



THE UNIVERSITY OF CHICAGO

Departments of Computer Science, Mathematics, Statistics, and the Computation Institute
SCIENTIFIC AND STATISTICAL COMPUTING SEMINAR

ERIC CANCES

CERMICS—Ecole des Ponts ParisTech

Quantum Monte Carlo Methods for Electronic Structure Calculation

FRIDAY, May 3, 2013, at 3:30 PM

Eckhart 133, 5734 S. University Avenue

ABSTRACT

In this talk, I will describe the mathematical foundations of Variational Monte Carlo (VMC) and Diffusion Monte Carlo (DMC) methods for computing the electronic ground state energy of a molecular system. I will sketch rigorous proofs of the tiling property for electronic ground states and of the fixed-node approximation inherent to the DMC method. I will also deal with numerical sampling for VMC.

Organizers:

Lek-Heng Lim, Department of Statistics, lekheng@galton.uchicago.edu,

Ridgway Scott, Departments of Computer Science and Mathematics, ridg@cs.uchicago.edu,

Jonathan Weare, Department of Mathematics and the Computation Institute, weare@math.uchicago.edu.

SSC Seminar URL: http://www.stat.uchicago.edu/seminars/SSC_seminars.shtml

If you wish to subscribe to our email list, please visit the following website:

<https://lists.uchicago.edu/web/arc/statseminars>.