Title:

Search of Transition Structures by means of Coevolutionary Genetic Algorithms

Abstract:

The search of transition structures can be considered one of the greatest chalanges of theoritcal chemistry, not only because of it's importance in the understanding of chemical reactions, such as those involved in the synthesis of materials, but also due to the problem's inherent dificulty. Actually, we're dealing with an extremely complex geometry optimization problem whose goal is to locate not a mere maximum (or minimum), but a first order saddle point on a Potential Energy Surface, which is characterized as being a minimum in all directions except that of the reaction path, in which it's a maximum. To date, there is no algorithm which guarantees convergence to a transition structure without being fed with a very close guess to the target. Our proposal is to apply a coevolutionary genetic algorithm to address this problem. In our approach, the only inputs to the algorithm are the reactants and the products geometries of the chemical reaction at hands. The evaluation of the candidate structures is done by the ab initio computational chemistry package Gaussian03. We have achieved extremely promising results in all the experiments conducted so far, which entirely agreed with previously known transition structures taken as benchmarks. The major appeal of our approach is that it needs no previous knowledge (close guesses) and thus, has the potential to still locate the transition structures when such information is not at our disposal.