Supervisor's assessment of the PhD candidate Anna Zhyrova

Anna Zhyrova started her PhD studies in December 2011. She started the project on the experimental analysis of the Belousov-Zhabotinsky reaction under mechanical and technical constraints. The motivation of this project were findings obtained in our early experiments which showed that different geometries of the reaction vessel cause different course of the reaction. Also, our team has developed a method of point information gain (PIG), point information gain entropy (PIE), and point information gain entropy density (PIED) calculation which enabled characterisation of multidimensional structured dataset in a way similar to the characterisation of the homogeneous solution by the physico-chemical parameter Gibbs energy. The task of Anna Zhyrova was challenging in all aspects.

The main condition for correct data analysis is to obtain correct data. A source of data for special distributions of intensities is a digital camera. Practically all data providing information on the spatial distribution of structures in chemical self-organising systems were photographic cameras, in some cases digital cameras. In all reported cases, the analysis was performed using 8-bit compressed images. The research of Anna Zhyrova was performed along with gradual understanding of the technical limitations of existent camera technology in our team.

The thesis of Anna Zhyrova is focused on the examination of the Belousov-Zhabotinsky reaction state trajectory in the space characterised by the point information gain entropy (PIE) and point information gain entropy density (PIED) state space. The general reason was to have a logical and reproducible natural multifractal dataset for examination of properties of these variables. The variable PIE and PIED were derived to provide the most general characteristics of a structured dataset. The most general assumption about such a dataset is that it is multifractal. For this reason, the Rényi entropy was used for calculation which is in close relation to the generalised dimension of the multifractal dataset. However, in the given experimental dataset, the values of PIE_α and $PIED_\alpha$ have to be understood only as heuristic measures as in a similar way when the concentrations of individual compounds represent heuristic measures of activities of these compounds. Or, reaching farther to the experimental reality, as intensities of individual spectral lines characterise concentrations and concentrations characterise activities. Among the possible ways how to make sense of the heuristic multidimensional dataset the principal component analysis was chosen.

The main part of the work of Anna Zhyrova was experimental. She performed a multitude of experiments and analysed them with great care using a PIE_α and $PIED_\alpha$ calculating software and standard tools of multivariate analysis. She was a great tester of our software and contributed to many developments. She also had to repeat the experiments frequently as the technology progressed. And the latest results, which are depicted also on the cover of the thesis and are technically correct as far as contemporary technology allows, are still awaiting publication. The best approximation to the free, i.e. mechanically unobstructed performance of the experiment is the experiment in a 200-mm Petri dish initiated by slow mixing using an orbital shaker. In this case, the effect of vessel's borders was observed only in the later stage of the reaction and the development of the structures may be completely analysed. All smaller

vessels and vessels of different shapes as well as different ways of mixing induced changes in the reaction course. The technical substantiation of the correct and reproducible performance and capture of the Belousov-Zhabotinsky reaction is the first big contribution of Anna Zhyrova.

The next step was the principle component analysis of the Belousov-Zhabotinsky reaction. From the first attempt, it was possible to find a combination of statistical weights to the different PIE_α and $PIED_\alpha$ values which constructed coordinates describing the dataset by three principle components for more than 90 % of the data. And, in this new space, it was possible to construct a trajectory which logically follows the course of the reaction.

The comparison of the latest results, which are unambiguously technically correct and also intelligible on the first sight, with the majority of results published in the thesis nicely illustrates the distortion introduced to the data by the photographic camera. From the beginning of the work on the thesis it was clear that it is necessary to work with so-called raw data format, i.e., typically 12-bit dataset stored by the camera. Until spring 2016, when we installed the camera with house-made control software, we were not aware how big distortion of the reality is caused by the transformation of the original 14-bit dataset to the 12-bit RAW dataset by those parts of the photographic camera which escape the control of the operator. Thus, finally, Anna Zhyrova obtained technically correct records of the numerous experiments which allow us to examine properties of PIE_α and $PIED_\alpha$ in the characterisation of a natural multifractal object evolving along a natural trajectory. This analysis provides exciting results and is still going on.

I feel obliged to apologise to Anna Zhyrova for giving her a seemingly simple but after all a very complicated task. She did a very valuable work which, to our understanding, has not been done at the level of technical correctness anywhere in the world over 60 years of the examination the chemical self-organisation. I fully recommend her thesis for the defence.

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