Langevin dynamic simulations of the energy landscape of rotary molecular motors

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Continuous rotation around one axis, which we use in many mechanical devices, is not seen in animals or other macroscopic biological systems. The reason is that tight contact is required between two parts, which still have to remain separated to move one with respect to the other. However, at the nanometer scale, Nature has found solutions to this topological problem and invented the wheel.
The bacterial flagellar motor is a nanoscopic rotary molecular motor responsible for the continuous rotation of the flagellum, a long extra-cellular appendage that provides thrust to bacteria, allowing them to swim in liquids. The motor is powerful and efficient, reaching rotational speeds of thousands of revolutions per second.
Despite almost two decades of single-molecule measurements, and the more recent resolution of the structure of most motor components, the mechanism of torque production in the motor remains poorly understood.
This project aims to 1) model and simulate the rotation of the motor within its membrane-embedded molecular bearing (Langevin dynamic simulations in Python), 2) compare such results to previously acquired single molecule experimental measurements and computationally derived measurements of the energy landscape, and 3) design the next generation experiments that may better reveal the underlying molecular mechanisms of rotation. If the candidate is interested, the stage could also include an experimental aspect: making single molecule measurements on the bacterial flagellar motor via methods that are well established in our team. Alternatively, or in addition, the theory and simulations could be extended to de novo synthetic rotors under creation by collaborators via protein design.