Locating Saddle Points of any Index on Potential Energy Surfaces by the Generalized Gentlest Ascent Dynamics

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The system of ordinary differential equations for the method of the gentlest ascent dynamics (GAD) is used to determine the saddle points of the PES of some molecules. The method has been proposed earlier by W.E and X.Zhou [Nonlinearity 24, 1831 (2011)]. It is a more general and abstract form of the long used eigenvector following. For the purpose we use diverse projection or reflection operators to given initial directions. We additionally use the metric of curvilinear internal coordinates. By a number of examples we explain the possibilities of a GAD curve: it can find the transition state of interest by a gentlest ascent, directly or indirectly.
We further propose generalized GAD formulas for the search of saddle points of a higher index. Discussed examples are the Wolfe-surface, the MB-potential, and a Lennard-Jones cluster.

Further references:

1. J.M.Bofill, W.Quapp, M.Caballero: CPL 583, 203-208 (2013)
"Locating transition states on potential energy surfaces by the Gentlest Ascent Dynamics"

2. W.Quapp, J.M.Bofill: TCA 133 (2014) 1510,
"Locating saddle points of any index on potential energy surfaces by the Generalized Gentlest Ascent Dynamics"

3. J.M.Bofill, W.Quapp, E.Bernuz: J Math Chem (2014) in press
"Some remarks on the Extended Gentlest Ascent Dynamics model"