Constrained Minimizations on Hyperspheres

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ABSTRACT

In the first part of this talk we present the implementation of a new efficient algorithm based on the trust-region method for hypersphere minimizations in the deMon2k program [1]. This algorithm allows restricted minimizations to be carried out on a hypersphere using the quasi-Newton method [2]. Applications on a variety of 31 chemical reactions demonstrate the robustness of the newly developed algorithm to perform saddle interpolations [3] and intrinsic reaction coordinate calculations.

In the second part of the talk the development and implementation of a single-ended transition state finder based on the new hypersphere minimization method will be discussed. To validate its effectiveness, this new method was tested on the Müller-Brown model surface to locate a transition state (TS) from a given local minimum. For the accurate description of the potential energy surface (PES) curvature, scaled normal coordinates (SNCs) are introduced [4,5]. These coordinates scale the PES based on the normal coordinates and their corresponding eigenvalues. Therefore, the use of SNCs follows more closely to the minimum energy path (MEP). To analyze the performance and stability of the SNCs, we present intrinsic reaction coordinate (IRC) calculations using the new hypersphere minimization method and the SNCs.

References

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