

Abstract Submitted
for the PSF13 Meeting of
The American Physical Society

A Study of the Effects of Basis Functions in Interpolating Moving Least Squares Methods for Fitting Potential Energy Surfaces YI SHI, DONALD THOMPSON, University of Missouri-Columbia — The interpolating moving least-squares (IMLS) method is an efficient means for potential energy surface fitting [R. Dawes, D. L. Thompson, A. F. Wagner, M. Minkoff, *J. Chem. Phys.*, **128**, 084107 (2008)]. To date no studies have been carried out on the effects of basis functions on the accuracy and fidelity of IMLS. Power functions are the only basis functions that have been used in IMLS. In our study, different basis functions have been used to fit different dimensional potential energy surfaces with IMLS. The efficiencies of various basis functions have been compared. The potential energy surfaces selected to fit are the Morse potential and an accurate analytical H_2O_2 potential energy surface. Our results show that other functions can be more efficient than power functions.

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Date submitted: 10 Oct 2013

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