

*CURRICULUM VITAE*

**Jesús A. Izaguirre**

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## 1 Current Position

2005- **Associate Professor (with tenure)**, Department of Computer Science and Engineering and Interdisciplinary Center for Network Science and Applications (iCeNSA), University of Notre Dame, Notre Dame, IN.

## 2 Higher Education

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EDUCATION/TRAINING			
INSTITUTION AND LOCATION	DEGREE	YEAR(s)	FIELD OF STUDY
Instituto Tecnológico de Monterrey (ITESM)	B.S.	1992	Electronic Systems Engineering
University of Illinois at Urbana-Champaign	M.S.	1996	Computer Science, specialization Computational Science and Engineering
University of Illinois at Urbana-Champaign	Ph.D.	1999	Computer Science

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### 3 Previous Positions

1992	Instructor, Department of Computer Science, Instituto Tecnológico de Monterrey (ITESM), México
1993	Research Programmer, National Center for Supercomputing Applications (NCSA), Urbana, IL
1997-99	Research Assistant, NIH Resource for Macromolecular Modeling and Bioinformatics, University of Illinois, Urbana, IL
1999-2005	Assistant Professor, Department of Computer Science and Engineering, University of Notre Dame, Notre Dame, IN
2006-2008	Visiting Professor, Institute for Computational and Mathematical Engineering, Stanford University, Stanford, CA

### 4 Distinctions and Other Activities

1992	Graduated second in class from ITESM, <i>with highest honors</i>
2002	NSF CAREER Award
2002	Departmental Faculty Undergraduate Teaching Award
2005	BP Foundation Outstanding Teacher of the Year for the College of Engineering, University of Notre Dame
2007-2008	Kaneb Fellow, University of Notre Dame
2006-	Member, Folding@Home Consortium, Stanford University
2007-2011	Standing Member, NIH BDMA Study Section

### 5 Scholarships and Fellowships

1987-95	Monterrey Tech (ITESM) fellowship
1992-97	Fulbright fellowship
May 2001	Visiting scholar, McCammon Research Group, University of California at San Diego
Summer 2003	Visiting research assistant professor, Beckman Institute, University of Illinois at Urbana Champaign
March 2005	Visiting scholar, Institute of Mathematics and its Applications (IMA), University of Minnesota Twin-Cities

### 6 Professional Memberships

- Association for Computing Machinery (ACM), Interest group on Algorithms and Computation Theory (SIGACT), Interest group on Programming Languages (SIGPLAN)

- The Institute of Electrical and Electronic Engineers (IEEE), IEEE Computer Society
- American Society of Engineering Education (ASEE)
- Society of Industrial and Applied Mathematics (SIAM), Activity Groups on Supercomputing, Computational Science and Engineering, and Life Sciences

## 7 Current Projects

**Long Timestep Molecular Dynamics.** My group develops numerical methods for achieving long timestep MD and reaching the millisecond timescale. These methods are combined with ensemble computing using Folding@Home, Markov State Models, and acceleration using general purpose GPUs. We distribute our methods through Protomol (<http://protomol.sourceforge.net>) and the GPU library OpenMM (<http://simtk.org/home/openmm>). Related to these problems is the development of scalable methods for computing reaction paths and generalized ensemble sampling using adaptive dimensionality reduction techniques. My main collaborators are Chris R. Sweet from the Center for Research Computing at Notre Dame and Prof. Vijay S. Pande at Stanford.

**Simulation of Protein Folding and Conformational Dynamics.** Using our enhanced methods, we are studying the effect of sequence on folding, particularly for WW domains, and trying to extend simulation capabilities to larger molecules on the millisecond timescale. Of particular interest is the effect of flexibility on catalytic activity, the effect of phosphorylation and other post translational modifications in structure and dynamics, and the connection between correlated motions and phylogenetic co-evolution. We are collaborating with several experimental labs in carrying out these studies.

**Prediction of domain-domain and protein-protein interactions and interfaces.** We are developing methods for improving the prediction of protein-protein interactions, and for finding sequence and structural signatures that explain specificity of interactions. Systems of interest include two component systems and GPCR - G-protein signaling pathways.

**Study of host-pathogen interactions.** We are characterizing interactions of the malaria parasite *Plasmodium falciparum* and red blood cells, particularly related to G-protein signaling and heat shock proteins. Our main collaborator is Prof. Kasturi Haldar at Notre Dame.

**Design of a new generation of insecticides.** We are attempting genome wide identification of insecticide targets through systems biology, molecular modeling, and molecular biology techniques. Our main collaborators are Profs. Frank Collins and Mary Ann McDowell at Notre Dame and Prof. Cate Hill at Purdue.

## 8 Publications

### References

- [1] F. Morcos, S. Chatterjee, C. McClendon, P. Brenner, R. Lopez-Rendon, J. Zintsmaster, M. Ercsey-Ravasz, C. R. Sweet, M. Jacobson, J. Peng, and J. A. Izaguirre. Modeling conformational ensembles of slow functional motions in pin1-ww. *PLoS Comput. Biol.* 6(12):e1001015, 2010.
- [2] J. A. Izaguirre, C. R. Sweet, and V. S. Pande. Multiscale dynamics of macromolecules using Normal Mode Langevin. *Pac. Symp. Biocomput.* 15:240–51, 2010.
- [3] F. Morcos, M. Sikora, M. Alber, D. Kaiser, and J. Izaguirre. Estimation of protein and domain interactions in the switching motility system of myxococcus xanthus. *Pac. Symp. Biocomput.* 15:157–65, 2010.
- [4] F. Morcos, M. Sikora, M. Alber, D. Kaiser, and J. A. Izaguirre. Belief propagation estimation of protein and domain interactions using algorithm. *IEEE Trans. Inf. Theory* 56:742–755, 2010.
- [5] T. Cickovski, S. Chatterjee, J. Wenger, C. R. Sweet, and J. A. Izaguirre. Mdlab: A molecular dynamics simulation prototyping environment. *J. Comp. Chem.*, 2010. doi 10.1002/jcc.21418.
- [6] C. Sweet, S. Hampton, R. Skeel, and J. Izaguirre. A separable shadow hamiltonian hybrid Monte Carlo method. *J. Chem. Phys.* 131:174106, 2009.
- [7] F. Morcos, C. Lamanna, N. V. Chawla, and J. A. Izaguirre. Determination of specificity residues in two component systems using graphlets. *Proc. International Conference on Bioinformatics & Computational Biology BIOCOMP 09*, 2009.
- [8] S. P. Kanaan, C. Huang, S. Wuchty, D. Z. Chen, and J. A. Izaguirre. Inferring protein-protein interactions from multiple protein domain combinations. *Methods Mol. Biol.* 541:43–59, 2009.
- [9] F. Morcos, C. Lamanna, M. Sikora, and J. Izaguirre. Cytoprophet: A Cytoscape plug-in for protein and domain interaction networks inference. *Bioinformatics* 19:2265–2266, 2008.
- [10] P. Brenner, J. M. Wozniak, D. Thain, A. Striegel, J. W. Peng, and J. A. Izaguirre. Biomolecular committor probability calculation enabled by processing in network storage. *Parallel Computing* 34:652–660, 2008.
- [11] C. R. Sweet, P. Petrone, V. S. Pande, and J. A. Izaguirre. Normal mode partitioning of Langevin dynamics for biomolecules. *J. Chem. Phys.* 128:1–14, 2008.

- [12] J. M. Wozniak, P. Brenner, D. Thain, A. Striegel, and J. A. Izaguirre. Making the best of a bad situation: Prioritized storage management in gems. *Future Generation Computer Systems* 24:10–16, Jan. 2008.
- [13] N. Chen, J. A. Glazier, J. A. Izaguirre, and M. S. Alber. A parallel implementation of the cellular Potts model for simulation of cell-based morphogenesis. *Comput. Phys. Commun.* 176:670, 2007.
- [14] P. Brenner, C. R. Sweet, D. VonHandorf, and J. A. Izaguirre. Accelerating the replica exchange method through an efficient all-pairs exchange. *J. Chem. Phys.* 126:074103, February 2007.
- [15] C. Huang, F. Morcos, S. P. Kanaan, S. Wuchty, D. Z. Chen, and J. A. Izaguirre. Predicting protein-protein interactions from protein domains using a set cover approach. *IEEE/ACM Trans. on Comp. Bio. and Bioinformatics* 4:78–87, Jan. 2007.
- [16] T. Cickovski, K. Aras, M. Swat, R. Merks, T. Glimm, H. H. M. S. Alber, J. A. Glazier, S. A. Newman, and J. A. Izaguirre. From genes to organisms via the cell: A problem solving environment for multicellular development. *Computing in Science and Engineering* 9:50, 2007.
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- [18] M. Sikora, F. Morcos, D. J. C. Jr., and J. A. Izaguirre. Bayesian inference of protein and domain interactions using the sum-product algorithm. *Proc. 2007 Information Theory and Applications Workshop*, 2007.
- [19] P. Brenner, J. M. Wozniak, D. Thain, A. Striegel, J. W. Peng, and J. A. Izaguirre. Biomolecular Path Sampling Enabled by Processing in Network Storage. *2007 IEEE International Parallel and Distributed Processing Symposium*, p. 256, 2007.
- [20] C. R. Sweet and J. A. Izaguirre. Backward error analysis of multiscale symplectic integrators and propagators. *Proc. Third International Conference Multiscale Materials Modeling MMM2006*, 2006.
- [21] F. Morcos, M. Boxem, N. Klitgord, M. Vidal, and J. A. Izaguirre. Prediction of domain interactions in *C. elegans*. *Proc. Workshop Computational Biophysics to Systems Biology CBSB06*, 2006.
- [22] S. S. Hampton, P. Brenner, A. Wenger, S. Chatterjee, and J. A. Izaguirre. Biomolecular sampling: Algorithms, test molecules, and metrics. *New Algorithms for Macromolecular Simulation*, vol. 49, pp. 103–121. Springer-Verlag New York, LNCS, 2006.

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a multimodel framework for simulation of morphogenesis. *Bioinformatics* 20:1129–1137, 2004, <http://bioinformatics.oupjournals.org/cgi/content/abstract/20/7/1129>, arXiv:<http://bioinformatics.oupjournals.org/cgi/reprint/20/7/1129.pdf>.

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- [35] S. S. Hampton and J. A. Izaguirre. Improved sampling for biological molecules using shadow hybrid Monte Carlo. *4th International Conference on Computational Science, Kraków, Poland*, vol. 3037, pp. 268–274. Springer-Verlag, LNCS, 2004.
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## 9 Software and other Publications

### References

- [1] MDSIMaid. Molecular Dynamics Simulation Aid. <http://mdsimaid.cse.nd.edu/>, Aug. 2004.

- [2] COMPUCCELL. COMPUCCELL: A framework for three-dimensional simulation of morphogenesis. <http://sourceforge.net/projects/compucecell/>, Sep. 2004. 350 downloads from Apr. 2003 - Feb. 2005.
- [3] PROTOMOL. PROTOMOL: An object oriented framework for molecular dynamics. <http://sourceforge.net/projects/protomol/>, Sep. 2004. 868 downloads from Sept. 2003 - Feb. 2005.
- [4] T. Cickovski and J. A. Izaguirre. BIOLOGO: A domain-specific language for morphogenesis. In preparation. Manuscript available at <http://www.nd.edu/~tcickovs/document.pdf>, 2005.
- [5] T. Cickovski, T. Matthey, and J. A. Izaguirre. Design patterns for scientific software. Tech. Rep. TR-2004-29, Univ. of Notre Dame, 2004. Preprint: <ftp://ftp.cse.nd.edu/pub/Reports/2004/TR-2004-29.pdf>.
- [6] A. Striegel, M. Shorts, E. Stuntebeck, D. Salyers, and J. A. Izaguirre. GIPSE: A toolset for streamlining the management aspects of the grid for simulation-based research. Tech. Rep. TR 04-16, University of Notre Dame, 2004.
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- [8] J. A. Izaguirre. *Longer Time Steps for Molecular Dynamics*. Ph.D. thesis, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA, 1999.

## 10 Postdoctoral Research Associates Supervised

1. Roberto López-Rendón, Ph.D. 2007, Universidad Autónoma de México, since 2008.
2. Chris Sweet, Ph.D. 2003, University of Leicester, 2005 - present.
3. Rajiv Chaturvedi, Ph.D. 2000, Indian Institute of Technology, 2001 - 2004.
4. Atul Bahel, Ph.D. 1998, New York University, 2000.

## 11 Ph.D. Theses Supervised

1. Faruck Morcos, Ph.D., March 2010, “Multiscale Protein Networks: Interactions, Two Component Systems and Kinetics”, (currently, Center for Theoretical Biological Physics, University of California San Diego)

2. Santanu Chatterjee, Ph.D., March 2010, “Coarse-Grained Methods for Long-Timescale Dynamics of Biomolecules”
3. Trevor Cickovski, Ph.D., March 2008, “Domain-Specific Languages in Computational Biology.” (currently, Dept. of Computer Science, Eckerd College)
4. Paul R. Brenner, Ph.D., July 2007, “Parallel Algorithms and Distributed Systems for Computational Biophysics.” (currently, Center for Research Computing, Notre Dame)
5. Scott S. Hampton, Ph.D., Oct. 2006, “Analysis of Shadow Hybrid Monte Carlo Methods.” (currently, Oak Ridge National Lab)
6. Chengbang Huang, Ph.D., Aug. 2005, “Multiscale Computational Methods for Morphogenesis and Algorithms for Protein-Protein Interaction.” (currently, Vice President, HSBC)
7. Qun (Marc) Ma, Ph.D., Aug. 2003, “Novel multiscale algorithms for molecular dynamics.”
8. Thierry Matthey, Ph.D., Nov. 2002, (co-advisor, main advisor Petter E. Bjorstad, Univ. of Bergen, Norway), “Framework Design, Parallelization and Force Computation in Molecular Dynamics.”

## 12 M.S. Theses Supervised

1. Kedar Aras, “Empirical Analysis of Design-Patterns - A Case Study in CompuCell3D”, October 2005
2. Trevor Cickovski, “BioLogo, a Domain-Specific Language for Morphogenesis”, December 2004
3. Scott Hampton, “Improved Sampling of Configuration Space of Biomolecules using Shadow Hybrid Monte Carlo method,” April 2004
4. Alice Ko, “MDSimAid: An Automatic Recommender for Optimization of Fast Electrostatic algorithms for Molecular Simulations”, Dec. 2002

## 13 Notable Professional Activities

- Member NIH Study Section Biological Data Management and Analysis, 2007 - 2011.
- Executive Committee, Interdisciplinary Center for the Study of Biocomplexity, Univ. of Notre Dame, Sept. 2001 - present

- Technical Program Committee, The Sixth IEEE Workshop on High Performance Computational Biology HiCOMB 2007
- Reviewer in NSF panels (ITR, CISE Algorithm grants, CCF, ACI, etc.)
- Reviewer for NIH National Institute of General Medical Sciences (NIGMS)
- Reviewer for Science, Biophysical Journal, J. Parallel Distributed Processing, IEEE Trans. on Software Engineering, Journal of Computational Physics, Multiscale Modeling and Simulation, Simulation Modelling Practice and Theory
- Reviewer for Algorithms for Macromolecules (AM3) 2004, Supercomputing 2004, ACM SAC 2003
- Session chair, SIAM CSE 2005, SIAM CSE 2003, ACM SAC 2003
- Co-organizer, two Notre Dame Biocomplexity Workshops, 2001, 2003
- Participant, Research@Indiana 2001-2004 displays at Supercomputing
- Member, Center for Nano Science and Technology, Univ. of Notre Dame, Sept. 2000 - present
- Judge, Regional Final, Siemens-Westinghouse Science, Math, and Technology competition, Fall 2004

## 14 Active Collaborations (grants or papers in last 24 months)

- Mark Alber, Notre Dame
- Russ Altman, Stanford University
- Frank Collins, Notre Dame
- Eric Darve, Stanford University
- Kasturi Haldar, Notre Dame
- Dale Kaiser, Stanford University
- Mary Ann McDowell, Notre Dame
- Vijay S. Pande, Stanford University
- Jeff Peng, Notre Dame
- Robert D. Skeel, Purdue University
- Douglas Thain, Notre Dame

## 15 Departmental and University Service

- Bioengineering Program Committee, College of Engineering, Fall 2005 - present
- Undergraduate Curriculum Committee of the CSE Dept., Univ. of Notre Dame, Sept. - Oct. 2001, Jan. 2005 - present.
- Faculty Advisor for the student chapter of the Mexican American Engineering Society (MAES)/Society of Hispanic Professional Engineers (SHPE), Univ. of Notre Dame, Sept. 1999 - present.
- Graduate Committee of the CSE Dept., Univ. of Notre Dame, Aug. 2000 - Dec. 2004
- Faculty Search Committee of the CSE Dept., Univ. of Notre Dame, Fall 2001
- Chair Search Committee for the CSE Dept., Univ. of Notre Dame, Aug. 2000 - May 2001.
- Ad-hoc Committee for Biology in the Engineering Curriculum, Univ. of Notre Dame, Sept. 2001 - Sept. 2002

## 16 Courses taught at Notre Dame

1. CSE 60531, Computational Biophysics and Systems Biology, Springs 2006, 2008, Fall 2009.
2. CSE 30332, Programming Paradigms, Spring 2010.
3. CSE 40232, Software Engineering, Spring 2008.
4. CSE 212, Fundamentals of Computing II, Spring 2003, 2004, 2005.
5. CSE 331, Data Structures, Fall 1999, 2000, 2001, 2002, 2003, 2005.
6. CSE 513, Numerical Methods, Fall 2000.
7. CSE 498E/598E, Computational Methods for Biomolecular Modeling, Spring 2000.
8. CSE 498K/598K, Computational Biology. Spring 2002, Fall 2004.
9. CSE 233, Functional Programming, Spring 2002.