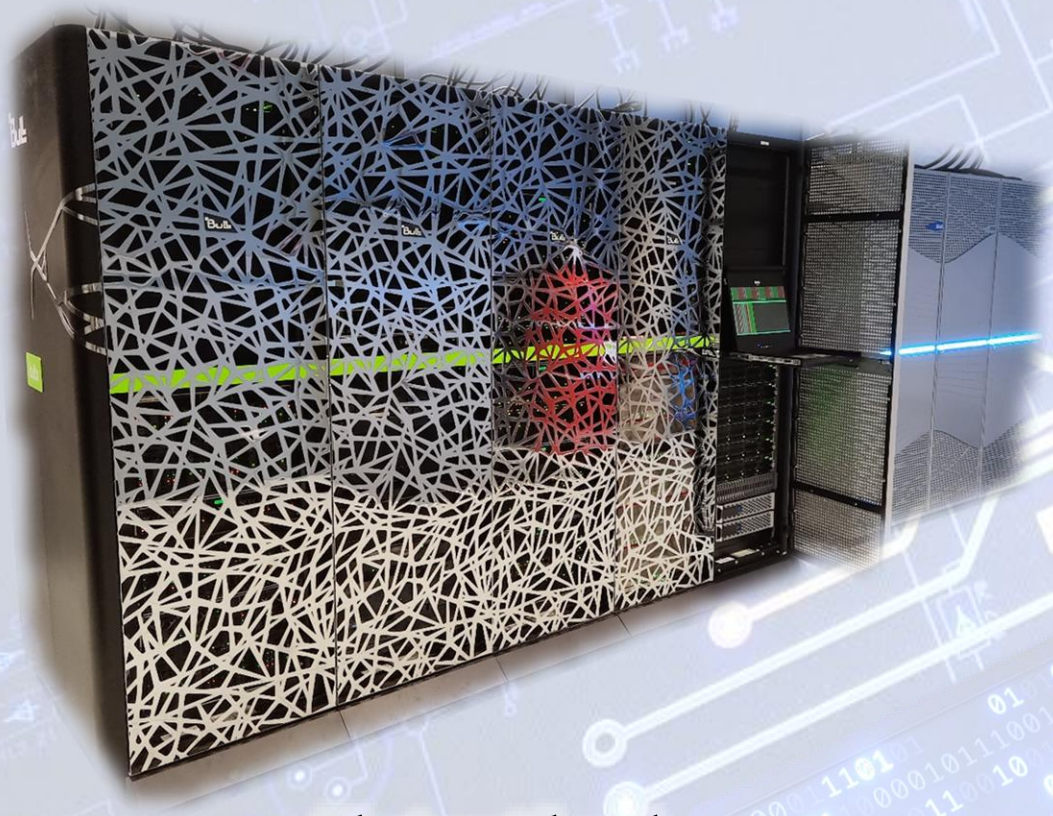
3RD EUROCC VILNIUS WORKSHOP ON USING HPC



Abstract book

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VILNIUS TECH

Lietuvos hidrometeorologijos tarnyba

Complete Non-adiabatic Exciton Hamiltonian for Photosynthetic Pigment-Protein Complexes

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One of the core processes of photosynthesis is the “collection of light” through multi-pigment light-harvesting antenna complexes. A vast diversity of photosynthetic pigments and light-harvesting complexes has evolved, what adapted the process to occur both in water and on land and it can be found in many bacteria, algae and plant species. In this work, we extend the standard exciton model typically used to calculate the Hamiltonian of the light-harvesting complexes. We incorporate the novel environment-induced non-adiabatic inter-molecular couplings and use the resulting Hamiltonian to calculate the variation of absorption spectra of two different light-harvesting complexes: Fenna-Matthews-Olson and fucoxanthin-chlorophyll binding protein using their crystallographic protein structures. To achieve this, pigments ground and first two excited states were modeled at QM level using GAUSSIAN[1] software with DFT/TD-DFT methodology with CAM-B3LYP functional and 6-31G(d) basis set, while their transition energies were adjusted due to electrostatic interaction with proteins. The non-adiabatic excitonic Hamiltonian was then used to calculate exciton relaxation rates, their lifetimes and the absorption spectra of the complexes. Spectra of pigments *in vacuo*, in a protein environment with different force-fields and in a protein environment with addition of ions in case of adiabatic and non-adiabatic (including ground state of pigments) couplings were compared. The results demonstrate that the excitonic non-adiabatic amplitudes lead to finite exciton lifetime, they shift absorption spectra to higher energies and induce variation of the spectral shape.

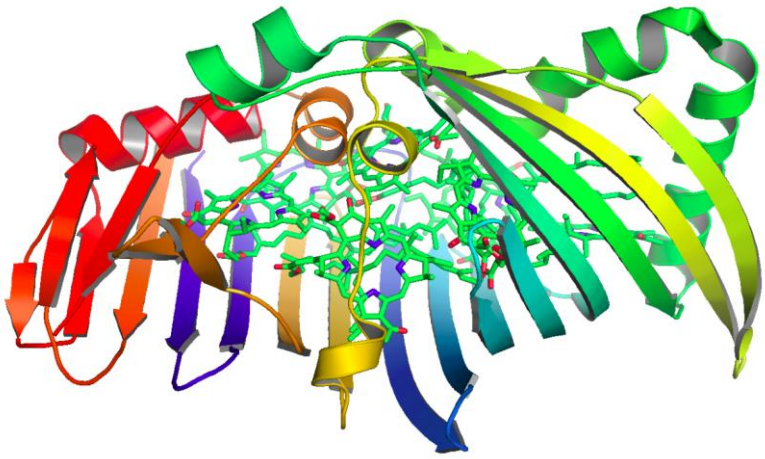

Fig. 1. FMO pigment-protein complex structure.

REFERENCES

[1] M. J. Frisch et al., GAUSSIAN 16, Gaussian Inc. Wallingford CT, (2016).