

TEMPLE UNIVERSITY MATHEMATICS COLLOQUIUM

Qiang Du

The Pennsylvania State University

will speak on

How to search for transition states/saddle points?

ABSTRACT: Exploring complex energy landscape is a challenging issue in many applications. Besides locating equilibrium states, it is often also important to identify the transition states given by saddle points. In this talk, we will discuss the mathematics and algorithms, in particular, the shrinking dimer dynamics, developed to compute transition states. Some applications will be considered, including the study of critical nuclei morphology in solid state transformations, optimal photonic crystal design and the generalized Thomson problem.

MONDAY, APRIL 1, 2013

LECTURE AT 4:00 PM

COFFEE, TEA, AND REFRESHMENTS FROM 3:40 PM

ROOM 617, WACHMAN BUILDING

DEPARTMENT OF MATHEMATICS