



# Collaborative Graduate Specialization in Computational Science and Engineering

## WEEKLY COLLOQUIUM

Tuesday, 29 January 2008

2:30-3:30 in RM101, Jeffery Hall

**Speaker:** Gary Slater, Professor of Physics  
Dean of Graduate Studies, University of Ottawa

**Title:** Diffusion and biased diffusion on a lattice: building models and replacing Monte Carlo simulations by “exact” numerical calculations

**Abstract:** Using lattice Monte Carlo simulations of random-walks to simulate diffusion problems is perhaps one of the very first things a computational physicist learns. He/she would then learn how to add a bias to the random walk in order to simulate systems where a net drift is also present. But how can such models represent reality when we know that the lattice is an artefact of the simulation method? In this presentation, I will first look at how one can define single Monte Carlo jumps that conserve the properties (diffusion coefficient and velocity) of the initial problem. We will see that biasing a random-walk is no trivial matter, especially in 3 or more dimensions. In the second part of the presentation, I will examine how one can replace the Monte Carlo simulations by exact numerical calculations that provide much better accuracy in less computing time – but with important memory requirements. Several applications will be discussed, such as electrophoretic sieving, thermodynamic ratchets and drug delivery. The algorithms presented here can be used in a wide variety of problems in the sciences and engineering.

**About the speaker:**

*In 1984 after receiving a Ph.D. from the Université de Sherbrooke, Gary Slater worked for six years at Xerox Research Centre of Canada in Mississauga. In 1990, he joined the Department of Physics at the University of Ottawa, where he was named Professor in 1996. From July 1997 to December 2000, Gary Slater was Vice-dean (Research) for the Faculty of Science and was then appointed Vice-dean of the Faculty of Graduate and Postdoctoral Studies (FGPS) from January 2002 through June 2004. He has been the Dean of the FGPS since January 2005.*

*Dr. Slater is a specialist in the physics of polymers and macromolecules. He is also interested in electrophoresis (a technique for separating biomolecules based on their differential velocity in an electric field), DNA sequencing, microfluidics and nanofluidics. In addition, he is interested in computer simulations and applications of the theory of diffusion in biophysics. In 2001, Dr. Slater received the Researcher of the Year Award from the University of Ottawa. Dr. Slater has been awarded the University of Ottawa Research Chair in Biological Physics in 2004.*

*Dr. Slater is currently a member of the NSERC Advisory Committee for the review of the Grant Selection process, a member of the Executive Committee, Ontario Council on Graduate Studies, and a member of the Board of Trustees of the High Performance Computing Virtual Laboratory (HPCVL).*