

# Scientific report for ESF grant 5698

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## **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 looked at first results and discuss future application areas. The results are promising and we made plans for future work.

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

We obtained quite promising results, which I will present during international conference ICPIG 2013. 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 results are very good and should be polished further.