mixing and chemical reactions in flow tube reactors lead to a structurally singular index-1 DAE system. In order to integrate the DAE system, consistent initial values must first be determined. It is well known that higher-index DAE systems can have hidden constraints. However, index-1 DAE systems may also have hidden constraints, and some of them are structurally singular. A method for calculating consistent initial values for such a class of DAE $F(t, y, \dot{y}) = 0$ is presented. Starting from consistent initial values for y, consistent initial values for the derivative $\dot{y}$ are determined. We derive the hidden constraints by differentiating suitable algebraic constraints and combine the result with the original DAE system to form an equation system, which can be solved to obtain initial consistent values for the original system. Automatic differentiation or finite difference techniques are used to evaluate these hidden constraints. Some practical application examples from the above mentioned fields are presented.

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