Principal Domains in Local Correlation Theory

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The computational efficiency of local correlation methods is strongly dependent on the size of the domain of functions used to expand local correlating orbitals such as orbital specific or pair natural orbitals. Here we define a principal domain of order m as the subset of m one-particle functions that provides the best support for a given n-electron wavefunction. Our chosen metric is the maximal overlap criteria, which was used by Löwdin to define natural orbitals. We present an efficient linear scaling greedy algorithm for obtaining principal domains of projected atomic orbitals and demonstrate its utility in the context of pair natural orbital local correlation theory.