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EMPLOYING REDUCED ORDER APPROACH FOR COMPUTING PROTEIN FOLDING VIA LANGEVIN EQUATION AND LYAPUNOV THEOREM

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Abstract. *Molecular structure computation involves an NP-complete algorithm. The order of the distance matrix is especially important, and reduced order processing is attempted to accelerate the folding computation. In my previous researches, the Ullman algorithm and the scoring function with force field simulation are used to reduce the dimensionality of the determinant and evaluate some important parameters for molecular docking acceleration. Additionally, the emergence of brand-new molecular structure processing is expected, and in particular, a simpler and more effective computation model can be established. This paper succeeds in using the Langevin Equation and Laplace's theorem for reducing molecular order, and employing Lyapunov theorem to delete some points that have local minimum energy for accelerating the calculation of protein folding.*
Keywords: Drug docking, Minimum energy, Protein folding, Molecular visualization

1. **Introduction.** Folding proteins are nanomachines before proteins can undertake their biochemical function; they assemble themselves, which is known as "folding". The process of protein folding, while essential to virtually all of biology, remains a mystery. Furthermore, when proteins do not fold correctly (i.e., "misfol"), serious effects can arise, including many well-known diseases, such as Alzheimer's, Mad Cow (BSE), CJD, ALS, and Parkinson's disease [1].

In order to perform protein function (e.g., enzymes or antibodies), proteins must take on a particular shape that assemble themselves before they do their work. One of the study goals is to simulate protein folding in order to understand how proteins fold so quickly and reliably, and to comprehend how to make synthetic polymers with these properties and find out the binding activity sites. Some diseases such as Alzheimer's disease, cystic fibrosis, BSE (Mad Cow disease), an inherited form of emphysema, and even many cancers are believed to result from protein misfolding [2]. Proteins misfolding can clump together that can often gather in the brain which is thought to lead to the symptoms of Mad Cow or Alzheimer's diseases.

Not only do proteins self-assemble fold but they do so surprisingly rapidly, sometimes in only a millionth of a second. While this time is very fast on a person's timescale, it is remarkably long for computers to simulate. In fact, a computer takes about a day to simulate a nanosecond (1/1,000,000,000 of a second). Unfortunately, proteins fold on a timescale of tens of microseconds (10,000 nanoseconds). Thus, a computer would take