

ACMS Applied Math Seminar

Michael Mascagni
Friday, April 21, 2017
154 Hurley Hall
3:15 – 4:15 PM



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

We will introduce 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 on 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 a joint work with Drs. Walid Keyrouz and Derek Juba from the Information Technology Laboratory at NIST.

The Department of Applied and Computational
Mathematics and Statistics

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