THE UNIVERSITY OF CHICAGO

Department of Statistics

SCIENTIFIC AND STATISTICAL COMPUTING SEMINAR

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Computational Geometry Aspects of Monte Carlo Approaches to PDE Problems in Biology, Chemistry, and Materials

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226 Jones Laboratory, 5747 South Ellis Avenue

ABSTRACT

We will introduce at some Monte Carlo methods for solving problems in electrostatics. These rely on evaluating functionals of the first-passage time of Brownian motion on geometries defined by the system of interest. We will use the Walk on Spheres (WOS) algorithm to quickly evaluate these functionals, and we will show how a computational geometric computation dominates this computation in complexity. We then consider computing the capacitance of a complicated shape, and use this as our model problem to find an efficient serial and parallel implementation. The capacitance computation is prototypical of many Monte Carlo approaches to problems in biology, biochemistry, and materials science.

This is joint work with Drs. Walid Keyrouz and Derek Juba from the Information Technology Laboratory at NIST.