Public Abstract

First Name:Yi

Middle Name:

Last Name:Shi

Adviser's First Name:Donald

Adviser's Last Name:Thompson

Co-Adviser's First Name:

Co-Adviser's Last Name:

Graduation Term:SS 2016

Department:Chemistry

Degree:PhD

Title:A Study Of Interpolating Moving Least-Squares Method On Fitting Potential Energy Surface

Trajectory calculation is commonly used in theoretical chemistry. Usually $10^5 - 10^7$ force calculations are required in trajectory calculations. If there is an analytical function as the potential energy surface (PES), the large number of force calculation is not a problem. However, it is very expensive if the large number of force is calculated by electronic structure methods. Instead, a PES can be fitted to some data points calculated from electronic structure method. It is cheap to calculate the large number of force using the fitted PES. The highly accurate PES fitting method, interpolating moving least-squares method (IMLS) is studied in current study. Three different IMLS methods are used to fit the potential energy surface of $\text{CO}_2 + \text{O}$ at the B3LYP/3-21G level. Trajectory calculation from the IMLS-fitted PES is in a good agreement with trajectory calculation using the force calculated from electronic structure method. The other two methods using IMLS are studied to fit specified range of the PES. Some preliminary results are obtained. Even though the electronic structure method used in the study is cheap, current study shows that the IMLS method can be used to fit data points from highly accurate electronic structure method for 4-atom PES. The current study shows that the large number of force in the trajectory calculation can be calculated using the IMLS-fitted PES fitting to data points calculated from highly accurate electronic structure method for 4-atom reaction.