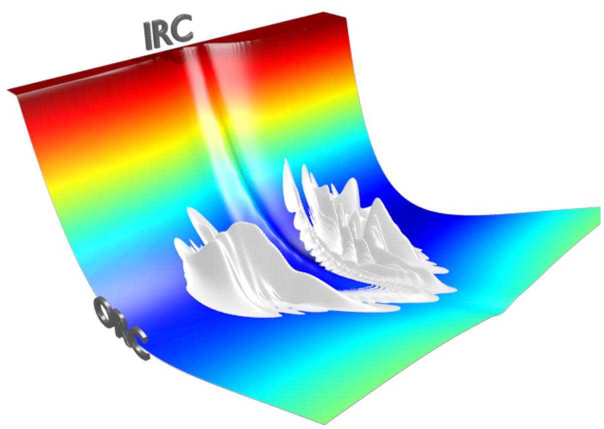
Master thesis project description:
“Radial basis functions for solving the Schrödinger equation in large quantum systems”

For the understanding of chemical reactions or the interactions with ultrashort laser pulses one has to treat molecules as quantum mechanical objects. The challenge with this very accurate theory is the curse of dimensionality which comes along with the concept of the wave function.
Radial basis function (RBF) approximation [1] seems to be a promising candidate for the solution of the Schrödinger equation in higher dimensions [2]. They serve as a mesh free description for the wave function which provides flexibility with respect to the computational domain. Moreover a good scaling behavior with the dimensionality is expected since only the distance between node points has to be calculated. However to obtain an efficient method the resulting matrices which are used in the algorithm must become sparse. To reduce the interactions in the computational domain and thus to obtain sparsity, two different methods are considered: RBFs in finite difference mode, which is a generalization of finite differences to scattered nodes, and the partition of unity approach, which is a type of domain decomposition approach.
Part of the thesis work should be to investigate the error and convergence behavior of at least one of both approaches.



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References:
[1] G. E. Fassauer, Meshfree Approximation Methods with MATLAB
[2] K. Kormann and E. Larsson, “Radial basis functions for the time-dependent Schrödinger equation”, AIP. Conf. Proc.: ICNAAM 2011, **1389**, 1323 (2011).