

CASSIAN D'CUNHA

13090 SW 80th St,
Miami, Florida –33183.

e-mail- cassian_dcunha@yahoo.com
Ph: 305-766-8667(C), 305-348-1198(O)

Education

Florida International University PhD: Chemistry & Biochemistry	Miami, Florida Present
Florida International University Master of Science: Computer Science	Miami, Florida Dec 2003
University of Mumbai Bachelor of Engineering: Chemical Engineering	Mumbai, India December 1999

Computer Skills

Programming	: C++, C, Shell programming, Pascal, Prolog, Clips.
RDBMS	: MS SQL Server7.0, MS Access.
Operating Systems	: LINUX, IRIX, Windows.
Other Applications	: CHARMM, AWK, Gaussian98, GopenMol, HyperChem, Spartan, Gnuplot, Rasmol, Molden, Q-Chem, Turbomole.

Projects

- **Setup, Configuration and Maintenance of a Beowulf Cluster**
 - Setup of a 30-dual-processor-node cluster.
 - Customization of parallel job submission to make it more flexible.
 - Have written a script that makes parallel jobs submitted on the cluster transparent to the user. It sets up a queue if all CPUs are busy and submits jobs when the required number of CPUs becomes free.

- **Computational Chemistry / Bioinformatics**
 - Implemented Geometric Hashing for pattern recognition of substructures in proteins.
 - Computer simulations of dynamics of protein backbone and side chains and gas-phase quantum mechanical calculations of the electronic structure of small organic molecules.
 - Methyl dynamics in crystalline amino acids: MD and NMR.
 - Ab initio study of abnormal Michael addition.
 - Correlation times and adiabatic barriers for methyl rotations in proteins.
 - Backbone flexibility of the small, doubly cross linked peptide α -conotoxin GI: MD and NMR.

Publications

- D. C. Chatfield, A. Augsten, C. D'Cunha, and S. E. Wong, "*Methyl dynamics in crystalline amino acids: MD and NMR*," J. Computational Chemistry. **24**, 1052-1058 (2003)
- D. C. Chatfield, A. Augsten, C. D'Cunha, E. Lewandowska, and S. F. Wnuk, "*Theoretical and Experimental Study of Regioselectivity of Michael Additions*," Euro. J. Organic Chemistry. 313-322 (2004)
- D. C. Chatfield, A. Augsten, and C. D'Cunha, "*Correlation times and adiabatic barriers for methyl rotations in proteins*," J. Molecular NMR. 1-9 (2004)