

Courant Institute of Mathematical Sciences
Mathematics Colloquium
April 11, 2011

Speaker: Malvin Kalos
Lawrence Livermore National Labs

Title: "Fermion Monte Carlo"

Abstract:

This talk will outline Monte Carlo methods that enable numerical solution of the many-body non-relativistic Schroedinger Equation. They permit computations with no uncontrolled approximations for the ground states of bosonic systems. Because the Pauli principle imposes a non-local constraint on the solution, extension to fermionic systems has proved much more difficult. The algorithmic barriers will be outlined, together with techniques that overcome them. The latter include the use of populations of pairs of random walkers that carry opposite algebraic signs; correlation of the diffusion of the pair; cancellation of pairs that become close; the use of different permutations to achieve statistical stability; and importance sampling.