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Molecular Finite Element Density Functional Calculations employing a Cusp Factor to enable convergence at the nuclei

FEM calculations have been performed in Cartesian coordinates in the finite element framework FEniCS[1], using the density functional approach for a number of small molecules. In order to aid convergence of the orbitals and total energies a suitable cusp factor F(**r**)=1+$\sum_{j=1}^{N_A} c_j \exp\left(-2Z_J r_j\right)$ with $r_j = |\mathbf{r}-\mathbf{R}_j|$ $.wasemployed, suchthattheresultingeffectivepotentialisnon-singularatallnucleiandwherethecoefficients\mathbf{c}_i$ are obtained by solving a linear system of equations. The finite element ansatz for the pseudo orbitals leads to a sparse generalized eigenvalue problem of dimension N up to 3.6 10^6, which was solved employing thethe Jacobi-Davidson method on a High Performance SMP Machine with 32 CPUs and 512 GB of memory.
The resulting total energies and densities were compared with those obtained using the Gaussian basis set package NWChem[2] and excellent agreement was found.

[1] Martin S. Alnæs, Jan Blechta, Johan Hake, August Johansson, Benjamin Kehlet, Anders Logg, Chris Richardson, Johannes Ring, Marie E. Rognes, and Garth N. Wells. The fenics project version 1.5. Archive of Numerical Software, 3(100), 2015.
[2] M. Valiev, E.J. Bylaska, N. Govind, K. Kowalski, T.P. Straatsma, H.J.J. Van Dam, D. Wang, J. Nieplocha, E. Apra, T.L. Windus, and W.A. de Jong. Nwchem: A comprehensive and scalable open-source solution for large scale molecular simulations. Computer Physics Communications, 181(9):1477 – 1489, 2010.

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