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SOLUTIONS SHEET 10

Exercise 29. Let everything be defined as on page 76/77 in the script by Prof. Sauter. Taylor expansion of $\mathbf{g}(h)$ around $h = 0$ yields (by already plugging in the simplifications of formula (4.24))

$$\begin{aligned}\mathbf{g}(h) =& \mathbf{g}(0) + \mathbf{g}'(0)h + \frac{1}{2}\mathbf{g}''(0)h^2 + O(h^3)\\ =& f\mathbf{1} + h\left(\partial_1 f + f\partial_2 f\right)\mathbf{c}\\ &+ \frac{1}{2}h^2\left((\partial_1^2 f + 2f\partial_1\partial_2 f + f^2\partial_2^2 f)\mathbf{c}^{\odot 2} + 2(\partial_2 f\partial_1 f + f(\partial_2 f)^2)\mathbf{A}\mathbf{c}\right) + O(h^3)\end{aligned}$$

Plugging this into the Runge-Kutta method yields

$$\begin{aligned}y_1 =& y_0 + hf\langle\mathbf{b},\mathbf{1}\rangle + h^2(\partial_1 f + f\partial_2 f)\langle\mathbf{b},\mathbf{c}\rangle\\ &+ \frac{1}{2}h^3(\partial_1^2 f + 2f\partial_1\partial_2 f + f^2\partial_2^2 f)\langle\mathbf{b},\mathbf{c}^{\odot 2}\rangle + h^3(\partial_2 f\partial_1 f + f(\partial_2 f)^2)\langle\mathbf{b},\mathbf{A}\mathbf{c}\rangle + O(h^4)\end{aligned}$$

Now we immediately see

$$\boxed{\langle\mathbf{b},\mathbf{c}^{\odot 2}\rangle = \frac{1}{3}} \qquad \boxed{\langle\mathbf{b},\mathbf{A}\mathbf{c}\rangle = \frac{1}{6}} \tag{1}$$

by comparing y_1 to

$$y(x_0 + h) = y_0 + y'(x_0)h + \frac{1}{2}y''(x_0)h^2 + \frac{1}{6}y'''(x_0)h^3 + O(h^4) \tag{2}$$

with

$$\begin{aligned}y'(x_0) =& f\\ y''(x_0) =& \partial_1 f + f\partial_2 f\\ y'''(x_0) =& \partial_1^2 f + 2f\partial_1\partial_2 f + \partial_1 f\partial_2 f + f\left(\partial_2 f\right)^2 + f^2\partial_2^2 f\end{aligned}$$

These are precisely the order conditions.
Remark: It should be $\mathbf{D_k}\partial_1\mathbf{F}(0, f\mathbf{1}) = -(\partial_2 f)\mathbf{A}$, otherwise there is a wrong sign.

Exercise 30.

a. By the theorem of *Guillou & Soulé* 1969, *Wright* 1970 [HLW02, p. 27] we have

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$$
\begin{aligned}
a_{11} &= \int_0^{c_1} \ell_1(\tau)d\tau = \int_0^{c_1} \frac{\tau - c_2}{c_1 - c_2} d\tau = \frac{c_1(c_1 - 2c_2)}{2(c_1 - c_2)} \\
a_{12} &= \int_0^{c_1} \ell_2(\tau)d\tau = \int_0^{c_1} \frac{\tau - c_1}{c_2 - c_1} d\tau = \frac{c_1^2}{2(c_1 - c_2)} \\
a_{21} &= \int_0^{c_2} \ell_1(\tau)d\tau = \int_0^{c_2} \frac{\tau - c_2}{c_1 - c_2} d\tau = \frac{c_2^2}{2(c_2 - c_1)} \\
a_{22} &= \int_0^{c_2} \ell_2(\tau)d\tau = \int_0^{c_2} \frac{\tau - c_1}{c_2 - c_1} d\tau = \frac{c_2(c_2 - 2c_2)}{2(c_2 - c_1)}
\end{aligned}
$$

and

$$
b_1 = \int_0^1 \ell_1(\tau)d\tau = \frac{1 - 2c_2}{2(c_1 - c_2)} \qquad b_2 = \int_0^1 \ell_2(\tau)d\tau = \frac{1 - 2c_1}{2(c_2 - c_1)}
$$

b. Since we have already determined b_1 and b_2 we can work with **Theorem 1.5 (Superconvergence)** [HLW02, p. 28]. We get

$$
b_1 + b_2 = \frac{1 - 2c_2}{2(c_1 - c_2)} + \frac{1 - 2c_1}{2(c_2 - c_1)} = \frac{1 - 2c_2}{2(c_1 - c_2)} - \frac{1 - 2c_1}{2(c_1 - c_2)} = 1 \tag{3}
$$

and thus the collocation method is at least of order 1 (with no restriction for c_1 and c_2). Further

$$
b_1c_1 + b_2c_2 = \frac{c_1 - 2c_1c_2}{2(c_1 - c_2)} + \frac{c_2 - 2c_1c_2}{2(c_2 - c_1)} = \frac{c_1 - 2c_1c_2}{2(c_1 - c_2)} - \frac{c_2 - 2c_1c_2}{2(c_1 - c_2)} = \frac{1}{2} \tag{4}
$$

and thus the collocation method is at least of order 2 (with no restrictions for c_1 and c_2). For order 3 however it must hold that

$$
b_1c_1^2 + b_2c_2^2 = \frac{1 - 2c_2}{2(c_1 - c_2)}c_1^2 - \frac{1 - 2c_1}{2(c_2 - c_1)}c_2^2 = \frac{(c_1^2 - c_2^2) - 2c_1c_2(c_1 - c_2)}{2(c_1 - c_2)} = \frac{c_1 + c_2}{2} - c_1c_2 \overset{!}{=} \frac{1}{3} \tag{5}
$$

Thus we get the restriction $\boxed{c_1 = \frac{2 - 3c_2}{3(1 - 2c_2)}}$ for order 3.

c. For order 4 it must hold that $b_1c_1^3 + b_2c_2^3 = \frac{1}{4}$. Thus by

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$$
\begin{aligned}
b_1c_1^3 + b_2c_2^3 &= \frac{1-2c_2}{2(c_1-c_2)}c_1^3 - \frac{1-2c_1}{2(c_1-c_2)}c_2^3 \\
&= \frac{c_1^3 - 2c_1^3c_2 - c_2^3 + 2c_1c_2^3}{2(c_1-c_2)} \\
&= \frac{\left(c_1^3 - c_2^3\right) - 2c_1c_2\left(c_1^2 - c_2^2\right)}{2(c_1-c_2)} \\
&= \frac{(c_1-c_2)\left(c_1^2 + c_1c_2 + c_2^2\right) - 2c_1c_2(c_1-c_2)(c_1+c_2)}{2(c_1-c_2)} \\
&= \frac{c_1^2 + c_1c_2 + c_2^2}{2} - c_1^2c_2 - c_1c_2^2
\end{aligned}
$$

we get the quadratic equation for c_1

$$(1-2c_2)\,c_1^2 + \left(c_2 - 2c_2^2\right)c_1 - \frac{1-2c_2^2}{2} = 0 \tag{6}$$

This gets kinda messy to evaluate. Hence I will use `MAPLE` to prevent calculation errors. Since equation 6 is a polynomial of degree 2 we get two roots and hence two conditions for c_1 dependent on c_2. Equate with above condition for order 3 we get

$$c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6} \qquad c_2 = \frac{1}{2} - \frac{\sqrt{3}}{6} \tag{7}$$

and thus by the order condition for order 3 corresponding

$$c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6} \qquad c_1 = \frac{1}{2} + \frac{\sqrt{3}}{6} \tag{8}$$

As can see in the file `ex_30_c.mw`. Thus there are precisely two collocation methods with $s = 2$ and order 4 (which one of is a *Gauss method*).

Exercise 31. By **Theorem 1.8** [HLW02, p. 32] the discontinuous collocation method is equivalent to a 4-stage Runge-Kutta method with $c_1 = 0$, $c_2 = \frac{1}{3}$, $c_3 = \frac{2}{3}$ and $c_4 = 1$. Also the condition $B(s-2)$ holds. This gives us

$$b_1 + b_2 + b_3 + b_4 = 1 \qquad b_1c_1 + b_2c_2 + b_3c_3 + b_4c_4 = \frac{1}{2} \tag{9}$$

or equivalently

$$b_2 + b_3 = \frac{3}{4} \qquad \frac{1}{3}b_2 + \frac{2}{3}b_3 = \frac{3}{8} \tag{10}$$

This immediately yields $b_2 = b_3 = \frac{3}{8}$. Now we can apply **Theorem 1.9 (Superconvergence)** [HLW02, p. 33] which states that the discontinuous collocation method has the same order as the underlying quadrature formula. The given discontinuous collocation method has the underlying quadrature formula on the interval $[0,1]$

$$I(f) = \frac{1}{8}f(0) + \frac{3}{8}f\left(\frac{1}{3}\right) + \frac{3}{8}f\left(\frac{2}{3}\right) + \frac{1}{8}f(1) \tag{11}$$

This is precisely the $\frac{3}{8}$-rule. The $\frac{3}{8}$-rule has the error term $h^5\frac{3}{80}f^{(4)}(\xi)$ for some $\xi \in]0,1[$ and thus is exact for all polynomials of degree 3. Since the order of a quadrature method

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is defined as degree of exactness plus one we have that the given discontinuous collocation method is of order 4.

Exercise 32. **a.** First of all we have to generalize the Störmer/Verlet method to a general partitioned method *. By introducing the velocity $v := \dot{q}$ we get from $\ddot{q} = f(q)$ the system $\dot{v} = f(q)$ and the Störmer/Verlet method admits a one-step formulation $\Phi_h : (q_n, v_n) \mapsto (q_{n+1}, v_{n+1})$ given by

$$\begin{aligned} v_{n+\frac{1}{2}} &= v_n + \frac{h}{2} f(q_n), \\ q_{n+1} &= q_n + h v_{n+\frac{1}{2}}, \\ v_{n+1} &= v_{n+\frac{1}{2}} + \frac{h}{2} f(q_{n+1}). \end{aligned} \tag{12}$$

The Störmer/Verlet method can also be interpreted as a *composition method* † Further we get by splitting formula 12 in the middle the scheme $\hat{\Phi}_h : (v_n, q_n) \mapsto (v_{n+\frac{1}{2}}, q_{n+\frac{1}{2}})$

$$\begin{aligned} v_{n+\frac{1}{2}} &= v_n + \frac{h}{2} f(q_n), \\ q_{n+\frac{1}{2}} &= q_n + \frac{h}{2} v_{n+\frac{1}{2}}. \end{aligned} \tag{14}$$

From the scheme 14 one has the *adjoint*‡ scheme $\hat{\Phi}_h^* : (v_{n+\frac{1}{2}}, q_{n+\frac{1}{2}}) \mapsto (v_{n+1}, q_{n+1})$ by formally replacing h by $-h$ and index shifting

$$\begin{aligned} q_{n+1} &= q_{n+\frac{1}{2}} + \frac{h}{2} v_{n+\frac{1}{2}}, \\ v_{n+1} &= v_{n+\frac{1}{2}} + \frac{h}{2} f(q_{n+1}). \end{aligned} \tag{16}$$

We see that the one-step formulation of the Störmer/Verlet method is the composition $\hat{\Phi}_h^* \circ \hat{\Phi}_h$. Now we want to generalize method 12 to *partitioned systems* of the form

$$\dot{q} = g(q, v) \qquad \dot{v} = f(q, v) \tag{17}$$

For that consider the extended formulae 14 and 16

$$\begin{aligned} v_{n+\frac{1}{2}} &= v_n + \frac{h}{2} f(q_n, v_{n+\frac{1}{2}}), \\ q_{n+\frac{1}{2}} &= q_n + \frac{h}{2} g(q_n, v_{n+\frac{1}{2}}). \end{aligned} \tag{18}$$

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*I will follow here the elegant paper of *Hairer, Lubich* and *Wanner* found here http://www.math.kit.edu/ianm3/lehre/geonumint2009s/media/gni_by_stoermer-verlet.pdf, last accessed May 18, 2016.

† Let Φ_h be a basic one-step method and $\gamma_1, \ldots, \gamma_s$ real numbers. Then we call its composition with stepsizes $\gamma_1 h, \gamma_2 h, \ldots, \gamma_s h$, i.e.,

$$\Psi_h = \Phi_{\gamma_s h} \circ \ldots \circ \Phi_{\gamma_1 h} \tag{13}$$

the corresponding *composition method* as defined in [HLW02, p. 43].

‡ This follows essentially [HLW02, pp. 38–39]. The *adjoint method* Φ_h^* of a method Φ_h is the inverse map of the original method with reversed time step $-h$, i.e.

$$\Phi_h^* := \Phi_{-h}^{-1} \tag{15}$$

In other words, $y_1 = \Phi_h^*(y_0)$ is implicitly defined by $\Phi_{-h}(y_1) = y_0$.

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$$
\begin{aligned}
q_{n+1} &= q_{n+\frac{1}{2}} + \frac{h}{2} g(q_{n+1}, v_{n+\frac{1}{2}}), \\
v_{n+1} &= v_{n+\frac{1}{2}} + \frac{h}{2} f(q_{n+1}, v_{n+\frac{1}{2}}).
\end{aligned} \tag{19}
$$

Composition of formula 19 and formula 18 yields

$$
\boxed{
\begin{aligned}
v_{n+\frac{1}{2}} &= v_n + \frac{h}{2} f(q_n, v_{n+\frac{1}{2}}), \\
q_{n+1} &= q_n + \frac{h}{2} \left(g(q_n, v_{n+\frac{1}{2}}) + g(q_{n+1}, v_{n+\frac{1}{2}}) \right), \\
v_{n+1} &= v_{n+\frac{1}{2}} + \frac{h}{2} f(q_{n+1}, v_{n+\frac{1}{2}}).
\end{aligned}
} \tag{20}
$$

Let us consider the partitioned initial value problem

$$
\dot{y} = f(y, z) \qquad \dot{z} = g(y, z) \tag{21}
$$

Applying formula 20 on the partitioned initial value problem 21 for $n = 0$ yields

$$
\begin{aligned}
z_{\frac{1}{2}} &= z_0 + \frac{h}{2} g(y_0, z_{\frac{1}{2}}), \\
y_1 &= y_0 + \frac{h}{2} \left(f(y_0, z_{\frac{1}{2}}) + f(y_1, z_{\frac{1}{2}}) \right), \\
z_1 &= z_{\frac{1}{2}} + \frac{h}{2} g(y_1, z_{\frac{1}{2}}).
\end{aligned} \tag{22}
$$

Plugging the first equation into the last one yields $z_1 = z_0 + \frac{h}{2}\left(g(y_0, z_{\frac{1}{2}}) + g(y_1, z_{\frac{1}{2}}) \right)$ from which immediately $\hat{b}_1 = \hat{b}_2 = \frac{1}{2}$, $\ell_1 = g(y_0, z_{\frac{1}{2}})$ and $\ell_2 = g(y_1, z_{\frac{1}{2}})$ follows. Further by $\ell_1 = g(y_0, z_{\frac{1}{2}}) = g(y_0 + ha_{11}k_1 + ha_{12}k_2, z_0 + h\hat{a}_{11}\ell_1 + \hat{a}_{12}\ell_2)$ follows $a_{11} = a_{12} = 0$ and by plugging the first equation into ℓ_1 we get that $\ell_1 = g(y_0, z_{\frac{1}{2}}) = g(y_0, z_0 + \frac{h}{2} \underbrace{g(y_0, z_{\frac{1}{2}})}_{= \ell_1})$ and thus $\hat{a}_{11} = \frac{1}{2}$, $\hat{a}_{12} = 0$. By plugging in the first equation into ℓ_2 we get $\ell_2 = g(y_1, z_{\frac{1}{2}}) = g(y_1, z_0 + \frac{h}{2} \underbrace{g(y_0, z_{\frac{1}{2}})}_{= \ell_1})$. Further plugging in the second equation yields

$$
\ell_2 = g(y_1, z_{\frac{1}{2}}) = g\left(y_0 + \frac{h}{2}\left(f(y_0, z_{\frac{1}{2}}) + f(y_1, z_{\frac{1}{2}}) \right), z_0 + \frac{h}{2} g(y_0, z_{\frac{1}{2}}) \right) \tag{23}
$$

which implies $\hat{a}_{21} = \frac{1}{2}$, $\hat{a}_{22} = 0$,$a_{21} = a_{22} = \frac{1}{2}$ with $k_1 = f(y_0, z_{\frac{1}{2}})$ and $k_2 = f(y_1, z_{\frac{1}{2}})$. Of interest is only k_2 to complete the Butcher tableau of the first Runge-Kutta method. By plugging in the definintion of y_1 into k_2 we get

$$
k_2 = f(y_1, z_{\frac{1}{2}}) = f\left(y_1 = y_0 + \frac{h}{2}\left(\underbrace{f(y_0, z_{\frac{1}{2}})}_{= k_1} + \underbrace{f(y_1, z_{\frac{1}{2}})}_{= k_2} \right), z_{\frac{1}{2}} \right) \tag{24}
$$

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and hence $a_{12} = a_{22} = \frac{1}{2}$. Since $c_i = \sum_{j=1}^{s} a_{ij}$ for all $i = 1, \dots, s$ we get that the first Runge-Kutta method is the implicit trapezoidal rule and the second Runge-Kutta method is given by

$$\begin{array}{c|cc} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

Hence the Störmer/Verlet method is a partitioned Runge-Kutta method.

b. Let $s = 2$. Then $c_1 = 0$ and $c_2 = 1$ for any Lobatto IIIA method. Thus we have again to use the theorem of *Guillou & Soulé* 1969*, Wright* 1970 [HLW02, p. 27] which gives us

$$a_{11} = \int_0^{c_1} \ell_1(\tau)d\tau = 0 \qquad a_{12} = \int_0^{c_1} \ell_2(\tau)d\tau = 0$$
$$a_{21} = \int_0^{c_2} \frac{\tau - c_2}{c_1 - c_2} d\tau = \frac{1}{2} \qquad a_{22} = \int_0^{c_2} \frac{\tau - c_1}{c_2 - c_1} d\tau = \frac{1}{2}$$

and

$$b_1 = \int_0^1 \ell_1(\tau)d\tau = \frac{1}{2} \qquad b_2 = \int_0^1 \ell_2(\tau)d\tau = \frac{1}{2} \tag{25}$$

Hence we get the Runge-Kutta method

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}$$

which is precisely the Butcher tableaux for the implicit trapezoidal rule.

References

[HLW02] Ernst Hairer, Christian Lubich, and Gerhard Wanner. *Geometric numerical integration : structure-preserving algorithms for ordinary differential equations*. Springer series in computational mathematics. Berlin, Heidelberg, New York: Springer, 2002.