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Design and construction of software for general linear methods

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Abstract

The ultimate goal in the study of numerical methods for ODEs is the construction of such methods which can be used to develop efficient and robust solvers. The theoretical study and investigation of stability and accuracy for a particular class of methods is a first step towards the development of practical algorithms.

This thesis is concerned with the use of general linear methods (GLMs) for this purpose. Whereas existing solvers use traditional methods, GLMs are more complex due to their complicated order conditions. A natural approach to achieve practical GLMs, is to first consider the advantages and disadvantages of traditional methods and then compare these with a particular class of GLMs. In this thesis, GLMs with IRKS– and F–properties are considered within the type 1 DIMSIMs class. The freedom of choice of free parameters in IRKS methods is used here to test the sensitivity and capability of the methods.

A complete ODE software package uses many numerical techniques in addition to the methods considered. These include error estimation, interpolation for continuous output, etc.. Existing ODE software is a combination of these techniques and much work has been done in the past to improve the capability of these traditional methods. The approach has been largely heuristic and empirical. These are developed by fitting all these techniques into one algorithm to produce efficient ODE software.

The design of the algorithm is the main interest in the thesis. An efficient solver will be in (h, p)-refinement mode. This design includes many decisions in the whole algorithm. These include selection of stepsize and order for the next step, rejection criteria, and selection of stepsize and order in case of rejection. To design such a robust algorithm, the Lagrange optimisation approach is used here. This approach for the selection of stepsize and order avoids the use of several heuristic choices and gives a new direction for developing reliable ODE software. Experiments with this design have been carried out on non–stiff, mildly–stiff and some discontinuous problems and are reported in this thesis.

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Dedication

This thesis is dedicated to my beloved late daughter Maha Ahmad who is the only human being I found, just loving me and gave me the meaning of love before she left us to heavens in November of 2013.

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Glossary

p order of the method. 12, 26

q stage order of the method. 12, 26

r number of elements in the data (Nordsieck) vector. 11, 26

s number of stages in the method. 11, 26

ARK almost Runge–Kutta method. 16, 92

DESIRE diagonally extended singly implicit Runge–Kutta effective order method. 22

DIMSIM diagonally implicit multistage integration method. i, 7, 16, 21, 22, 24, 25, 27, 28, 30, 32, 35, 45, 127

DIRK diagonally implicit Runge–Kutta method. 7, 8, 23, 24

FSAL first stage as last. 23, 35

IRKS inherent Runge–Kutta stability. i, xiii, xv, xvi, 9, 15, 17–19, 25, 31–37, 40, 41, 45, 52, 62, 65, 68, 69, 73, 81–91, 93–101, 104, 126–129

SIRK singly implicit Runge–Kutta method. 4, 5, 7, 8, 22, 25, 31, 36

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