Mathematics Department Colloquium

Organizer: Maciej Zworski

Thursdays, 4:10–5:00pm, 60 Evans

March 17 **Eric Vanden-Eijnden**, Courant Institute

Metastability in complex systems: Reaction coordinate, free energy, and rates

Many problems in physics, material sciences, chemistry and biology can be abstractly formulated as a system that navigates over a complex energy landscape of high or infinite dimensions. Well-known examples include phase transitions of condensed matter, conformational changes of biopolymers, and chemical reactions. The state of these systems is confined for long periods of time in metastable regions in configuration space and only rarely switches from one region to another. The separation of time scale is a consequence of the disparity between the effective thermal energy and typical energy barrier in these systems, and their dynamics effectively reduces to a Markov chain on the metastables regions. The analysis and computation the transition pathways and rates between the metastable states is a major computational challenge, especially when the energy landscape exhibits multiscale features. I will review recent work done by scientists from several disciplines on probing such energy landscapes, introduce concepts such as reaction coordinate and free energy, and show how these concepts can be made mathematically precise. I will then present a new method, the string method, that has proven to be very effective for some complex systems in material science and chemistry.