PhD position - Department of Mathematics, University of Innsbruck

We are looking to fill a PhD position in the project 'Hierarchical dynamical low-rank approximation for the chemical master equation'. The successful applicant will be employed as a 'Doctoral candidate' within the doctoral college DK CIM [2] and will work on algorithmic improvements of hierarchical dynamical low-rank algorithms, their efficient implementation, and application to biochemical reaction networks. Potential candidates are encouraged to directly contact the PI of the project (lukas.einkemmer@uibk.ac.at). Applications can be submitted via https://lfuonline.uibk.ac.at/public/karriereportal.details?asg_id_in=12596 and more details on the dissertation project can be found below.

[1] https://www.uibk.ac.at/mathematik/na/
[2] https://www.uibk.ac.at/dk-cim/index.html.en

The full, legally binding call for application (in German) including the salary can be found here: https://lfuonline.uibk.ac.at/public/karriereportal.details?asg_id_in=12596

Project summary:
Understanding the processes that determine the behavior of tumor cells is an important aspect of cancer research and drug development. Due to the enormous complexity of a cell, it is virtually impossible to gain an understanding without the help of computer simulation based on mathematical models. The models used are formulated as reaction networks and the corresponding dynamics are governed by the chemical master equation (CME). The main problem in performing accurate simulations of such systems is that the dimension of the phase space is equal to the number of species considered.

The exponential growth of computational effort in the number of dimensions (the so-called curse of dimensionality) makes such simulations extremely expensive. As a result, collecting detailed statistics for many large-scale biological systems still requires resources beyond what current and, most likely, future (super)computers can provide. Therefore, it is state of the art to omit the stochastic information given by the chemical master equation and to describe the biological system by its average behavior. However, it is well known that such an approach misses a range of important phenomena that are critical to understanding cell dynamics.
In this doctoral thesis, we will develop an efficient hierarchical DLR approximation for the chemical master equation. Such an approach splits the network into two (or more) subnetworks. A reaction within such a subnetwork is treated exactly while the interaction between them is treated by the low-rank approximation.

The process is then repeated (if necessary, depending on the size and characteristics of the network) in a hierarchical manner. Since most reaction networks in cell biology have a modular structure, they fit very well within such a hierarchical low-rank approach. A further challenge is how to automatically partition the network. That is, how to choose the subnetworks such that the error and thus the computational effort is minimized. This has to be done on a problem per problem basis and therefore automation of this task is crucial. The numerical algorithms developed will be implemented as part of our open-source DLR framework Ensign, which can effectively exploit modern computer hardware such as graphic processing units (GPUs).