計算生物物理研究室

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Overview of Computational Biophysics Lab

Biophysics is a field of study that aims to understand biological phenomena using the principles and tools of physics. Every living organism must be following the laws of physics; however, our understanding of biological systems is still limited due to their complexity. B laboratory focuses on studying biomolecules such as proteins and nucleotides that perform many vital cellular functions, and whose dysfunctions result in severe diseases. To understand diseases and develop treatments, the functional mechanisms of these complex biomolecules must be elucidated. A crucial step in this process is the characterization of their structures and dynamics. We use computational techniques, often in collaboration with experimental groups, to study these biomolecules.

Our current research focuses on:

Molecular Dynamics Simulation to study Biological Functions

Biomolecules are highly dynamics due to their interactions with other molecules (small chemical or biological molecules). Such dynamics are essential for their functions; however, at the atomic level, direct observation of their motions is still difficult with current experimental techniques. Molecular dynamics simulation is a powerful computational technique to obtain additional insights as it can provide atomistic level details of molecular motions. In this approach, a potential energy function represents the physicochemical properties of biomolecules. Newton's equation of motion is then numerically solved using high-performance computers to obtain a complete description of atomic motions. We study biomolecules using molecular dynamics simulations to discover new insights that are not accessible from experimental studies. Recent studies include circadian clock proteins as well as multiple enzymes.

Hybrid Approaches - Computational Modeling and Experimental Data

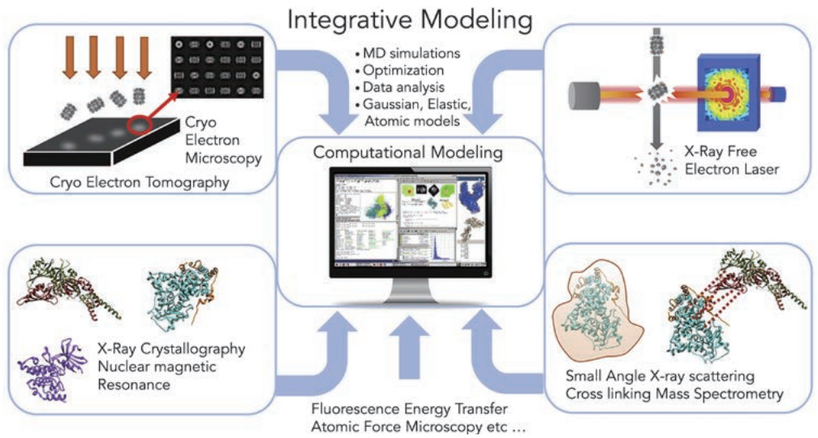
Information on the 3-dimensional (3D) structures and dynamics of biomolecules is essential to understand their functions' mechanisms. X-ray crystallography and cryo-electron microscopy (cryo-EM) provide 3D structures of protein complexes. However, such 3D structures represent frozen snapshots of the molecule and cannot alone provide all the information on the conformational dynamics responsible for biological functions. Other experimental techniques can provide information closer to physiological conditions, room temperature, and in solution (Small Angle X-ray Scattering, Atomic Force Microscopy, Fluorescence Energy Transfer, X-ray Free Electron Lasers); however, the resolution of the data is still limited for constructing detailed atomic models of biomolecules. Each experimental technique has its own strengths and weakness. Therefore, the integrative use of multiple experimental data is essential for an in-depth understanding of biomolecular dynamical mechanisms under physiological conditions. We develop new computational modeling techniques, which utilize concepts of mechanics in physics and combine them with various experimental data (hybrid approach) to model the structure and dynamics of biomolecules. Multi-scale modeling, which describes the system at different levels of detail, is used to study various biological systems. Accurate descriptions of molecular mechanics and computational algorithms for efficient sampling are critical components to these projects.

タンパク質中の熱・エネルギー移動機構

生きている細胞の中では，沢山の生体分子たちが休むことなく働き，生命活動を支えています．遺伝子の設計図に基づいてポリペプチド鎖が合成されると，タンパク質は天然構造に折り畳まり，アミノ酸残基はお互いに相互作用をし始めます．B研究室では，この相互作用を理解することでタンパク質の動作原理を追求しています．凝縮系物理学と生物物理学の概念を融合するユニークな手法を用いて，タンパク質中の熱・エネルギーの移動機構を調べ，アミノ酸残基の間のコミュニケーションの様子を探っています．独自のコンピュータープログラムを駆使して，これまでに，タンパク質がシグナルを伝達するメカニズム等の問題を解明してきました．この分野では欧州や米国のチームと並んで世界の研究を牽引しています．「物理の言葉で生命を語る」をモットーにして，新しい生物物理学を生み出す「特異点」を目指しています．

光合成反応初期過程の研究

生物が生物らしく活動する力の源は，生体エネルギー変換というダイナミックな働きが重要になります．地球に降り 注ぐ太陽光が生物界で最も基本的なエネルギー源であり，光合成生物はそれを吸収し，集め，電子移動反応という化学反応によって，電気化学エネルギーという生物が利用できるエネルギーに変換します．B研では，光合成反応の初期過程である，光エネルギーを吸収し電子を取り出すまでに発生する，励起エネルギー移動/電子移動反応に焦点を当てて，そのメカニズムの解明を行っています．これらの反応はすべて光合成反応中心タンパク質中で起こります．そこで，反応中心タンパク質の構造情報を基に，溶液中などで起こる化学反応論や非平衡統計物理学を駆使して，光合成反応の特徴を明らかにします．B研究室は，この分野では世界的に実績ある理論的研究を進めています．



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教授：1／准教授：1／助教：1／DC：2／MC：5