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BioSim Talk #11

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Institute for Protein Science, Osaka U. (Suita Campus)
2nd floor conference room (#202)

Introduction to Molecular Dynamics Software, GENESIS

Through advances in experimental research, the structures of biological macromolecules, such as proteins, have been elucidated, revealing that some of structural changes play a crucial role in their biological functions. However, understanding the details of these structural changes remains a challenging task experimentally.
Molecular dynamics (MD) simulation is a computational method that calculates atomistic motions by solving Newton's equations of motion. With advancements in computational hardware and algorithms, MD simulations of biomolecules have become widely utilized. Nevertheless, their applicability is often constrained by the substantial computational resources they require.
Dr. Yuji Sugita and his team at RIKEN have developed GENESIS, a state-of-the-art MD software package. As one of the developers, I have contributed to its optimization and enhancement. GENESIS integrates unique parallelization and acceleration schemes, enabling large-scale, high-speed calculations on supercomputers such as "Fugaku." Furthermore, it supports various advanced ensemble methods, including replica exchange, making it highly versatile for diverse research applications.
In this lecture, I will introduce GENESIS, its features, and its fundamental usage.

Link for online participation via Zoom:
Meeting ID: 863 8759 7799
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