

Final Report  
of the  
STSM at Budapest University of Technology  
and Economics

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## **Purpose of the STSM**

This Short Term Scientific Meeting was a visit whose main aim was to collaborate with Professor Boglárka G.-Tóth at the Budapest University of Technology and Economics, Hungary, on Interval Analysis Techniques used in Nonlinear Programming in order to solve Inverse Problems. I had been working with her in the past, so the scientific plan was to carry on with the topics previously studied and to develop new tools which may lead to publications in prestigious and high-impact journals in Operations Research.

## **Description of the work carried out during the STSM**

Global optimization of inverse problems with ordinary differential equations (ODEs) in the constraints are key methods in energy production, in particular in those focusing on chemical reaction networks. One problem which we already investigated is how to find the chemical kinetic model that best describes a given reaction network. When there are many such models, it is not easy to choose the real one.

The optimization problem we wanted to solve is to find the time instant  $t$  that maximizes the difference of possible chemical kinetic models. In order to get a reliable result, we aimed to use a Branch and Bound algorithm and interval analysis techniques. Due to the chemical laws, the evaluation of the objective function implies to solve ordinary differential equations (ODEs). That increases dramatically the computational time of the algorithm.

## **Description of the main results obtained**

We have first made a deep analysis on the literature in order to find existing open-source software that allow us to solve ODEs in a short period of time reliably. The chosen software was VNODE-LP written by Ned Nedialkov at the McMaster University in Canada. It is developed in C++ and allow us to solve Initial Value Problems in a reasonable time. Furthermore, it gives apriori interval bounds of the solution that can be used for the Branch and Bound strategy. The algorithm implemented in the software does not allow us to provide the stepsize which is used in the resolution of the ODE but it computes it automatically. For this reason, we had to define our own procedures so that the stepsize can be specified. Some equations are tested with this new method obtaining satisfactory results in case when the stepsize is small enough.

Secondly, new bounds for the Branch and Bound method are designed. These bounds are based on the first order Taylor approximation. For this purpose an ODE with a larger dimension (it includes the solution of the equation and its derivative) must be solved. We have compared both bounds in some instances, and we can conclude that in most of the cases the Taylor approximation is better than the one obtained by the algorithm, however at a higher computational cost.

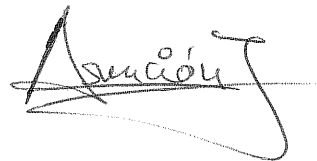
### **Future collaboration with the host institution**

The first point will be to finish the research topics already open. The Branch and Bound method should be tested with more examples and we have to make improvements in its design in order to extend it to other models. I am optimistic about future cooperation with Boglárka G. Tóth in order to study, not only this type of problems, but also others in which Interval Analysis can be applied.

### **Foreseen publications resulting from the STSM**

It is my hope that, the research done during my stay leads at least one paper in prestigious journals on Operations Research.

Sevilla, 2nd of March, 2015.



M. Asunción Jiménez-Cordero  
Visitor, University of Seville

## **Confirmation by the host institution of the successful execution of the STSM**

I have read the final report written by Asunción Jiménez-Cordero describing her STSM visit at the Budapest University of Technology and Economics to collaborate with my research group. I am extremely satisfied with the results of the visit. We have successfully cooperated in some challenging MINLP problems, and I hope this fruitful cooperation will continue in the future as well. We will write and submit a paper discussing the results obtained from her visit and then we will plan further research lines, possibly involving other researchers as well.

Budapest, 4th of March, 2015.



Boglárka G.-Tóth  
Host, Budapest University of Technology and Economics