JULIO ENRIQUE CASTRILLON CANDAS

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December 8, 2004

Re: Assistant Professor

Dear

I am interested in applying to the Assistant Professor position at the Biocomplexity Institute, Indiana University, Bloomington. After completing a Ph.D. in Electrical Engineering and Computer Science at the *Massachusetts Institute of Technology (MIT)*, I was awarded a highly competitive ICES Post Doctoral Fellowship to conduct research in **Scientific Computing** applied to **Molecular Biology** coupled with **Scientific Visualization** at the Computational Visualization Center (CVC*). I am currently working under the supervision of Professor Chandrajit Bajaj, Director of the CVC.

Bio-molecular Complexes (BCs) form the machinery responsible for most biological processes and are relevant to understanding many diseases, such as cancer and metabolic disorders. Knowledge of these structures would provide not only the mechanistic descriptions for how macromolecules act in an assembly, but more importantly tools in developing therapeutic interventions related to disease. The goal of my research is to answer the following Bio-molecular questions:

- How do we identify, represent, match and visualize Large Biomolecular Complexes (LBCs) structures efficiently and fast?
- How do these structures interact?

My approach involves the development of *Multi-Resolution and Radial Basis Functions* (MR) theory to optimize computational modeling and information processing techniques, in particular, for large-scale complex physical systems. More precisely, MR theory is leading to:

- Feature preserving molecular representations of LBC.
- Fast and stable extraction of suitable representations of LBCs suitable for large-scale visualization and information processing.
- Fast biomolecular convolution codes for structure identification and docking.
- Simulation of biophysical phenomena

This research leads to computational molecular tools (written in C++) to process and analyze multi-dimensional data sets that allow fast and accurate docking and matching of large protein structures. We have currently reached computational speeds of 100 times faster and 50 times less memory with a .1% energy and 1.5% peak location detection error. We have also achieved visualization of molecules consisting of 1,000,000+ atoms at near interactive speeds on a common desktop. These tools have been developed in conjunction with my references:

- Dr. C. Bajaj (Postdoctoral Advisor and Head of the Computational Visualization Center (CVC) at the University of Texas)
- Dr. A. Olson (Head of the Molecular Graphics Laboratory at The Scripps Research Institute. CA)
- Dr. W. Chiu (Head of the National Center for Macromolecular Imaging, Baylor College of Medicine, TX).

^{*}The Center is under the joint auspices of the Institute for Computational Engineering and Sciences (ICES) and the Department of Computer Sciences at the University of Texas at Austin.

Other references include:

- Dr. Kevin Amaratunga (Ph.D. Advisor, MIT)
- Dr. Gilbert Strang (MIT)
- Dr. Pavel Bochev (Sandia National Laboratories)

More detailed information on my research can be found on my website at http://www.ices.utexas.edu/~julio/index.html. Note also, that current manuscripts will be updated in the website.

My research capabilities are complemented with experience writing research proposals. This year I have participated in the writing of three National Institutes of Health (NIH) proposals. The proposals are titled as follows:

- A New Approach to Rapid Protein-Protein Docking (top 7% score, funding pending)
- Hierarchical Methods for Large Bio-molecular Complexes (pending)
- Software Maintenance for Bio-molecular Complexes (pending)

In addition to my research interests, I have substantial teaching and advisory experience. I have many years experience as a Teaching Assistant and Recitation Instructor. I have also managed large groups of Teaching Assistants and am currently advising Ph.D. students on thesis topics. I would be pleased to meet and discuss your research needs and how I may address them.

Sincerely,

Julio E. Castrillon Candas

Curriculum Vitae

Julio E. Castrillón-Candás

ICES Postdoctoral Fellow
Institute for Computational and Engineering Sciences
Computational Visualization Center, Department of Computer Science
201 East 24th Street, ACES 2.412, 1 University Station C0200
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PRINCIPAL FIELDS OF INTEREST

Large scale multidimensional computational modeling such as numerical analysis/methods, scientific computing and signal processing applied to Bioinformatics, Molecular Structural Identification, Protein Docking and Scientific Visualization. Particular interest in hierarchal representation, simulation and visualization of highly complex systems/objects.

EDUCATION

Institution	Degree	Date
Massachusetts Institute of Technology	Ph.D (Elec. Eng. and Comp. Sc.)	2001
Massachusetts Institute of Technology	M.S. (Elec. Eng. and Comp. Sc.)	1996
Instituto Tecnológico de Monterrey	IEC	1992

RESEARCH EXPERIENCE

Lab	Position	Date
CVC (ICES), Formerly TICAM	Post Doctoral Fel-	March 2003 -
	low	Present

Recipient of an Institute for Computational Engineering and Sciences (ICES) Post Doctoral Fellowship to conduct research in Computational Molecular Biology coupled with Scientific Visualization at the Computational Visualization Center (CVC). The Center is under the joint auspices of the Institute for Computational Engineering and Sciences (ICES) and the Department of Computer Sciences (CS) at the University of Texas at Austin. I am currently working under the supervision of Professor Chandrajit Bajaj, who is the head of CVC.

Lab	Position	Date
Intelligent Engineering Systems Labo-	Post. Doc. Assoc.	June 2001 - Decem-
ratory (MIT)		ber 2001

Research position. Developing new novel multi scale numerical methods, including hierarchal boundary Elements, generalized hierarchal finite elements, and 3D reduced order complexity Singular Value Decomposition Algorithms. Other duties include advising Ph.Ds students.

Lab	Position	Date
Intelligent Engineering Systems Labo-	Research Assistant	Fall 1998 - Spring
ratory		2001

Developed a new wavelet basis over irregular meshes with applications to computational modeling. Combines the flexibility of Finite Element Methods with the fast decorrelation, localization and entropy reduction properties of wavelets. These new wavelet constructions lead to a practical implementation of wavelets for solving PDEs with complex 3D geometries. Other research areas in computational modeling include data and graphics compression. (Research sponsored by NSF).

Lab	Position	Date	;
Intelligent Engineering Systems Labo-	Research Assistant	Spr.	1998 - Sum.
ratory		1998	

Virtual Workbench Project: Implementation of web tools for remote experimentation. (Research sponsored by Ford Motor Company as part of the Virtual Engineering Initiative).

Lab	Position	Date
Laboratory for Electromag. and Elect.	Research Assistant	Fall 1994 - Spring
Sys.		1997

Fast computation of finite time Grammians and development of reduced order models, with applications to power systems.

CONSULTING

Employer	Position	\mathbf{Date}
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Siproco, Mexico City Consultant June 1993-August 1993

DGI, ITESM-CEM, Mexico City Social Service, Research As. 1991-1992

AWARDS

Award
ICES Post Doctoral Fellowship (University Of Texas, Austin)

Fall 2002

Fulbright scholarship Awarded (Offered, but not accepted)

Spring 1993

Graduate with Honors, ITESM-CEM December 1992

First Prize, Institute wide engineering competition, ITESM-CEM Fall 1991

ORGANIZATION MEMBERSHIPS AND REVIEWER

Organization

Society for Industrial and Applied Mathematics (SIAM)

Sigma Xi

Reviewer for IEEE Transactions on Signal Processing

Reviewer for IEEE Transactions on Circuits and Systems

SKILLS

C++/ MATLAB/ Unix/ Linux

MIT TEACHING EXPERIENCE

Term ST2001	Subject Number 1.130/18.327	Title Wavelets and Filter Banks	Role TA (Recitation instructor) Taught Recitations, grading and hwk review
ST2000	1.130/18.327	Wavelets and Filter Banks	Teaching Assistant Taught Recitations, grading and hwk review
FT1999	6.003	Signal and Systems	Head Teaching Assistant Organized 4 T.As. for hwks, tutorials
ST1999	1.130/18.327	Wavelets and Filter Banks	Teaching Assistant Taught Recitations, grading and hwk review
FT1998	6.003	Signal and Systems	Head Teaching Assistant Organized 4 T.As. for hwks, tutorials
SP1998	6.002	Circuits and systems	Head Teaching Assistant Organized 11 T.As. for Labs, hwks, tutorials
FT1997	6.003	Signal and Systems	Head Teaching Assistant Organized 4 T.As. for hwks, tutorials
ST1997	6.002	Circuits and systems	Teaching Assistant Labs, hwks, tutorials
FT1996	6.003	Signal and Systems	Teaching Assistant Labs, hwks, tutorials
ST1996	6.002	Circuits and systems	Teaching Assistant Labs, hwks, tutorials

REFERENCES

Chandrajit Bajaj (Postdoctoral Advisor)

Professor of Computer Sciences
Director of CVC,
Computer Sciences Dept. & ICES
ACES 2.324A, 24th & Speedway
University of Texas at Austin
Austin, TX 78712
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Art Olson

Professor of Molecular Biology Molecular Graphics Laboratory Department of Molecular Biology, MB-5 The Scripps Research Institute 10550 North Torrey Pines Road La Jolla, CA 92037-1000 (858) 784-9702, (858) 784-2860 olson@scripps.edu

Wah Chiu

Professor of Biochemistry and Molecular Biology Director, National Center for Macromolecular Imaging Baylor College of Medicine One Baylor Plaza, Houston, Texas 77030 (713) 798-6985 (713) 798-1625 (Fax) wah@bcm.tmc.edu

Kevin Amaratunga (Ph.D Advisor)

Associate Professor of Civil and Env. Eng. Department of Civil and Environmental Eng. Massachusetts Institute of Technology 77 Mass Ave Room 1-274 Cambridge MA, 02139 617 258 0217 kevina@mit.edu

Gilbert Strang

Professor of Mathematics
Department of Mathematics
Massachusetts Institute of Technology
77 Mass Ave Room 2-240
Cambridge MA, 02139
617 253 4383
gs@math.mit.edu

Dr. Pavel Bochev

P.O. Box 5800, MS 1110 Computational Math and Algorithms Sandia National Laboratories Albuquerque, NM 87185-1110 505-844-1990 pbboche@sandia.gov

PUBLICATION IN REFEREED JOURNALS

- [1] Julio E. Castrillón-Candás, Chandrajit Bajaj and Jun Li, "Sparsification and Stabilization of Radial and Anisotropic Basis Functions", ICES Technical Report.
- [2] Julio E. Castrillón-Candás, Chandrajit Bajaj and Vinay K. Siddavanahalli. "An adaptive Compact Fourier Representation Method for Protein-Protein Docking", *ICES Technical Report*.
- [3] C. Bajaj, J.E. Castrillón-Candás and Z. Xu, "Hierarchical and compressed volumetric representations of molecular structures", *ICES Technical Report*.
- [4] W. Luo, J. E. Castrillón-Candás, H. Zarbl and W. G. Thilly (2004). "Inducible DNA Repair Accounts for Time Dependent resistance of Human AHH-1 Cells to Mutation by PAH", Submitted to Mutation Research.
- [5] S. D Heedene , K Amaratunga and J.E. Castrillon-Candas, "Generalized Hierarchical Bases: a Wavelet-Ritz-Galerkin Framework for Lagrangian FEM" , To appear in *Engineering Computations*.
- [6] J. E. Castrillon-Candas and K. Amaratunga, "Spatially Adapted Multiwavelets and Sparse Representation of Integral Operators on General Geometries", *SIAM Journal on Scientific Computing*, 24,5, 1530-1566, 2003.
- [7] J. E. Castrillon-Candas and K. Amaratunga, "Fast Computation of Continuous Karhunen-Loeve Eigenfunctions using Wavelets", *IEEE Transactions on Signal Processing*, 50, 1, 78-86, January 2002.
- [8] K. Amaratunga and J. E. Castrillon-Candas: "Surface Wavelets: A Multiresolution Signal Processing Tool for 3D Computational Modeling". *International Journal of Numerical Methods in Engineering*, 52, 3, 239-271, September 2001.

CONFERENCES

- [1] J. E. Castrillon-Candas and K. Amaratunga "Spatially Adaptive MultiWavelet Representation on Unstructured Grids with Applications to Multidimensional Computational Modeling", First MIT Conference on Computational and Solid Mechanics, Cambridge, USA June 2001.
- [2] J. E. Castrillon-Candas and K. Amaratunga "Interpolating Wavelets on Unstructured Grids for the Fast Computation of 3D Integral Problems", Proceedings of SPIE Wavelet Applications VII, 4056, 421-432, Orlando, FL, April 2000.

- [3] K. Amaratunga and J. E. Castrillon-Candas, "Wavelets Transforms on 3D Unstructured Grids for the Fast Computation of Integral Equations", IT SIAM 2000 Annual Meeting, Mini symposium on Multi scale Methods for Conservation Laws, Bihari and Amaratunga organizers, San Juan, Puerto Rico, July 2000.
- [4] K. Amaratunga and J. E. Castrillon-Candas, "3D Fast Multiresolution Computation of Partial Differential Equations", IT Proceedings of Electromagnetic Code Consortium (EMCC) 2000 Annual Meeting, St Louis, MO, May 2000.