Development of the maximum probability domains method

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Proposal

1.1 Introduction and motivation

In the last few years it has been proposed to analyze arbitrary wave functions by searching the regions of space for which the probability to find a given number of electrons, ν, is maximal [1-4]. These regions of space, and by extension the associated interpretative method, are thus called «maximum probability domains» (MPDs). When ν = 2, it relates to the Lewis' concept of electron pairs, and thus provides a natural connection between quantum mechanics and the traditional way of thinking of chemists. The motivation of this discussion meeting would be to gather in the same location, time and space, several european reseachers actively working each on their side on the development of this method, related concepts, and/or programs, in order to initiate a small network of researchers combining forces on this topic.

1.2 State of the art

Researchers in the UPMC (LCT and LJLL) have been working lately on the development of a level set algorithm for domain optimizations suited to the three-dimensional space problem and the use of adaptive non-regular grids. A new modular prototype program around these algorithm and numerical techniques is in development. These new techniques appear to be very promising, as potentially allowing a more controlled and efficient optimization of the domains, in particular

regarding the difficulty of this multiple solution problem. The other participants participants have been working on their side on different aspects related to probabilities analysis, programs, and/or concepts related to probability-based analysis.[5–10]

1.3 References

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1.4 Objectives

The goal of these meeting will be, for the different participants, to present in details the recent work around this topic, with enough time to details the technical aspects of the work. Large time will be devoted to current challenges and difficulties. In particular, the following challenges will be discussed and tackled:

- Improvement of the current algorithms: numerical efficiency problems, fast-marching methods, and error control ;
- Extension to the analysis of analytical wave functions beyond single-determinant;
- Multi-domain optimization ;
- Development of a shape second derivative, for characterization of true maxima ;
- Development of related concepts for the analysis of the chemical bond.

1.5 Participant List

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