Order Conditions for Numerical Methods for Partitioned Ordinary Differential Equations

E. Hairer
Institut für Angewandte Mathematik, Universität Heidelberg, Im Neuenheimer Feld 294, D-6900 Heidelberg 1, Germany (Fed. Rep.)

Summary. Motivated by the consideration of Runge-Kutta formulas for partitioned systems, the theory of "P-series" is studied. This theory yields the general structure of the order conditions for numerical methods for partitioned systems, and in addition for Nyström methods for $y''=f(y, y')$, for Rosenbrock-type methods with inexact Jacobian (W-methods). It is a direct generalization of the theory of Butcher series [7, 8]. In a later publication, the theory of P-series will be used for the derivation of order conditions for Runge-Kutta-type methods for Volterra integral equations [1].

Subject Classifications: AMS(MOS): 65L05; CR: 5.17

1. Introduction

With the Runge-Kutta theory of Butcher [4, 5] or with the theory of Hairer and Wanner [7, 8] one can construct the order conditions for Runge-Kutta methods, Rosenbrock methods, etc. In recent years, several authors have considered procedures which use different methods for different parts of the partitioned differential system, usually an implicit procedure for the stiff part and an explicit method for the non-stiff part (so called "mixed", "partially implicit" or "compound" methods [6, 10, 12]). Our aim is to extend the theory of [7, 8] to partitioned differential equations. It turned out that with this extended theory (P-series) one could not only derive the order conditions for mixed Runge-Kutta methods, but also for many numerical methods such as W-methods [13], Nyström methods for $y''=f(y, y')$ [9] and Runge-Kutta-type methods for Volterra integral equations of the second kind [1]. The presentation of the theory of P-series and its application to some methods will be the content of this paper.

1 Note that the "partitioning" of Runge-Kutta methods into "internal" and "external" stages has been introduced by Burrage and Butcher [2] in order to create a satisfactory framework for their theory of algebraic stability and is, of course, a completely different notion.
Let us consider the partitioned system of differential equations

\[
\begin{align*}
Y'_a &= f_a(Y_a, y_b, \ldots) \\
Y'_b &= f_b(y_a, y_b, \ldots) \\
\dot{y}_n &= f_n(y_a, y_b, \ldots) \\
\end{align*}
\]  

(1)

where \( y_a \in \mathbb{R}^{n_a}, \ y_b \in \mathbb{R}^{n_b}, \ n = n_a + n_b + \ldots, \ y := (y_a, y_b, \ldots)^T, \ f(y) = (f_a(y), f_b(y), \ldots)^T \) and \( \mathcal{A} = \{a, b, \ldots\} \) is a finite index-set. For graphic reasons, letters instead of numbers are used as indices. For simplicity of the notations and formulations of the theorems we assume that \( f: U \rightarrow \mathbb{R}^n \) is arbitrarily often differentiable, where \( U \) is an open set in \( \mathbb{R}^n \). If we consider the Taylor series expansion of the exact solution of (1) passing through the initial value

\[
y(x_0) = y_0 = (y_a^{(0)}, y_b^{(0)}, \ldots)^T,
\]

(2)

we have to compute the higher derivatives of \( y(x) \). We demonstrate this for the first component \( y_a(x) \).

\[
y_a(x_0) = y_a^{(0)} \\
y'_a(x_0) = f_a \\
y''_a(x_0) = \frac{\partial^2 f_a}{\partial y_a^2} f_a + \frac{\partial^2 f_a}{\partial y_b^2} f_b + \ldots \\
y^{(3)}_a(x_0) = \frac{\partial^3 f_a}{\partial y_a^3} (f_a, f_a) + \frac{\partial^3 f_a}{\partial y_a^2 \partial y_b} (f_a, f_b) + \frac{\partial^3 f_a}{\partial y_a \partial y_b^2} f_a \\
+ \frac{\partial f_a}{\partial y_a} f_a + \frac{\partial f_a}{\partial y_b} f_b + \frac{\partial^2 f_a}{\partial y_a \partial y_b} (f_b, f_a) + \frac{\partial^2 f_a}{\partial y_b^2} (f_b, f_b) \\
+ \frac{\partial f_a}{\partial y_a} f_a + \frac{\partial f_a}{\partial y_b} f_b + \frac{\partial f_a}{\partial y_b} f_b + \ldots
\]

(3)

The summands on the right hand side (called elementary differentials in definition 9) have to be evaluated at the initial value \( y_0 \). In a similar way as it has been done in ([7], p. 293–294), we associate to every elementary differential a graph with double-labelled nodes.

\[\text{Fig. 1}\]