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Supplementary Document: Higher-Order Time Integration for Deformable Solids

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A. Method coefficients

This section gives method coefficients for the schemes introduced for evaluation in the main paper. In the following, we consider methods to solve systems of ordinary differential equations (ODEs) of the form

$$\dot{\boldsymbol{y}} = \boldsymbol{g}(t, \boldsymbol{y}) \,. \tag{1}$$

A.1. DIRK methods

Diagonally implicit RK (DIRK) methods can be written as

$$\begin{aligned} \boldsymbol{y}^{n+1} &= \boldsymbol{y}^n + \Delta t \sum_i^s b_i \boldsymbol{G}_i \,, \\ \boldsymbol{G}_i &= \boldsymbol{g}(t^n + c_i \Delta t, \boldsymbol{y}^n + \Delta t \sum_{j=1}^{i-1} a_{ij} \boldsymbol{G}_j + a_{ii} \Delta t \boldsymbol{G}_i) \,. \end{aligned} \tag{2}$$

A thorough review of the theoretical background, implementation details and numerical experiments w.r.t. DIRK methods was presented by Kennedy and Carpenter [KC16]. In the following, the coefficients for the methods are written as Butcher tableaus of the form

$$\begin{array}{c|c} \boldsymbol{c} & A \\ \hline & \boldsymbol{b}^T \end{array}$$

A.1.1. SDIRK2 and SDIRK3

SDIRK2 (two-stage, second-order) and SDIRK3 (three-stage, third-order) were the first methods designated as DIRK methods [Ale77]. An embedded second-order method for error-estimation for SDIRK3 was presented shortly afterwards [Cas79]. It was noted that both methods are stiffly-accurate and L-stable [KC16]. Note that these names are also often used in the literature for other methods. The coefficients given below, however, are the only coefficients exhibiting all the listed properties.

SDIRK2 The butcher tableau for SDIRK2 is given by

$$\begin{array}{c|cc} \gamma & \gamma & 0 \\ 1 & 1-\gamma & \gamma \\ \hline & 1-\gamma & \gamma \end{array}$$

with $\gamma = \frac{1}{2}(2-\sqrt{2})$.

SDIRK3 The butcher tableau for SDIRK3 is given by

$$\begin{array}{c|ccc} \gamma & \gamma & 0 & 0 \\ c_2 & (c_2-\gamma) & \gamma & 0 \\ 1 & (1-b_2-\gamma) & b_2 & \gamma \\ \hline & (1-b_2-\gamma) & b_2 & \gamma \end{array}$$

with

$$b_2 = \frac{-3\alpha^2}{4\beta} \,, \quad c_2 = \frac{2-9\gamma+6\gamma^2}{3\alpha} \,,$$

and

$$\alpha = 1-4\gamma+2\gamma^2 \,, \quad \beta = -1+6\gamma-9\gamma^2+3\gamma^3 \,,$$

where $\gamma = 0.435866521508458999416019\!5$, which is the root of

$$x^3 - 3x^2 + \frac{3}{2}x - \frac{1}{6} = 0$$

in the interval $(\frac{1}{6}, \frac{1}{2})$, see [Ale77].

A.1.2. The TR-BDF2 EDIRK family

The TR-BDF2 integrator, originally proposed by Banks et al. [BCF*85], performs a fractional substep from t^n to $t^n + \gamma\Delta t$ with the trapezoidal rule for $\gamma \in (0,1)$ and then uses the variable step size BDF2 method (see [HW92]) with the states at t^n and $t^{n+\gamma}$. This family of methods parametrized by γ can be written as an EDIRK method with three stages. Particular choices for γ found in the literature are:

- $\gamma = 2-\sqrt{2}$, originally proposed by Banks et al. [BCF*85] as this leads to identical coefficients for the Jacobians of both implicit stages. Bonaventura and Della Rocca [BDR17] derive that this is an optimal choice in the context "strong stability preserving" (SSP) methods and that the method has a stage order of two (which is not possible for SDIRK methods, only for methods with an explicit first stage, see [KC16]). According to Butcher and Chen [BC00], this is the only choice for which the family is L-stable.
- $\gamma = 1/2$, as introduced to nonlinear structural dynamics by Bathe [Bat07], and used in computer graphics by Xu and Barbič [XB17]. We do not see a reason to prefer this choice of γ over the former.

The Butcher tableau for the family is given by (see [BDR17]):

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \gamma & \frac{\gamma}{2} & \frac{\gamma}{2} & 0 \\ 1 & \frac{1}{2(2-\gamma)} & \frac{1}{2(2-\gamma)} & \frac{1-\gamma}{2-\gamma} \\ \hline & \frac{1}{2(2-\gamma)} & \frac{1}{2(2-\gamma)} & \frac{1-\gamma}{2-\gamma} \end{array}$$

A.1.3. SDIRK-NCS23 and SDIRK-NC34

SDIRK-NCS23 (two-stage, third-order) and SDIRK-NC34 (three-stage, fourth-order) were some of the first DIRK methods that were investigated for their nonlinear stability and are algebraically stable and A-stable. It was noted that SDIRK-NCS23 is not stiffly-accurate [KC16] (as this is not possible for a two-stage method with order higher than two).

SDIRK-NCS23 The butcher tableau for SDIRK-NCS23 is given by

$$\begin{array}{c|cc} \gamma & \gamma & 0 \\ 1-\gamma & 1-2\gamma & \gamma \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$$

with $\gamma = \frac{3+\sqrt{3}}{6}$.

SDIRK-NC34 The butcher tableau for SDIRK3 is given by

$$\begin{array}{c|ccc} \gamma & \gamma & 0 & 0 \\ \frac{1}{2} & \frac{1}{2}-\gamma & \gamma & 0 \\ 1-\gamma & 2\gamma & 1-4\gamma & \gamma \\ \hline & b_1 & b_2 & b_3 \end{array}$$

with

$$b_1 = \frac{1}{6(1-2\gamma)^2}, \quad b_2 = \frac{2(1-6\gamma+6\gamma^2)}{3(2\gamma-1)^2}, \quad b_3 = b_1,$$

where

$$\gamma = \frac{3+2\sqrt{3}\cos(\frac{\pi}{18})}{6}.$$

A.1.4. SDIRK(3,3,4,5) and SDIRK(4,3,4,7)

SDIRK(3,3,4,5) and SDIRK(4,3,4,7) are derived as methods suited well for ODEs with oscillating solutions [FGR97]. They follow the naming scheme DIRK(s,p,p_{disp},p_{diss}) where s is the number of stages, p the classical order of accuracy, p_{disp} the dispersion order and p_{diss} the dissipation order. Both methods are A-stable and were tested with a low dimensional, nonlinear oscillatory problem in the original publication.

SDIRK(3,3,4,5) The butcher tableau for SDIRK(3,3,4,5) is given by

$$\begin{array}{c|ccc} \gamma & \gamma & 0 & 0 \\ c_2 & c_2-\gamma & \gamma & 0 \\ c_3 & 0 & c_3-\gamma & \gamma \\ \hline & 0 & 1-b_3 & b_3 \end{array}$$

with

$$\begin{aligned} \gamma &= 1.068579021301629, \\ b_3 &= 0.6696236404609742, \\ c_2 &= 0.08902038200616, \\ c_3 &= 0.7027675575254050. \end{aligned}$$

SDIRK(4,3,4,7) The butcher tableau for SDIRK(4,3,4,7) is given by

$$\begin{array}{c|cccc} \gamma & \gamma & 0 & 0 & 0 \\ c_2 & c_2-\gamma & \gamma & 0 & 0 \\ c_3 & 0 & c_3-\gamma & \gamma & 0 \\ c_4 & 0 & 0 & c_4-\gamma & \gamma \\ \hline & 0 & 0 & 1-b_4 & b_4 \end{array}$$

with

$$\begin{aligned} \gamma &= 1.2805797612753055, \\ b_4 &= 0.4453994092277531, \\ c_2 &= 0.3489302860638736, \\ c_3 &= 0.7586985719573739, \\ c_4 &= 0.1778747841442887. \end{aligned}$$

A.2. Rosenbrock methods

For an implicit system

$$M\dot{\boldsymbol{y}} = \boldsymbol{g}(t,\boldsymbol{y}), \tag{3}$$

Hairer and Wanner [HW96] propose a formulation for Rosenbrock methods that is optimized for computational efficiency given by

$$\begin{aligned} \boldsymbol{y}^{n+1} &= \boldsymbol{y}^n + \sum_i^s m_i \boldsymbol{G}_i, \\ \left(\frac{1}{\gamma_{ii}\Delta t}M - \frac{\partial \boldsymbol{g}}{\partial \boldsymbol{y}}\right)\boldsymbol{G}_i &= \boldsymbol{g}(t^n + \alpha_i\Delta t, \boldsymbol{y}^n + \sum_j^{i-1} a_{ij}\boldsymbol{G}_j) \\ &\quad + M\sum_j^{i-1}\frac{c_{ij}}{\Delta t}\boldsymbol{G}_j + \gamma_i\Delta t\frac{\partial \boldsymbol{g}}{\partial t}, \end{aligned} \tag{4}$$

where a_{ij}, c_{ij}, m_i and γ_{ij} and $\gamma_i = \sum_j^i \gamma_{ij}$ are the coefficients identifying a particular Rosenbrock scheme. In the literature, sometimes other formulations of Rosenbrock methods are used such that one has to take care to correctly transform the coefficients for the implementation.

A.2.1. ROS3PL

ROS3PL is a four-stage, third-order method that is L-stable and stiffly accurate. The authors derived it as a W-method that permits inexact Jacobians and claim that it is robust against order reduction [CLW09]. In addition, it has an embedded method for error estimation. The coefficients for the formulation shown above are

given by $\gamma = 0.435866521508459$ and

$$\begin{aligned}\gamma_1 &= 0.435866521508459\\ \gamma_2 &= -0.064133478491541\\ \gamma_3 &= 0.111028172512505\\ \gamma_4 &= 0.0\end{aligned}$$

The coefficients m_i yield the original third-order method, while replacing them with $\hat{m}_i$ yields the embedded second-order method

$$\begin{aligned} m_1 &= 2.463070773030053 & \hat{m}_1 &= 2.346947683513665\\ m_2 &= 1.147140180139521 & \hat{m}_2 &= 0.456530569451895\\ m_3 &= 0.0 & \hat{m}_3 &= 0.056949243945495\\ m_4 &= 1.0 & \hat{m}_4 &= 0.738684936166224\end{aligned}$$

The other required coefficients are given by

$$\begin{aligned} a_{11} &= 0.0\\ a_{21} &= 1.147140180139521\\ a_{22} &= 0.0\\ a_{31} &= 2.463070773030053\\ a_{32} &= 1.147140180139521\\ a_{33} &= 0.0\\ a_{41} &= 2.463070773030053\\ a_{42} &= 1.147140180139521\\ a_{43} &= 0.0\\ a_{44} &= 0.0\end{aligned}$$

and

$$\begin{aligned} c_{11} &= -2.294280360279042\\ c_{21} &= -2.631861185781065\\ c_{23} &= -2.294280360279042\\ c_{31} &= -1.302364158113095\\ c_{32} &= 2.769432022251304\\ c_{33} &= -2.294280360279042\\ c_{41} &= -1.552568958732400\\ c_{42} &= 2.587743501215153\\ c_{43} &= -1.416993298352020\\ c_{44} &= -2.294280360279042\end{aligned}$$

Note the sign change of the coefficients c_{ij} w.r.t. to the original publication, as we use a slightly different formulation of the Rosenbrock method here.

A.2.2. ROS3PRL2

More recent publications have shown that previously used conditions to prevent order reduction for very stiff problems were not sufficient. Rang [Ran15] derives new variants of commonly used third-order methods including ROS3PL and, amongst others, presents ROS3PRL2 that is shown to preserve third-order accuracy in numerical experiments. In our experiments, however, we were not able to obtain stable results with this method. Therefor, we will not reproduce the coefficients here.

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