

Departamento de Informática

Constraints and Bioinformatics



CENTRIA



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Chemistry graduate, has a MsC in Artificial Intelligence and a PhD in structural biochemistry. Currently working on structural bioinformatics and protein docking whenever teaching obligations allow.

Objectives

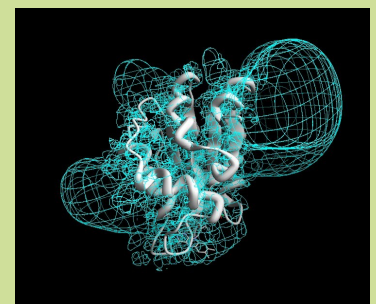
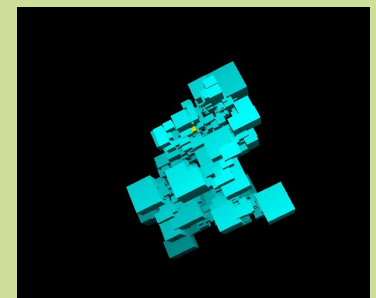
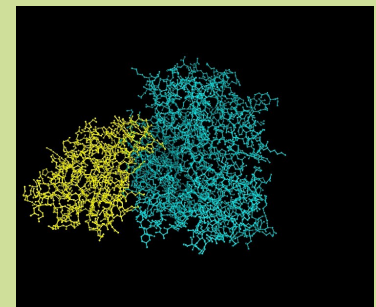
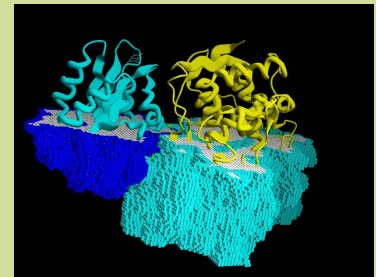
- To improve protein docking algorithms with constraint propagation and by incorporating constraints derived from experimental data and coevolution indicators.
- To improve the detection of coevolution in Multiple Sequence Alignments.
- To improve the computation of protein structures with constraint programming.
- To improve the display of structural, physical and biochemical data.

Methodology

This approach focuses mainly on applying techniques from Artificial Intelligence to bioinformatics problems, in particular constraint programming and machine learning methods. However, since both Artificial Intelligence and Biotechnology are fields which tend to transgress classical boundaries, there are significant contributions from other fields such as computer graphics, scientific computing, information science and software engineering.

Expected Results

- Better modeling algorithms for predicting protein-protein interaction in transient complexes.
- An algorithm to refine Multiple Sequence Alignments using constraint programming and incorporating coevolution indicators to determine where the assumption of independent mutations does not hold.
- The Open Chemera Library, an open source toolbox containing libraries and applications implementing these new algorithms and auxiliary tools for modeling and visualization.



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