2020 HGF – OCPC – Programme

for the involvement of postdocs in bilateral collaboration projects

Title of the project:

Development of adaptive machine-learning and tensor-network approximations for quantum simulations of nuclear motion dynamics in weakly bound clusters

Helmholtz Centre, division/group:

DESY, CFEL Controlled Molecule Imaging (FS-CFEL-CMI)

Project leader:

Dr. Andrey Yachmenev

Contact Information of Project Supervisor:

andrey.yachmenev@cfel.de, +494089986304

Web-address:

http://controlled-molecule-imaging.org
https://www.desy.de

Department/Group:

Center for Free Electron Laser Science (CFEL)
Controlled Molecule Imaging Group

Programme Coordinator (Email, telephone and telefax)

Dr. Frank Lehner
DESY Head of Directorates Office
Phone: +49 40 8998 3612
Email: frank.lehner@desy.de

Description of the project (max. 1 page)**:**

first principles simulations of the hydrogen-bond dynamics in molecular complexes with water is one of the most interesting, computationally challenging, and accuracy demanding problems in computational physics. Accurate simulations of molecular and chemical dynamics in weakly-bound complexes with water are crucial for the development of improved experimental protocols, elucidation of acquired data, and the unraveling of the underlying chemistry motifs. The development

of rigorous variational approaches to nuclear motion dynamics of polyatomic molecules enables the accurate theoretical modeling of simple cluster systems. However, the exponential scaling of the computational burden with the number of degrees of freedom, i.e., cluster size, renders the computational costs of existing variational methods unaffordable for clusters composed of more than two molecules.

The goal of this project is to explore and implement the paradigms of *tensor-network* and *machine-learning* to mitigate or break the curse of dimensionality in variational calculations of larger clusters.

The development of methods that allow to mitigate or even break the curse of dimensionality is currently a very active filed of research. One of the most successful paradigms, that has in recent years been developed in numerical linear algebra, is based on the approximation of high-dimensional objects by low-rank tensor decompositions, the so-called tensor network (TN) representations. To make efficient use of TN, the variational methodologies for solution of the nuclear time-dependent Schrödinger equation need to be reformulated for the tensor algebra in a framework of massively parallel computations.

More recent concepts to circumvent the curse of dimensionality rely on geometrical and topological methods for nonlinear dimensionality reduction and on kernel-based approximation methods. In either case, such methods need to be motivated by *some* physical or chemical intuition. The main idea is to choose the ingenious reduced set of dimensions (coordinates) that are most significant for the dynamics of interest. The curvilinear valence-bond coordinates have shown to work best for molecules with strong covalent bonds, however they are not prompted to describe floppy motions in complexes only weakly bound by hydrogen bonds, dispersion forces, or dipole-dipole interactions. Assuming that a better set of coordinates exist, it is desirable to develop an adaptive method and the corresponding algorithms to identify and separate the significant coordinates from the negligible once. Such a reduced set will result in computational savings without compromising the desired accuracy. Most recent concepts successfully developed for the problems of nonlinear dimensionality reduction rely on manifold learning algorithms, such as isomap or Riemannian normal coordinates (RNC). Moreover, kernel-based approximation methods provided powerful algorithms for adaptive data analysis and machine learning. Successful application of the machine learning to molecular dynamics problem will require development of non-standard kernels based on molecular descriptors, which is an interesting and challenging task on its own.

The TN methods using matrix product states and matrix product operators count among the most successful approached to numerically simulating the many-body quantum systems. One of the challenges that need to be addressed to foster tensor algebra in the nuclear quantum dynamics is to reconsider the Krylov subspace algorithms for the TN formalism of matrix product operators. The Krylov methods are crucially important in quantum dynamics, as they are extensively used to perform linear algebra operations on sparse matrices.

Description of existing or sought Chinese collaboration partner institute (max. half page)**:**

We would like to collaborate with the group of Pavlo Dral at State Key Laboratory of Physical Chemistry of Solid Surfaces (PCOSS), Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, Department of Chemistry College of Chemistry and Chemical Engineering Xiamen University. The group of Pavlo Dral are experts in the development and applications of machine-learning algorithms to the problems of quantum chemistry, which are closely related to the challenges addressed in this project.
Hover, independent applications are also welcome.

Required qualification of the post-doc:

- PhD in physics, theoretical chemistry, applied mathematics, computer science, or related field
- Experience with programming, e.g., C, C++, Python, (Fortran)
- Additional skills with machine-learning, linear algebra, tensor-network methods
- Language requirement: fluency in English