

***Isomeric trees with applications to Runge-Kutta methods***

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Classical Runge–Kutta methods, up to the work of Nyström, were derived to achieve a required order for scalar problems, even though they often retained the same asymptotic accuracy for high-dimensional problems. By writing trees in terms of products of what will be referred to as atomic factors, the distinction between scalar and vector conditions is seen to be equivalent to identifying permuted products with the same factors. These interrelated trees are said to be “isomeric”.

The number of conditions for order  $p$ , in the scalar and vector cases, are shown in the table below. Also shown are the number of free parameters for an  $s$  stage method, where  $s$  corresponds to the minimum number of stages to achieve order  $p$ .

$p$	scalar	vector	$s$	parameters
1	1	1	1	1
2	2	2	2	3
3	4	4	3	6
4	8	8	4	10
5	16	17	6	21
6	31	37	7	28

For  $p = 5$ , methods exist which have this order for a scalar problem, but not for a vector problem.

The first method of order 6, derived by A. Huřa, used  $s = 8$  stages, so that there would be 36 parameters, which were expected, at that time, to be necessary to satisfy the 31 conditions for a scalar problem.