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Taylor series based solution of nonlinear-quadratic ODE systems

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1. INTRODUCTION

The "Modern Taylor Series Method" (MTSM) is the numerical integration method that can numerically solve ordinary differential equations (ODEs). The method calculates terms of the Taylor series recurrently for each integration step. The number of calculated terms is generally different for every step and it depends on a defined accuracy of the calculation. Model implementation of MTSM (TKSL software package, Kunovský (1994)), is limited by maximal number of equations and double accuracy.Therefore the method is currently being tested and reimplemented in MATLAB.

Several papers focus on computer implementation of the Taylor series method in a variable-order and variable-step context (see, for instance, Abad et al. (2015), the TIDES software or in Jorba and Zou (2005)). The reduction of rounding errors Rodríguez and Barrio (2012) and utilization of multiple arithmetic Barrio et al. (2011) improves the applicability of Taylor series based algorithms.

This paper demonstrates that the MTSM, specialized to directly solving nonlinear-quadratic ODE systems, solves non-stiff and in some cases stiff systems very fast (in comparison with MATLAB implementation of explicit and implicit ode solvers) and outperforms standard solvers in the considered benchmark problems. This paper is closely connected with Šátek et al. (2015) where effective solution of linear ODE systems using MSTM was introduced.

2. SCHEME FOR QUADRATIC ODES

In this article, we have focused on effective solution of special case of nonlinear-quadratic systems of ODEs. The nonlinear-quadratic systems of ODEs is any first-order ODE that is quadratic in the unknown function. For such system Taylor series based numerical method can be implemented in very effective way.

The best-known and most accurate method of calculating a new value of a numerical solution of ordinary differential equation $y' = f(t, y),\ \ y(0) = y_0$ is to construct the Taylor series Hairer et al. (1987).

The $n-$th order method uses n Taylor series terms in the explicit form

$$\begin{aligned} y_{i+1} &= y_i + hf(t_i, y_i) + \frac{h^2}{2!} f^{[1]}(t_i, y_i) + \cdots \\ &+ \frac{h^n}{n!} f^{[n-1]}(t_i, y_i). \end{aligned} \tag{1}$$

Equation (1) for nonlinear-quadratic systems of ODEs can be rewritten in the form

$$\boldsymbol{y}' = \mathbf{A}\boldsymbol{y}^2 + \mathbf{B}\boldsymbol{y_{jk}} + \mathbf{C}\boldsymbol{y} + \mathbf{b}\,, \tag{2}$$

where $\mathbf{A} \in \mathbb{R}^{ne\times ne}$ is the matrix for pure quadratic term, $\mathbf{B} \in \mathbb{R}^{ne\times ne(ne-1)/2}$ is the matrix for mixed quadratic term, $\mathbf{C} \in \mathbb{R}^{ne\times ne}$ is the Jacobian matrix for linear part of the system and $\mathbf{b} \in \mathbb{R}^{ne}$ is the right-hand side for the forces incoming to the system. The unknown function $\boldsymbol{y}^2$ represents the vector of multiplications $(y_1y_1, y_2y_2, \ldots, y_{ne}y_{ne})^T$; the unknown function $\boldsymbol{y_{jk}}$ represents the vector of mixed terms multiplications $(y_{j_1}y_{k_1}, y_{j_2}y_{k_2} \ldots, y_{j_{ne(ne-1)/2}}y_{k_{ne(ne-1)/2}})^T$. The indices j, k come from combinatorics $C(ne, 2)$ and symbol ne stands for the number of equations in ODE system. For simplification we suppose that the constant matrices $\mathbf{A}, \mathbf{B}, \mathbf{C}$ and the constant vector $\mathbf{b}$ are used in system (2).

Higher derivatives of such systems (2) can be effectively computed in MATLAB software MathWorks (2017) using matrix-vector multiplication, e.g. higher derivative $\boldsymbol{y}^{[p]}$ for pure quadratic term with matrix $\mathbf{A}$ should be expressed as

$$\boldsymbol{y}^{[p]} = \mathbf{A}\left(\sum_{i=0}^{p-2} \boldsymbol{y}^{[p-1-i]}.*\boldsymbol{y}^{[i]}\binom{p-1}{i} + \boldsymbol{y}.*\boldsymbol{y}^{[p-1]}\right), \tag{3}$$

where the operation '.*' stands for *element-by-element* multiplication, i.e. $\boldsymbol{y}^{[p_1]}.*\boldsymbol{y}^{[p_2]}$ is vector $(y_1^{[p_1]}y_1^{[p_2]}, \ldots, y_{ne}^{[p_1]}y_{ne}^{[p_2]})^T$. The binomial coefficients $\binom{p-1}{i}$ can be effectively precomputed using Pascal triangle, for more information see *pascal* function in MATLAB software.

3. NUMERICAL EXPERIMENTS

All algorithms are implemented in Matlab 2015a and computations are partially performed on SALOMON supercomputer at IT4Innovations VŠB-TU Ostrava

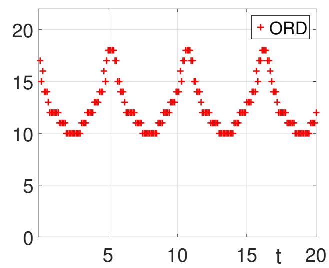

Fig. 1. Order of MTSM for B1 non-stiff problem

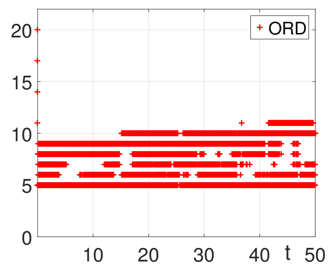

Fig. 2. Order of MTSM for D4 stiff problem

IT4Innovations (2017). Relative and absolute tolerance for all computations was set to 10^{-7}. Classical double precision arithmetic has been used in our examples and maximum order of Taylor series was set to $ORD = 60$.

Vectorized MATLAB code of explicit Taylor series **expTay** with a variable order and variable step size scheme for nonlinear-quadratic systems of ODEs (2) has been implemented. This algorithm was compared on a set of "non-stiff" nonlinear-quadratic systems (see Enright and Pryce (1987)) with vectorized MATLAB explicit **ode** solvers. Benchmark results are shown in table 1 (each reported runtime is taken as a median value of 100 computations). Ratios of computation times $ratio = \boldsymbol{ode/expTay} > 1$ indicate faster computation of the MTSM in all cases (see used orders in Fig. 1).

Table 1. Time of solutions (non-stiff systems): explicit Taylor **expTay** and MATLAB explicit **ode** solver comparison

problem	**ode23** *ratio*	**ode45** *ratio*	**ode113** *ratio*	**expTay** [s]
B1	30.67	2.05	1.57	0.0323
B3	14.79	1.65	1.34	0.00965
B5	29.54	2.17	1.28	0.0201
E4	17.1	2.12	2.19	0.00276

The MTSM, due to the higher order, has some positive properties for stability of the solution. Thanks to these properties it can be effectively used for solution of moderately stiff problems. In table 2 one can see the comparisons **expTay** method with implicit MATLAB **ode** solvers (see used orders in Fig. 2).

Table 2. Time of solutions (stiff systems): explicit Taylor **expTay** and MATLAB implicit **ode** solver comparison

problem	**ode15s** *ratio*	**ode23s** *ratio*	**ode23t** *ratio*	**ode23tb** *ratio*	**expTay** [s]
C1	1.07	21.21	14.99	14.53	0.0849
C2	1.03	20.05	14.05	13.34	0.0823
D1	0.23	24.75	2.9	2.33	0.569
D3	2.12	19.55	19.4	17.28	0.065
F3	1.2	15.31	13.14	11.75	0.0359

4. CONCLUSION

The Taylor series scheme (after MATLAB vectorization) seems to be very efficient for solution of some types of nonlinear-quadratic ODEs. In many cases it significantly outperforms standard solvers on the considered benchmark problems. Detailed information and more results will be presented at the conference.

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