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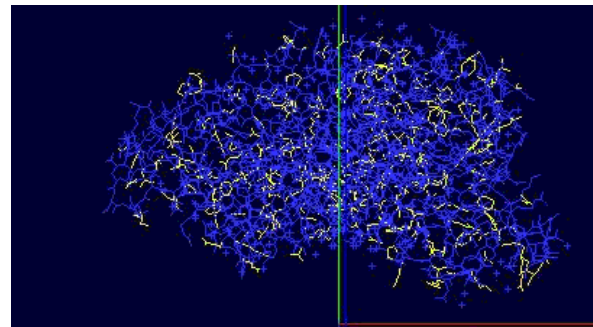
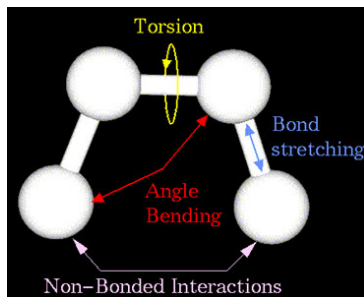
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Ras Nache, 13th June 2010

Master Thesis / Bachelor Thesis

Test of an algorithm for the Protein Sidechain Positioning (SCP) problem based on Lagrangian Relaxation (LR) and Development of appropriate Graphical User Interface (GUI)



Energy = Stretching Energy + Bending Energy + Torsion Energy + Non-Bonded Interaction Energy. The Total Energy has to be minimized

3D model (backbone + sidechains) of a whole protein (here: Phytase from *Klebsiella terrigena* with Deep View / Swiss pdb-viewer 3.7)

In cooperation with the Institute of Simulation of Biological Systems, University of Tübingen, Germany, a new algorithm for sidechain positioning (SCP) of proteins based on Lagrangian relaxation (LR) has been developed at IGEEH, Karlsruhe (see www.aecenar.com/publications) with the Molecular Modeling Toolkit BALL. This algorithm has been implemented, but there are still some bugs. Also tests on test sets have to be undergone and an appropriate User Interface has to be programmed. These working packages are offered to be done as student research thesis (Master thesis or bachelor thesis).

Keywords: Bioinformatics, Molecular Modeling, Discrete Optimization, Lagrangian Relaxation

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