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MOLECULAR SIMULATION VIA LYAPUNOV PRINCIPLE AND NURBS CURVES

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Abstract. *A Lyapunov principle to explore the Computer-aided drug design (CADD) is proposed. Based on NCBI' 97 reports, the most significant challenge is the docking procedure. In this work, Lyapunov stability theorem is used to discuss and analyze the numbers of binding sites in the drug design and to enhance the docking performance. These novel techniques are significantly based on the concept of minimum energy and optimal geometry search strategies to ensure the stability of protein–ligand interactions. This study also applies the Lyapunov stability theorem to discuss the molecular orbit adjustment of molecular dynamics equations when the equilibrium point moves away from the initial state with zero input in molecule infinite time t. From the view point of the minimum energy, we have used the Non-Uniform Rational B-Splines (NURBS) curves to accelerate the molecular docking system by the short route. Furthermore, the folding of various proteins is discussed. And the force field is also analyzed. Finally, simulation results are given to show the feasibility and effectiveness of this study.*
Keywords: Lyapunov, NURBS, Drug docking, CADD

1. **Introduction.** The most important application of molecular docking is virtual screening for drug discovery and improvement. Molecular docking explores how two or more molecular structures interact, and is like solving a 3-dimensional puzzle. In molecular docking, this work aims to predict the structures of the intermolecular complex formed between two or more molecules. Molecular docking is a nonlinear dynamics chaos system; the indirect and direct Lyapunov theorems are used to find the optimal solution with low cost and to accelerate the docking by using Lyapunov approach. The docking problem involves many degrees of freedom. One molecule has six degrees of translational and rotational freedom relative to the other, as well as the conformational degrees of freedom of each molecule [3].

Four different optimal geometry search strategies are introduced for locating the binding sites of the minimum energy in the receptor structure. Then, the following results were obtained: the Monte Carlo Algorithm is randomly calculated and has the lowest precise ratio; the Simulated Annealing Algorithm is randomly calculated and liable to local minimum error; the Genetic Algorithm performs better than the above two, but its selection is still random and the result of performances is not high efficient when the docking system is in running various compound and ligand. In this work, the Lyapunov stability theorem is employed to reduce the number of binding sites to enhance the docking performance, and the NURBS knot and weight are modified to cut down the docking