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CS 360 Parallel and Distributive Computation
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April 23, 2024

Use of GPGPUs in Molecular Dynamics for Drug Discovery

Molecular Dynamics (MD) is a computational technique based on Newtonian physics that allows us to analyze interactions between molecules. Using mathematical models called force fields, it simulates the motion of atoms and molecules, capturing the dynamic nature of molecular systems, including temperature, pressure, bonds, angles, dihedrals, and non-bonded interactions between atoms. This technique proves to be vital in drug discovery as it allows scientists to analyze nuances of drug binding, enzymatic reactions, and the stability of drug-target complexes. This level of detailed, complex simulation is crucial in designing effective drugs.

MD was first discovered in the 1970s and has become revolutionary in drug discovery. It has been significantly improved using high-performance computing. GPGPUs have significantly accelerated molecular dynamics simulations, improving the time to compute the per-frame trajectories of individual atoms by orders of magnitude. MD simulations leverage the vector and matrix processing capabilities of GPGPU to speed up the process.

GPGPUs significantly speed up force field calculations, such as Lennard-Jones and Coulombic forces, improving non-bonded interactions. Integration methods like Verlet and Leapfrog, crucial for molecular dynamics simulations, are well-suited for parallelization, resulting in improved efficiency. Moreover, they enhance the performance of constructing and updating neighbor lists, which are essential for large simulations. Additionally, GPGPUs efficiently calculate long-range electrostatics using techniques such as Particle Mesh Ewald (PME) and Smooth Particle Mesh Ewald (SPME), contributing to the acceleration of simulations. These advancements in GPGPU technology are revolutionizing computational chemistry and drug discovery, paving the way for more efficient and accurate simulations.

Open-source Software:

1. OpenMM
2. Gromacs
3. Amber

References

1. This is a great video introducing the concept of MD for drug discovery: https://www.youtube.com/watch?v=9PBmL8F0Hd4
2. https://www.azolifesciences.com/article/What-Role-Does-Molecular-Dynamics-play-in-Drug-Discovery.aspx

3. https://www.tandfonline.com/doi/full/10.1080/17460441.2018.1465407
4. https://www.hpcwire.com/2023/03/20/accelerating-drug-discovery-and-development-with-gpu-powered-high-performance-computing/
5. I used ChatGPT to find information about the algorithms implemented on GPGPUs and the open-source software titles.