ExotiMO Package Specification
Version 0.1

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Contents

Part I

Introduction

1 Purpose

ExotiMO is a new quantum chemistry package that is intended for modeling of systems of arbitrary numbers and types of classical and quantum particles, and this document is intended to be both a "good"[2] functional (*i.e.*requirements) specification and a technical specification of Version 1.0 of the ExotiMO package. This specification will be updated for future versions of ExotiMO.

The current draft is a work-in-progress and therefore incomplete.

2 Acknowledgments

Hopefully the list of contributors to the ExotiMO package and its specification will grow long in the future. For now, it's just me, Paul Adamson.

Chapel is a derivative of a number of quantum chemistry codes and takes ideas directly from them, especially GAMESS, pyQuante, and NWChem.

The structure and approach of this specification draws heavily from that of the language in which it is written, Chapel. Much thanks to the Chapel team for making the source code for the Chapel specification available.

3 Notation

Special notations are used in this specification to denote ExotiMO Chapel code and to denote ExotiMO syntax.

ExotiMO Chapel code is represented with a fixed-width font where keywords are bold and comments are italicized.

Example.

```
for i in D do   // iterate over domain D
  writeln(i);   // output indices in D
```

ExotiMO syntax is represented with standard syntax notation in which productions define the syntax of the package. A production is defined in terms of non-terminal (*italicized*) and terminal (non-italicized) symbols. The complete syntax defines all of the non-terminal symbols in terms of one another and terminal symbols.

A definition of a non-terminal symbol is a multi-line construct. The first line shows the name of the non-terminal that is being defined followed by a colon. The next lines before an empty line define the alternative productions to define the non-terminal.

Example. The production

bool−literal:
  true
  false

defines *bool−literal* to be either the symbol **true** or **false**.

In the event that a single line of a definition needs to break across multiple lines of text, more indentation is used to indicate that it is a continuation of the same alternative production.

As a short-hand for cases where there are many alternatives that define one symbol, the first line of the definition of the non-terminal may be followed by "one of" to indicate that the single line in the production defines alternatives for each symbol.

Example. The production

unary−operator: *one of*
  + − ~ !

is equivalent to

unary−operator:
  +
  −
  ~
  !

As a short-hand to indicate an optional symbol in the definition of a production, the subscript "opt" is suffixed to the symbol.

Example. The production

formal:
formal−tag identifier formal−type$_{opt}$ *default−expression*$_{opt}$

is equivalent to

formal:
formal−tag identifier formal−type default−expression
formal−tag identifier formal−type
formal−tag identifier default−expression
formal−tag identifier

4 Organization

This specification is organized as follows:

- Part I. Introduction
  - Chapter 1, Purpose, describes the purpose of this document.
  - Chapter 2, Acknowledgements, offers a note of thanks to people and projects.
  - Chapter 3, Notation, introduces the notation that is used throughout this document.
  - Chapter 4, Organization, describes the contents of each of the parts and chapters within this document.
- Part II. Functional (*i.e.*Requirements) Specification
  - Chapter 5, Scope, describes the scope of the ExotiMO package.
- Part III. Technical Specification

Part II

Functional (*i.e.* Requirements) Specification

5 Scope

5.1 Introduction

ExotiMO is a software package that is intended for *ab initio* molecular quantum chemistry studies, and is suited for modeling of systems of arbitrary numbers and types of classical (*e.g.*nucleonic) and quantum (*e.g.*electronic, muonic) particles. This specification is relevant to version 1.0 of the package. Future versions will have additional features.

> *TODO:* Describe the inspiration behind this approach to developing ExotiMO (Cook, Handbook of Computational Quantum Chemistry [1]). Write this after the basic architecture and approach to documentation (WEB?) is determined.

The package is structured in such a way that it will serve three main purposes simultaneously:

- **Library**: ExotiMO can be viewed as a suite of data and Chapel code that can be used to develop new quantum chemistry applications. ExotiMO classes (*e.g.*the contracted Gaussian basis function class), functions (*e.g.*the two-electron integral function), and data (*e.g.*the STO-3G basis set) can be accessed by simply adding the appropriate `use module` statement to your Chapel code and passing the `-compopts '-M $EXOTIMO_HOME/src'` option to the `chpl` compiler.
- **Executable**: Makefiles are provided to generate executables to be used as "black boxes" with properly formatted input files to run the supported calculations described below.
- **Textbook**: This specification and the documented source code is written in such a way that an aspiring code developer can use ExotiMO to learn various techniques in quantum chemistry.

> *TODO:* Revisit the above description of the structure after the basic requirements for ExotiMO classes, functions, and code documentation are developed.

> *TODO:* Determine how best to serve the "Textbook" purpose through documentation, citing, and code readability.

Briefly, ExotiMO can compute self-consistent field (SCF) wavefunctions at the Restricted Hartree-Fock (RHF) level. Second-order Møller-Plesset (MP2) correlation corrections to RHF wavefunctions is available. Gradients of classical particle and basis function center positions are available for automatic geometry optimization.

Many basis sets are stored internally.

Computations are performed using direct techniques. Although not the primary focus of version 1.0, the package is written in the Chapel programming language, and it is meant to be massively parallel "from the ground up."

For sytems containing electrons and one positron, to facilitate comparison with experiment, the two-photon annihilation rate and the two-photon momentum density (TPMD) are availble as wavefunction properties.

Open issue. Should one of the primary focuses of ExotiMO be to connect with experiment wherever possible?

Part III

Technical Specification

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Bibliography

[1] D. B. Cook. *Handbook of Computational Quantum Chemistry*. Dover, 2005.

[2] Joel Spolsky. Painless functional specifications. `http://www.joelonsoftware.com/articles/fog0000000036.html`. Accessed: 2014-12-29.