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How localized is "local?" Efficiency vs. accuracy of $O(N)$ domain decomposition in local orbital based all-electron electronic structure theory VILE HAVU, VOLKER BLUM, MATTHIAS SCHEFFLER, Fritz-Haber Institut der MPG — Numeric atom-centered local orbitals (NAO) are efficient basis sets for all-electron electronic structure theory. The locality of NAO's can be exploited to render (in principle) all operations of the self-consistency cycle $O(N)$. This is straightforward for 3D integrals using domain decomposition into spatially close subsets of integration points, enabling critical computational savings that are effective from ∼tens of atoms (no significant overhead for smaller systems) and make large systems (100s of atoms) computationally feasible. Using a new all-electron NAO-based code,[1] we investigate the quantitative impact of exploiting this locality on two distinct classes of systems: Large light-element molecules [Alanine-based polypeptide chains $(Ala)_n$], and compact transition metal clusters. Strict NAO locality is achieved by imposing a cutoff potential with an onset radius r_c, and exploited by appropriately shaped integration domains (subsets of integration points). Conventional tight $r_c \leq 3$Å have no measurable accuracy impact in $(Ala)_n$, but introduce inaccuracies of 20-30 meV/atom in Cu_n. The domain shape impacts the computational effort by only 10-20 % for reasonable r_c.

[1] V. Blum, R. Gehrke, P. Havu, V. Havu, M. Scheffler, *The FHI Ab Initio Molecular Simulations (aims) Project*, Fritz-Haber-Institut, Berlin (2006).

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