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December 28, 2004

Biocomplexity Faculty Search Committee
c / o Prof. Rob de Ruyter van Steveninck
Department of Physics
Indiana University
Swain Hall West 117
Bloomington, IN 47405-7105

Dear Dr. Rob de Ruyter van Steveninck:

This is a reference letter of academic accomplishments of Dr. Julio Castrillon-Candas, to very strongly support his faculty application.

Julio received his Ph.D. in 2001 from the Electrical Engineering & Computer Science Department, Massachusetts Institute of Technology, on the topic of spatially adaptive wavelet representations on unstructured grids, under the supervision of Ph.D. advisor Dr. Amaratunga. This development of multi-resolution boundary and finite element representations, summarized in the two papers in IJNME, 2001 and SIAM -SISC 2003, are fundamental and provide the computational framework for several applications involving the solution of integral and differential equations. This was my primary attraction as I was looking for a postdoc with computational mathematics experience, to work with in developing efficient computational representations of biomolecules that would yield fast solutions to the protein-protein docking, and the protein – 3D Map docking problems. The scoring function for a good match in each of the two docking applications, is a multi-dimensional Integral equation, and the problem reduces to computing this integral equation fast, as the search is over six dimensional real space or higher.

The protein-protein docking is actually a hierarchy of problems, with an attempt to progressively model the interaction of two proteins, as they come together or dock. The simplest scoring function is based on shape complementarity and attempts to model the fit of one protein in the complementary space of the other. This search for the best shape

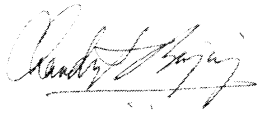
fit is over six dimensional space for rigid proteins, and increases in dimensionality with the relative flexibility or deformability of the involed proteins. Julio's contributions to the solution of this problem was instrumental in the development of a fast Fourier based method of rapidly computing the solution of the docking problem. In conjunction with my Ph.d. student, Vinay Siddavanahalli, Julio additionally adapted and implemented a method of irregular discrete FFT published by Potts and Steidel, to provided an efficient protein-protein shape docking solution. This primary shape complementarity docking scheme is extensible to enhanced electrostatics complementarity docking. This work is summarized in a paper, Julio is preparing for submission to a journal, this month. This method also forms the kernel of our collaboration with Dr. Art Olson and Dr. Michel Sanner of The Scripps Research Institute in the joint development of a new generation fast docking code, for public use.

Julio's second major contribution as a postdoc in my group, has been in the development of a wavelet based preconditioner and sparsifier used in the accurate and efficient construction of a radial basis spline representation of volumetric maps reconstructed from electron microscopy. This three dimensional multi-wavelet is constructed using a lifting scheme, with polynomial vanishing moments, and based on extensions of Julio's Ph.D. work. This is summarized in a paper being prepared for journal submission. In conjunction with my Ph.d. student, Jun Li, this method has also been implemented in C++, and is going to be made publicly available. The radial basis spline representation is extremely useful as a representation to match and fit (dock) high-resolution crystal structures into low or medium resolution reconstructed maps of protein structures and other macromolecular complexes.

Julio has also contributed to refining an earlier wavelet based compressed representation scheme with fast decompression, that my group had been developing as an efficient representation of biomolecular complexes for direct and interactive volume visualization. This has been summarized in a paper, and submitted to Structure for publication. The compression/decompression has been implemented by my Ph.d. student Zaiqing Xu, in C++ and the code has been made publicly available.

Julio's is on track to becoming an accomplished researcher and has all the required background to make very significant contributions. He works well with students, and has a natural affinity to teaching. I recommend him very highly to you.

Sincerely,



Chandrajit L. Bajaj