

## Chapter 20

# Adaptive Simulated Annealing Algorithm to Solve Bio- Molecular Optimization

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### ABSTRACT

*Energy minimization is a paramount zone in the field of computational and structural biology for protein modeling. It helps in mending distorted geometries in the folded functional protein by moving its atoms to release internal constraints. It attempts to hold back to zero value for the net atomic force on every atom. But to overcome certain disadvantages in energy minimization, Simulated Annealing (SA) can be helpful. SA is a molecular dynamics technique, where temperature is gradually reduced during the simulation. It provides the best configuration of bio-molecules in shorter time. With the advancement in computational knowledge, one essential but less sensitive variant of SA: Adaptive Simulated Annealing (ASA) algorithm is beneficial, because it automatically adjusts the temperature scheme and abrupt opting of step. Therefore it benefits to prepare stable protein models and further to investigate protein-protein interactions. Thus, a residue-level study can be analyzed in details for the benefit of the entire biota.*

### INTRODUCTION

It is an essential techniques into the manifold approaches and analysis for the entire developmental idea into the field of in silico structural biology, via energy minimization. Energy minimization is the phenomena to investigate the arrangement of a atomic cluster within vacuum. As per some *in silico* replica of chemical interactions, like quantum mechanics, the zero is the value for the gross atomic force on every atoms (Peng, Ayala & Schlegel, 1996). A single unique molecule, an ion, or a state of transition or even a cluster of all the aforementioned parameters prepare the respective atomic cluster.

For an instance, for optimizing the geometry of a water molecule, the length of the bonds between hydrogen and oxygen as well as the angles between the hydrogen, oxygen and hydrogen (H-O-H) are

DOI: 10.4018/978-1-5225-0058-2.ch020

perceived to reduce the overall force. Otherwise they would pull atoms together or push them apart (Peng, Ayala & Schlegel, 1996)

Therefore, energy minimization also is an important step for protein molecular modeling. It is capable to mend the deformed geometries in the folded functional protein by moving its atoms to release internal constraints. Therefore, as it optimizes the geometry of the protein structure, it is often called energy optimization (Rachid & Normand, 2011). It is also often called geometry optimization (Rachid & Normand, 2011). It helps in hunting the set up for an assortment for the positioning of the respective atomic cluster (Rachid & Normand, 2011).

Tracing forward the concept of chemical bonding in the field of computational modeling, acceptable zero value is kept for the total inter-atomic force on each atom as well as the potential energy surface holds a stationary point (Frank, 1999). Broadly, an optimization algorithm explores the area nearby, generates a random initial solution and attempts to provide the best inference. If the newly obtained inference is superior and improved in nature in comparison to the previous one that was already present, only then, the algorithm moves to it, accepting it as the best solution at that stage (Eduardo et.al, 2011). Energy optimization can be performed following several techniques and optimization algorithms, including genetic algorithms; steepest descent, conjugate gradient and more (Eduardo et.al., 2011). The complications in an energy minimization arises when the energy comprises a preceding term which takes into report the geometrical parameters of the objects like biological macromolecules that are to be energy minimized (Eduardo et.al, 2011).

To overcome this problem, Simulated Annealing (SA): a unique case of Molecular Dynamics simulation can be utilized. This method maintains no data structure of conflicts; instead it picks a neighbor at random and either rejects or accepts the new assignment (Černý, 1985). In this method, maintenance of temperature is obtained on reducing during the progress of the simulation (Černý, 1985). The system is generally heated, followed by cooling (Černý, 1985). The system thereby surmounts energetic barriers to obtain ceratin conformations with energies much lower than the local-minimum energy brought into being by diminishing the energy. This improved the equilibration. Furthermore, at lower temperature, greater amount of rational simulations of dynamics are thus obtained (Kirkpatrick, Gellat & Vecchi, 1983). Therefore, this Simulated Annealing (SA) technique aims to extract the best configuration of the proteins or other bio-molecules by providing some good minimization in a small span (Kirkpatrick, Gellat & Vecchi, 1983). The stable states of the bio-molecular system are corresponded by the minimum energy arrangements of the atoms. There might exist a very large number of minima with shallow dips on the energy surface. These are called the regions of local minima. Among all the regions the minimum one with the least energy is termed as the global energy minima. It is in this global energy minima, where, the overall structure attains the most stable conformation (Kirkpatrick, Gellat & Vecchi, 1983). For varying temperature situations, essential parameters are essential to regulate the temperature scheme and carry out abrupt assortment of the resepective step. The one and only, such alternative of SA is Adaptive Simulated Annealing (ASA) algorithm. In this algorithm, the temperature schedule as well as the choice for the abrupt steps is involuntarily adjusted with respect to the observed movement. Therefore, compared to canonical SA, ASA is much more well-organized and less susceptible to consumer defined parameters (Ingber, 1983; Ingber, 1989).

These energy optimization studies are utilized to model a protein to its most firm and a steady conformation and then make that protein undergo insilico interactions through molecular docking techniques to obtain a docked complex. The energy optimization of the docked complex is also performed following

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