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Application of High-Performance Computing in Nanomedicine: Lipid based nanocarriers and biogenic nanoparticles

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High-performance computing (HPC) is an increasingly influential field with the potential to transform various industries, with nanomedicine being one of the key beneficiaries. Nanomedicine is the integration of nanotechnology into medical practices, encompassing the diagnosis, treatment, and prevention of diseases. Among the various nanoparticles used in this field, lipid-based nanocarriers stand out as versatile tools. Comprised of lipids, the fundamental components of cell membranes, lipid-based nanocarriers are employed to transport drugs, genes, and therapeutic agents to target cells and tissues within the human body. HPC plays a pivotal role in advancing this field by aiding in the development of novel lipid-based nanocarriers and optimizing their drug delivery mechanisms. Biogenic nanoparticles, which are naturally produced by living organisms ranging from microbes to animals, have immense potential within nanomedicine. Their applications span drug delivery, imaging, and tissue engineering. To delve deeper into the behaviour of lipid membranes and their interactions with nanocarriers and biogenic nanoparticles, computational tools such as coarse-grained molecular dynamics (CGMD) are indispensable. CGMD simulations model groups of atoms as single beads, enabling the analysis of large biological systems, which would be impractical with traditional all-atom molecular dynamics (MD) simulations. To facilitate these simulations, the CHARMM-GUI platform provides a user-friendly interface for setting up and executing MD simulations using the CHARMM force field. Specifically, CHARMM-GUI Martini Maker allows researchers to configure a variety of lipid membrane systems, including planar bilayers, micelles, and vesicles. By harnessing HPC resources for the design of new lipid-based nanocarriers and biogenic nanoparticles, optimizing therapeutic agent delivery, and investigating the interaction between these nanomaterials and biological entities, the potential for breakthroughs in nanomedicine is vast. This synergy of HPC and nanomedicine holds promise for enhancing healthcare solutions and revolutionizing disease treatment and prevention strategies.

Student or Postdoc?

No. Not a student nor Postdoc.

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