Title: Analysis of a simple one-dimensional analogue of carbon nanotube growth

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Abstract:
Carbon nanotubes (CNTs) have exceptional mechanical, electronic, and thermal properties, which make them ideal for a variety of applications. In this presentation, we describe mathematical models that allow for greater understanding and control of the CNT synthesis process. We first describe an atomistic model of CNT growth, which focuses on carbon-carbon interactions and approximates the interaction of carbon atoms with the substrate and catalyst. This model is used to motivate a simplified one-dimensional atomistic model that preserves some features of the full model. Like the full model, this simple model has one global energy minimum and many competing local minima. We simulate this system and compare the non-equilibrium probability distributions with the equilibrium distribution. We calculate transition rates between the basins of different local minima, and use these in a master equation to calculate non-equilibrium distributions when atoms are added to the system. To allow for further analysis, we approximate the rate matrix by a matrix with two parameters – a slow rate and a fast rate. We present the equilibrium distribution, hitting times, and eigenvalues of this matrix and describe how they depend on the rate parameters and the number of atoms in the chain. Finally, we describe the insights this simplified model provides regarding CNT growth.