QCEngine Documentation

Release v0.9.0+0.g8e45c01.dirty

The QCArchive Development Team

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CONTENTS:

Quantum chemistry program executor and IO standardizer (QCSchema) for quantum chemistry.

CHAPTER

ONE

PROGRAM EXECUTION

A simple example of QCEngine's capabilities is as follows:

```
>>> import qcengine as qcng
>>> import qcelemental as qcel

>>> mol = qcel.models.Molecule.from_data("""
O  0.0  0.000  -0.129
H  0.0 -1.494  1.027
H  0.0  1.494  1.027
""")

>>> input = qcel.models.ResultInput(
    molecule=mol,
    driver="energy",
    model={"method": "SCF", "basis": "sto-3g"},
    keywords={"scf_type": "df"}
    )
```

These input specifications can be executed with the `compute` syntax along with a program specifier:

```
>>> ret = qcng.compute(input, "psi4")
```

The results contain a complete record of the computation:

```
>>> ret.return_result
-74.45994963230625

>>> ret.properties.scf_dipole_moment
[0.0, 0.0, 0.6635967188869244]

>>> ret.provenance.cpu
Intel(R) Core(TM) i7-7820HQ CPU @ 2.90GHz
```

CHAPTER

TWO

BACKENDS

Currently available compute backends for single results are as follow:

- Quantum Chemistry:
  - Terachem
  - Molpro
  - Psi4
- AI Evaluation:
  - TorchANI
- Molecular Mechanics:
  - RDKit

In addition, several procedures are available:

- Geometry Optimization:
  - geomeTRIC

CHAPTER

THREE

CONFIGURATION DETERMINATION

In addition, QCEngine can automatically determine the following quantites:

- The number of physical cores on the system and to use.
- The amount of physical memory on the system and the amount to use.
- The provenance of a computation (hardware, software versions, and compute resources).
- Location of scratch disk space.
- Location of quantum chemistry programs binaries or Python modules.

Each of these options can be specified by the user as well.

```
>>> qcng.get_config()
<JobConfig ncores=2 memory=2.506 scratch_directory=None>

>>> qcng.get_config(local_options={"scratch_directory": "/tmp"})
<JobConfig ncores=2 memory=2.506 scratch_directory='/tmp'>

>>> os.environ["SCRATCH"] = "/my_scratch"
>>> qcng.get_config(local_options={"scratch_directory": "$SCRATCH"})
<JobConfig ncores=2 memory=2.506 scratch_directory='/my_scratch'>
```

CHAPTER

FOUR

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Getting Started

4.1 Installing QCEngine

You can install `qcengine` with `conda`, with `pip`, or from source.

4.1.1 Conda

You can install or update `qcengine` using conda:

```
conda install qcengine -c conda-forge
```

This command installs `qcengine` and its dependencies. The `qcengine` package is maintained on the conda-forge channel.

4.1.2 Pip

`qcengine` may be installed with `pip`:

```
pip install qcengine
```

4.1.3 Install from Source

To install `qcengine` from source, clone the repository from github:

```
git clone https://github.com/MolSSI/QCEngine.git
cd qcengine
python setup.py install
```

or use `pip` for a local install:

```
pip install -e .
```

We recommend building a development environment with the following lines:

```
cd qcengine
python devtools/scripts/conda_env.py -n=qcngdev -p=3.6 devtools/conda-envs/psi.yaml
conda activate qcngdev
```

This will build out a new environment with several compute backends for `qcengine` which provides a platform to test and develop the code.

Test

Test a `qcengine` local install with `pytest`:

```
cd qcengine
pytest -v
```

4.2 Community

The QCArchive is an open community sponsored by The Molecular Sciences Software Institute. However, this is a community-driven project which requires feature requests, user feedback, and code support. There are a variety of ways to help support the QCArchive project as seen below.

4.2.1 Discussion

- QCArchive Slack is a great place to get feedback and advice from the community. Click here to get started.
- The QCArchive GitHub repositories contain future roadmaps, current code updates, and a list of issues that are being worked and provide an excellent overview of the development status of the project. See the following links:
  - QCSchema
  - QCElemental
  - QCEngine
  - QCFractal

4.2.2 Work with us!

The QCArchive project is actively looking for early collaborations to use our tools, help us shake out the bugs, and be evangelists within the computational molecular science community for this code ecosystem. In return you will receive the following benefits:

- Work directly with a MolSSI Software Scientist who will discuss your problem and provide ideas.
- Develop the requirements and potential solutions for your use case within the QCArchive ecosystem.
- Setup monthly meetings to ensure your project stays on track.
- Highlight your project within the QCArchive ecosystem.

If you are interested in working with us, please send an email to QCArchive@molssi.org and we will set up a meeting to discuss specifics.

User Interface

4.3 Single Compute

QCEngine's primary purpose is to consume the MolSSI QCSchema and produce QCSchema results for a variety of quantum chemistry, semiempirical, and molecular mechanics programs. Single QCSchema representation comprises of a single `energy`, `gradient`, `hessian`, or `properties` evaluation.

4.3.1 Input Description

An input description has the following fields:

- `molecule` - A QCSchema compliant dictionary or Molecule model.
- `driver` - The `energy`, `gradient`, `hessian`, or `properties` option.
- `model` - A description of the evaluation model. For quantum chemistry this is typically `method` and `basis`. However, non-quantum chemistry models are often a simple `method` as in `method = 'UFF'` for forcefield evaluation.
- `keywords` - a dictionary of keywords to pass to the underlying program. These are program-specific keywords.

An example input is as follows:

```
>>> import qcengine as qcng
>>> import qcelemental as qcel

>>> mol = qcel.models.Molecule.from_data("""
O  0.0  0.000  -0.129
H  0.0 -1.494  1.027
H  0.0  1.494  1.027
""")

>>> inp = qcel.models.ResultInput(
    molecule=mol,
    driver="energy",
    model={"method": "SCF", "basis": "sto-3g"},
    keywords={"scf_type": "df"}
    )
```

4.3.2 Computation

A single computation can be evaluated with the `compute` function as follows:

```
>>> ret = qcng.compute(inp, "psi4")
```

By default the job is given resources relating to the compute environment it is in; however, these variables can be overridden:

```
>>> ret = qcng.compute(inp, "psi4", local_options={"memory": 2, "ncores": 3})
```

4.3.3 Results

The results contain a complete record of the computation:

```
>>> ret.return_result
-74.45994963230625

>>> ret.properties.scf_dipole_moment
[0.0, 0.0, 0.6635967188869244]

>>> ret.provenance.cpu
Intel(R) Core(TM) i7-7820HQ CPU @ 2.90GHz
```

A short description of the fields is as follow:

- `return_result` - the direct return of the `driver` input. That is energy and gradient for a driver `energy` and `gradient` call, respectively.
- `properties` - Values associated with the `return_result` such as the `scf_one_electron_energy`.
- `stdout` - The `stdout` or log of a programs run.
- `provenance` - A description of the calling program, version, wall time, etc.

A complete description of the input is also available in the output:

```
>>> ret.driver
energy
```

4.3.4 Fields

A list of all fields is available through the `fields` property on the input and output:

```
>>> ret.fields
['molecule', 'driver', 'model', 'id', 'schema_name', 'schema_version', 'keywords',
 'extras', 'provenance', 'return_result', 'success', 'properties', 'stdout', 'stderr',
↪ 'error']
```

4.4 Environment Detection

QCEngine can inspect the current compute environment to determine the resources available to it.

4.4.1 Node Description

QCEngine can detect node descriptions to obtain general information about the current node.

```
>>> qcng.config.get_node_descriptor()
<NodeDescriptor hostname_pattern='*' name='default' scratch_directory=None
                memory=5.568 memory_safety_factor=10 ncores=4 jobs_per_node=2>
```

4.4.2 Config

The configuration file operated based on the current node descriptor and can be overridden:

```
>>> qcng.get_config()
<JobConfig ncores=2 memory=2.506 scratch_directory=None>

>>> qcng.get_config(local_options={"scratch_directory": "/tmp"})
<JobConfig ncores=2 memory=2.506 scratch_directory='/tmp'>

>>> os.environ["SCRATCH"] = "/my_scratch"
>>> qcng.get_config(local_options={"scratch_directory": "$SCRATCH"})
<JobConfig ncores=2 memory=2.506 scratch_directory='/my_scratch'>
```

4.4.3 Global Environment

The global environment can also be inspected directly.

```
>>> qcng.config.get_global()
{
    'hostname': 'qcarchive.molssi.org',
    'memory': 5.568,
    'username': 'user',
    'ncores': 4,
    'cpuinfo': {
        'python_version': '3.6.7.final.0 (64 bit)',
        'brand': 'Intel(R) Core(TM) i7-7820HQ CPU @ 2.90GHz',
        'hz_advertised': '2.9000 GHz',
        ...
    },
    'cpu_brand': 'Intel(R) Core(TM) i7-7820HQ CPU @ 2.90GHz'
}
```

Developer Documentation

- *QCEngine API*
- *Changelog*
- *Development Guidelines*

4.5 QCEngine API

4.5.1 qcengine Package

Base file for the dqm_compute module.

Functions

compute(input_data, program[, raise_error, ...])	Executes a single quantum chemistry program given a QC Schema input.

Continued on next page

Table 1 – continued from previous page

compute_procedure(input_data, procedure[, ...])	Runs a procedure (a collection of the quantum chemistry executions)
get_config(*[, hostname, local_options])	Returns the configuration key for qcengine.
get_molecule(name)	Returns a QC JSON representation of a test molecule.
get_procedure(name)	Returns a procedures executor class
get_program(name[, check])	Returns a program's executor class
list_all_procedures()	List all procedures registered by QCEngine.
list_all_programs()	List all programs registered by QCEngine.
list_available_procedures()	List all procedures that can be exectued (found) by QCEngine.
list_available_programs()	List all programs that can be exectued (found) by QCEngine.
register_program(entry_point)	Register a new ProgramHarness with QCEngine.
unregister_program(name)	Unregisters a given program.

compute

qcengine.**compute**(*input_data: Union[Dict[str, Any], ResultInput], program: str, raise_error: bool = False, local_options: Optional[Dict[str, Any]] = None, return_dict: bool = False*) → Result

Executes a single quantum chemistry program given a QC Schema input.

The full specification can be found at: http://molssi-qc-schema.readthedocs.io/en/latest/index.html#

Parameters

- **input_data** (*Union[Dict[str, Any], 'ResultInput']*) – A QCSchema input specification in dictionary or model from QCElemental.models
- **program** (*str*) – The program to execute the input with.
- **raise_error** (*bool, optional*) – Determines if compute should raise an error or not.
- **retries** (*int, optional*) – The number of random tries to retry for.
- **local_options** (*Optional[Dict[str, Any]], optional*) – A dictionary of local configuration options
- **return_dict** (*bool, optional*) – Returns a dict instead of qcelemental.models.ResultInput

Returns A computed Result object.

Return type Result

compute_procedure

qcengine.**compute_procedure**(*input_data: Union[Dict[str, Any], BaseModel], procedure: str, raise_error: bool = False, local_options: Optional[Dict[str, str]] = None, return_dict: bool = False*) → BaseModel

Runs a procedure (a collection of the quantum chemistry executions)

Parameters

- **input_data** (*dict or qcelemental.models.OptimizationInput*) – A JSON input specific to the procedure executed in dictionary or model from QCElemental.models
- **procedure** (*{"geometric"}*) – The name of the procedure to run

- **raise_error** (*bool, option*) – Determines if compute should raise an error or not.
- **local_options** (*dict, optional*) – A dictionary of local configuration options
- **return_dict** (*bool, optional, default True*) – Returns a dict instead of qcelemental.models.ResultInput

Returns A QC Schema representation of the requested output, type depends on return_dict key.

Return type dict, Optimization, FailedOperation

get_config

qcengine.**get_config**(*, *hostname: Optional[str] = None*, *local_options: Dict[str, Any] = None*) → qcengine.config.JobConfig

Returns the configuration key for qcengine.

get_molecule

qcengine.**get_molecule**(*name*)

Returns a QC JSON representation of a test molecule.

get_procedure

qcengine.**get_procedure**(*name: str*) → ProcedureHarness

Returns a procedures executor class

get_program

qcengine.**get_program**(*name: str*, *check: bool = True*) → ProgramHarness

Returns a program's executor class

Parameters **check** – `True` Do raise error if program not found. `False` is handy for the specialized case of calling non-execution methods (like parsing for testing) on the returned `Harness`.

list_all_procedures

qcengine.**list_all_procedures**() → Set[str]

List all procedures registered by QCEngine.

list_all_programs

qcengine.**list_all_programs**() → Set[str]

List all programs registered by QCEngine.

list_available_procedures

qcengine.**list_available_procedures**() → Set[str]

List all procedures that can be exectued (found) by QCEngine.

list_available_programs

qcengine.**list_available_programs**() → Set[str]
List all programs that can be exectued (found) by QCEngine.

register_program

qcengine.**register_program**(*entry_point: ProgramHarness*) → None
Register a new ProgramHarness with QCEngine.

unregister_program

qcengine.**unregister_program**(*name: str*) → None
Unregisters a given program.

4.5.2 qcengine.compute Module

Integrates the computes together

Functions

compute(input_data, program[, raise_error, ...])	Executes a single quantum chemistry program given a QC Schema input.
compute_procedure(input_data, procedure[, ...])	Runs a procedure (a collection of the quantum chemistry executions)

compute

qcengine.compute.**compute**(*input_data: Union[Dict[str, Any], ResultInput], program: str, raise_error: bool = False, local_options: Optional[Dict[str, Any]] = None, return_dict: bool = False*) → Result
Executes a single quantum chemistry program given a QC Schema input.

The full specification can be found at: http://molssi-qc-schema.readthedocs.io/en/latest/index.html#

Parameters

- **input_data** (*Union[Dict[str, Any], 'ResultInput']*) – A QCSchema input specification in dictionary or model from QCElemental.models
- **program** (*str*) – The program to execute the input with.
- **raise_error** (*bool, optional*) – Determines if compute should raise an error or not.
- **retries** (*int, optional*) – The number of random tries to retry for.
- **local_options** (*Optional[Dict[str, Any]], optional*) – A dictionary of local configuration options
- **return_dict** (*bool, optional*) – Returns a dict instead of qcelemental.models.ResultInput

Returns A computed Result object.

Return type Result

compute_procedure

qcengine.compute.**compute_procedure**(*input_data: Union[Dict[str, Any], BaseModel], procedure: str, raise_error: bool = False, local_options: Optional[Dict[str, str]] = None, return_dict: bool = False*) → BaseModel

Runs a procedure (a collection of the quantum chemistry executions)

Parameters

- **input_data** (*dict or qcelemental.models.OptimizationInput*) – A JSON input specific to the procedure executed in dictionary or model from QCElemental.models
- **procedure** (*{"geometric"}*) – The name of the procedure to run
- **raise_error** (*bool, option*) – Determines if compute should raise an error or not.
- **local_options** (*dict, optional*) – A dictionary of local configuration options
- **return_dict** (*bool, optional, default True*) – Returns a dict instead of qcelemental.models.ResultInput

Returns A QC Schema representation of the requested output, type depends on return_dict key.

Return type dict, Optimization, FailedOperation

4.5.3 qcengine.config Module

Creates globals for the qcengine module

Functions

get_config(*[, hostname, local_options])	Returns the configuration key for qcengine.
get_provenance_augments()	
global_repr()	A representation of the current global configuration.

get_config

qcengine.config.**get_config**(*, *hostname: Optional[str] = None*, *local_options: Dict[str, Any] = None*) → qcengine.config.JobConfig

Returns the configuration key for qcengine.

get_provenance_augments

qcengine.config.**get_provenance_augments**() → Dict[str, str]

global_repr

qcengine.config.**global_repr**() → str

A representation of the current global configuration.

Classes

NodeDescriptor(**data)	Description of an individual node

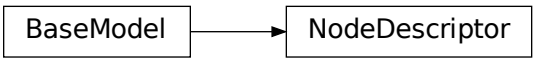
NodeDescriptor

class qcengine.config.**NodeDescriptor**(***data*)

Bases: pydantic.main.BaseModel

Description of an individual node

Class Inheritance Diagram



4.5.4 qcengine.util Module

Several import utilities

Functions

compute_wrapper([capture_output, raise_error])	Wraps compute for timing, output capturing, and raise protection
get_module_function(module, func_name[, ...])	Obtains a function from a given string
model_wrapper(input_data, model)	Wrap input data in the given model, or return a controlled error
handle_output_metadata(output_data, metadata)	Fuses general metadata and output together.

compute_wrapper

qcengine.util.**compute_wrapper**(*capture_output: bool = True*, *raise_error: bool = False*) → Dict[str, Any]

Wraps compute for timing, output capturing, and raise protection

get_module_function

qcengine.util.**get_module_function**(*module: str*, *func_name: str*, *subpackage=None*) → Callable[[...], Any]

Obtains a function from a given string

Parameters

- **module** (*str*) – The module to pull the function from
- **func_name** (*str*) – The name of the function to acquire, can be in a subpackage
- **subpackage** (*None, optional*) – Explicitly import a subpackage if required

Returns **ret** – The requested functions

Return type function

Example

Import numpy.linalg.eigh f = get_module_function("numpy", "linalg.eigh") f(np.ones((2, 2)))

model_wrapper

qcengine.util.**model_wrapper**(*input_data: Dict[str, Any], model: BaseModel*) → BaseModel
Wrap input data in the given model, or return a controlled error

handle_output_metadata

qcengine.util.**handle_output_metadata**(*output_data: Union[Dict[str, Any], BaseModel], metadata: Dict[str, Any], raise_error: bool = False, return_dict: bool = True*) → Union[Dict[str, Any], BaseModel]
Fuses general metadata and output together.

Returns **result** – Output type depends on return_dict or a dict if an error was generated in model construction

Return type dict or pydantic.models.Result

4.5.5 qcengine.programs Package

Functions

get_program(name[, check])	Returns a program's executor class
list_all_programs()	List all programs registered by QCEngine.
list_available_programs()	List all programs that can be exectued (found) by QCEngine.
register_program(entry_point)	Register a new ProgramHarness with QCEngine.
unregister_program(name)	Unregisters a given program.

get_program

qcengine.programs.**get_program**(*name: str, check: bool = True*) → ProgramHarness
Returns a program's executor class

Parameters **check** – `True` Do raise error if program not found. `False` is handy for the specialized case of calling non-execution methods (like parsing for testing) on the returned `Harness`.

list_all_programs

qcengine.programs.**list_all_programs**() → Set[str]
List all programs registered by QCEngine.

list_available_programs

qcengine.programs.**list_available_programs**() → Set[str]
List all programs that can be exectued (found) by QCEngine.

register_program

qcengine.programs.**register_program**(*entry_point: ProgramHarness*) → None
Register a new ProgramHarness with QCEngine.

unregister_program

qcengine.programs.**unregister_program**(*name: str*) → None
Unregisters a given program.

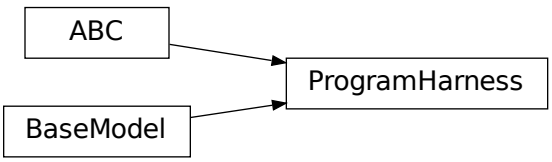
Classes

ProgramHarness(**kwargs)

ProgramHarness

class qcengine.programs.**ProgramHarness**(***kwargs*)
Bases: pydantic.main.BaseModel, abc.ABC

Class Inheritance Diagram



4.6 Changelog

4.6.1 v0.9.0 / 2019-08-14

New Features

- (GH#120) Engine now takes advantage of Elemental's new Msgpack serialization option for Models. Serialization defaults to msgpack when available (`conda install msgpack-python [-c conda-forge]`), falling back to JSON otherwise. This results in substantial speedups for both serialization and deserialization actions and should be a transparent replacement for users within Engine and Elemental themselves.

Enhancements

- (GH#112) The `MolproHarness` has been updated to handle DFT and CCSD(T) energies and gradients.
- (GH#116) An environment context manager has been added to catch NumPy style parallelization with Python functions.
- (GH#117) MOPAC and DFTD3 can now accept an `extras` field which can pass around additional data, conforming to the rest of the Harnesses.
- (GH#119) Small visual improvements to the docs have been made.
- (GH#120) Lists inside models are now generally converted to numpy arrays for internal storage to maximize the benefit of the new Msgpack feature from Elemental.
- (GH#133) The GAMESS Harness now collects the CCSD as part of its output.

Bug Fixes

- (GH#127) Removed unused imports from the NWChem Harvester module.
- (GH#129) Missing type hints from the `MolproHarness` have been added.
- (GH#131) A code formatting redundancy in the GAMESS input file parser has been removed.

4.6.2 v0.8.2 / 2019-07-25

Bug Fixes

- (GH#114) Make compute and compute_procedure not have required kwargs while debugging a Fractal serialization issue. This is intended to be a temporary change and likely reverted in a later release

4.6.3 v0.8.1 / 2019-07-22

Enhancements

- (GH#110) Psi4's auto-retry exception handlers now catch more classes of random errors

Bug Fixes

- (GH#109) Geometric auto-retry settings now correctly propagate through the base code.

4.6.4 v0.8.0 / 2019-07-19

New Features

- (GH#95, GH#96, GH#97, and GH#98) The NWChem interface from QCDB has been added. Thanks to @vivacebelles and @jygrace for this addition!
- (GH#100) The MOPAC interface has now been added to QCEngine thanks help to from @godotalgorithm.

Enhancements

- (GH#94) The gradient and molecule parsed from a GAMESS calculation output file are now returned in `parse_output`
- (GH#101) Enabled extra files in TeraChem scratch folder to be requested by users, collected after program execution, and recorded in the `Result` object as extras.
- (GH#103) Random errors can now be retried a finite, controllable number of times (current default is zero retries). Geometry optimizations automatically set retries to 2. This only impacts errors which are categorized as `RandomError` by QCEngine and all other errors are raised as normal.

Bug Fixes

- (GH#99) QCEngine now manages an explicit folder for each Psi4 job to write into and passes the scratch directory via `-s` command line. This resolves a key mismatch which could cause an error.
- (GH#102) DFTD3 errors are now correctly returned as a `FailedOperation` instead of a raw `dict`.

4.6.5 v0.7.1 / 2019-06-18

Bug Fixes

- (GH#92) Added an `__init__.py` file to the `programs/tests` directory so they are correctly bundled with the package.

4.6.6 v0.7.0 / 2019-06-17

Breaking Changes

- (GH#85) The resource file `programs.dftd3.dashparam.py` has relocated and renamed to `programs.empirical_dispersion_resources.py`.
- (GH#89) Function `util.execute` forgot str argument `scratch_location` and learned `scratch_directory` in the same role of existing directory within which temporary directories are created and cleaned up. Non-user-facing function `util.scratch_directory` renamed to `util.temporary_directory`.

New Features

- (GH#60) WIP: QCEngine interface to GAMESS can run the program (after light editing of rungms) and parse selected output (HF, CC, FCI) into QCSchema.

- (GH#73) WIP: QCEngine interface to CFOUR can run the program and parse a variety of output into QCSchema.
- (GH#59, GH#71, GH#75, GH#76, GH#78, GH#88) Molpro improvements: Molpro can be run by QCEngine; and the input generator and output parser now supports CCSD energy and gradient calculations. Large thanks to @sjrl for many of the improvements
- (GH#69) Custom Exceptions have been added to QCEngine's returns which will make parsing and diagnosing them easier and more programmatic for codes which invoke QCEngine. Thanks to @dgasmith for implementation.
- (GH#82) QCEngine interface to entos can create input files (dft energy and gradients), run the program, and parse the output.
- (GH#85) MP2D interface switched to upstream repo (https://github.com/Chandemonium/MP2D v1.1) and now produces correct analytic gradients.

Enhancements

- (GH#62, GH#67, GH#83) A large block of TeraChem improvements thanks to @ffangliu contributions. Changed the input parser to call qcelemental to_string method with bohr unit, improved output of parser to turn stdout into Result, and modified how version is parsed.
- (GH#63) QCEngine functions `util.which`, `util.which_version`, `util.parse_version`, and `util.safe_version` removed after migrating to QCElemental.
- (GH#65) Torchani can now handle the ANI1-x and ANI1-ccx models. Credit to @dgasmith for implementation
- (GH#74) Removes caching and reduces pytorch overhead from Travis CI. Credit to @dgasmith for implementation
- (GH#77) Rename `ProgramExecutor` to `ProgramHarness` and `BaseProcedure` to `ProcedureHarness`.
- (GH#77) Function `util.execute(..., outfiles=[])` learned to collect output files matching a globbed filename.
- (GH#81) Function `util.execute` learned list argument `as_binary` to handle input or output files as binary rather than string.
- (GH#81) Function `util.execute` learned bool argument `scratch_exist_ok` to run in a preexisting directory. This is handy for stringing together execute calls.
- (GH#84) Function `util.execute` learned str argument `scratch_suffix` to identify temp dictionaries for debugging.
- (GH#90) DFTD3 now supports preliminary parameters for zero and Becke-Johnson damping to use with SAPT0-D

Bug Fixes

- (GH#80) Fix "psi4:qcvars" handling for older Psi4 versions.

4.6.7 v0.6.4 / 2019-03-21

Bug Fixes

- (GH#54) Psi4's Engine implementation now checks its key words in a case insensitive way to give the same value whether you called Psi4 or Engine to do the compute.
- (GH#55) Fixed an error handling routine in Engine to match Psi4.
- (GH#56) Complex inputs are now handled better through Psi4's wrapper which caused Engine to hang while trying to write to `stdout`.

4.6.8 v0.6.3 / 2019-03-15

New Features

- (GH#28) TeraChem is now a registered executor in Engine! Thanks to @ffangliu for implementing.
- (GH#46) MP2D is now a registered executor in Engine! Thanks to @loriab for implementing.

Enhancements

- (GH#46) `dftd3`'s workings received an overhaul. The `mol` keyword has been replaced with `dtype=2`, full Psi4 support is now provided, and an MP2D interface has been added.

Bug Fixes

- (GH#50 and GH#51) Executing Psi4 on a single node with multiprocessing is more stable because Psi4 temps are moved to scratch directories. This behavior is now better documented with an example as well.
- (GH#52) Psi4 calls are now executed through the `subprocess` module to prevent possible multiprocessing issues and memory leak after thousands of runs. A trade off is this adds about 0.5 seconds to task start-up, but its safe. A future Psi4 release will correct this issue and the change can be reverted.

4.6.9 v0.6.2 / 2019-03-07

Enhancements

- (GH#38 and GH#39) Documentation now pulls from the custom QC Archive Sphinx Theme, but can fall back to the standard RTD theme. This allows all docs across QCA to appear consistent with each other.
- (GH#43) Added a base model for all `Procedure` objects to derive from. This allows procedures' interactions with compute programs to be more unified. This PR also ensured GeomeTRIC provides Provenance information.

Bug Fixes

- (GH#40) This PR improved numerous back-end and testing quality of life aspects. Fixed `setup.py` to call `pytest` instead of `unittest` when running tests on install. Some conda packages for Travis-CI are cached to reduce the download time of the larger computation codes. Psi4 is now pinned to the 1.3 version to fix build-level pin of libint. Conda-build recipe removed to avoid possible confusion for everyone who isn't a Conda-Forge recipe maintainer. Tests now rely exclusively on the `conda env` setups.

4.6.10 v0.6.1 / 2019-02-20

Bug Fixes

- (GH#37) Fixed an issue where RDKit methods were not case agnostic.

4.6.11 v0.6.0 / 2019-02-28

Breaking Changes

- (GH#36) **breaking change** Model objects are returned by default rather than a dictionary.

New Features

- (GH#18) Add the `dftd3` program to available computers.
- (GH#29) Adds preliminary support for the `Molpro` compute engine.
- (GH#31) Moves all computation to `ProgramExecutor` to allow for a more flexible input generation, execution, output parsing interface.
- (GH#32) Adds a general `execute` process which safely runs subprocess jobs.

Enhancements

- (GH#33) Moves the `dftd3` executor to the new `ProgramExecutor` interface.
- (GH#34) Updates models to the more strict QCElemental v0.3.0 model classes.
- (GH#35) Updates CI to avoid pulling CUDA libraries for `torchani`.
- (GH#36) First pass at documentation.

4.6.12 v0.5.2 / 2019-02-13

Enhancements

- (GH#24) Improves load times dramatically by delaying imports and cpuutils.
- (GH#25) Code base linting.
- (GH#30) Ensures Psi4 output is already returned and Pydantic v0.20+ changes.

4.6.13 v0.5.1 / 2019-01-29

Enhancements

- (GH#22) Compute results are now returned as a dict of Python Primals which have been serialized-deserialized through Pydantic instead of returning un-processed Python objects or json-compatible string.

4.6.14 v0.5.0 / 2019-01-28

New Features

- (GH#8) Adds the TorchANI program for ANI-1 like energies and potentials.
- (GH#16) Adds QCElemental models based off QCSchema to QCEngine for both validation and object-based manipulation of input and output data.

Enhancements

- (GH#14) Migrates option to Pydantic objects for validation and creation.
- (GH#14) Introduces NodeDescriptor (for individual node description) and JobConfig (individual job configuration) objects.
- (GH#17) NodeDescriptor overhauled to work better with Parsl/Balsam/Dask/etc.

4.7 Development Guidelines

Core development guidelines go here.

PYTHON MODULE INDEX

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