

Chapter 1

BDF Discretizations

Consider the first order DAE

$$F(y, y', t) = 0 \quad (1.1)$$

A BDF discretization reads

$$y_{n+1} = \phi(y_n, \dots, y_{n-k}) + h\beta y'_{n+1} \quad (1.2)$$

where $\phi(y_n, \dots, y_{n-k})$ depends on previous states only and k is the order of the BDF method. Replacing for y' as a function of y

$$y'_{n+1} = \frac{y_{n+1} - \phi(y_n, \dots, y_{n-k})}{h\beta} \quad (1.3)$$

Replacing into (1.1) and dropping subscripts

$$F\left(y, \frac{y - \phi}{h\beta}, t\right) = 0 \quad (1.4)$$

with the the Jacobian

$$J^y = F_y + \frac{1}{h\beta} F_{y'} \quad (1.5)$$

Consider the stabilized index-2 DAE of motion

$$M(q, t)u' + \Phi_q^\top \lambda - S^1(q, q', t) = 0 \quad (1.6)$$

$$q' - u - \Phi_q^\top \mu = 0 \quad (1.7)$$

$$\Phi(q, t) = 0 \quad (1.8)$$

$$\Phi_q u + \Phi_t = 0 \quad (1.9)$$

Let $y = (u^\top \quad q^\top \quad \lambda^\top \quad \mu^\top)^\top$ and

$$F = \begin{pmatrix} M(q,t)u' + \Phi_q^\top \lambda - S^1(q,u,t) \\ q' - u - \Phi_q^\top \mu \\ \Phi(q,t) \\ \Phi_q u + \Phi_t \end{pmatrix} = 0 \quad (1.10)$$

$$F_{y'} = \begin{pmatrix} M & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (1.11)$$

$$F_y = \begin{pmatrix} -S_u^1 & (M(q,t)u' + \Phi_q^\top \lambda - S^1(q,u,t))_q & \Phi_q^\top & 0 \\ -I & -(\Phi_q^\top \mu)_q & 0 & -\Phi_q^\top \\ 0 & \Phi_q & 0 & 0 \\ \Phi_q & (\Phi_q u)_q + \Phi_{q,t} & 0 & 0 \end{pmatrix} \quad (1.12)$$

Replacing expressions (1.11) and (1.12) into (1.5)

$$J^y = \begin{pmatrix} \frac{1}{h\beta}M - S_u^1 & (M(q,t)u' + \Phi_q^\top \lambda - S^1(q,u,t))_q & \Phi_q^\top & 0 \\ -I & \frac{1}{h\beta}I - (\Phi_q^\top \mu)_q & 0 & -\Phi_q^\top \\ 0 & \Phi_q & 0 & 0 \\ \Phi_q & (\Phi_q u)_q + \Phi_{q,t} & 0 & 0 \end{pmatrix} \quad (1.13)$$

Now, consider solving for y' in (1.1) [3]. Replacing (1.2) into (1.1) and dropping subscripts

$$F(\phi + h\beta y', y', t) = 0 \quad (1.14)$$

with the the Jacobian

$$J^{y'} = h\beta F_y + F_{y'} \quad (1.15)$$

With $y = (u^\top \quad q^\top \quad \lambda^\top \quad \mu^\top)^\top$, and

$$F = \begin{pmatrix} M(q,t)u' + \Phi_q^\top \lambda - S^1(q,u,t) \\ q' - u - \Phi_q^\top \mu \\ \frac{1}{h\beta}\Phi(q,t) \\ \frac{1}{h\beta}(\Phi_q u + \Phi_t) \end{pmatrix} = 0 \quad (1.16)$$

$$F_{y'} = \begin{pmatrix} M & 0 & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (1.17)$$

$$F_y = \begin{pmatrix} -S_u^1 & (M(q,t)u' + \Phi_q^\top \lambda - S^1(q,u,t))_q & \Phi_q^\top & 0 \\ -I & -(\Phi_q^\top \mu)_q & 0 & -\Phi_q^\top \\ 0 & \frac{1}{h\beta} \Phi_q & 0 & 0 \\ \frac{1}{h\beta} \Phi_q & \frac{1}{h\beta} ((\Phi_q u)_q + \Phi_{q,t}) & 0 & 0 \end{pmatrix} \quad (1.18)$$

Hence,

$$J^{y'} = \begin{pmatrix} M - h\beta S_u^1 & h\beta(M(q,t)u' + \Phi_q^\top \lambda - S^1(q,u,t))_q & h\beta \Phi_q^\top & 0 \\ -h\beta I & I - h\beta(\Phi_q^\top \mu)_q & 0 & -h\beta \Phi_q^\top \\ 0 & \Phi_q & 0 & 0 \\ \Phi_q & (\Phi_q u)_q + \Phi_{q,t} & 0 & 0 \end{pmatrix} \quad (1.19)$$

As a result of scaling the constraints in (1.16) by $\frac{1}{h\beta}$, and solving for y' instead of solving for y , the Jacobian $J^{y'}$ remains very well-conditioned when $h \rightarrow 0$. Hence, the formulation is not susceptible to fail at very small step-sizes, h .

Chapter 2

HASTIFF: Index Reduction using the Hiller-Anantharaman Formulation

Equation (1.16) defines a Stabilized Index-2 (SI2) formulation [2], similar to GSTIFF SI2, but more stable due to

1. The scaling of the constraint equations by $\frac{1}{h\beta}$.
2. Solving for y' instead of solving for y .

As a result of the above manipulations of the formulation, the Jacobian remains well-conditioned for very small step-sizes, $h \rightarrow 0$.

Replacing the Lagrange multiplier pair λ and μ with a pair of differentiated Lagrange multipliers, ψ' and χ' , respectively

$$F(y, y', t) = \begin{pmatrix} q' - u + \Phi_q^\top \chi' \\ Mu' + \Phi_q^\top \psi' - S^1 \\ \Phi_q u + \Phi_t \\ \Phi(q, t) \end{pmatrix} = 0 \quad (2.1)$$

the DAE index drops to index-1 and the result is the uniform index-1 Hiller Anantharaman formulation [1, 4, 5], which is a Stabilized Index-1 (SI1) formulation.

Re-arranging components and scaling the constraint equations by $\frac{1}{h\beta}$

$$F(y, y', t) = \begin{pmatrix} Mu' + \Phi_q^\top \psi' - S^1(q, u, t) \\ q' - u - \Phi_q^\top \chi' \\ \frac{1}{h\beta} \Phi(q, t) \\ \frac{1}{h\beta} (\Phi_q u + \Phi_t) \end{pmatrix} = 0 \quad (2.2)$$

where $y = (u^\top \ q^\top \ \psi^\top \ \chi^\top)^\top$. Solving for y' , the obtained Jacobian is

$$J^{y', HA} = \begin{pmatrix} M - h\beta S_u^1 & h\beta(M(q, t)u' + \Phi_q^\top \psi' - S^1(q, u, t))_q & \Phi_q^\top & 0 \\ -h\beta I & I - h\beta(\Phi_q^\top \chi')_q & 0 & -\Phi_q^\top \\ 0 & \Phi_q & 0 & 0 \\ \Phi_q & (\Phi_q u)_q + \Phi_{q,t} & 0 & 0 \end{pmatrix} \quad (2.3)$$

The stabilized index-1 form of this formulation is preferred, because it is more stable numerically than any index-2 formulation [2]; i.e., potentially fewer bigger time-steps could be taken.

The HASTIFF integrator supports both SI1/SI2 formulations, SI1 being the default one. The remaining of the HASTIFF defaults agree with GSTIFF SI2 defaults. Also, same as GSTIFF I3 and SI2, HASTIFF supports both the classical and the modified correctors.

Bibliography

- [1] M. Anantharaman and M. Hiller. Numerical Simulation of Mechanical Systems Using Methods for Differential Algebraic Equations. *International Journal for Numerical Methods in Engineering*, 32:1531–1542, 1991.
- [2] E. Hairer and G. Wanner. *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems*. Springer-Verlag, second revised edition edition, 1996.
- [3] N. Khude, L.O. Jay, A. Schaffer, and D. Negrut. A DISCUSSION OF LOW ORDER NUMERICAL INTEGRATION FORMULAS FOR RIGID AND FLEXIBLE MULTIBODY DYNAMICS. In Proceedings of IEDTC07, editor, *Proceedings of the 6th ASME International Conference on Multibody Systems, Nonlinear Dynamics and Control, September 4-7, 2007, Las Vegas, Nevada, USA*, 2007.
- [4] A. Schaffer. *ON THE ADJOINT FORMULATION OF DESIGN SENSITIVITY ANALYSIS OF MULTIBODY DYNAMICS*. PhD thesis, University of Iowa, 2005.
- [5] Andrei Schaffer. Stabilized Index-1 Differential-Algebraic Formulations for Sensitivity Analysis of Multibody Dynamics. *J. Multi-body Dynamics*, 220 Part K.:141–156, 2006.