# Physics Colloquium

## Michigan Technological University

**Thursday, February 17, 2011, 4:00 pm**

**Room 139, Fisher Hall**

### Kinetic Monte Carlo and Master Equation Approaches to Solving a System of Rates

**Douglas Banyai**

**Advisor: Dr. John Jaszczak**

**Abstract:** Last week we saw Partha and Saikat characterize the transport properties of molecular junctions from first principles. This week I will describe ways to calculate the transport properties of a class of systems that contain multiple such junctions and are too big for an ab initio treatment. We will look at a specific condition under which the standard methods for finding a Thevenin equivalent for the system fails, and introduce a semi-classical model to account for the differences. This model will allow us to calculate the rates at which we expect electrons to traverse individual junctions, but these rates need to be integrated to find the current through the entire device. Kinetic Monte Carlo and the master equation approach are two ways to do this.

A master equation (ME) describes how the probability for a system to be in a given state changes in time. In certain simple systems, the steady state solution can be found very efficiently and from this, properties of the system can be calculated. Kinetic Monte Carlo (KMC) is a powerful method for calculating both transient and steady state properties, and can handle more complex systems than the ME method. I will describe the theory and implementation of both the ME and KMC algorithms, and show example results from a toy model.

### Characterization of First Hadronic Interaction of Extensive Air Shower Using Pierre Auger Observatory

**Tolga Yapici**

**Advisor: Dr.Brian Fick**

**Abstract:** The lack of information about the hadronic interaction at high energies (E>10^{18} eV) results in high degrees of uncertainty in extensive air shower simulations. With the current level of technology, it is impossible for particle accelerators to retrieve the information at high energies. The important information about the interactions can be probed using the Pierre Auger Observatory data with the help of sophisticated methods, such as Neural Networks.

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