Niedoida User’s Guide

September 20, 2007
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Part I

Getting started
Chapter 1

Introduction

Niedoida[1] is a general-purpose quantum-chemical and microelectrostatic package, at the moment in the pupal state. For up-to-date information about niedoida check http://www.chemia.uj.edu.pl/~niedoida/en/.

The niedoida package consists of two programs, niedoida and elektrycerz. They implement the quantum-chemical and the microelectrostatic calculations, respectively.
Chapter 2

Installation

This chapter covers all the information necessary to compile and install niedoida.

2.1 Prerequisites

Before you start compiling niedoida, you need a few additional software packages necessary to compile it. The full list of dependencies is

- **Tools**
  - python version 2.4 ([http://www.python.org/](http://www.python.org/))
  - scons version 0.96 ([http://www.scons.org/](http://www.scons.org/))
  - \(\TeX\) system, eg. teTeX ([http://www.tug.org/teTeX/](http://www.tug.org/teTeX/))

- **Libraries**
  - boost version 1.32.0 ([http://www.boost.org/](http://www.boost.org/))
  - HDF5 version 1.6.3.patch ([http://hdf.ncsa.uiuc.edu/HDF5/](http://hdf.ncsa.uiuc.edu/HDF5/))
  - TAO (Toolkit for Advanced Optimization)[2] version 1.9
  - PETSc[3, 4, 5] version 2.3.3

2.2 Compilation

niedoida build system is based on the scons software construction tool. More information about scons can be found at [http://www.scons.org/](http://www.scons.org/).

To compile niedoida, run scons in the main directory of the program. If needed, scons may be parametrized with compilation options.

It is possible to set several compilation options. They may specify compilation mode and list of directories being searched by the compiler to fulfill external
dependencies. Full list of options, and their default values can be obtained by running `scons -h` in the main directory of the program.

Running `scons` generates all libraries and programs comprising `niedoida`, and full documentation in the PDF format.

Basic tests of most of the components can be performed by running `scons check`.

2.3 Installation

The recommended way of installing `niedoida` involves building binary packages and then installing them in the target system using standard package management tools.

`niedoida` build system allows for creation of binary RPM and DEB packages. The DEB packages are built by running `scons deb` in the main directory of the program. The resulting files can be found in the `packages/deb` subdirectory. The RPM packages are built by running `scons rpm`. The resulting files can be found in the `packages/rpm` subdirectory.

The `niedoida` packages depend on the following external third-party libraries:

- boost version 1.32.0
- LAM/MPI version 7.1.1
- HDF5 version 1.6.3.patch
Chapter 3

The Fine Print

Niedoida and associated documentation is distributed according to the license allowing you to use it only for conducting scientific research, and without any warranty. For details see Appendix A.

For each publication using results obtained by running niedoida, we request citation including the name of the program, it’s version and all authors. For the current version the required citation is:

@Misc{niedoida02,  
author = {Grzegorz Mazur and Marcin Makowski and Witold Piskorz and Łukasz Wiklik and Mariusz Sterzel and Mariusz Radoń and Barbara Jagoda-Wiklik, Waldemar Kulig and Daniel Błażewicz},  
title = {Niedoida 0.2},  
year = 2007}

Additionally, binary distribution of niedoida is using, among others, HDF5, TAO, PETSc and Boost libraries. Their licenses are reproduced in Appendices B, C, D and E, respectively.
Part II

Niedoida
3.1 Capabilities

niedoida allows for SCF calculations at the Hartree-Fock level of theory. The implemented schemes are

- RHF,
- UHF,
- ROHF (in Longuet-Higgins-Pople approximation\cite{6, 7}).

For all these methods, the following properties are available:

- energy,
- molecular orbitals,
- Mulliken\cite{8, 9, 10, 11}, Löwdin, Hirshfeld, Voronoi and Bader population analyses,
- Mayer\cite{12, 13}, Gopinathan-Jug and Nalewajski-Mrozek\cite{14, 15, 16} bond order analyses.

Moreover, niedoida implements selected post-HF calculations

- CIS,
- MP2.
Chapter 4

Invoking niedoida

The chapter covers all the information necessary to prepare input data and run niedoida. It is assumed that the program is already installed and configured.

4.1 Command-line interface

niedoida provides typical command-line interface. It allows for running the program with input being read either from file, or from the standard input.

Running niedoida without any arguments causes the program to read input from the standard input, and write results to the standard output. If an argument is provided, it is treated as the input file name. In this case results are written to a file. The results file is created in the same directory and has the same name as the input file, but the extension is changed to .log.

4.2 Configuration file

Default configuration is stored in niedoida during compilation. When running niedoida, it reads the global configuration file (if it exists) and then local configuration file (if it exists). Setting a configuration parameter in any of them overrides the previous value.

Configuration files format is free-form. Spaces, tabs and line breaks are uniformly treated as whitespaces, except for literal strings and comments. Configuration file may contain parameter definitions and comments.

Global configuration file is named niedoida.cfg, and is stored in directory <prefix>/share/niedoida. Default path to the global configuration file is /usr/local/share/niedoida.

Local configuration file is named niedoida.cfg, and is searched for in the same directory in which the input file is located. If input is read from standard input, local configuration file is searched for in the current working directory.

4.2.1 Configuration settings

basis_set  Parameters set defining where and in which format atomic basis sets descriptions are stored. Each entry has the following form
and the whole set

```
basis_set = {
    <entry_1>,
    <entry_2>,
    ...
    <entry_n>
};
```

**scratch_dir** Parameter defining in which directory temporary files are created. Default is /tmp.

## 4.3 Input description

The input format is free-form. Spaces, tabs and line breaks are uniformly treated as whitespaces, except for literal strings and comments. Input may contain parameter definitions and comments.

### 4.3.1 Comments

Comments may appear anywhere in the input. They either start with the `//` string, and end at the end of the line, or start with the `/*` string and end with the `*/` string. An example comment is shown in Example 6.1.

Comments do not influence the calculations in any way.

```
// A single line comment

/* Another single line comment */

/* A multi-line
   comment
*/
```

Example 4.1: Comments

### 4.3.2 Parameter definitions

Parameters control calculations performed by **niedoida**. By setting them to specific values you decide what and how is calculated when the program is run.

Parameters may be of simple, compound or list type. All parameter definitions have the form

```
<parameter_name>=<parameter_value>;
```
4.3. INPUT DESCRIPTION

The order of parameter definitions is not significant.\(^1\)

**Simple parameters**

Simple parameter values are integer or real numbers, identifiers, or literal strings. Examples are shown in Example 4.2.

// a string parameter
title = "an example job";

// an identifier parameter
run_type = single_point;

// an integer parameter
charge = -1;

// a real parameter
energy_threshold = 1e-6;

---

Example 4.2: Simple parameters

**Compound parameters**

Compound parameters are collections of other parameters. Their definitions have the form

```plaintext
<compound_parameter_name> = {
  <parameter_name_1> = <parameter_value>;
  <parameter_name_2> = <parameter_value>;
  // ...
  <parameter_name_n> = <parameter_value>;
};
```

where the embedded parameters may be of any type.

An example is shown in Example 4.3.

**List parameters**

List parameters are collections of values. Their definitions have the form

```plaintext
<list_parameter_name> = {
  <value_1>,
  <value_2>,
  // ...
  <value_n>
};
```

An example is shown in Example 4.4.

---

\(^1\)Except for the inputs where the same parameter appears more than once. In such cases only the last definition is effective. This (mis)feature should not be relied upon, and it is planned that in the future versions of niedoida an attempt to define the same parameter more than once will be reported as error.
scf = {
    method = rhf;
    energy_threshold = 1e-6;
    density_threshold = 1e-6;
    convergence_accelerator = diis;
};

Example 4.3: A compound parameter

atoms = {
    o 0.0000000 0.24618131 0.0000000,
    h 1.4326629 -0.95521837 0.0000000,
    h -1.4326629 -0.95521837 0.0000000
};

Example 4.4: A list parameter

4.4 Parameters

All of the parameters in this section are optional, except for basis_set and atoms.

Skipping an optional parameter means that the default value is assigned to it. Note: default values are constant, and do not depend on other parameters values. No attempt is made to adjust skipped parameters to those specified in input. This means, for example, that setting multiplicity to 1, and not specifying the SCF method different from the default one (RHF) is reported as input error.

4.4.1 Top level

Parameter title

Type string

Default

Title of the job.

Parameter run_type

Type enum (single_point, geometry_optimization)

Default single_point

Type of the job.
### 4.4 PARAMETERS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>basis_set</td>
<td>string</td>
<td></td>
<td>Name of the atomic basis set. For the mapping between the basis set name and actual definition of the basis set see Section 4.2.1.</td>
</tr>
<tr>
<td>charge</td>
<td>integer</td>
<td>0</td>
<td>Molecular charge.</td>
</tr>
<tr>
<td>multiplicity</td>
<td>positive integer</td>
<td>1</td>
<td>Multiplicity of electronic state.</td>
</tr>
<tr>
<td>atoms</td>
<td>list</td>
<td></td>
<td>List of the atoms comprising the system and their coordinates. See Sec. 4.4.2</td>
</tr>
<tr>
<td>scf</td>
<td>compound</td>
<td></td>
<td>Set of parameters controlling the SCF process. See Sec. 4.4.3</td>
</tr>
<tr>
<td>units</td>
<td>compound</td>
<td></td>
<td>Specifies the (physical) units system to use for reading input and printing results. See Sec. 4.4.4</td>
</tr>
</tbody>
</table>

Parameter **basis_set**

Type string

Default

Name of the atomic basis set. For the mapping between the basis set name and actual definition of the basis set see Section 4.2.1.

Parameter **charge**

Type integer

Default 0

Molecular charge.

Parameter **multiplicity**

Type positive integer

Default 1

Multiplicity of electronic state.

Parameter **atoms**

Type list

Default

List of the atoms comprising the system and their coordinates. See Sec. 4.4.2

Parameter **scf**

Type compound

Default

Set of parameters controlling the SCF process. See Sec. 4.4.3

Parameter **units**

Type compound

Default

Specifies the (physical) units system to use for reading input and printing results. See Sec. 4.4.4
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Default</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Parameter limits</td>
<td>compound</td>
<td></td>
<td>Set of parameters controlling system usage. ?? See Sec. 4.4.5</td>
</tr>
<tr>
<td>Parameter integrals</td>
<td>compound</td>
<td></td>
<td>Integration options. See Sec. 4.4.6</td>
</tr>
<tr>
<td>Parameter theory</td>
<td>enum (hf, hf-vwn, slater, svwn)</td>
<td>hf</td>
<td>Bloody theory.</td>
</tr>
<tr>
<td>Parameter moller_plesset</td>
<td>compound</td>
<td></td>
<td>Second order Møller-Plesset options. See Sec. 4.4.7</td>
</tr>
<tr>
<td>Parameter cis</td>
<td>compound</td>
<td></td>
<td>Single CI options. See Sec. 4.4.8</td>
</tr>
<tr>
<td>Parameter properties</td>
<td>compound</td>
<td></td>
<td>Specifies which properties should be calculated from the SCF wavefunction.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>See Sec. 4.4.9</td>
</tr>
</tbody>
</table>
4.4. PARAMETERS

Parameter output

Type compound

Default

Output options. See Sec. 4.4.10

4.4.2 atoms

Parameter atoms contains set of atoms from which the molecule is built. It is a list parameter 4.3.2.

Each atom is described in following format:
[weight] symbol[_label] x y z

where weight is a atomic weight of element, symbol is a chemical symbol (case insensitive), label is arbitrary string and x y z are position coefficient of atoms. Parameters in square brackets are optional

```plaintext
atoms = {
    16 0 0.0000 0.0000 0.1141,
    H_alpha 0.0000 0.7803 -0.4563,
    1 H_beta 0.0000 -0.7803 -0.4563
}
```

Example 4.5: Molecule specification

4.4.3 scf

Parameter method

Type enum (rhf, rohf, uhf)

Default rhf

Specifies the type of SCF process.

Parameter max_no_iterations

Type positive integer

Default 30

Maximal number of iterations.
Parameter energy_threshold
Type positive real
Default $10^{-5}$
SCF is not considered converged until the energy difference between two consecutive steps is larger than the threshold.

Parameter density_threshold
Type positive real
Default $10^{-5}$
SCF is not considered converged until the density difference between two consecutive steps is larger than the threshold.

Parameter convergence_accelerator
Type enum (none, diis, oda)
Default diis
The convergence accelerator to use in SCF process.

Parameter shift_1
Type positive real
Default 0
Activates level shifting. In case of RHF it denotes the shift of virtual orbital energies with respect to the occupied orbitals. In case of ROHF it gives the energy shift of singly occupied orbitals with respect to the doubly occupied orbitals. Finally in case of UHF it denotes the shift of virtual orbital energies with respect to the occupied orbitals for $\alpha$ spin. Warning! Using level shifting may lead to unphysical results.

Parameter shift_2
Type positive real
Default same as shift_1
In case of ROHF it gives the energy shift of virtual orbitals with respect to the singly occupied orbitals. In case of UHF it denotes the shift of virtual orbital energies with respect to the occupied orbitals for $\beta$ spin. Skipping this parameter means that it is equal shift_1.
### 4.4. PARAMETERS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Type</th>
<th>Default</th>
</tr>
</thead>
<tbody>
<tr>
<td>initial_guess</td>
<td>enum (fragments, core_hamiltonian, from_file)</td>
<td>fragments</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Type of initial guess.</td>
</tr>
<tr>
<td>initial_guess_filename</td>
<td>enum</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Default</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Name of the file from which MO coefficients are read when initial_guess = from_file.</td>
</tr>
<tr>
<td>occupations</td>
<td>enum (aufbau, fermi)</td>
<td>aufbau</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Determines how occupation numbers are assigned to molecular orbitals during the SCF procedure. Allowed values are aufbau (occupations based on Aufbau principle) and fermi (smearing of electrons due to Fermi-Dirac distribution of fixed width).</td>
</tr>
<tr>
<td>degeneracy_threshold</td>
<td>positive real</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Applies only if occupations = aufbau. Then, if the value was given electrons are uniformly smeared in orbitals which energy difference with HOMO is less than the value. If no value was given occupation numbers are always integer, irrespective of possible HOMO quasi-degeneracy.</td>
</tr>
<tr>
<td>smear</td>
<td>positive real</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Applies only if occupations = fermi. If so, electrons are distributed according to Fermi-Dirac formula with $kT$ equal smear. Actual Fermi level value is assumed to be $(E_{HOMO} + E_{LUMO})/2$.</td>
</tr>
</tbody>
</table>
4.4.4 units

Parameter energy
Type enum (eV, hartree)
Default eV
Energy unit to use.

Parameter length
Type enum (bohr, angstrom)
Default bohr
Length unit to use.

Parameter storage
Type enum (byte, kilobyte, megabyte, gigabyte)
Default megabyte
Storage unit to use.

4.4.5 limits

Parameter cpu_time
Type positive real?
Default 7200
Maximal time of processor running. ?

4.4.6 integration

Parameter engine
Type enum (naive, os1)
Default os1
Type of integration engine.
4.4. PARAMETERS

Parameter threshold
Type positive real
Default $10^{-10}$
Integration miscount.

Parameter cache_size
Type positive integer
Default 16
Storage capacity.

Parameter storage
Type enum (none, local, shared, in_core)
Default none?
The way of integrals storage.

4.4.7 mp2

Parameter order
Type natural
Default 0
Order of perturbation theory calculations.

Parameter memory_pool
Type natural
Default 64

Parameter no_frozen
Type natural
Default 0
Number of frozen molecular orbital.
Parameter no_deleted
Type natural
Default 0
Number of deleted virtual orbitals.

4.4.8 cis

Parameter multiplicity
Type enum (singlet, triplet, both)
Default both
Requested multiplicity of excited states.

Parameter no_frozen
Type natural
Default 0
Number of frozen molecular orbital.

Parameter no_deleted
Type natural
Default 0
Number of deleted virtual orbitals.

Parameter no_states
Type natural
Default 0
Number of states.
4.4.9 properties

Parameter population_analysis
Type compound
Default
Specifies which population analysis should be performed. This compound argument is a collection of simple parameters having the form: `<population_analysis_name> = <bool_value>`, where `<population_analysis_name>` is a name of population analysis and `<bool_value>` should be non-zero to switch the proper analysis on or 0 to switch it off. See Sec. 4.4.9.

Parameter bond_order_analysis
Type compound
Default
Specifies which bond order analysis should be performed. This compound argument is a collection of substitution of form: `<bond_order_analysis_name> = <bool_value>`, where `<bond_order_name>` is a name of bond order analysis and `<bool_value>` should be non-zero to switch the proper analysis on or 0 to switch it off. See Sec. 4.4.9

Parameter max_multipole_moment_order
Type natural
Default ?
Maximal order of multipole moment.???

population_analyses

Parameter mulliken
Type boolean
Default 1
Controls whether Mulliken population analysis is performed.

Parameter lowdin
Type boolean
Default 1
Controls whether Löwdin population analysis is performed.
Parameter **hirshfeld**
*Type* boolean
*Default* 0
Controls whether Hirshfeld population analysis is performed.

Parameter **voronoi**
*Type* boolean
*Default* 0
Controls whether Voronoi population analysis is performed.

Parameter **bader**
*Type* boolean
*Default* 0
Controls whether Bader population analysis is performed.

**bond_order**

Parameter **mayer**
*Type* boolean
*Default* 1
Enable Mayer bond order analysis.

Parameter **gopinathan_jug**
*Type* boolean
*Default* 1
Enable Gopinathan-Jug bond order analysis.

Parameter **nalewajski**
*Type* boolean
*Default* 1
Enable Nalewajski bond order analysis.
4.5. EXAMPLES

4.4.10 output

Parameter binary
Type boolean
Default 0

Binary form of output.

Parameter molden
Type boolean
Default 0

Generate the MOLDEN output. For more information about MOLDEN see http://www.cmbi.kun.nl/molden/molden.html.

4.5 Examples

Example 4.6 shows an input for energy calculations of water molecule. Let’s analyze it closer.

```plaintext
title = "water molecule";

Sets the job title. It does not influence the calculations, but is reproduced in the output. Therefore, it can be used to convey information which makes it easier to identify or analyze output later.

run_type = single_point;

Causes the calculations to be performed only for geometry given in input. It is the default, so skipping the line would not change the calculations.

basis_set = "sto-3g";

Sets the atomic orbitals basis to be used in calculations.

units = {
    length = bohr;
    energy = hartree;
};

Determines units used to interpret input, and units which will be used in output. In this case all lengths and energies are in atomic units.
Determines the stoichiometry and geometry of the molecule for which calculations should be performed. In this case it is a water molecule, and geometry is close to optimal.

Example 4.6: Water molecule
Example 4.7: Ammonia molecule
Part III

Elektrycerz
Chapter 5

Introduction

elektrycerz implements the SCPF[17] method of the polarization energy calculations.
Chapter 6

Invoking elektrycerz

The chapter covers all the information necessary to prepare input data and run elektrycerz. It is assumed that the program is already installed and configured.

6.1 Command-line interface

elektrycerz provides typical command-line interface. To run elektrycerz an argument should be provided. The argument is treated as the input-file name. Results of calculations are written to the output file. The output file is created in the same directory and has the same name as the input file, but the extension is changed to .log.

6.2 Input description

The input format is free-form. Spaces, tabs and line breaks are uniformly treated as whitespaces, except for literal strings and comments. Input may contain parameter definitions and comments.

6.2.1 Comments

Comments may appear anywhere in the input. They either start with the // string, and end at the end of the line, or start with the /* string and end with the */ string. An example comment is shown in Example 6.1.

Comments do not influence the calculations in any way.

6.2.2 Parameter definitions

Parameters control calculations performed by elektrycerz. By setting them to specific values you decide what and how is calculated when the program is run.

Parameters may be of simple, compound or list type. All parameter definitions have the form

<parameter_name>=<parameter_value>;

The order of parameter definitions is not significant.\(^1\)

\(^1\)Except for the inputs where the same parameter appears more than once. In such cases
Example 6.1: Comments

6.3 Parameters

All parameters are optional, except for molecules. Skipping an optional parameter means that the default value is assigned to it. Note: default values are constant, and do not depend on other parameters values. No attempt is made to adjust skipped parameters to those specified in input.

Parameter title

Type: string
Default
Title of the job.

Parameter threshold

Type: positive real
Default: $10^{-5}$
Required accuracy.

Parameter solver

Type: enum (cg, jacobi, minres)
Default: cg
Algorithm to be used to solve the SCPF equations.

only the last definition is effective. This (mis)feature should not be relied upon, and it is planned that in the future versions of elektrycerz an attempt to define the same parameter more than once will be reported as error.
Parameter damping_factor

Type real in the range (0; 1)

Default 0.5

Damping factor. Used only for jacobi solver.

Parameter model

Type enum (intermolecular, intramolecular)

Default intermolecular

Defines the model of microelectrostatic calculations. In the intermolecular there are no interactions between submolecules belonging to the same molecule. In the intramolecular model, submolecule may interact with every other submolecule, even with those belonging to the same molecule. For this model an explicit list of non-interacting submolecules may be specified.

Parameter molecules

Type list

Default

Defines the system for which calculations will be performed. The list consists of entries describing molecules. Every molecule is defined as a list of submolecules. A submolecule is defined by its position, polarizability, and, optionally, the charge. For the intramolecular model a list of non-interacting submolecules may be specified.
CHAPTER 6. INVOKING ELEKTRYCERZ
Chapter 7

Examples
Example 7.1: Four fullerene molecules, each represented as a single submolecule
Appendix A

License

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Appendix F

Pearls of Wisdom

C++: an octopus made by nailing extra legs onto a dog.
     -- Anonymous

FORTRAN was the language of choice for the same reason that three-legged races are popular.
     -- Ken Thompson

There's no Moore law for the productivity of programmers.
     -- Robert Dewar

* Me: My brain is burnt out after trying to follow what the iterators have to do.
  * Joerg: That's Dr. Stepanov's gift for us ;-)  
     -- Boost developer

DFT is assuming a local external potential ....
     -- Bernd Schimmelpfennig

Failure is not an option. It comes bundled with your Microsoft product.
     -- Derek Harkness

A bug in the code is worth two in the documentation.
     -- Anonymous

If the only thing you know is a hammer, everything looks like a nail.
     -- Anonymous

We always know what we're doing -- we're superheroes, we're C++ programmers.
     -- Aaron W. LaFramboise

The use of COBOL cripples the mind; its teaching should, therefore, be regarded as a criminal offence.
     -- Edsger W. Dijkstra, SIGPLAN Notices, Volume 1
Inefficient abstractions are a dime a dozen.

-- Andrei Alexandrescu
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