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Review article

The development of molecular docking and molecular dynamics and their application in the field of chemistry and computer simulation

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ABSTRACT

With the rapid development of modern life science, computational Molecular docking has gradually become one of the core disciplines and methods of modern life science research. Computational docking studies the relationship between the structure and pharmacodynamics of biological macromolecules and the interaction between biological macromolecules and ligands. It promotes the development of protein engineering, protein design, and computer-aided drug design with powerful and various docking software in predicting the three-dimensional structure and dynamic characteristics of proteins from protein sequences. Nowadays, this computing power can be provided by the GPU through the use of a general-purpose computing model on GPUs. This article presents two approaches to parallelizing the descriptive algorithms on the GPU to solve the molecular docking problem and then evaluating them in terms of the computation time achieved. The proposed approaches are effective in accelerating molecular docking on GPUs compared to a single-core or multicore CPU. Besides introducing parallelization approaches, we propose a new descriptive algorithm based on the bee swarm algorithm to solve the molecular docking problem as an alternative to traditional descriptive algorithms such as the genetic algorithm.

Keywords: Molecular Docking Simulation, Drug Design; ligands, Software.

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INTRODUCTION

Molecular docking and molecular dynamics modeling are significant aspects of computational chemistry that continue to be used in the development of medicine. Molecular docking and molecular dynamics technology can explain the interaction between molecules in great detail and vividly explain the mechanism of the interaction, which is useful in drug development. It has also become an important research method for explaining biological mechanisms [1].

Molecular docking and molecular dynamics are also valuable tools for predicting biomacromolecule complexes' binding type and interaction mode and providing a valuable reference base and theoretical support for future investigations. Molecular docking and molecular dynamics approaches have become the most crucial and widely used tools in elaborating biological and molecular systems, particularly in predicting molecular simulation or even atomic complexes. Given the significance of the two methodologies, we give a preliminary introduction to molecular docking and molecular dynamics research methods for reference [2].

Molecular docking

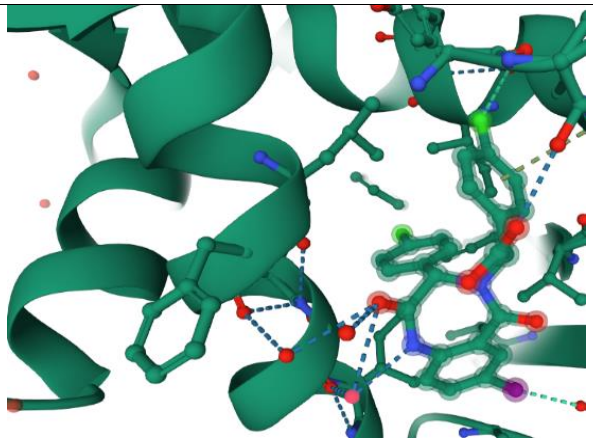
General Principles of Molecular Docking Technology

The Molecular Docking Method(MDM), sometimes named Computer-Assisted Drug Design, refers to a method that uses the computer-simulated placement of ligands that are tiny molecules in the binding region of large target molecules (receptors) like the lock-and-key model. Then, when the ligand and receptor are joined in their active region, calculate physical and chemical characteristics to estimate the binding affinity and mode (conformation) and then discover the interaction of the lowest energy conformation [3].

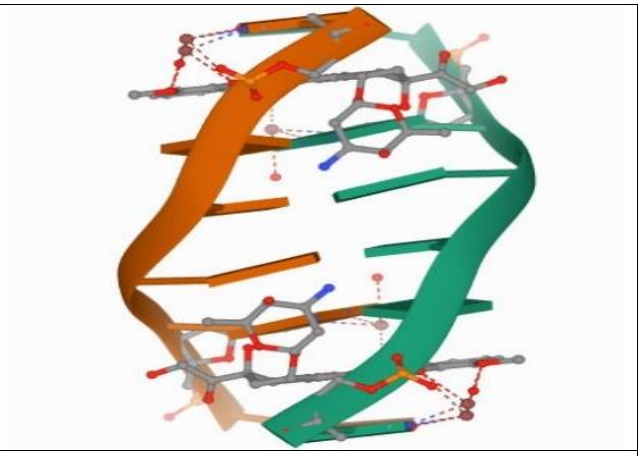
When the ligand and the receptor bind, there are electrostatic, hydrogen bond interactions, van derails & hydrophobic interactions with each other. The binding of ligands and receptors must meet the principle of mutual matching. The geometric shape of the ligand and receptor is complementary and matched, and the electrostatic interaction is complementary, the hydrogen bond interaction is complementary, and the hydrophobic interaction

The interaction is complementary and matched (Figure 1).

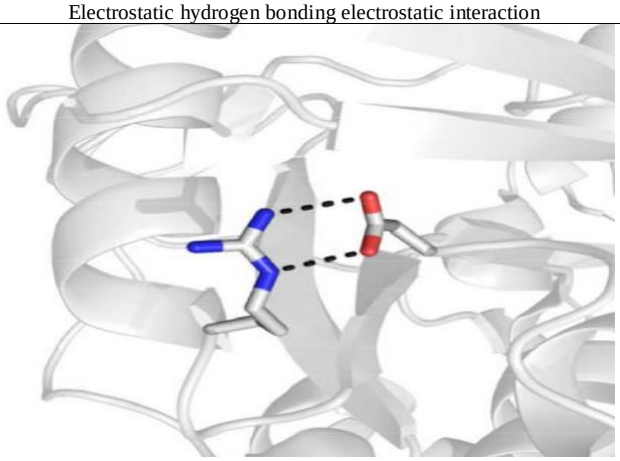
Figure 1: Schematic diagram of the binding and interaction between the ligand and the receptor.



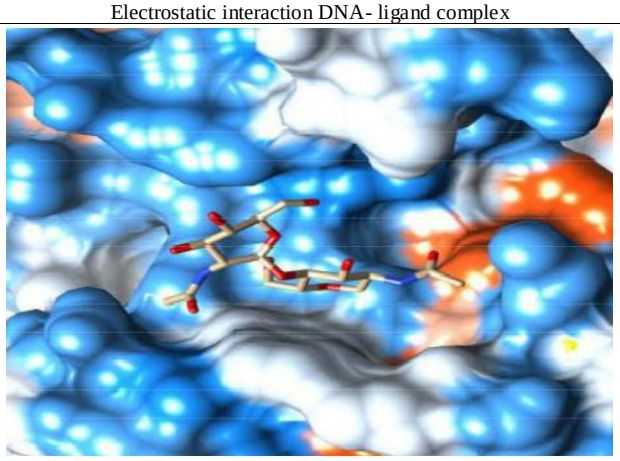
Electrostatic hydrogen bonding electrostatic interaction



Electrostatic interaction DNA- ligand complex



Salt bridge



Hydrophilic Surface

Molecular docking algorithms comprise the following two categories: search techniques, which determine the acceptable conformation of receptor-ligand complexes, and the scoring function, which assesses binding affinity and ligand location [4].

Classification of molecular docking

However, whether the docking molecule conformation changes, molecular docking, according to the degree of flexibility between the ligand and receptor, is divided into rigid, flexible, and semi-flexible docking.

Rigid Molecular docking

During this process, the research system operates, but the configuration remains unchanged. It is well suited to studying comparatively large systems, such as protein and its interaction with other proteins and nucleic acid docking [3].

Semi-flexible docking

The research system (docking software), particularly the configuration of the ligand, is allowed to change to a certain degree during the docking process. It is ideal for managing to dock between large and small molecules. Small molecules' conformation may typically be altered during docking, whereas large molecules are stiff [5].

Flexible docking

The confirmation of the research system can be flexibly modified during the docking procedure. To compute the exact interaction between molecules, this docking type is used. Because the system's conformation might vary during the computation procedure, the calculation amount is the largest [6,7].

Pre-processing of molecular docking

Small-molecule processing

After constructing the structure of small molecule compounds using the classical chemical composition method, use quantitative software to calculate the molecular charge distribution, the molecular orbital, and the reaction activation energy to optimize the structure of small molecules (Figure 2).

Protein Processing

For protein processing, the main objective is to integrate information on hydrogenation, charge addition, disulfide bonding, and protonation status. The greatest difficulty lies in how to deal with the protonation status of HIS amino acids around small molecules. At present, there is no unified method in the world. (Figure 3) [8].

Figure 2: Schematic diagram of the processing of small molecules (energy minimization using the Chem 3D program)

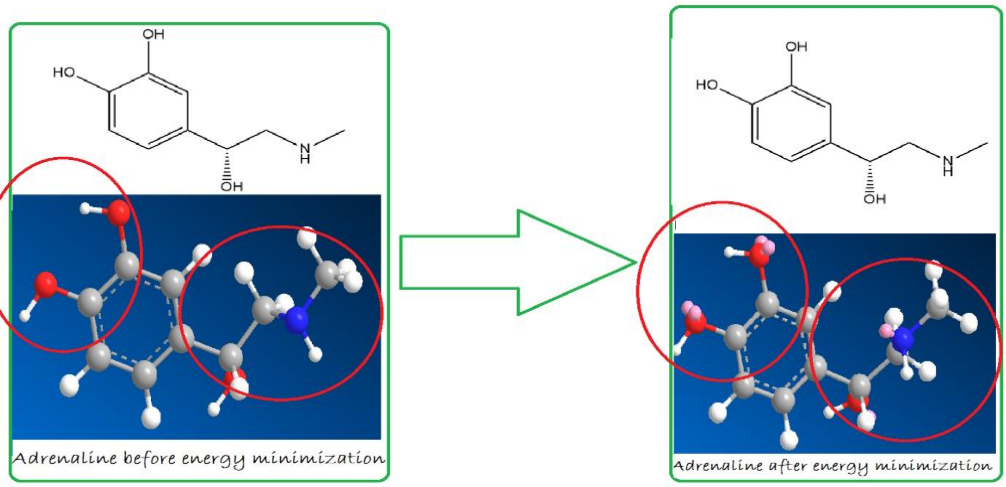


Figure 3: Schematic diagram of protein processing and interactions with small molecular

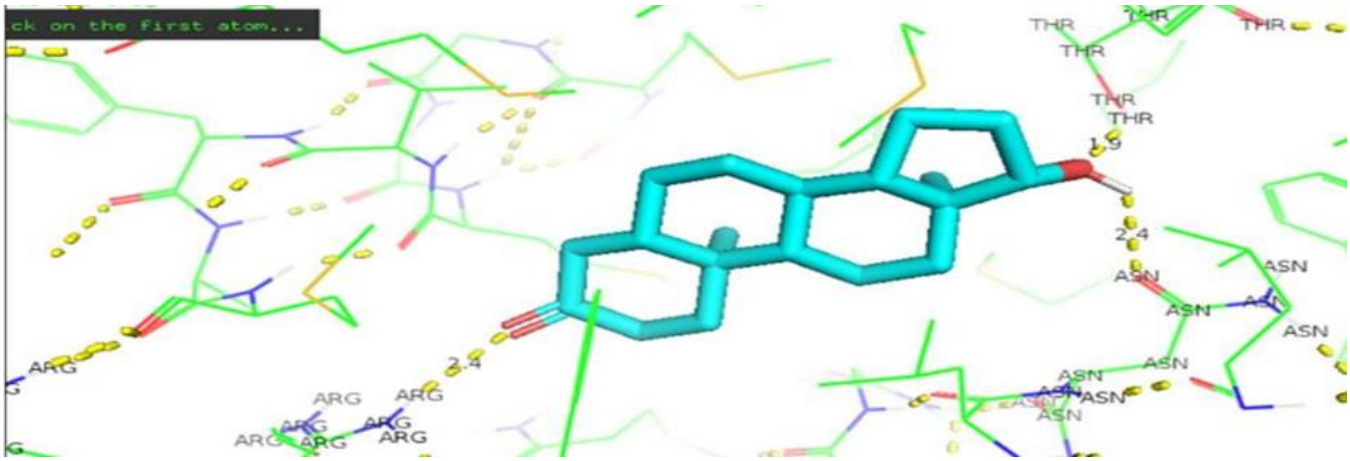
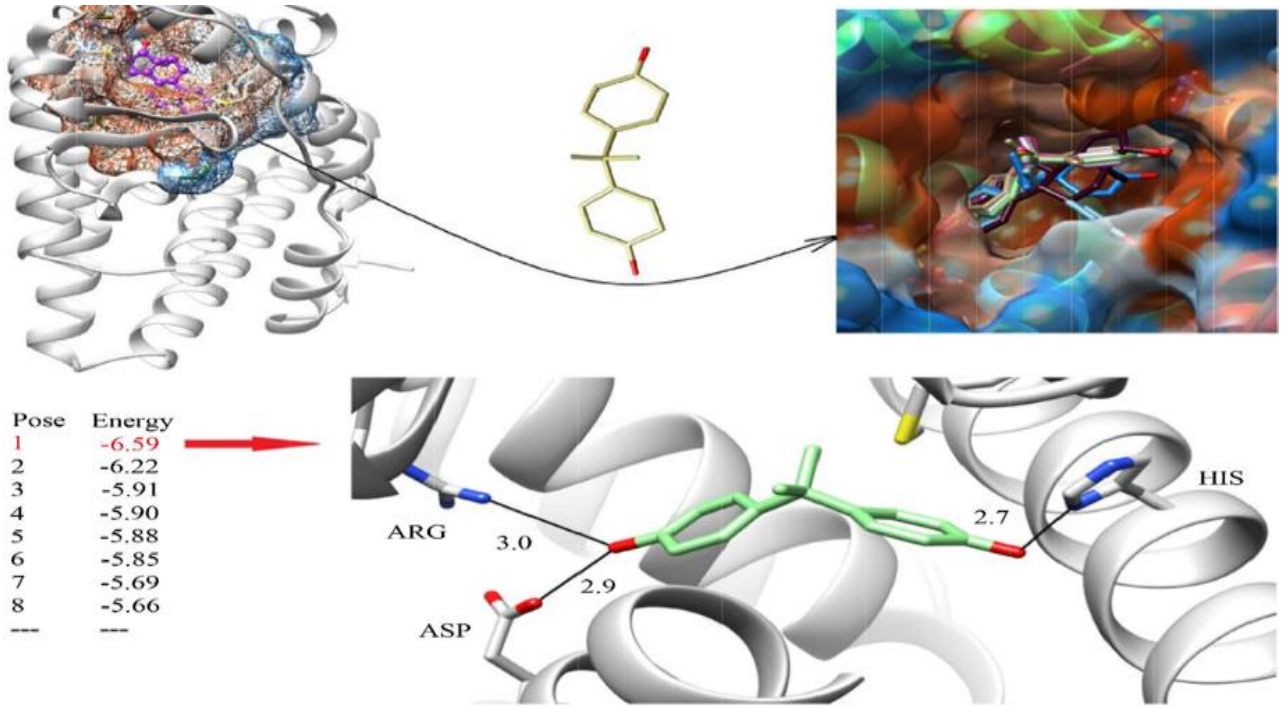


Figure 4: Analysis of docking results of protein-ligand molecules



They involve-spatial matching and energy scoring between molecules. According to the energy ranking, the preliminary optimal structure and the binding mode between the molecules are finally obtained (Figure 4).

The "Protein-ligand" docking software is complicated; the main software includes Auto dock, Vina, Dock, and other software, as shown in Table 1

Molecular docking diagram

Molecular docking is an identification process amongst two or more molecules involving spatial matching and energy scoring between molecules. The initial optimal structure and binding pattern between molecules are obtained according to the energy ranking (Figure 4), including Autodock, Vina, Dock, Rosetta, GOLD, Glide, and Z-DOCK, some of them and their properties shown in (table 1) [9,10].

Table 1: Programs and software used in molecular docking and ligand-protein stimulation

Program name	Scope of application	Algorithms and Features
AutoDock	Protein-Small Molecule	Lamarck Genetic Search Algorithm offers a free license, one of the best molecular docking programs that predict the binding strength between the ligand and the molecular.
AutoDock Vina	Protein Small Molecule	Compared to the previous Previse versions of Auto Dock, the updated version's success rate and computation speed are quite good. Significant enhancement, simple parameter configuration, ease of use, and integration ability on a multicore computer.
DOCK	Protein Small Molecule	Fragment growth method, using the matching protocol in the space with a geometric overview, with an evaluation of possible force field (AMBER) and potential energy evaluation with scoring function.
Glide	Protein Small Molecule	Commercial software, fast and accurate molecular docking program for high-throughput database screening, MC search algorithm, Hierarchical screening to search for potential binding sites
GOLD	Protein Small Molecule	Commercial software, GA search, ligand flexibility, partial consideration of protein flexibility, automatic alignment The access program is one of the optimum docking and visualization interface.
MDock	Protein Small Molecule	Consider the protein using multiple proteins and small-molecule conformations in the docking process. The Flexibility of Quality and small molecules; using knowledge-Based Atomic Score Function for Statistical Potential
PIPER	Protein-protein	Fast Fourier transform search, knowledge-based atomic scoring function for statistical potential, applied to ClusPro Server [3]
DOT	Protein-protein/DNA/RNA	The scoring function in the fast Fourier transforms [3].
HADDOCK	Protein-protein/ DNA/ RNA/ small molecular	Docking methods are analytical and experimental (for example, NMR chemical shifts and point mutations), etc.)
PatchDock	Protein-protein/ DNA/ small molecule	Geometric hashing can search for the conformational space based on geometrics. Matching docking program
RosettaDock	Protein-protein/ DNA/ RNA/ small molecular	MC search, scoring function based on the empirical energy function
ZDOCK	Protein-protein	FFT search and use RDOCK to filter and sort
PyRx	Ligand protein interactions	Use visual screening and visual docking based on Autodock vina and Autodock tools

Application of molecular docking

In the past 10 years, with the continuous advance of technologies such as X-ray crystallography and high-throughput sequencing, more and more protein crystal structures have been confirmed, and their corresponding genetic information has also been announced.

Therefore, understanding the structures and function of cellular elements such as receptors, proteins, and other functional macromolecules continues to deepen, resulting in more and more drug targets. With the vigorous development of computational science, the application and promotion of molecular docking and virtual screening technology in the discovery and design of the drug.

Today, computing technology has become one of the important methods in drug design. Researchers can quickly and accurately describe the interaction between drugs and targets through computer-simulated molecular docking operations—function, shortening the drug development cycle [2,11].

Reverse molecular docking technology is a new specific application of molecular docking. It uses small-molecule compounds to perform molecular docking in a target database with a three-dimensional structure and search for large-scale biological organisms that may be combined through spatial and energy-matching evaluation. Molecules, and then predict the potential theoretical target of the drug. Therefore, the emergence of reverse molecular docking technology provides a new way to discover drug targets and clarify the mechanism of action [3,13].

Molecular docking methods are also widely used in nondrug discovery. For example, protein engineering (refers to people who will change the structure and function of proteins or design new proteins), bioremediation, and biosensors (biological macromolecules such as antibodies). Receptor proteins and enzymes, etc., because of their specific binding ability to substrates, as biometric elements, have been widely used in biosensors to monitor pollutants in the environment), nanoscience (nanomaterials and protein interactions), and so on [9,11].

Molecular dynamics simulation calculation

Overview of molecular dynamics simulation

Suppose molecular docking is likened to a picture. In that case, molecular dynamics simulation is like a dynamic movie composed of frames, rich and colorful, full of fun, and people cannot help it!

Molecular dynamics (MD) uses theoretical theories and computational tools to model or replicate the microscopic dynamics of molecular motion. Molecular dynamics always assumes that the movement of atoms obeys a certain equation. This equation can be Newton's, Lagrangian, or Hamilton's, showing that the atom's motion is related to a certain trajectory. When the quantum impact of nucleons and the Born-Oppenheimer adiabatic approximation are ignored, these molecular dynamics theories are possible [12,15].

Materials research, biology, and drug design extensively use molecular dynamics modeling. As small as a single chemical molecule or as large as a complex biological or material system, kinetic simulation can be studied.

Classic MD simulation can reach tens of thousands of atoms on a general computer, and the simulation time can be reached in nano-seconds.

The study of molecular dynamics may depict the dynamic behavior of molecules on a computer screen, making it easier to comprehend the system development process under certain conditions. Molecular dynamics methods may be used to determine the heat transition in glass, thermal expansion, crystal formation, movement of the particles, expanding phase, dynamics relax (relax), and the system's change process under the impact of an external field are all factors to consider.

However, when traditional research cannot provide the needs of a research project, computer-aided drug design can give crucial information because a huge number of proteins have been identified and placed on a special website that is easy to access, the PDB protein data bank. However, computer simulation cannot completely replace experimental work and can serve as a useful reference for scientists. It also directs experiments and confirms specific theoretical assumptions, allowing theories and experiments to progress[13,14].

Basic principles of molecular dynamics simulation

Today, the computational technique describes and stimulates several things around us. One of its most important simulations is that of using molecular dynamics (MD) studies and rules to the dynamic performance of molecular, such as binding of molecular, protein, and its conformation, as the 3D method and evaluating the function by simulation box (ligands, proteins, and any explicit waters) as flexible [11].

The molecular dynamics algorithm is the finite difference method (a technique for determining the mathematical model of a partition or ordinary dynamic systems and solving other equations fixing). Simulated simple systems, with the first application in 1957 to study collisions between hard spheres[13], McCammon *et al.*,[7]; in 1977, the first 3d structures of a macromolecular was done by using molecular dynamic stimulation; It is a 9.2 ps modeling of a 58-reactive bovine pancreas trypsin inhibitor (BPTI) with a primitive molecular dynamic ability.

Molecular docking simulation produces atomic motions over time by integrating Newton's equations of motion (traditional mechanics), as shown in the calculation below [14].

$$\frac{d^2 r_i(t)}{dt^2} = \frac{F_i(t)}{m_i}$$

Were the $F_i(t)$ being the force applied to molecular i in special times *t*, whereas the $r_i(t)$ reflects the location of molecular i in a time –t finally the (m_i)mass(weight) of the molecular (Figure 5).

Time, in particular, is divided into time steps (*t*), which are used to move the system forward in time. However, several integration algorithms that use a discrete-time mathematical estimate to derive from Newton's equations are now available.

Where ri(t) is the position of the molecular, vi(t) is the velocity or acceleration of the molecule, and ai (t) is the time, whereas ri(t+δt) is the position, vi(t+δt) is the velocity of the atom and ai(t+δt) is the acceleration of atom at time t+δt.\.

The acceleration is calculated from the forces acting on atom i according to Newton's second law,

and forces are calculated from the force field according to the following equation.

$$a_i(t) = \frac{d^2 r_i(t)}{dt^2} = \frac{F_i(t)}{m_i} = -\frac{dV(r(t))}{m_i dr_i(t)}$$

Here V(r(t)) is the force's recovered possible energy value (figure 5). The force fields that are used most frequently in the dynamics of molecules are CHARMM [14], AMBER [15], OPLS, and GROMOS [11].

Important Concepts in Molecule Simulation of Molecular Dynamics

Periodic boundary conditions

Only a small part of the actual substance is simulated so that the simulated system becomes an infinite molecular system with the same properties. This part periodically exists in the three-dimensional space and represents the entire system[17].

Potential function

The potential function describes how molecules react (molecules). The interaction behavior of atoms governs the interaction behavior of atoms and fundamentally dictates all of the material's qualities. The potential function clearly describes this impact. The choice of a potential function influences the simulation outcomes in molecular dynamics simulation.

Figure 5: illustrates the equation of position and velocity of the molecular

$$r_i(t+\delta t) = r_i(t) + v_i(t)\,\delta t + \frac{1}{2}a_i(t)\,\delta t^2$$

$$v_i(t+\delta t) = v_i(t) + \frac{1}{2}\left[a_i(t) + a_i(t+\delta t)\right]\delta t$$

ri(t)- position of the molecular
vi(t)- velocity of molecule
ai (t)- time
ri(t+δt)- position
vi(t+δt) velocity
ai(t+δt) is acceleration of atom
(t+δt)time differance.

Figure 6: Molecular dynamics and calculations

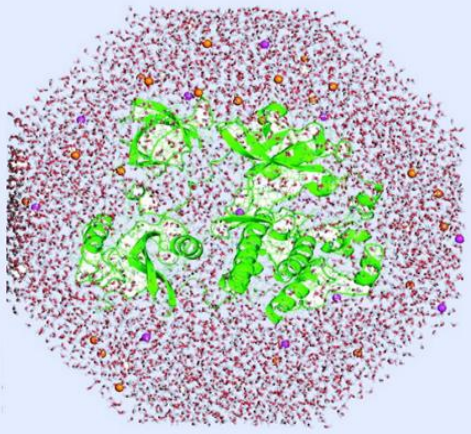
potential energy: $V(r(t))$

velocity: $v_i(t) = \frac{dr_i(t)}{dt}$

acceleration: $a_i(t) = \frac{d^2r_i(t)}{dt^2} = \frac{F_i(t)}{m_i}$

force: $F_i(t) = -\frac{dV(r(t))}{dr_i(t)}$

position: $r_i(t) = (x_i(t), y_i(t), z_i(t))$



Ensemble

A collection of a large number of autonomous systems with identical features and structures in multiple motion states under particular macro-environments. When statistical methods are employed to characterize the statistical regularity of thermodynamic systems, the idea of an ensemble is introduced.

The canonical ensemble is a process that gathers the ensemble, which is made up of N particles that come into contact with a large heat source at T and achieve thermal equilibrium. It can also be imagined as this: Take a large number of M identical systems with a volume of V and a particle number of N to form an ensemble, any one of which can be used as the system under study, and the rest M 1 Each system plays the role of a constant temperature bath, and there is an energy exchange between the systems, and they are in heat balance together.

The micro-canonical ensemble, known as the NVE ensemble, signifies that the system's atomic number N, volume V, and energy E remain constant.

The isothermal and pressure ensemble is an extension of the canonical ensemble and a statistical mechanics ensemble, and this ensemble is a system with constant temperature and pressure.

The system in each set can exchange energy and volume with other systems. However, each system's total energy and volume in the ensemble are fixed, and each system has the same number of particles [16].

Integration step

The primary idea behind molecular dynamics calculations is to leverage the natural motion of the molecule to extract samples in phase space for statistical calculations when the molecular system's initial motion state is known. The integration step is the sampling interval. The principle of selecting an appropriate integration step length is that the integration step length is less than one-tenth of the fastest movement period in the system. It saves time and ensures that the calculation is accurate [18].

Application of Molecular Dynamics Simulation

The spectrum of applications for molecular dynamics simulation has widened in recent years. For example, we used docking and dynamics of molecules (MD) modeling to investigate the

interaction mechanism between fentanyl molecules and opioid receptors.

First, use the AutoDock4.0 program to connect fentanyl compounds to the homologously modeled opioid μ receptor structure. Then, use the GROMACS program package to analyze 12 fentanyl agonists and opioid μ receptor proteins in an aqueous system [16,20]. The complex was studied by MD simulation to optimize the structure of the docking complex. Finally, in the APBS software, the MM-PBSA method was utilized to calculate the free energy of binding between the fentanyl derivatives and the opioid receptor, and the resulting receptor complex was determined. The binding constant (Ki) agrees with its experimental value and predicts the activity ranking of the compounds [20,21].

Moreover, Nguyen Trong et al., 2021 used molecular dynamics combined with the multi-body potential of embedded atoms to simulate Ni nano-cluster's heating and melting process with different radii [20]. Furthermore, Voeltzel N et al. used molecular dynamics simulation and quantum chemistry calculation methods to study different ionic liquids and got the structural properties, spectral properties (infrared spectroscopy, Raman spectroscopy), and catalytic reaction mechanism of ionic liquids [21]. Interestingly, many researchers worldwide have used molecular docking and molecular dynamics to treat the COVID-19 pandemic infection [23,24]. Radwan et al. used molecular dynamics methods to simulate the antibiotic ceftriaxone against the pathogenic proteins of SARS-CoV-2 [22,25].

Application in the field of computational chemistry

Application in the field of computational chemistry **i**s part of the chemistry science mainly interested in using a computer to solve mathematical equations and describe and find out the properties and values of molecules that may be physical properties such as boiling point or melting point, etc [26,27]. Or chemical interactions, molecular properties, the result of interaction, and the binding capacity and type of binding. Sometimes, this information may not resolve or take lots of time to solve these properties or equations; however, nowadays, the computer simulation method gives results of interactions in accurate value that may be more accurate than experimental methods. In theory, fairly precise theoretical calculations can be performed on any molecule, and these proper methods are also included in many computing software [28].

Other problems that so

Predicting the start condition and point of chemical synthesis.

Study chemical reaction mechanism and explain reaction phenomenon

The sub-disciplines of computational chemistry mainly include

Computer representation of atoms and molecules

Computer-assisted storage and search of chemical information data [29].

Study the relationship among the structure of chemicals and binding, and other properties, which are sometimes called -Quantitative Structure (Activity or Property) Relationship (QSAR)(QSPR) respectively)

Theoretical interpretation of chemical structures based on force simulations

Computer Aided Compound Synthesis

Computer Aided Characteristic Molecular Design (e.g., Computer Aided Drug Design)The first principal method (ab initio), also known as the total initial calculation, frequently refers to a quantum mechanics-based concept entirely developed from the idea and has no practical value [30]. It is a relatively precise calculation method because it does not use experimental data other than basic physical constants, atomic weights, or empirical or semi-empirical parameters to solve the Schrodinger equation. Most first-principles procedures entail approximation, commonly resulting from fundamental mathematics reasoning, such as switching to simpler functional forms or employing approximate integral methods [31].

Most first-principles methods use the Born-Oppenheimer approximation, which separates the motion of electrons and the motion of nuclei to simplify the Schrödinger equation [32]. Calculations are often carried out in two steps: electronic structure calculations and chemical kinetics calculations

Electronic structure

The electronic structure can be obtained by solving the steady-state Schrödinger equation (also known as the time-free Schrödinger equation). The solution process is often approximated using a basis set obtained by the linear atomic orbitals (LCAO) combination. With this approximation, the Schrodinger equation can be transformed into a "simple" eigenvalue equation of the electronic Hamiltonian. The solution to this equation is a discrete set. The solved eigenvalues are a molecular structure-function, and this correspondence is called a potential energy surface [33].

Hartree-Fock is the most common type of first-principles electronic structure equations. Every electron goes in the average potential of the remaining electrons in the Hartree-Fock model, but the positions of these electrons are not known. When electrons are relatively close together, even though the Coulomb interactions between electrons are taken into account via the averaging method, the electron repulsion is overstated in Hartree-Fock. The variational approach is required to solve the Hartree-Fock equation, and the obtained approximation energy is always equal to or greater than the real energy. The Hartree-Fock energy approaches the Hartree-Fock limit energy indefinitely as the basis function increases [34,35].

Quantum Monte Carlo (QMC) is another approach to solving electron-related problems. In quantum Monte Carlo, the ground state wave function of the system is written explicitly as the associated wave

function. The wave function is an explicit function of the electron-electron distance. Quantum Monte Carlo uses the Monte Carlo method to numerically analyze the integral [36]. Quantum Monte Carlo calculations are time-consuming but may be the most accurate first-principles method.

Many common functionals of density functional theory (DFT) contain parameters fitting experimental data. However, density functional theory is often used as a first-principles method to solve the electronic structure of molecules. Density functional theory uses electron density rather than wave function to describe system energy. In DFT calculations, one term of the Hamiltonian, the exchange-correlation functional, takes an approximate form [37,39].

The results of the first-principles electronic structure method can approach the exact value infinitely when the approximation used is sufficiently tiny. However, the difference from the real number does not always decrease monotonically as the approximation lowers, and simple calculations can sometimes produce more accurate answers. The main disadvantage of first-principles computing is that it is computationally intensive, often requiring large amounts of computing time, memory, and disk space. The computational cost of the HF method grows with N4 (N is the number of basic functions) with the size of the system – it takes 16 times longer to calculate a system twice as large – the electron correlation method grows faster (DFT computations are about N3 growth, by contrast, is the most efficient electron-related method) [40,41].

Computational chemistry

Computational chemistry approaches can similarly use to solve problems in the solid state. An energy band structure is commonly used to represent a crystal's electrical structure. The orbital energies calculated using first principles and semi-empirical approaches can then be used to calculate the band structure [41].

Chemical kinetics

This entry requires the participation and assistance of editors who are proficient or familiar with the subject matter.

After separating the nuclear coordinate variables from the electronic variables under the Born-Oppenheimer approximation, the wave packets associated with the nuclear degrees of freedom are propagated through the evolution operator associated with the full Hamiltonian of the time-dependent Schrödinger equation. In another method based on energy eigenstates, the time-dependent Schrödinger equation is solved by scattering theory. Potential energy surfaces describe interatomic interaction potential; in general, potential energy surfaces are coupled to each other through vibrational coupling terms [42].

The main methods used to solve the propagation of wave packets in molecules include

1. Molecular dynamics uses Newton's laws of motion to study the time-dependent properties of systems, including vibrations or Brownian motion. In most cases, some description of classical mechanics is often added. The combination of molecular dynamics and density functional theory is called the Car-Parrinello method [32,42].

Semi-empirical method

Electronic structure

Semi-empirical methods omit or approximate some terms in the Hartree-Fock calculation (e.g., two-electron integrals). Semi-empirical calculations use a series of parameters fitted from experimental results to correct errors introduced by these approximations. Sometimes these parameters are fitted from first-principles estimates.

The empirical method is a further approximation of the semi-empirical method. The practical method does not include the two-electron part of the Hamiltonian. Classical methods include the Huckel method proposed by Eric Huckel for π-electron systems and the extended Huckel method proposed by Roald Hoffman [42]. Semi-empirical calculations are much faster than first-principles calculations. However, semi-empirical methods may give completely wrong results if the calculated molecules do not closely resemble the molecular structures used to parameterize the technique [31,42-45].

Semi-empirical methods are most widely used in organic chemistry because organic molecules are moderately sized and mainly composed of a few kinds of atoms.

Similar to empirical methods, semi-empirical methods can also be divided into two broad categories

A semi-empirical method limited to the π-electron system

A semi-empirical approach limited to valence electron systems

Most current methods belong to the second category of semi-empirical methods [48,49].

Molecular Mechanics Methods

Studying complex molecular phenomena might reduce the need for quantum mechanical computations in several circumstances. Quantum mechanical models use classical mechanical models, such as harmonic oscillators, to represent the energies of molecules. The molecular mechanics model's constants are derived from experimental evidence or first-principles calculations. Molecular force fields are the optimum results of parameters and equations [45].

The computational success of molecular mechanics approaches is dependent on parametric compound libraries. When applied to the same molecule type, a force field designed for that molecule type can only provide reliable results [46].

CONCLUSIONS

Molecular docking and its use of molecular dynamics have become necessary for computational chemistry, playing an important role in biology, medicine, pharmacology, agronomy, and environmental science. Molecular docking and molecular dynamics are

important parts of computational biology, and their development depends on the development and penetration of various interdisciplinary subjects. At the same time, the rapid development of different interdisciplinary topics also creates favorable conditions for the development of computational biology.

With the deepening of human genome research and proteomic research, molecular docking and molecular dynamics technology will face greater challenges in the future, especially the huge demand for artificial intelligence technology and computing resources, which will continue to promote the continuous development of these two technologies. Progress and change will also become more mature and perfect in revealing the mysteries of life. The contribution of molecular docking and molecular dynamics technology to the development of biology will also promote the continuous generation of new interdisciplinary subjects and jointly promote life sciences into a new realm.

Molecular docking and molecular dynamics technologies provide important tools for predicting biomacromolecule complexes' type and mode of interaction and offer useful references and theoretical support for further experiments. In elaborating biological and molecular mechanisms, especially in predicting and simulating the structure of complexes at the molecular or even atomic level, molecular docking and molecular dynamics techniques have become the most critical and widely used methods. The importance and intricacy of molecular docking and dynamics technologies have steadily become apparent as biological data grows. The higher the need for participation and use of these two technologies, the more complex the biological problems must be solved. Computational chemistry, particularly molecular docking, and molecular dynamics technology, is rapidly becoming life science's most dynamic scientific research tool.

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