

# Multi Domain Finite Element Calculations for Molecules Using the FEniCS Framework and Iso-Parametric Elements

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## Abstract

We consider a molecule consisting of  $M$  atoms and  $N$  electrons which is described by the Hamiltonian

$$H = - \sum_{i=1}^N \nabla_i^2 + \sum_{i>j=1}^N \frac{2}{|\mathbf{r}_i - \mathbf{r}_j|} - \sum_{i=1}^N \sum_{j=1}^M 2 \frac{Z_j}{|\mathbf{r}_i - \mathbf{R}_j|} + \sum_{i>j=1}^M 2 \frac{Z_i Z_j}{|\mathbf{R}_i - \mathbf{R}_j|}$$

Applying the method of Finite Elements to such a system runs into difficulties if only Cartesian coordinates are used, since the Coulomb potentials due to the nuclei lead to numerical challenges when numerically evaluating matrix elements and the convergence of the finite element method will be suboptimal.

However, subdividing the computational domain in to  $M$  spheres  $\Omega_i$  defined by

$$|\mathbf{r} - \mathbf{R}_i| \leq r_{MTi}$$

around the nuclei at  $\mathbf{R}_i$  and the interstitial remainder  $\Omega$ , using spherical coordinates in the spheres and Cartesian coordinates in  $\Omega$ , the problems with the Coulomb Potentials are avoided. This approach is in analogy to the muffin tin approach used in computational solid state physics, for example by the LAPW method[1].

In the present contribution a formalism for implementing density functional calculations for molecules using a multi domain finite element approach is outlined and some initial results for small molecules are given. The finite element method is applied using the FEniCS Framework[2] and custom coded iso-parametric finite elements[3] for boundary layers to facilitate the continuity of the orbitals between the spheres and the interstitial domain.

## References

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