

A posteriori analysis to guarantee electronic structure calculations

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The field of computational chemistry is booming . While so far, very few collaborations exist between quantum chemists and mathematicians (in any case much less in this area than in the context of computational fluid mechanics or structures), things are changing rapidly and the interactions between the two communities grow significantly , each community understanding what the other can provide. The purpose of this talk is to present mathematical models and some work on the a priori and a posteriori analysis for discretization of ab initio models like Hartree -Fock or Kohn-Sham . Recent results on a posteriori analysis identify the contributions to the error of the various ingredients involved in the approximation of a solution : (i) approximation of the model (Schrödinger versus Hartree Fock or density functional) (ii) due to approximation of the space and the discretization method - variational or not (with the inclusion of many non- linearities), (iii) of the algorithm for solving the discrete system (always recursive and converging but where the limit is never reached in practice), to discern areas for improvement to increase the accuracy of calculations.

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