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Big data, high performance computing and Pharmaceutical innovations

In the pharmaceutical research, high throughput scientific experiments, high performance computations, automated information acquisition and office automation, and scientific publications and patent literatures, are four sources that produce big data. The biomedical big data brings greater challenges because conventional hardware and software are unable to handle it due to limited memories and extreme computing complexity. With cloud high performance computing (cHPC) technology, the challenges can be resolved by parallelizing existing chemoinformatics and bioinformatics programs. Biomedical big data is usually scattered, incomplete, low signal/noise ratio, and involving in sophisticated relations among objects. Combining multiple machine learning approaches, such as, naive Bayesian learning, support vector machine and recursive petitioning, are used in biomedical big data mining projects. This talk outlines current progress in biomedical big data processing technology including parallelized and GPU-accelerated molecular dynamics simulation technology, enhanced molecular docking technology, new parallelized algorithms for shape-based virtual screening, free energy landscape calculations, and machine learning algorithms for pharmaceutical innovations.

Biography

Jun Xu has completed his PhD from University of Science & Technology of China and Post-doctoral studies from Australian National University and McGill University. He is the founding Director of Research Center for Drug Discovery (RCDD), which consisits of Bio/Chemo-informatics lab, Drug Design lab, Phyto/Medicinal Chemistry lab, Structure Biology lab, and Drug Screening lab. He has published more than 80 papers in reputed journals and has been serving as an Editorial Board Member of a number of reputed international journals.

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