Title:	A New Algorithm for Finding Critical Points of Potential Energy Surfaces
Authors:	Krishan, Bal (/jspui/browse?type=author&value=Krishan%2C+Bal)
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Abstract:	The problem of finding critical points of real N-dimensional functions is of great practical interest in physics and chemistry, particularly in molecular dynamics. Newton Raphson method is a widely used first derivative method used to find zeros of a function which converges to a root quadratically provided the initial guess lies close to the root. This method can be used to find critical points of a function by finding the zeros of its derivative. However, sensitive dependence on initial points limits the applications of this method as this require prior knowledge about function and its critical points and several modified Newton's methods have been developed to overcome this difficulty. In this paper, we show that the use of complex variables in Newton's method provide extra degrees of freedom which help it to move from region/basin of one critical point to other. Optimization of various complex scaled test functions show that the method converges to different critical points upon varying the complex scaling parameter. Also, in most circumstances, complex scaled Newton's method found more critical points than ordinary Newton's method. This method can be useful for finding critical points on PESs which can be complexified by scaling the reaction coordinate during ab-initio molecular calculations.
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