Efficiency of the energy transfer in the FMO complex using hierarchical equations on Graphics Processing Units

TOBIAS KRAMER, CHRISTOPH KREISBECK, University of Regensburg, Germany, MIRTA RODRIGUEZ, IEM CSIC, Madrid, Spain, BIRGIT HEIN, University of Regensburg, Germany — We study the efficiency of the energy transfer in the Fenna-Matthews-Olson complex solving the non-Markovian hierarchical equations (HE) proposed by Ishizaki and Fleming in 2009, which include properly the reorganization process. We compare it to the Markovian approach and find that the Markovian dynamics overestimates the thermalization rate, yielding higher efficiencies than the HE. Using the high-performance of graphics processing units (GPU) we cover a large range of reorganization energies and temperatures and find that initial quantum beatings are important for the energy distribution, but of limited influence to the efficiency. Our efficient GPU implementation of the HE allows us to calculate nonlinear spectra of the FMO complex. References see www.quantumdynamics.de