SPECIAL PHYSICAL MATHEMATICS SEMINAR

KINETIC MONTE CARLO APPLICATIONS TO SOME MATERIALS SCIENCE PROBLEMS: A NEW ALGORITHM BASED ON FIRST PASSAGE GREENS FUNCTIONS

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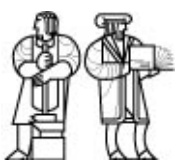
ABSTRACT:

We discuss some materials science applications of kinetic Monte Carlo techniques. These include the annealing of systems that have been subjected to ion implantation or radioactive decay, including silicon devices and materials for nuclear fusion reactors. In addition, we discuss models of polycrystalline thin film deposition. These problems often involve the laborious calculation of numerous diffusion hops for mobile particles or defects that are more or less isolated, and for which there are exact analytical expression for the probability distribution of the particle position. By employing these results, we expect to obtain a huge speedup of the simulations, often several orders of magnitude.

FRIDAY, DECEMBER 2, 2005
2:30 PM
Building 2, Room 105

Refreshments at 3:30 PM in Room 2-349.



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