Microscopic modelling of the highly efficient intra- and inter-antennae energy transfer to the reaction centre in plant photosystem II

Reporting

Project Information

MicroMod-PSII

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Periodic Reporting for period 1 - MicroMod-PSII (Microscopic modelling of the highly efficient intra- and inter-antennae energy transfer to the reaction centre in plant photosystem II)

Reporting period: 2017-04-01 to 2019-03-31

Summary of the context and overall objectives of the project

The research project MicroMod-PSII focussed on natural photosynthesis in plants. The development of photosynthesis was one of the key steps for the evolution of higher forms of life on earth providing nutrition to the predominant majority of living organisms. During photosynthesis, light energy from the sun is collected by antenna proteins and processed via multiple steps by highly specialized protein machineries. In the first step, so-called antenna proteins capture the light and transmit its energy to the reaction center of photosystem II. The latter performs the initial transformation to store the energy in a chemical way. The capturing and transmission of light energy is a delicate process which requires specialized molecules – the chlorophylls – and moreover, a precise arrangement of these chlorophylls. The protein machineries involved in photosynthesis arrange hundreds of chlorophylls in such an optimized way that almost every excitation event is successfully transmitted to the reaction center. Remarkably, this high efficiency occurs in a flexible material – the leafs – which has to continuously adapt to the light conditions.
Artificial photosynthesis has been trying to adapt the concept of nature for many years. However, in contrast to natural photosynthesis, artificial devices still suffer from multiple loss pathways which reduce their efficiency. Any reduction or suppression of these loss pathways to improve the overall efficiency would advance the energy transition to renewable energy.
MicroMod-PSII set out to investigate structural fluctuations of the protein machineries involved in photosynthesis. For example, vibrations of proteins or interactions with neighbouring molecules cause small atom movements which slightly change the structure. These slight changes cause structural fluctuations. The goal of MicroMod-PSII was to unravel how the proteins manage to perform photosynthesis with high efficiency despite their structural fluctuations. This is of interest because the structural fluctuations alter the arrangement of the chlorophylls involved in light capturing and transmission. Altered chlorophyll arrangements result in changed conditions for light capturing and energy transmission. A complete suppression of these fluctuations is not possible in living organisms. A better understanding how highly efficient photosynthesis is possible in the presence of structural fluctuations can lead to an improvement of artificial photosynthesis.

Work performed from the beginning of the project to the end of the period covered by the report and main results achieved so far

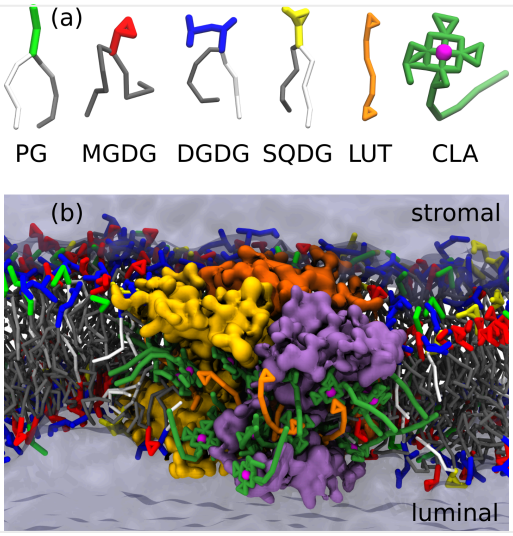
In this research project, different computational techniques were combined to gain insights into the fluctuations of photosynthetic proteins and their impact on the efficiency of photosynthesis. The major aims of the project were:
1. To build coarse-grained models of the protein machineries involved in plant photosynthesis.
2. To study and characterize the structural fluctuations of the protein machineries in their natural environment – the thylakoid membrane – on the microsecond time scale.
3. To gain new insights about the impact of the proteins' structural fluctuations on their photosynthetic properties.
With respect to (1), I optimized a protein model for the antenna protein light-harvesting complex II (LHCII) in the framework of the coarse-grained Martini model. The Martini model still operates at

almost atomistic resolution but offers an about 1000-fold speed-up compared to atomistic simulations. To improve the capability of the model, I used a combination of the Martini model with an approach to describe contact-specific dynamics in proteins, so-called Gō models. To make this method applicable for the large-scale simulations of this research project, I developed two major improvements. These improvements were crucial to efficiently use the method on supercomputers which are indispensable for this kind of research.
The new protein model of light-harvesting complex II allowed studying in detail its structural fluctuations in order to achieve aim (2). I could show that the chlorophylls embedded in the antenna protein are sensitive to their position within the protein: The closer they are to the membrane interface, the higher are their structural fluctuations. Moreover, the chlorophylls are also sensitive to the environment of the protein. If the antenna protein interacts with other proteins, e.g. proteins to which the light energy should be transmitted, the chlorophylls close to the interface get stabilized. The simulations also unravelled the preferred lipid environment of LHCII, its lipid fingerprint.
The diversity of the chlorophyll arrangements obtained from the performed coarse-grained simulations served as basis to work towards aim (3). Using tools from machine learning, I extracted representative arrangements. These arrangements representing the full diversity present in the coarse-grained simulations were used to calculate the light absorption properties of the proteins by means of quantum mechanical simulations. The employed method relies on excitonic Hamiltonians which take into account the chlorophyll arrangements. My simulations have shown that the different chlorophyll arrangements exhibit different light absorption which potentially could be measured in experiments.
The obtained results were disseminated in different ways: First, I presented my results at 14 scientific conferences in form of five talks and nine poster presentations. This included national meetings like the “DutchBiophysics” as well as leading international conferences like the “XXI International Conference on Ultrafast Phenomena”. Second, parts of the results are already published in two peer-reviewed articles, one preprint, and two conference papers. More peer-reviewed articles are in progress. Third, I will present part of my research results to a non-scientific broader audience in a public talk at the Nationalpark-Haus in St. Peter-Ording, Germany.

Progress beyond the state of the art and expected potential impact (including the socio-economic impact and the wider societal implications of the project so far)

During this research project, I developed improvements for a recently presented method to simulate proteins using the coarse-grained force field Martini. While the initial version of the model made the use of supercomputers practically impossible due to technical issues with the parallelization, the improved version can now be used in highly parallelized simulations on supercomputers. A program to prepare the model for any given protein structure is currently in its beta test phase and will be published soon. As of then it will also be made publicly available at www.cgmartini.nl.
To the best of my knowledge, the results of MicroMod-PSII show for the first time the interplay between microsecond protein dynamics of photosynthetic proteins and their optical signals. A detailed

understanding of this interplay in natural photosynthesis can potentially result in future improvements of artificial photosynthesis and therefore promote the use of renewable energy.



Coarse-grained simulation box of light-harvesting complex II in the thylakoid membrane.

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