



**FACULTY
OF MATHEMATICS
AND PHYSICS**
Charles University

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Doctoral Thesis – Advisor’s reference

Miroslav Kratochvíl: High-performance exploration and querying of selected multi-dimensional spaces in life sciences

There are two main topics of the thesis: Structure-based search and visualization of multi-dimensional data. Both the topics arose from real-life problems in chemistry, biology, and medicine while the author was, in both cases, a valuable member of interdisciplinary scientific teams. As a result, the thesis is not a classical monography in computer science but rather a piece of applied computer science in the two fields of chemical search and biomedical visualization.

Nevertheless, there is still a lot of pure computer science behind the scenes – the graph theory that forms the base of structure search as well as the Self-Organizing Maps involved in the visualization. Above these theoretical foundations, the thesis focuses on the computational performance of the software involved – the inverted indexes for the search and a parallel implementation for the Self-Organizing Maps. Finally, there is also a software-engineering part related to the integration of both systems into the software ecosystems being developed in their respective communities.

Besides the underlying computer science, the main value of the thesis is its interdisciplinary character and the fact that its results are immediately useful in the chemical and biomedical research. It also shows that the author is not only a computer scientist but has also acquired the necessary understanding of the other science fields involved in the respective areas.

In addition, a part of the underlying work by the author was also successfully employed in information retrieval, as evidenced by the winning entry of the SOM method in the Video Browser Showdown, part of the respected MMM 2020 conference.

All the theory, methods, software, and experiments presented in the thesis were already published, mostly in respected interdisciplinary journals. As it may be expected in such research, all the articles have several authors; however, the author of this thesis was always the main contributor in the computing part and, in most cases, also the main author of the article. This fact justifies the organization of the thesis, which is partly composed from reprints of these articles.

The author was also involved in international research community, including an internship in the Bioinformatics group of Prof. Reinhard Schneider in Luxembourg.

The author has also demonstrated his pedagogical skills during several seasons of teaching C++ and Haskell, always receiving enthusiastic remarks in students' polls.

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I think that the thesis, the publications, the scientific activity as well as teaching duties show that Miroslav Kratochvíl is a valuable member of academia. Therefore, I recommend the thesis for defense as well as awarding the PhD degree to the author.

David Bednárek
advisor