To the History and the Development of two Papers

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This short text concerns the two 1998 papers:

[1] Wolfgang Quapp, Michael Hirsch, Olaf Imig and Dietmar Heidrich: Searching for Saddle Points of Potential Energy Surfaces by Following a Reduced Gradient, J. Comput. Chem. **19**, (1998), 1087-1100 (my most cited paper).
[2] Wolfgang Quapp, Michael Hirsch and Dietmar Heidrich: Bifurcation of Reaction Pathways: the Set of Valley Ridge Inflection Points of a Simple Three-dimensional Potential Energy Surface, Theor. Chem. Acc. **100**, (1998), 285-299.

In 1997, the breakdown of the state of the GDR, and the following chaotic transformations slowly came to an end, also at the University of Leipzig. However, our loosely connected research group of theoretical chemists and mathematicians suffered a loss: a colleague from Maths was going from us in an ugly dispute. Such a cooperation is, of course, always complicated, and this man did not have enough patience. Later, he came out with a new method with strange side effects. It works, but not well, and the description which the author gave could not be correct.

I am familiar with this problem from other cases in theoretical chemistry due to my many years of collaboration.

I therefore wonder how the computer actually performs its calculations? How can the method work if the description is incorrect? I ask for the real procedure behind the developer's illusion.

We discussed the problem, we understood it, and we were able to solve it without the original creator. In this case we came down at what the later so called Newton trajectories (NT) [1,2]. The fundamental idea is that a curve is searched for where the gradient at every point of a potential points into the same direction. This method replaces and improves upon the 'distinguished coordinate method' [3-5].

[3] Klaus Müller and L.D. Brown: Location of Saddle Points and Minimum Energy Paths by a Constrained Simplex Optimisation Procedure, Theor. Chim. Acta, **53**, (1979), 75-93.
[4] I. H. Williams and G. M. Maggiora: Use and Abuse of the Distinguished-Coordinate Method For Transition-State Structure Seraching, J. Mol. Struct. (Theochem), **89**, (1982), 365-378.
[5] D.Heidrich: An Introduction to the Nomenclature and Usage of the Reaction Path Concept, in: The Reaction Path in Chemistry, (Ed.: D.Heidrich), Kluwer Academic Press, Dordrecht, 1995, p.1-10.

The papers [1,2] had, so to say, rediscovered the wheel. However, mathematicians were already familiar with the theory [6]. For this reason, we later renamed the reduced gradient following (RGF) into Newton trajectories.

[6] Immo Diener: Globale Aspekte des kontinuierlichen Newtonverfahrens, Habilitation, Göttingen, 1991; and H.Th. Jongen, P. Jonker and F. Twilt: Nonlinear Optimization in Finite Dimensions, Kluwer Academic Publ., Dordrecht Boston London, 2000.

NTs can be used to find all stationary points on a potential surface because they connect such points [1,2,7], as well as bifurcation points of valleys.
[7] R. Crehuet, J. M. Bofill and J. M. Anglada: A new Look at the Reduced-gradient-following Path, Theor. Chem. Acc., **107**, (2002), 130-139.

There are many applications of the method to different problems. See the list of my papers. Still later, the method was applied to mechanochemistry [8], a very natural application (which we discovered very late!).
[8] W.Quapp and J. M. Bofill: A contribution to a theory of mechanochemical pathways by means of Newton trajectories, Theoret. Chem. Acc., **135**, (2016), 113.

Currently (2025), the old, flawed distinguished coordinate method is being revived through the use of the so-called CoGEF method. Thus, a not overly difficult mathematical method that follows the NTs, is being replaced by an even simpler, but often false going method, thus incorrect. Uncontrollable jumps across the potential surface often appear, which are turning points well known for Newton trajectories.

And some chemists reject my hints.