AKTION project no. 69p22 - final report

Content

Synopsis

The AKTION project no. 69p22 ("Modern Taylor Series Method and Parallel Implementation of Numerical Methods for Large Systems") has been carried out by groups of the Brno University of Technology (BUT) and the Vienna University of Technology (VUT) in the time frame 10th February 2014 – 30th April 2015. All project activities and goals according to the project plan have been carried out and fulfilled, and in fact even significantly more exchange activities could be carried out than originally planned. This generated an enlarged impact in terms of education (a special university course could be established at VUT) as well as in the scientific tasks. Researchers and students from various research fields came together and inspired multi-disciplinary discussions related to the project's core content – the Modern Taylor Series Method (MTSM). Some of these scientific aspects include the numeric solution of partial differential equations (Finite Elements, Finite Differences, Galerkin approximations), Taylor series properties, or massively-parallel scientific computing issues. Their relations to the MTSM have been studied and their consideration led to a wider understanding of the method. Summing up, the project has been a rewarding experience for all project participants – both in scientific and social/cultural dimensions. More than that, it shows important aspects for future studies and possible follow-up projects.

Project Participants

The following persons have used the funding allocated to cover their costs of travel and stay:

List of participants (BUT)

- Academics : Jiří Kunovský, Václav Šátek
- Students : Filip Kocina, Gabriela Nečasová, Jan Chaloupka, Petr Veigend, Alžběta Martinkovičová, Václav Valenta

List of participants (VUT)

- Academics: Martin Kozek, Alexander Schirrer
- Students: Michaela Killian, Emir Talic, Nico Didcock, Nikolas Euler-Rolle, Elisabeth Luchini, Elvira Thonhofer, Maja Miletic

Project Outcomes and Activities

Achievement of Principal Project Goals

- Close cooperation, both in scientific and in personal aspects has been initiated and established between BUT and VUT.
- Modern Taylor Series algorithms have been development and extended, especially targeting the efficient integration of stiff and high-order systems, as well as systems with discontinuous dynamics. The application of MTSM to stiff systems, discontinuous dynamics, and high-order systems could be demonstrated by new developments and first implementation onsets. Numeric tests unveiled key bottlenecks in the current software packages and enables targeted continued software development of MTSM solvers. Concepts to support and efficiently solve systems with discontinuous dynamics have been studied and cast into proof-of-concept implementations. Furthermore, the development of implicit MTSM showed significant benefits over explicit onsets in stiff problems.
- Ph.D. students of both institutions have been brought together for discussions, education, as well as social activities. They introduced many valuable aspects to the scientific discourse by relating their respective dissertation research work to Modern Taylor Series onsets, and vice-versa, they could benefit from mutual exchange and a common discussion platform in their path towards their dissertations.
- Specialized ECTS-recognized lectures and courses, held by researchers of both institutions have been organized and frequented by graduate students as well as undergraduates. These courses also included seminar-style parts to amplify the exchange of ideas in open discussions.

Technical Achievements

The research teams of both universities were supported by two long-term internships of postdoctoral fellow Dr. Vaclav Satek at TU Vienna (covered by this AKTION project as well as project CZ.1.07/2.3.00/30.0055, "New creative teams in priorities of scientific research" led by VŠB-Technical University of Ostrava). In this setup, the team researched methodologies and developed solutions for application problems modelled by high-order differential equations via the MTSM method and its variants. Surprisingly good results have surfaced: already the first draft implementation of solving a high-order mechatronic application problem with MTSM in MATLAB has outperformed MATLAB's standard (state-of-the-art) ODE solvers (ode23, ode45) by runtime factors of 2 and more, while yielding higher precision.

The treated application problem from mechanical engineering is the model of a railway catenary in dynamic contact with a pantograph current collector multi-mass model. The numeric formulation leads to large systems of ordinary differential equations (obtained by finite-difference approximation of the describing partial differential equations in space). Various problem sizes, up to about 200 variables, have been studied and analysed, yielding highly promising results.

Next, the focus has been laid on efficiency improvement, treatment of stiff systems and the preparation of the publication of the method's performance in a high-impact journal. Code optimization enabled additional, significant performance improvements. Also, the implicit variant of the solver provides high performance and outperforms MATLAB's standard (state-of-the-art) implicit ODE solvers (e.g., ode15s, ode23s) by runtime factors of 100 and more, depending on the test problem.

The publication of these significant results has been conceptually prepared (structure, literature review), test cases have been defined, and the paper body has been drafted as of the end of the AKTION project. One suitable benchmark application problem is the mentioned model of a railway catenary in dynamic contact with a pantograph current collector multi-mass model. The resulting high-order systems of ordinary differential equations (including the modelling of the pantograph contact) could be handled in an implicit manner efficiently which justifies testing the implicit solver with this particular example.

Technical Goal	Achievement	Status
Assessment of MTSM-solver interface with MATLAB	Identified bottlenecks in interface, decision to implement concrete MTSM solution directly in MATLAB	Fulfilled
Develop MTSM solution for high-order application problem	App. problem solved, accuracy and cpu time better than with state-of-the-art reference ODE solvers	Fulfilled
Efficiency improvement of the linear systems MTSM solver in MATLAB	Code optimization and streamlining has been done, resulting in a significant further speedup compared to initial implementation	Fulfilled
Development of stiff systems MTSM solver for linear systems in MATLAB	Implicit solver has been developed for linear systems, code optimizations have been propagated from explicit solver codebase, high performance could be achieved in first tests	Fulfilled
Conceptual preparation of journal article on the achieved MTSM	Results have been structured, article concept has been developed, a detailed literature study has been	Fulfilled

algorithm performance	performed, and simulation tasks for code demonstration have been identified

Project Activities

The project activities notably include:

- Short lectures held by J. Kunovsky (BUT), V. Satek (BUT) at VUT
- Short lectures held by M. Kozek (VUT) and A. Schirrer (VUT) at BUT
- Bi-lateral, scientific presentation series given by participating students at BUT and VUT
- Course "Efficient numerical integration methods" at VUT with numerous participants

- Algorithmic studies of partial differential equation (PDE) approximation methods to high-order ordinary differential equations (ODEs), ODE solution by the MTSM, and extension of the MTSM approach by suitable pre-processing techniques to address PDE problems with varying structure, high order, discontinuities, and stiffness.
- Development of test problems to demonstrate and test these features.
- Quantification of MTSM performance, numeric properties, limitations, and strengths in these application areas.
- Analysis of applicability of the MTSM to various application problem settings, such as flexible vibrations of train overhead lines, computational fluid dynamics problems, or heat network system models.

- Joint consultations and creation of the TKSL-MATLAB software

- Review on the Doctoral Thesis of Diplomingenieur Maxime Deregnaucourt titled „Efficient Data-Driven Modelling of Constrained Nonlinear Processes"

Joint Publication Work

ICNAAM 2014 conference:

Multiple Integral Computations Using Taylor Series
Chaloupka J., Kunovský J., Martinkovičová A., Šátek V., Thonhofer E.
In: Proceedings of the 12th International Conference of Numerical Analysis and Applied Mathematics, Rhodes: American Institute of Physics, 2014, ISBN 978-0-7354-1287-3

Abstract. The paper is a part of student cooperation in AKTION project (Austria-Czech) and deals with possibilities of numerical solution of initial value problems of ordinary differential equations (ODEs). The Taylor series method with automatic computation of higher Taylor series terms is used for solution of multiple integrals.
A Multiple integral of a continuous function of n variables can be computed by n-ary integration of the function fixing the remaining variables. These simple integrals can be solved as a ODEs, thus introducing a problem of parallel solving of a growing number of equations with respect to n and the required precision.

New Trends in Taylor Series Based Computations
Kocina F., Kunovský J., Marek M., Nečasová G., Schirrer A., Šátek V.
In: Proceedings of the 12th International Conference of Numerical Analysis and Applied Mathematics, Rhodes: American Institute of Physics, 2014, ISBN 978-0-7354-1287-3

Abstract. The paper is a part of student cooperation in AKTION project (Austria-Czech) and concentrates on the numerical solution of partial differential equations (PDEs) using high-order forward, backward and symmetrical formulas. As an example, the hyperbolic PDE is analyzed. The paper is based on the numerical solution of ordinary differential equations by the Taylor series method and on the simulation language TKSL that has been created to test the properties of the technical initial problems and to test an algorithm for Taylor series method. The idea of parallel computations using special integrators is also a part of the paper.

MATHMOD 2015 conference:

Taylor Series Based Solution of Linear ODE Systems and MATLAB Solvers Comparison
Šátek V., Kocina F., Kunovský J., Schirrer A.
In: *MATHMOD VIENNA 2015 - 8th Vienna Conference on Mathematical Modelling*. Vienna: ARGE Simulation News, 2015, ISBN 978-3-901608-46-9

Abstract. The Modern Taylor Series Method (MTSM) is employed here to solve initial value problems of linear ordinary differential equations. An automatic computation of higher Taylor series terms and an efficient, vectorized coding of explicit and implicit schemes enables a very fast computation of the solution to specified accuracy. For a set of benchmark problems from literature, the MTSM significantly outperforms standard solvers.
Finally, ideas of parallelizing the MTSM computations are discussed.

Multiple Integral Computations Using Taylor Series
Nečasová G., Kunovský J., Šátek V., Chaloupka J., Veigend P.
In: *MATHMOD VIENNA 2015 - 8th Vienna Conference on Mathematical Modelling*. Vienna: ARGE Simulation News, 2015, ISBN 978-3-901608-46-9

Abstract. The paper is a part of student cooperation in AKTION project (Austria-Czech) and concentrates on numerical computations using high-order forward, backward and symmetrical formulas. As an example, the hyperbolic PDE is analyzed, together with multiple integral computations. A multiple integral of a continuous function of n variables can be computed by n-ary integration of the function fixing the remaining variables.

Brno, 10. 7. 2015

Doc. Ing. Jiří Kunovský, CSc.