

# BI-CO MATHEMATICS COLLOQUIUM

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## *“Sampling from Rough Energy Landscapes”*

*Monday, November 8, 2021*

*Talk at 4:00 – Hilles 109*

### **Abstract:**

In high dimensional problems, classical method for numerical integration become computationally inefficient, leading us to consider the Monte Carlo method, an algorithm based on sampling from an appropriately chosen probability distribution. In physics and chemistry, such high dimensional problems readily occur when one examines the interactions of a large number of atoms interacting through an energy landscape at finite temperature; these are the so called Boltzmann distributions.

In this talk, I will introduce Monte Carlo sampling for such distributions, and examine distinct challenges that appear when the landscape is, in some sense, “rough.” We develop and examine sampling strategies that are insensitive to this roughness, and analyze how the roughness can impede the performance of other sampling strategies. Numerical experiments confirm our predictions. This is joint work with Petr Plechac (U. Delaware).