THE SOLUTION OF INDEX-ONE DIFFERENTIAL-ALGEBRAIC PROBLEMS WITH A DICHOTOMICALLY STABLE INTEGRATOR

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As has previously been established, a dichotomically stable discretization is important when solving stiff boundary-value problems in ordinary differential equations (ODEs). A dichotomically stable implicit Runge-Kutta method, of order 4, has been implemented in a variable step-size initial-value integrator (SYMIRK). By elimination of the value at the intermediate stage, the 3-stage Lobatto IIIA method may be written in symmetric form as a single formula:

$$\mathbf{X}_{i+1} - \mathbf{X}_i - h\left[\tfrac{1}{6}\mathbf{X}'_{i+1} + \tfrac{2}{3}\mathbf{F}\left\{\tfrac{1}{2}(\mathbf{X}_{i+1} + \mathbf{X}_i) - \tfrac{h}{8}(\mathbf{X}'_{i+1} - \mathbf{X}'_i)\right\} + \tfrac{1}{6}\mathbf{X}'_i\right] = \mathbf{0}. \qquad (1)$$

An explicit third-order method is also required, both as a predictor, and to provide a local error indicator, and in the case of equal step sizes, the 4-step extrapolation formula $\mathbf{X}^p_{i+1} = 4\mathbf{X}_i - 6\mathbf{X}_{i-1} + 4\mathbf{X}_{i-2} - \mathbf{X}_{i-3}$ has the correct asymptotic behaviour, both for small step sizes in the boundary layers, and for large step sizes outside the boundary layers.

In the case of differential-algebraic equations (DAEs) of the form $\mathbf{F}(\mathbf{x}', \mathbf{x}, t) = \mathbf{0} \in I\!R^n$, it is not possible to reduce the Lobatto IIIA formulae to the single equation (1), but instead, the two equations:

$$\begin{aligned} \mathbf{F}\left(\mathbf{X}'_{i+\frac{1}{2}}, \mathbf{X}_i + \tfrac{5}{24}h\mathbf{X}'_i + \tfrac{1}{3}h\mathbf{X}'_{i+\frac{1}{2}} - \tfrac{1}{24}h\mathbf{X}'_{i+1}, t_{i+\frac{1}{2}}\right) &= \mathbf{0}, \\ \mathbf{F}\left(\mathbf{X}'_{i+1}, \mathbf{X}_i + \tfrac{1}{6}h\mathbf{X}'_i + \tfrac{2}{3}h\mathbf{X}'_{i+\frac{1}{2}} + \tfrac{1}{6}h\mathbf{X}'_{i+1}, t_{i+1}\right) &= \mathbf{0}, \end{aligned} \qquad (2)$$

must be solved for the derivatives $\mathbf{X}'_{i+\frac{1}{2}}$, $\mathbf{X}'_{i+1}$. The iteration matrix for modified Newton iteration is then in $I\!R^{2n\times 2n}$, and is non-singular for an index-one system. The local error indicator may be obtained in the normal way, by comparing $\mathbf{X}_{i+1}$ to its predicted value, but in addition to predictors for the variables $\mathbf{X}_{i+1}$, $\mathbf{X}_{i+\frac{1}{2}}$, predictors are also needed for the derivatives.

The ODE integrator (SYMIRK) has been adapted in this way, for the solution of index-one DAEs, and the resulting integrator (SYMDAE) has been inserted into the multiple-shooting code (MSHDAE) developed by R. Lamour for differential-algebraic boundary-value problems. The standard version of MSHDAE uses a BDF integrator, which is not dichotomically stable, and for some stiff test problems this fails to integrate across the interval of interest; the dichotomically stable integrator SYMDAE encounters no difficulty. Indeed, for such problems, the modified version of MSHDAE produces an accurate solution, and within limits imposed by computer word length, the efficiency of the solution process improves with increasing stiffness. For some non-stiff problems, the solution is also entirely satisfactory.

An optimal control problem from chemical engineering has been formulated as a differential-algebraic problem, involving a singular arc where the system is of index three. By introducing a singular perturbation, this may be considered as the limiting case of a stiff index-one differential-algebraic boundary-value problem. Results will be reported on the application of the modified version of MSHDAE to this optimal-control problem.