CURRICULUM VITAE

Christopher R. Sweet

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1 Current Position

August 2009-2010 — Research Assistant Professor,
Department of Mathematics,
University of Notre Dame,
Notre Dame, USA.

Concurrently

Computational Scientist,
Center for Research Computing,
University of Notre Dame,
Notre Dame, USA.

2 Higher Education

EDUCATION/TRAINING			
INSTITUTION AND LOCATION	DEGREE	YEAR(s)	FIELD OF STUDY
University of Leicester	B.Sc.	1998-2001	Mathematics
University of Leicester	Ph.D.	2001-2004	Applied Mathematics

3 Previous Positions

April 2009-August 2009	Postdoctoral Research Associate, Department of Mathematics, University of Notre Dame, Notre Dame, USA.
2005-April 2009	Research Assistant Professor, Department of Computer Science and Engineering, University of Notre Dame, Notre Dame, USA.
2004-2005	Lecturer in Applied Mathematics, Department of Mathematics, University of Leicester, Leicester, UK.
1987-1998	Research and Development Director Geotechnical Instruments Ltd, Leamington Spa, UK.
1981-1987	Managing Director Probec Electronics, Leicester, UK.

4 Distinctions, Honors, and Awards

1998	British Design Council, Millennium Product Award

5 Refereed Journal Papers

[1] C.R.Sweet, B.J.Leimkuhler. The Canonical Ensemble via Symplectic Integrators using Nosé and Nosé-Poincaré chains. J. Chem. Pys. **121**, 108-126, 2004.

[2] C.R.Sweet, B.J.Leimkuhler. A Hamiltonian Formulation for Recursive Multiple Thermostats in a Common Timescale. SIAM J. on Applied Dynamical Systems **4**, 187-216, 2005.

[3] Paul Brenner, Christopher R. Sweet, Dustin VonHandorf, and Jesús A. Izaguirre. Accelerating the replica exchange method through an efficient all-pairs exchange. J. Chem. Phys. **126**, 126-132, 2007.

[4] Christopher R. Sweet, Paula Petrone, Vijay S. Pande and Jesús A. Izaguirre. Normal Mode Partitioning of Langevin Dynamics for Biomolecules. J. Chem. Phys. **128-11**, 1-14, 2008

[5] Christopher R. Sweet, Scott S. Hampton, Robert D. Skeel and Jesús A. Izaguirre. Separable Shadow Hybrid Monte Carlo Method. J. Chem. Phys. **131**, 174106 (2009)

[6] Trevor Cickovski, Santanu Chatterjee, Jacob Wenger, Christopher R. Sweet, Jesús A. Izaguirre. MDLab: A Molecular Dynamics Simulation Prototyping Environment. J. Comp. Chem. 2009.

6 Refereed Conference Proceedings

[1] E.Barth, B.J.Leimkuhler, C.R.Sweet. Approach to Thermal Equilibrium in Biomolecular Simulation. New Algorithms for Macromolecular Simulation, Springer Berlin Heidelberg. **49**, 125-140, 2006

[2] T. Cickovski, C. Sweet and J. A. Izaguirre. MDL, A Domain-Specific Language for Molecular Dynamics. In IEEE Proceedings of 40th Annual Simulation Symposium, Norfolk, VA. 256-266, 2007.

[3] Christopher R. Sweet and J. A. Izaguirre. Backward error analysis of multiscale symplectic integrators and propagators, Proc. Third International Conference Multiscale Materials Modelling MMM2006, Freiburg, Germany. September 2006.

[4] Jesús A. Izaguirre, Chris R. Sweet, and Vijay S. Pande. Multiscale dynamics of macromolecules using Normal Mode Langevin. Pac. Symp. Biocomput. 2010:240-51.

[5] Jesús A. Izaguirre and Christopher R. Sweet. Adaptive dimensionality reduction of stochastic differential equations for protein dynamics. Proc. Second International Workshop on Model Reduction in Reacting Flows, April 2009, Notre Dame, IN.

7 Papers Under Revision

[1] Christopher R. Sweet, Scott S. Hampton, Jesús A. Izaguirre. Optimal implementation of the Shadow hybrid Monte Carlo method. Submitted to *SIAM J. on Scientific Computing*.

[2] Christopher R. Sweet, Jesús A. Izaguirre. Backward Error Analysis of the Verlet-I MTS method.

[3] C.R.Sweet, B.J.Leimkuhler. Higher Order Symmetric Variable Stepsize Methods. Submitted to *Numerische Mathematik*.

[4] C.R.Sweet, Jesús A. Izaguirre. Simulating Conformational Changes using Dynamically Updated Normal Modes.

[5] Faruck Morcos, Santanu Chatterjee, Christopher L. McClendon, Paul R. Brenner, Roberto Lopez-Rendon, John Zintsmaster, Maria Ercsey-Ravasz, Chris R. Sweet, Matthew P. Jacobson, Jeffrey W. Peng, and Jesús A. Izaguirre. Modeling the conformational ensembles of NMR relaxation dispersion: molecular dynamics study of slow functional motions in the Pin1-WW domain.. Submitted. 2009.

[6] Santanu Chatterjee, Christopher R. Sweet, and Jesús A. Izaguirre. String Method with Collective Variables from Normal Modes: Application to Alanine Dipeptide. Submitted. 2009.

8 Other Publications

[1] C.R.Sweet. Hamiltonian Thermostatting Techniques for Molecular Dynamics Simulation. Ph.D. thesis, University of Leicester, Leicester, UK, 2004.

[2] C. R. Sweet, S. S. Hampton, and J. A. Izaguirre. Optimal implementation of the shadow hybrid Monte Carlo method. Technical Report TR-2006-09, University of Notre Dame, 2006.

[3] UK Patent 8922422.4/US Patent 5027655
Patent on a 'Sonic Dipmeter' to allow contactless and continuous monitoring of water levels in dip wells, 1986.

[4] UK Patent/US Patent
Patent on a 'Variable Path Length' cell to allow widely differing gasses of differing concentrations to be analyzed, using non-dispersive Infrared techniques, within the same instrument.

9 Selected Invited Lectures

1. *BIRS Workshop on Mathematical Issues in Molecular Dynamics*, Banff Research Station, University of Victoria, Canada, June 4, 2005.

2. *Molecular simulation: Algorithmic and Mathematical aspects*, Prestissimo Workshop 2004, Institut Henri Poincaré, Paris, December 1, 2004.

3. *International Conference on Scientific Computation and Differential Equations*, Scicade 2003, Trondheim, Norway. June 2003.

10 Undergraduate Research Projects Supervised

1. Justin Kent, "OpenGL visualization of constrained dynamics", Spring 2005.

2. Graham Bonner, "Simulation of perturbed Kepler orbits", Fall 2004-Spring 2005.

11 Courses taught

- MA3011, Applied Numerical Mathematics. Third year 20 credit undergraduate module on numerical methods and analysis, Leicester University, Fall 2004.

- MA7711, Research Presentation. M.Sc. course in Latex, Web design and Presentation, Leicester University, Spring 2005.

- MA2502, Presentations in Applied Mathematics. Second year 10 credit undergraduate course in presenting mathematics, Leicester University, Summer 2005.

- Math 20210, Computer Programming and Problem Solving, University Notre Dame, Spring 2010.

12 Outline of career as Research and Development Director of Geotechnical Instruments Ltd

Responsible for the Development Department and product development within the company. The department varied in size but generally consisted of 2-4 Electronics Engineers, 2 Software Engineers, 1 Mechanical Engineer and 1-2 Technicians. In addition I attended the monthly Board meetings and was involved in formulating the direction and policies of the company. Despite my management duties, I retained a 'hands on' approach and continued to be personally involved in the design and development of most of the key Infra-red products for the company. I moved the company more

towards the Gas Analysis side of the business, taking 85% of the UK landfill gas market for monitoring products and gaining major contracts in USA with the Pacific Energy Corp. in California and Siemens-Plessey in Europe.

In 1998 a CO2 Personal Monitor, which I personally designed, was chosen by the British Design Council to be one of the first 200 'Millennium Products'. An announcement was made by Tony Blair, the UK Prime Minister, on 02/04/1998 launching the scheme where eventually 2000 products were selected to represent British ingenuity and creativity, and a selection of them were displayed in the Millennium Dome the following year.

In 1989 I took part in a Management buy-out, when we acquired the company from its original owners. Geotechnical Instruments went on to become the 4th-5th largest Civil Engineering instrumentation company in the world and was sold to Setpoint Technology, from South Africa, in 1998. At this point I resumed my academic career at Leicester University.

13 References

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