AKTION project no. 64p13 - final report

# Synopsis

The AKTION project no. 64p13 (“Efficient Application of Modern Taylor Series Methods to Stiff and High-Order 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 2nd July 2012 – 30th June 2013. 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, Josef Dalík, Karel Mikulášek
* Students : Václav Vopěnka, Filip Kocina, Lenka Turoňová, Patricia Humenná, Hana Pluháčková, Jan Chaloupka, Alena Obluková, Alžběta Martinkovičová

## List of participants (VUT)

* Academics : Martin Kozek, Alexander Schirrer
* Students : Raphael Priesner, Stefan Grosswindhager, Michaela Killian, Markus Deutsch, Emir Talic, Nico Didcock, Nikolas Euler-Rolle

# 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 developed 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.

## Project Activities

The project activities notably include:

* Short lectures held by J. Kunovsky (BUT), V. Satek, and J. Dalik (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 onset 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 attendancy of VUT and BUT participants at the HPCSE 2013 workshop (“High Performance Computing in Science and Engineering”) in Czech Republic (<http://spomech.vsb.cz/hpcse/>)
* Joint consultations and creation of the TKSL-MATLAB software

## Joint Publication Work

ICNAAM 2012 conference:

[Stiffness in Technical Initial Problems](http://www.fit.vutbr.cz/%7Esatek/pubs.php?id=10088&shortname=1)

Kunovský, J., Šátek, V., Vopěnka, V., Schirrer, A.

In: Proceedings of the 10th International Conference of Numerical Analysis and Applied Mathematics, Kos, GR, AIP, 2012, s. 4, ISBN 978-0-7354-1091-6, ISSN 1551-7616

**Abstract.** Technical initial problems are defined as initial problems where the right-hand side functions of the system are those occurring in the technical practice, that is functions generated by adding, multiplying and superposing elementary functions. Such systems can be expanded into systems with only rationals operations on the right-hand sides of the equations. In such a case the Taylor series terms can easily be calculated . Test examples are presented in the paper. Stiffness in technical initial problems can be eliminated by the TKSL software and solved by the direct use of the explicit and implicit Taylor series methods.

HPCSE 2013 conference:

Modern Taylor Series Method

Kunovský, J., Šátek, V.

presented as poster

### Publications in review process:

ICNAAM 2013 conference:

Adaptive solution of Laplace equation

Václav Valenta, Václav Šátek, Jiří Kunovský and Patricia Humenná

**Abstract:** The paper is a part of student cooperation in AKTION project (Austria-Czech). Method of aposteriori error estimation based on weighted averaging to improve initial triangulation to get better solution of the planar elliptic boundary-value problem of second order and numerical illustrations of the method are presented in the paper.

Taylor Series Based Computations and MATLAB ODE Solvers Comparisons

Václav Šátek, Jiří Kunovský, Filip Kocina and Jan Chaloupka

**Abstract:** The paper is a part of student cooperation in AKTION project (Austria-Czech). Taylor series method for solving differential equations represents a non-traditional way of a numerical solution. Even though this method is not much preferred in the literature, experimental calculations done at the Department of Intelligent Systems of the Faculty of Information Technology of TU Brno have verified that the accuracy and stability of the Taylor series method exceeds the currently used algorithms for numerically solving differential equations.

The paper deals with possibilities of numerical solution of Initial Value Problems of Ordinary Differential Equations (ODEs) - using the Taylor series method with automatic computation of higher Taylor series terms.

The explicit and implicit scheme of Taylor series method is compared with numerical solvers implemented in MATLAB software. The computation time and accuracy of our approach are compared with that of MATLAB ode solvers on a set of ODEs test examples.

ICNAAM 2013 conference (continued):

Parallel Computations Based on Automatic Transformation of Ordinary Differential Equations

Jan Kopřiva, Jiří Kunovský, Václav Šátek, Martina Drozdová and Alexander Schirrer

**Abstract:** The paper is a part of student cooperation in AKTION project (Austria-Czech).

Theoretical work on the numerical solution of ordinary differential equations by the Taylor series method has been going on for a number of years. The simulation language TKSL has been created to test the properties of the technical initial problems and to test an algorithm for Taylor series method.

The Residue Number System (RNS) has great potential for accelerating arithmetic operation, achieved by breaking operands into several residues and computing with them independently.

INFORMATICS 2013 conference:

Parallel system based on the RNS

Jan Kopriva, Jiri Kunovky, Martina Drozdova, Vaclav Satek, Michaela Killian

**Abstract:** The Residue number system (RNS) is an unposition system based on a modular arithmetic. The main benefit of this system is the binary computation without using a carry bit (well-known for example in hardware representation). Parallel computation can easily be completed. The second benefit of this system is the integer computation without rounding off. This paper proposes our parallel system, which is able to use RNS and makes arithmetic operation using CPU and the GPU. Widely used transformations from binary numbers to RNS and back are presented in the paper.

Numerical integration in the RNS

Jan Kopriva, Jiri Kunovsky, Filip Kocina, Vaclav Satek, Emir Talic

**Abstract**: The Residue Number System (RNS) usually uses the integer numbers. The computation is exact from this reason. As some problems like solutions of ordinary differential equations (ODE) are unsolvable without modification, this paper proposes a transformation from the integer binary RNS to the floating point

binary RNS. The computation using the floating point numbers is exact after the transformation. Solutions of ODEs are presented in the paper. One-step integration methods (Euler, Heun, Runge-Kutta) are adapted to RNS to solve simple ODEs with exact precision.