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Molecules are made from atoms and their electrons. The nuclei tend to push themselfes away, the electrons hold together the molecule. The energy of that process can be formulated as a function of the nuclei: it is a high dimensional surface over the configuration space of the nuclear geometry. Chemists are interested in the minimums of that surface. That are the stable molecules. The next interesting structures are deep lying valleys between the minimums. That are possible candidates for chemical reactions. Especially, chemists are interested in the saddle points of such reaction pathways. But the calculation of saddles is an old task. A further, next interesting structure is a bifurcation of a reaction valley. The calculation of such events is a current task in theoretical chemistry.

Our lab is developing methods that will find bifurcation points on molecular surfaces. We use the definition of a special kind of curves, so-called Newton trajectories (NT). They are curves which have the property that their tangent points in every node of the curve into the same direction. Such NTs bifurcate in bifurcation points of valleys. Thus, if we find a bifurcating NT we have automatically found a bifurcation event on the surface.

In this project, you will incorporate computer experiments from our lab with a row of small and medium sized molecules. The goal is the exploration of the surface of a further special molecule of current chemical interest, in coorporation with theoretical chemists. To calculate numerically NTs, you need gradient and Hesse matrix of the surface, and you have to understand a little differential geometry, because the internal coordinates of a molecule are length and angle, thus curvilinear coordinates.

This is a computational project, and previous knowledge of Linux-based operating systems and Fortran programming is helpful. You will be working closely with a student in the lab which has collected former computational experimental data, and the current software of our programs. Scientific results will be discussed and presented in the lab, and possibilities for publication will be evaluated at the completion of the project.

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