ExotiMO

General Exotic Particle Molecular Orbital System

# Motivation

There are several motivations for developing a new code to treat systems containing exotic particles. Currently, the only mainstream quantum chemistry code that is capable of computing wavefunctions for more than one light particle is GAMESS. This functionality in GAMESS is provided through modifications to the NEO package, which was originally developed for including quantum protons in calculations.

There is a fundamental difference with the way that quantum protons are included in molecular orbital (MO) calculations compared to exotic particles. Namely, basis function centers (BFCs) for light particles should usually be placed on classically treated nuclei, while BFCs for quantum protons are located away from classical nuclei. The mechanics for handling BFCs in NEO is not optimal for light particles, and would require a complete redesign to do that properly.

There are instances in exotic particle quantum chemistry where it would be nice to be able to compute wavefunctions for systems containing more than two types of light particles (e.g. a system containing a muon, two electrons, and a quantum proton). With the modifications to NEO to handle exotic particles, GAMESS can compute wavefunctions for systems containing only \textit{two} types of quantum particles (e.g. electrons and positrons, electrons and protons, \textit{or} positrons and protons). A new code could be designed from the ground up to include as many different types of quantum particles as desired (within limits of computational resources, of course).

GAMESS is a large and complicated code, written in FORTRAN, to which it is somewhat difficult to add modifications or new functionality. NEO is not parallel, and systems with exotic particles require large basis sets for accurate treatment.

# Program Philosophy

Some definitions:

1. quantum particle: particle for which a Slater determinant is included in the solution to the Schrödinger equation
2. basis function center: location in three-dimensional space at which basis functions for one or more types of quantum particle are placed
3. atom: basis function center that also has a classically-treated particle with a positive or negative charge and a non-zero mass

The code will allow the user to specify:

* as many types of quantum particles (e.g. muons, positrons, protons, electrons) as desired
* basis function centers can be placed anywhere, and they can contain basis functions for any or all of the quantum particles in the problem
* basis function centers can be placed on classical particles (e.g. heavy nuclei), but not necessarily
* common basis sets for multiple basis function centers or different basis sets for each

We will use the Chapel

# Math Behind the Code

# References

[1] M.W. Schmidt, K.K. Baldridge, J.A. Boatz, S.T. Elbert, M.S. Gordon, J.H. Jensen, S. Koseki, N. Matsunaga, K.A. Nguyen, S. Su, T.L. Windus, M. Dupuis, and J.A.M. Jr, “General atomic and molecular electronic structure system,” *Journal of Computational Chemistry*, vol. 14, 1993, pp. 1347-1363.

[2] P.E. Adamson, X.F. Duan, L.W. Burggraf, M.V. Pak, C. Swalina, and S. Hammes-Schiffer, “Modeling Positrons in Molecular Electronic Structure Calculations with the Nuclear-Electronic Orbital Method,” *The Journal of Physical Chemistry A*, vol. 112, Feb. 2008, pp. 1346-1351.

[3] “Chapel Programming Language Homepage.”