

CURRICULUM VITAE

Jesús A. Izaguirre

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1 Current Position

- 2006- **Visiting Professor**, Institute for Computational and Mathematical Engineering, Stanford University, Stanford, CA
- 2005- **Associate Professor (with tenure)**, Department of Computer Science and Engineering, University of Notre Dame, Notre Dame, IN

2 Higher Education

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

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

4 Distinctions, Honors, and Awards

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

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
- New York Academy of Sciences

7 Current Grants and Sponsored Programs

PI: *CompBio: Simulation of self-emerging properties of coupled biochemical and cellular networks in social behavior of Myxobacteria*, NSF CCF-0622940, Sep. 1 2006 - Aug. 30 2008, \$300,000, 50% effort. Co-PI: Mark Alber, Mathematics.

PI: *Grid-enabled Integration of Experimental Data and Simulation for Flexible Protein Docking* (NSF Biological Databases and Informatics (DBI-0450067), Mar. 1, 2005 - Feb. 28, 2008, \$809,367 total; 34% effort; J. Peng, Chemistry, Co-PI; A. Striegel, Computer Science and Engineering, Co-PI). Also NSF REU supplement for \$22,500.

PI: *CAREER: Scalable Mathematical and Computational Models for Biomolecular Modeling*, Feb. 1, 2002 - Feb. 29, 2008 – \$384,918 (Award No. 0135195). Also NSF REU supplements for \$30,500.

Co-PI: *High performance computational cluster* (Notre Dame, 2003-present, \$200,000; 50% effort) Through a faculty renovation grant with PI M. Scheutz we acquired a 44 dual-processor nodes of high performance compute nodes connected through fast Myrinet interconnect.

8 Refereed Journal Papers

- [1] Faruck Morcos, Charles Lamanna, Marcin Sikora, and Jesús Izaguirre. Cytoprophet: A Cytoscape plug-in for protein and domain interaction networks inference. *Bioinformatics*, 19:2265–2266, 2008.
- [2] Paul Brenner, Justin M. Wozniak, Douglas Thain, Aaron Striegel, Jeff W. Peng, and Jesús A. Izaguirre. Biomolecular committor probability calculation enabled by processing in network storage. *Parallel Computing*, 34:652–660, 2008.
- [3] Christopher R. Sweet, Paula Petrone, Vijay S. Pande, and Jesús A. Izaguirre. Normal mode partitioning of Langevin dynamics for biomolecules. *J. Chem. Phys.*, 128:1–14, 2008.

- [4] 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.
- [5] 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.
- [6] Paul Brenner, Chris R. Sweet, Dustin VonHandorf, and Jesús A. Izaguirre. Accelerating the replica exchange method through an efficient all-pairs exchange. *J. Chem. Phys.*, 126:074103, February 2007.
- [7] Chengbang Huang, Faruck Morcos, Simon P. Kanaan, Stefan Wuchty, Danny Z. Chen, and Jesús 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.
- [8] T. Cickovski, K. Aras, M. Swat, R.M.H. Merks, T. Glimm, H.G.E. Hentscheland 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.
- [9] T. Cickovski, C. Huang, R. Chaturvedi, T. Glimm, H. G. E. Hentschel, M. S. Alber, J. A. Glazier, S. A. Newman, and J. A. Izaguirre. A framework for three-dimensional simulation of morphogenesis. *IEEE/ACM Trans. on Comp. Bio. and Bioinformatics*, 2(4):273–288, 2005.
- [10] Jesús A. Izaguirre, Scott S. Hampton, and Thierry Matthey. Parallel multigrid summation for the N-body problem. *J. Paral. Distrib. Comp.*, 65:949–962, 2005.
- [11] Michael S. Crocker, Scott S. Hampton, Thierry Matthey, and Jesús A. Izaguirre. MDSimAid: Automatic parameter optimization in fast electrostatic algorithms. *J. Comp. Chem.*, 26:1021–1031, 2005.
- [12] R. Chaturvedi, C. Huang, B. Kazmierczak, T. Schneider, J. A. Izaguirre, S. A. Newman, J. A. Glazier, and M. S. Alber. On multiscale approaches to 3-dimensional modeling of morphogenesis. *J. Roy. Soc. Interface*, 2:237–253, 2005.
- [13] Jesús A. Izaguirre and Scott S. Hampton. Shadow hybrid Monte Carlo: An efficient propagator in phase space of macromolecules. *J. Comput. Phys.*, 200(2):581–604, 2004.
- [14] Thierry Matthey, Trevor Cickovski, Scott S. Hampton, Alice Ko, Qun Ma, Matthew Nyerges, Troy Raeder, Thomas Slabach, and Jesús A. Izaguirre. PROTOMOL: An object-oriented framework for prototyping novel algorithms for molecular dynamics. *ACM Trans. Math. Softw.*, 30(3):237–265, 2004.

- [15] J. A. Izaguirre, R. Chaturvedi, C. Huang, T. Cickovski, J. Coffland, G. Thomas, G. Forgacs, M. S. Alber, G. Hentschel, S. A. Newman, and J. A. Glazier. CompuCell, a multimodel framework for simulation of morphogenesis. *Bioinformatics*, 20:1129–1137, 2004.
- [16] Q. Ma and J. A. Izaguirre. Targeted mollified impulse — a multiscale stochastic integrator for long molecular dynamics simulations. *Multiscale Model. Simul.*, 2(1):1–21, 2003.
- [17] Q. Ma, J. A. Izaguirre, and R. D. Skeel. Verlet-I/r-RESPA/Impulse is limited by nonlinear instability. *SIAM J. Sci. Comput.*, 24(6):1951–1973, 2003.
- [18] R. D. Skeel and J. A. Izaguirre. An impulse integrator for Langevin dynamics. *Mol. Phys.*, 100(24):3885–3891, 2002.
- [19] J. A. Izaguirre, D. P. Catarello, J. M. Wozniak, and R. D. Skeel. Langevin stabilization of molecular dynamics. *J. Chem. Phys.*, 114(5):2090–2098, 2001.
- [20] J. A. Izaguirre, S. Reich, and R. D. Skeel. Longer time steps for molecular dynamics. *J. Chem. Phys.*, 110(19):9853–9864, 1999.

9 Refereed Conference Proceedings

- [1] Trevor Cickovski, Chris Sweet, and Jesús A. Izaguirre. MDL, A domain-specific language for molecular dynamics. In *Proc. 40th Annual Simulation Symposium*, 2007.
- [2] Marcin Sikora, Faruck Morcos, Daniel J. Costello Jr., and Jesús A. Izaguirre. Bayesian inference of protein and domain interactions using the sum-product algorithm. In *Proc. 2007 Information Theory and Applications Workshop*, 2007.
- [3] 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. In *2007 IEEE International Parallel and Distributed Processing Symposium*, page 256, 2007.
- [4] Chris R. Sweet and Jesús A. Izaguirre. Backward error analysis of multiscale symplectic integrators and propagators. In *Proc. Third International Conference Multiscale Materials Modeling MMM2006*, 2006.
- [5] Faruck Morcos, Mike Boxem, Niels Klitgord, Marc Vidal, and Jesús A. Izaguirre. Prediction of domain interactions in *C. elegans*. In *Proc. Workshop Computational Biophysics to Systems Biology CBSB06*, 2006.

- [6] Scott S. Hampton, Paul Brenner, Aaron Wenger, Santanu Chatterjee, and Jesús A. Izaguirre. Biomolecular sampling: Algorithms, test molecules, and metrics. In Benedict Leimkuhler, Christophe Chipot, Ron Elber, Aatto Laaksonen, Alan Mark, Tamar Schlick, Christoph Schütte, and Robert Skeel, editors, *New Algorithms for Macromolecular Simulation*, volume 49 of *LNCS*, pages 103–121, Secaucus, NJ, USA, 2006. Springer-Verlag New York.
- [7] Justin Wozniak, Paul Brenner, Doug Thain, Aaron Striegel, and Jesús A. Izaguirre. Applying feedback control to a replica management system. In *Proc. of 38th South-eastern Symposium on System Theory*, 2006.
- [8] D. Thain, S. Klous, J. Wozniak, P. Brenner, A. Striegel, and J. A. Izaguirre. Separating abstractions from resources in a tactical storage system. In *Proceedings of Supercomputing 2005*, Seattle, WA, Nov. 2005.
- [9] J. M. Wozniak, P. Brenner, D. Thain, A. Striegel, and J. A. Izaguirre. Generosity and gluttony in gems: Grid enabled molecular simulations. In *IEEE International Symposium on High Performance Distributed Computing Proceedings*, 2005. In Press.
- [10] J. M. Wozniak, A. Striegel, D. Salyers, and J. A. Izaguirre. GIPSE: Streamlining the management of simulation on the grid. In *Proc. of the 38th Annual Simulation Symposium ANSS 05*, 2005. Preprint: http://www.nd.edu/~izaguirr/papers/wozniakj_gipse.pdf.
- [11] R. Chaturvedi, C. Huang, J. A. Izaguirre, S. A. Newman, J. A. Glazier, and M. S. Alber. A hybrid discrete-continuum model for 3-D skeletogenesis of the vertebrate limb. In Peter M. A. Sloot, Bastien Chopard, and Alfons G. Hoekstra, editors, *Cellular Automata: 6th International Conference on Cellular Automata for Research and Industry, ACRI 2004, Amsterdam, The Netherlands, October 25-28, 2004*, volume 3305 of *Lecture Notes in Computer Science*, pages 543–552. Springer Verlag, Berlin Heidelberg, 2004. Preprint: <http://www.nd.edu/~izaguirr/papers/Chat0xb.pdf>.
- [12] Scott S. Hampton and Jesus A. Izaguirre. Improved sampling for biological molecules using shadow hybrid Monte Carlo. In M. Bubak, G. D. von Albada, and P. M. A. Sloot; J. J. Dongarra, editors, *4th International Conference on Computational Science, Kraków, Poland*, volume 3037 of *LNCS*, pages 268–274. Springer-Verlag, New York, 2004.
- [13] R. Chaturvedi, J. A. Izaguirre, C. Huang, T. Cickovski, P. Virtue, G. Thomas, G. Forgacs, M. S. Alber, H. G. E. Hentschel, S. A. Newman, and J. A. Glazier. Multi-model simulations of chicken limb morphogenesis. In *Lecture Notes in Computational Science*, volume 2659, pages 39–49. Springer-Verlag, Berlin, 2003.

- [14] T. Matthey, A. Ko, and J. A. Izaguirre. ProtoMol, an object-oriented framework for algorithmic development. In *Computational Science—ICCS 2003, International Conference, Melbourne, Australia and St. Petersburg, Russia*, pages 50–59. Springer-Verlag, Berlin, 2003. Lecture Notes Computational Science 2659.
- [15] Q. Ma and J. A. Izaguirre. Long time step molecular dynamics using targeted langevin stabilization. In *Proceedings of the ACM Symposium on Applied Computing (SAC 03), Melbourne, FL*, pages 178–182, New York, 2003. ACM.
- [16] Qun Ma, Jesús A. Izaguirre, and Robert D. Skeel. Nonlinear instability in multiple time stepping molecular dynamics. In *Proceedings of the ACM Symposium on Applied Computing (SAC 03), Melbourne, Fl*, pages 167–171, Melbourne, Florida, Mar. 2003. ACM Press.
- [17] J. A. Izaguirre, Q. Ma, T. Matthey, J. Willcock, T. Slabach, B. Moore, and G. Vi-amontes. Overcoming instabilities in Verlet-I/r-RESPA with the mollified impulse method. In T. Schlick and H. H. Gan, editors, *Proceedings of 3rd International Workshop on Methods for Macromolecular Modeling*, volume 24 of *Lecture Notes in Computational Science and Engineering*, pages 146–174. Springer-Verlag, New York, 2002.
- [18] J. A. Izaguirre. *Generalized Mollified Multiple Time Stepping Methods for Molecular Dynamics*, volume 177 of *NATO Science Series: Series III Computer and Systems Sciences*, pages 34–47. IOS Press, Amsterdam, The Netherlands, Jan. 2001. Preprint: <http://www.nd.edu/~izaguirr/papers/eilat.pdf>.
- [19] T. Matthey and J. A. Izaguirre. ProtoMol: A molecular dynamics framework with incremental parallelization. In *Proc. of the Tenth SIAM Conf. on Parallel Processing for Scientific Computing (PP01)*, Proceedings in Applied Mathematics, Philadelphia, Mar. 2001. Society for Industrial and Applied Mathematics. Preprint: <http://www.nd.edu/~izaguirr/papers/proto.pdf>.
- [20] Shannon Kuntz, Richard Murphy, Mike Niemier, J. A. Izaguirre, and Peter Kogge. Petaflop computing for protein folding. In *Proc. of the Tenth SIAM Conf. on Parallel Processing for Scientific Computing (PP01)*, Proceedings in Applied Mathematics, Philadelphia, Mar. 2001. Society for Industrial and Applied Mathematics. Preprint: <http://www.nd.edu/~izaguirr/papers/protopim.pdf>.
- [21] Milind Bhandarkar, Gila Budescu, William F. Humphrey, Jesus A. Izaguirre, Sergei Izrailev, Laxmikant V. Kalé, Dorina Kosztin, Ferenc Molnar, James C. Phillips, and Klaus Schulten. BioCoRE: A collaboratory for structural biology. In Agostino G. Bruzzone, Adelinde Uchrmacher, and Ernest H. Page, editors, *Proceedings of the SCS International Conference on Web-Based Modeling and Simulation*, pages 242–251, San Francisco, California, 1999.

- [22] R. D. Skeel and J. A. Izaguirre. The five femtosecond time step barrier. In P. Deuffhard, J. Hermans, B. Leimkuhler, A. Mark, S. Reich, and R. D. Skeel, editors, *Computational Molecular Dynamics: Challenges, Methods, Ideas*, volume 4 of *Lecture Notes in Computational Science and Engineering*, pages 303–318. Springer-Verlag, Berlin Heidelberg New York, Nov. 1998.
- [23] J. A. Izaguirre. Empirical evaluation of graph partitioning algorithms. In *Proceedings of the National Computer Science Encounter*, pages 44–50, México, 1997. Sociedad Nacional de Computación. Preprint: <http://www.nd.edu/~izaguirr/papers/enc97.pdf>.

10 Software and other Publications

- [1] MDSIM Aid. Molecular Dynamics Simulation Aid. <http://mdsimaid.cse.nd.edu/>, Aug. 2004.
- [2] COMPUCELL. COMPUCELL: 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] Trevor Cickovski and Jesús A. Izaguirre. BIOLOGO: A domain-specific language for morphogenesis. In preparation. Manuscript available at <http://www.nd.edu/~tcickovs/document.pdf>, 2005.
- [5] Trevor Cickovski, Thierry Matthey, and Jesús A. Izaguirre. Design patterns for scientific software. Technical Report 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. Technical Report TR 04-16, University of Notre Dame, 2004.
- [7] J. A. Izaguirre, T. Matthey, J. Willcock, Q. Ma, B. Moore, T. Slabach, and G. Viarmontes. A tutorial on the prototyping of multiple time stepping integrators for molecular dynamics. Available from <http://www.cse.nd.edu/~lcls/Protomol.html>, 2001.
- [8] J. A. Izaguirre. *Longer Time Steps for Molecular Dynamics*. PhD thesis, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA, 1999.

11 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.

12 Ph.D. Theses Supervised

1. Trevor Cickovski, Ph.D., March 2008, “Domain-Specific Languages in Computational Biology.”
2. Paul R. Brenner, Ph.D., July 2007, “Parallel Algorithms and Distributed Systems for Computational Biophysics.”
3. Scott S. Hampton, Ph.D., Oct. 2006, “Analysis of Shadow Hybrid Monte Carlo Methods.”
4. Chengbang Huang, Ph.D., Aug. 2005, “Multiscale Computational Methods for Morphogenesis and Algorithms for Protein-Protein Interaction.”
5. Qun (Marc) Ma, Ph.D., Aug. 2003, “Novel multiscale algorithms for molecular dynamics.”
6. 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.”
7. Santanu Chatterjee, Ph.D. candidate.
8. Faruck Morcos, in progress.

13 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

14 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

15 Active Collaborations (grants or papers in last 24 months)

- Mark Alber, Notre Dame
- Alexandre Chorin, Berkeley
- Daniel J. Costello, Jr., Notre Dame
- Eric Darve, Stanford University

- James Glazier, Indiana University Bloomington
- Dale Kaiser, Stanford University
- Stuart Newman, New York Medical College
- Vijay S. Pande, Stanford University
- Jeff Peng, Notre Dame
- Robert D. Skeel, Purdue University
- Aaron Striegel, Notre Dame
- Douglas Thain, Notre Dame
- Mark Vidal, Harvard University
- Art Votter, Los Alamos National Laboratory

16 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

17 Courses taught at Notre Dame

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