

Scientific report for ESF grant 5697

Aram Markosyan

1. Purpose of the visit

The purpose of the visit was to continue work on PumpKin package and look at first results with Dr. Francisco J. Gordillo Vázquez, Granada, Spain.

2. Description of the work carried out during the visit

During the first visit to Dr. J. Gordillo Vázquez, Dr. A. Luque and I specified exact topic “determining of all significant pathways in chemical reaction systems”. After long discussions we come up with an algorithm and I started a practical implementation of it. The work is still in progress. The motivation was the following: when the output of a complex chemical model is analysed, a typical topic is the determination of pathways, i.e., reaction sequences, that produce or destroy a chemical species of interest.

During this visit we already start to look at first results and discuss future application areas. The first results were quite promising and we made plans for future work.

3. Description of the main results obtained

We obtained quite promising preliminary results indicating that algorithm is working. PumpKin software is already fully written.

4. Future collaboration with host institution

We are in active collaboration now. In future we plan one more visit to host institution in order to discuss the results and future publications.

5. Projected publications / articles resulting or to result from the grant

As mentioned in the sections 3 and 4, the first results are very good and should be polished further.