QCEngine Documentation

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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
>>> """)

>>> model = qcel.models.AtomicInput(
>>>     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(model, "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:
  - adcc
  - Entos
  - Molpro
  - Psi4
  - Terachem
- Semi-Emperical:
  - MOPAC
  - xtb
- AI Potential:
  - TorchANI
- Molecular Mechanics:
  - RDKit
- Analytical Corrections:
  - DFTD3

In addition, several procedures are available:

- Geometry Optimization:
  - geomeTRIC
  - Pyberny

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

PROGRAM AND PROCEDURE INFORMATION

Available programs and procedures may be printed using the *CLI*:

```
>>> qcengine info
>> Version information
QCEngine version:    v0.11.0
QCElemental version: v0.11.0

>> Program information
Available programs:
mopac v2016
psi4 v1.3.2
rdkit v2019.03.4

Other supported programs:
cfour dftd3 entos gamess molpro mp2d nwchem terachem torchani
...
```

CHAPTER

FIVE

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Getting Started

- *Install QCEngine*

5.1 Install QCEngine

You can install qcengine with `conda` or with `pip`.

5.1.1 Conda

You can install qcengine using conda:

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

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

5.1.2 Pip

You can also install QCEngine using `pip`:

```
>>> pip install qcengine
```

5.1.3 Test the Installation

Note: QCEngine is a wrapper for other quantum chemistry codes. The tests for QCEngine will only test the wrapper for a given code if its detected in the `$PATH` or current Python Environment, otherwise the tests for that package are skipped. Keep this in mind if you see many `skip` or `s` codes output from PyTest.

You can test to make sure that Engine is installed correctly by first installing `pytest`.

From `conda`:

```
>>> conda install pytest -c conda-forge
```

From `pip`:

```
>>> pip install pytest
```

Then, run the following command:

```
>>> pytest --pyargs qcengine
```

5.1.4 Developing from Source

If you are a developer and want to make contributions Engine, you can access the source code from github.

User Interface

- *Single Compute*
- *Environment Detection*
- *Command Line Interface*

5.2 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.

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

5.2.2 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})
```

5.2.3 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
```

5.2.4 Input Fields

class qcelemental.models.**AtomicInput**(*, *id: str = None*, *schema_name: qcelemental.models.results.ConstrainedStrValue = 'qcschema_input'*, *schema_version: int = 1*, *molecule: qcelemental.models.molecule.Molecule*, *driver: qcelemental.models.common_models.DriverEnum*, *model: qcelemental.models.common_models.Model*, *keywords: Dict[str, Any] = {}*, *protocols: qcelemental.models.results.AtomicResultProtocols = AtomicResultProtocols(wavefunction=<WavefunctionProtocolEnum.none: 'none'>, stdout=True, error_correction=ErrorCorrectionProtocol(default_policy=True, policies=None), native_files=<NativeFilesProtocolEnum.none: 'none'>)*, *extras: Dict[str, Any] = {}*, *provenance: qcelemental.models.common_models.Provenance = None*)

The MolSSI Quantum Chemistry Schema

Parameters

- **id** (*str, Optional*) – The optional ID for the computation.
- **schema_name** (*ConstrainedStrValue, Default: qcschema_input*) – The QCSchema specification this model conforms to. Explicitly fixed as qcschema_input.
- **schema_version** (*int, Default: 1*) – The version number of `schema_name` to which this model conforms.
- **molecule** (`Molecule`) – The molecule to use in the computation.

- **driver** (*{energy,gradient,hessian,properties}*) – Allowed computation driver values.
- **model** (`Model`) – The computational molecular sciences model to run.
- **keywords** (*Dict[Any], Default: {}*) – The program-specific keywords to be used.
- **protocols** (`AtomicResultProtocols`, Optional) – Protocols regarding the manipulation of computational result data.
- **extras** (*Dict[Any], Default: {}*) – Additional information to bundle with the computation. Use for schema development and scratch space.
- **provenance** (`Provenance`, Optional) – Provenance information.

5.2.5 Returned Fields

class qcelemental.models.**AtomicResult**(**, id: str = None, schema_name: qcelemental.models.results.ConstrainedStrValue = 'qcschema_output', schema_version: int = 1, molecule: qcelemental.models.molecule.Molecule, driver: qcelemental.models.common_models.DriverEnum, model: qcelemental.models.common_models.Model, keywords: Dict[str, Any] = {}, protocols: qcelemental.models.results.AtomicResultProtocols = AtomicResultProtocols(wavefunction=<WavefunctionProtocolEnum.none: 'none'>, stdout=True, error_correction=ErrorCorrectionProtocol(default_policy=True, policies=None), native_files=<NativeFilesProtocolEnum.none: 'none'>), extras: Dict[str, Any] = {}, provenance: qcelemental.models.common_models.Provenance, properties: qcelemental.models.results.AtomicResultProperties, wavefunction: qcelemental.models.results.WavefunctionProperties = None, return_result: Union[float, qcelemental.models.types.Array, Dict[str, Any]], stdout: str = None, stderr: str = None, native_files: Dict[str, Any] = None, success: bool, error: qcelemental.models.common_models.ComputeError = None*)

Results from a CMS program execution.

Parameters

- **id** (*str, Optional*) – The optional ID for the computation.
- **schema_name** (*ConstrainedStrValue, Default: qcschema_output*) – The QCSchema specification this model conforms to. Explicitly fixed as qcschema_output.
- **schema_version** (*int, Default: 1*) – The version number of `schema_name` to which this model conforms.
- **molecule** (`Molecule`) – The molecule to use in the computation.
- **driver** (*{energy,gradient,hessian,properties}*) – Allowed computation driver values.
- **model** (`Model`) – The computational molecular sciences model to run.
- **keywords** (*Dict[Any], Default: {}*) – The program-specific keywords to be used.

- **protocols** (`AtomicResultProtocols`, Optional) – Protocols regarding the manipulation of computational result data.
- **extras** (*Dict[Any], Default: {}*) – Additional information to bundle with the computation. Use for schema development and scratch space.
- **provenance** (`Provenance`) – Provenance information.
- **properties** (`AtomicResultProperties`) –

  Named properties of quantum chemistry computations following the MolSSI QCSchema.

  All arrays are stored flat but must be reshapable into the dimensions in attribute `shape`, with abbreviations as follows:

  – nao: number of atomic orbitals = calcinfo_nbasis

  – nmo: number of molecular orbitals
- **wavefunction** (`WavefunctionProperties`, Optional) – Wavefunction properties resulting from a computation. Matrix quantities are stored in column-major order. Presence and contents configurable by protocol.
- **return_result** (*Union[float, Array, Dict[Any]]*) – The primary return specified by the `driver` field. Scalar if energy; array if gradient or hessian; dictionary with property keys if properties.
- **stdout** (*str, Optional*) – The primary logging output of the program, whether natively standard output or a file. Presence vs. absence (or null-ness?) configurable by protocol.
- **stderr** (*str, Optional*) – The standard error of the program execution.
- **native_files** (*Dict[Any], Optional*) – DSL files.
- **success** (*bool*) – The success of program execution. If False, other fields may be blank.
- **error** (`ComputeError`, Optional) – Complete description of the error from an unsuccessful program execution.

5.2.6 FAQ

1. Where is scratch so I can access the CMS code's files?

   The QCArchive philosophy is that you shouldn't go looking in scratch for CMS-code-written files since the scratch directory is deleted automatically by QCEngine and even if preserved may be subject to autodeletion if run from a cluster. Instead, QCEngine brings back the primary input and output and any ancillary files from which it can harvest results. Whether these are returned to the user in `AtomicResult` can be controlled through protocols in the input like `atomicinput.protocols.stdout = True` and eventually (https://github.com/MolSSI/QCElemental/pull/275) `atomicinput.protocols.native_files = "all"`.

   Nevertheless, you can, of course, access the scratch directory and CMS-code-written files. Pass an existing directory to the compute command (this directory will be parent) and tell it to not delete after the run: `qcng.compute(..., local_options={"scratch_directory": "/existing/parent/dir", "scratch_messy": True})`.

2. sdfs

5.3 Environment Detection

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

5.3.1 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>
```

5.3.2 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'>
```

5.3.3 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'
}
```

5.3.4 Configuration Files

The computational environment defaults can be overridden by configuration files.

Configuration files must be named `qcengine.yaml` and stored either in the directory from which you run QCEngine, a folder named `.qcarchive` in your home directory, or in a folder specified by the `DQM_CONFIG_PATH` environmental variable. Only one configuration file will be used if multiple are available. The `DQM_CONFIG_PATH` configuration file takes precedence over the current directory, which takes precedence over the `.qcarchive` folder.

The configuration file is a YAML file that contains a dictionary of different node configurations. The keys in the YAML file are human-friendly names for the configurations. The values are dictionaries that define configurations for different nodes, following the `NodeDescription` schema:

class qcengine.config.**NodeDescriptor**(*, *hostname_pattern: str*, *name: str*, *scratch_directory: str = None*, *memory: float = None*, *memory_safety_factor: int = 10*, *ncores: int = None*, *jobs_per_node: int = 2*, *retries: int = 0*, *is_batch_node: bool = False*, *mpiexec_command: str = None*)

Description of an individual node

When running QCEngine, the proper configuration for a node is determined based on the hostname of the node and matching the `hostname_pattern` to each of the configurations defined in `qcengine.yaml`.

An example `qcengine.yaml` file that sets the scratch directory for all nodes is as follows:

```
all:
  hostname_pattern: "*"
  scratch_directory: ./scratch
```

5.3.5 Cluster Configuration

A node configuration file is required when using node-parallel tasks on a compute cluster. The configuration file must contain a description of the command used to launch MPI tasks and, in some cases, the designation that a certain node is a compute node. See the descriptions for `mpiexec_command` and `is_batch_node` in the `NodeDescriptor` documentation for further details.

5.4 Command Line Interface

QCEngine provides a command line interface with three commands:

- `qcengine info` displays information about the environment detected by QCEngine.
- `qcengine run` runs a program.
- `qcengine run-procedure` runs a procedure.

5.4.1 Info Command

Command Invocation

```
qcengine info <options>
```

Command Description

This command prints information about the QCEngine environment.

Arguments

`category` The information categories to show. Choices include:

- `version`: Print version of QCEngine and QCElemental.
- `programs`: Print detected and supported programs.
- `procedures`: Print detected and supported procedures.
- `config`: Print host, compute, and job configuration
- `all`: Print all available information.

By default, all available information is printed.

5.4.2 Run Command

Command Invocation

```
qcengine run <program> <data>
```

Command Description

This command runs a program on a given task and outputs the result as a JSON blob.

Arguments

`program` The program to run.

`data` Data describing the task. One of:

- A JSON blob.
- A file name.
- '-', indicating data will be read from STDIN.

5.4.3 Run-Procedure Command

Command Invocation

```
qcengine run-procedure <program> <data>
```

Command Description

This command runs a procedure on a given task and outputs the result as a JSON blob.

Arguments

`procedure` The procedure to run.

`data` Data describing the task. One of:

- A JSON blob.
- A file name.
- '-', indicating data will be read from STDIN.

Programs

- *Program Overview*
- *Molecular Mechanics*

5.5 Program Overview

The general capabilities available through QCEngine for each program can be found below:

5.5.1 Quantum Chemistry

Program	Production	E	G	H	Properties	Wavefunction
adcc		✓			✓	
CFOUR		✓	✓		✓	
Qcore (Entos)		✓	✓	✓		✓
GAMESS		✓	✓		✓	
MRChem	✓	✓			✓	
Molpro	✓	✓	✓		✓	
NWChem		✓	✓	✓	✓	
Psi4	✓	✓	✓	✓	✓	✓
Q-Chem		✓	✓	✓		
Terachem		✓	✓			
Terachem PBS		✓	✓			
Turbomole		✓	✓			

5.5.2 Semi-Empirical

Program	Production	E	G	H	Properties	Wavefunction
MOPAC	✓	✓	✓		✓	
xtb		✓	✓		✓	

5.5.3 AI Potential

Program	Production	E	G	H	Properties
TorchANI	✓	✓	✓		✓

5.5.4 Molecular Mechanics

Program	Production	E	G	H	Properties
OpenMM		✓	✓		✓
RDKit	✓	✓	✓		✓

5.5.5 Analytical Corrections

Program	Production	E	G	H	Properties
DFTD3	✓	✓	✓		
DFTD4	✓	✓	✓		
gCP		✓	✓		

5.6 Semiempirical Quantum Mechanics

For semiempirical quantum mechanics (SQM) engines to fit the AtomicInput/Result schema the following convention is used:

- Method: The unique method name (PM7 or GFN2-xTB) including the parametrisation information is provided, no basis is needed

As for quantum mechanical methods a minimal Molecule object is sufficient as input.

Note: Semiemprical engines might not handle the concept of ghost atoms correctly, check carefully how the used engine handles ghost atoms. To be sure remove ghost atoms from input to semiempirical engines beforehand.

5.6.1 Example

For example, running a calculation with the GFN2-xTB method using the `xtb` engine would work like any other QM engine with

```
>>> import qcelemental as qcel
>>> mol = qcel.models.Molecule(
...     symbols=["O", "H", "H"],
...     geometry=[
...         [ 0.00000000000000, 0.00000000000000,-0.73578586109551],
...         [ 1.44183152868459, 0.00000000000000, 0.36789293054775],
...         [-1.44183152868459, 0.00000000000000, 0.36789293054775],
...     ],
... )
...
>>> model = qcel.models.AtomicInput(
...     molecule=mol,
...     driver="energy",
...     model={"method": "GFN2-xTB"},
... )
...
>>> import qcengine as qcng
>>> ret = qcng.compute(model, "xtb")
>>> ret.return_result
-5.070451354836705
```

5.6.2 MOPAC

The following semiempirical Hamiltonians are supported with the MOPAC engine.

Method	Basis
mndo	None
am1	None
pm3	None
rm1	None
mndod	None
pm6	None
pm6-d3	None
pm6-dh+	None
pm6-dh2	None
pm6-dh2x	None
pm6-d3h4	None
pm6-3dh4x	None
pm7	None
pm7-ts	None

5.6.3 xtb

The following extended tight binding Hamiltonians are available with the `xtb` engine.

Method	Basis	Reference
GFN2-xTB	None	10.1021/acs.jctc.8b01176
GFN1-xTB	None	10.1021/acs.jctc.7b00118
GFN0-xTB	None	10.26434/chemrxiv.8326202.v1

5.7 Molecular Mechanics

For Molecular Mechanics (MM) engines to fit the AtomicInput/Result schema the following convention is used:

- Method: The force field used such as MMFF94, GAFF, OpenFF-1.0.0.
- Basis: The typing engine used to find the required paramters.

For all MM computations the input Molecule object must have connectivity and this will not be automatically assigned for you.

5.7.1 Example

```
>>> mol = qcel.models.Molecule(
>>>     symbols=["O", "H", "H"],
>>>     geometry=[[0, 0, 0], [0, 0, 2], [0, 2, 0]],
>>>     connectivity=[[0, 1, 1], [0, 2, 1]],
>>> )

>>> model = qcel.models.AtomicInput(
>>>     molecule=mol,
>>>     driver="energy",
>>>     model={"method": "openff-1.0.0", "basis": "smirnoff"},
>>> )
>>> ret = qcng.compute(model, "openmm")
>>> ret.return_result
0.011185654397410195
```

5.7.2 OpenMM

Currently OpenMM only supports the smirnoff typing engine from the `openff-toolkit`. Currently available force fields are the following:

Method	Basis
smirnoff99Frosst-1.1.0	smirnoff
openff-1.0.0	smirnoff
openff_unconstrained-1.0.0	smirnoff

Other forcefields may be available depending on your version of the `openff-toolkit`, see their docs for more information.

5.7.3 RDKit

RDKit force fields currently do not require a typing engine and the basis is omitted in all computations. Currently available force fields are the following:

Method	Basis
UFF	None
MMFF94	None
MMFF94s	None

5.7.4 xtb

Experimental access to force fields are available with the `xtb` engine. Note that the `xtb` engine will not require nor use a topology information provided in the input schema.

Method	Basis	Reference
GFN-FF	None	10.1002/anie.202004239

Developer Documentation

- *QCEngine API*
- *Changelog*

5.8 QCEngine API

5.8.1 qcengine Package

Base file for the dqm_compute module.

Functions

compute(input_data, program[, raise_error, ...])	Executes a single CMS program given a QCSchema input.
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], qcelemental.models.results.AtomicInput]*, *program: str*, *raise_error: bool = False*, *local_options: Optional[Dict[str, Any]] = None*, *return_dict: bool = False*) → qcelemental.models.results.AtomicResult

Executes a single CMS program given a QCSchema input.

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

Parameters

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

Returns A computed AtomicResult 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", "berny"}*) – 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.AtomicInput

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

Return type dict, OptimizationResult, FailedOperation

get_config

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

Classes

MDIServer(mdi_options, program, molecule, ...)	

MDIServer

class qcengine.**MDIServer**(*mdi_options: str*, *program: str*, *molecule*, *model*, *keywords*, *raise_error: bool = False*, *local_options: Optional[Dict[str, Any]] = None*)
Bases: object

Methods Summary

recv_coords([coords])	Receive a set of nuclear coordinates through MDI and assign them to the atoms in the current molecule
recv_elements([elements])	Receive a set of atomic numbers through MDI and assign them to the atoms in the current molecule
recv_masses([masses])	Receive a set of nuclear masses through MDI and assign them to the atoms in the current molecule
recv_multiplicity([multiplicity])	Receive the electronic multiplicity through MDI
recv_total_charge([charge])	Receive the total system charge through MDI
run_energy()	Run an energy calculation
send_coords()	Send the nuclear coordinates through MDI
send_elements()	Send the atomic number of each nucleus through MDI
send_energy()	Send the total energy through MDI
send_forces()	Send the nuclear forces through MDI
send_masses()	Send the nuclear masses through MDI
send_multiplicity()	Send the electronic multiplicity through MDI
send_natoms()	Send the number of atoms through MDI
send_node()	Send the name of the current node through MDI

continues on next page

Table 3 – continued from previous page

send_total_charge()	Send the total system charge through MDI
start()	Receive commands through MDI and respond to them as defined by the MDI Standard
stop()	Stop listening for MDI commands
update_molecule(key, value)	Update the molecule

Methods Documentation

recv_coords(*coords: Optional[numpy.ndarray] = None*) → None
Receive a set of nuclear coordinates through MDI and assign them to the atoms in the current molecule

Parameters **coords** (*np.ndarray, optional*) – New nuclear coordinates. If None, receive through MDI.

recv_elements(*elements: Optional[List[int]] = None*)
Receive a set of atomic numbers through MDI and assign them to the atoms in the current molecule

Parameters **elements** (`list` of `int`, optional) – New element numbers. If None, receive through MDI.

recv_masses(*masses: Optional[List[float]] = None*) → None
Receive a set of nuclear masses through MDI and assign them to the atoms in the current molecule

Parameters **masses** (`list` of `float`, optional) – New nuclear masses. If None, receive through MDI.

recv_multiplicity(*multiplicity: Optional[int] = None*) → None
Receive the electronic multiplicity through MDI

Parameters **multiplicity** (*int, optional*) – New multiplicity of the system. If None, receive through MDI.

recv_total_charge(*charge: Optional[float] = None*) → None
Receive the total system charge through MDI

Parameters **charge** (*float, optional*) – New charge of the system. If None, receive through MDI.

run_energy() → None
Run an energy calculation

send_coords() → numpy.ndarray
Send the nuclear coordinates through MDI

Returns **coords** – Nuclear coordinates

Return type np.ndarray

send_elements()
Send the atomic number of each nucleus through MDI

Returns **elements** – Element of each atom

Return type `list` of `int`

send_energy() → float
Send the total energy through MDI

Returns **energy** – Energy of the system

Return type float

send_forces() → numpy.ndarray
Send the nuclear forces through MDI

Returns **forces** – Forces on the nuclei

Return type np.ndarray

send_masses() → numpy.ndarray
Send the nuclear masses through MDI

Returns **masses** – Atomic masses

Return type np.ndarray

send_multiplicity() → int
Send the electronic multiplicity through MDI

Returns **multiplicity** – Multiplicity of the system

Return type int

send_natoms() → int
Send the number of atoms through MDI

Returns **natom** – Number of atoms

Return type int

send_node() → str
Send the name of the current node through MDI

Returns **node** – Name of the current node

Return type str

send_total_charge() → float
Send the total system charge through MDI

Returns **charge** – Total charge of the system

Return type float

start() → None
Receive commands through MDI and respond to them as defined by the MDI Standard

stop() → None
Stop listening for MDI commands

update_molecule(*key: str*, *value*)
Update the molecule

Parameters

- **key** (*str*) – Key of the molecular element to update
- **value** – Update value

Class Inheritance Diagram

5.8.2 qcengine.compute Module

Integrates the computes together

Functions

compute(input_data, program[, raise_error, ...])	Executes a single CMS program given a QCSchema 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], qcelemental.models.results.AtomicInput]*, *program: str*, *raise_error: bool = False*, *local_options: Optional[Dict[str, Any]] = None*, *return_dict: bool = False*) → qcelemental.models.results.AtomicResult

Executes a single CMS program given a QCSchema input.

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

Parameters

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

Returns A computed AtomicResult 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", "berny"}*) – 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.AtomicInput

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

Return type dict, OptimizationResult, FailedOperation

5.8.3 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: Optional[Dict[str, Any]] = None*) → qcengine.config.TaskConfig

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(*, hostname_pattern, name, ...)	Description of an individual node

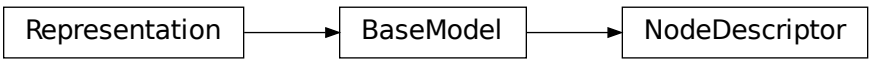
NodeDescriptor

class qcengine.config.**NodeDescriptor**(*, *hostname_pattern: str*, *name: str*, *scratch_directory: str = None*, *memory: float = None*, *memory_safety_factor: int = 10*, *ncores: int = None*, *jobs_per_node: int = 2*, *retries: int = 0*, *is_batch_node: bool = False*, *mpiexec_command: str = None*)

Bases: pydantic.main.BaseModel

Description of an individual node

Class Inheritance Diagram



5.8.4 qcengine.util Module

Several import utilities

Functions

compute_wrapper([capture_output, raise_error])	Wraps compute for timing, output capturing, and raise protection
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.
create_mpi_invocation(executable, task_config)	Create the launch command for an MPI-parallel task
execute(command[, infiles, outfiles, ...])	Runs a process in the background until complete.

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

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.AtomicResult

create_mpi_invocation

qcengine.util.**create_mpi_invocation**(*executable: str*, *task_config: qcengine.config.TaskConfig*) → List[str]

Create the launch command for an MPI-parallel task

Parameters

- **executable** (*str*) – Path to executable
- **task_config** (*TaskConfig*) – Specification for number of nodes, cores per node, etc.

execute

qcengine.util.**execute**(*command: List[str]*, *infiles: Optional[Dict[str, str]] = None*, *outfiles: Optional[List[str]] = None*, ***, *as_binary: Optional[List[str]] = None*, *scratch_name: Optional[str] = None*, *scratch_directory: Optional[str] = None*, *scratch_suffix: Optional[str] = None*, *scratch_messy: bool = False*, *scratch_exist_ok: bool = False*, *blocking_files: Optional[List[str]] = None*, *timeout: Optional[int] = None*, *interupt_after: Optional[int] = None*, *environment: Optional[Dict[str, str]] = None*, *shell: Optional[bool] = False*, *exit_code: Optional[int] = 0*) → Tuple[bool, Dict[str, Any]]

Runs a process in the background until complete.

Returns True if exit code <= exit_code (default 0)

Parameters

- **command** (*list of str*)
- **infiles** (*Dict[str] = str*) – Input file names (names, not full paths) and contents. to be written in scratch dir. May be {}.
- **outfiles** (*List[str] = None*) – Output file names to be collected after execution into values. May be {}.
- **as_binary** (*List[str] = None*) – Keys of *infiles* or *outfiles* to be treated as bytes.
- **scratch_name** (*str, optional*) – Passed to temporary_directory
- **scratch_directory** (*str, optional*) – Passed to temporary_directory
- **scratch_suffix** (*str, optional*) – Passed to temporary_directory
- **scratch_messy** (*bool, optional*) – Passed to temporary_directory
- **scratch_exist_ok** (*bool, optional*) – Passed to temporary_directory
- **blocking_files** (*list, optional*) – Files which should stop execution if present beforehand.
- **timeout** (*int, optional*) – Stop the process after n seconds.
- **interupt_after** (*int, optional*) – Interupt the process (not hard kill) after n seconds.
- **environment** (*dict, optional*) – The environment to run in
- **shell** (*bool, optional*) – Run command through the shell.
- **exit_code** (*int, optional*) – The exit code above which the process is considered failure.

Raises **FileExistsError** – If any file in *blocking* is present

Examples

execute multiple commands in same dir >>> success, dexe = qcng.util.execute(['command_1'], infiles, [], scratch_messy=True) >>> success, dexe = qcng.util.execute(['command_2'], {}, outfiles, scratch_messy=False, scratch_name=Path(dexe['scratch_directory']).name, scratch_exist_ok=True)

5.8.5 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(*, name, scratch, ...)	

ProgramHarness

class qcengine.programs.**ProgramHarness**(*, *name: str*, *scratch: bool*, *thread_safe: bool*, *thread_parallel: bool*, *node_parallel: bool*, *managed_memory: bool*, *extras: Dict[str, Any] = None*)
Bases: pydantic.main.BaseModel, abc.ABC

Methods Summary

build_input(input_model, config[, template])	
compute(input_data, config)	
execute(inputs[, extra_outfiles, ...])	
found([raise_error])	Checks if the program can be found.
get_version()	Finds program, extracts version, returns normalized version string.
parse_output(outfiles, input_model)	

Methods Documentation

build_input(*input_model: AtomicInput*, *config: TaskConfig*, *template: Optional[str] = None*) → Dict[str, Any]

abstract compute(*input_data: AtomicInput*, *config: TaskConfig*) → AtomicResult

execute(*inputs: Dict[str, Any]*, *extra_outfiles: Optional[List[str]] = None*, *extra_commands: Optional[List[str]] = None*, *scratch_name: Optional[str] = None*, *timeout: Optional[int] = None*) → Tuple[bool, Dict[str, Any]]

abstract static found(*raise_error: bool = False*) → bool
Checks if the program can be found.

Parameters **raise_error** (*bool, optional*) – If True, raises an error if the program cannot be found.

Returns Returns True if the program was found, False otherwise.

Return type bool

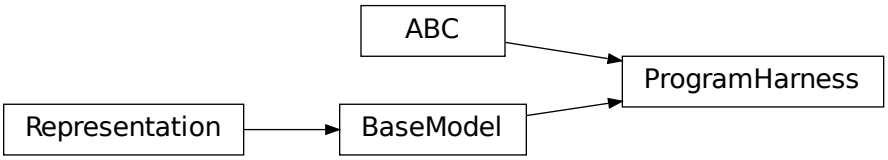
get_version() → str
Finds program, extracts version, returns normalized version string.

Returns Return a valid, safe python version string.

Return type str

parse_output(*outfiles: Dict[str, str]*, *input_model: qcelemental.models.results.AtomicInput*) → qcelemental.models.results.AtomicResult

Class Inheritance Diagram



5.9 Changelog

5.9.1 v0.23.0 / 2022-03-10

Enhancements

- (GH#351) Torsiondrive procedure refactored to make it easier for users to implement a parallel version via subclassing and overwriting the *_spawn_optimizations* method. @jthorton

5.9.2 v0.22.0 / 2022-01-25

Bug Fixes

- (GH#338) Correctly export version to tarballs created by git-archive. @mbanck, @loriab
- (GH#339) QCEngine now tolerant of *cpuinfo* failure to populate *brand_raw*, *brand*. @dotsdl, @loriab, @WardLT

5.9.3 v0.21.0 / 2021-11-22

Enhancements

- (GH#321) CFOUR, GAMESS, NWChem, Psi4, DFTD3, MP2D, gCP - learned to return certain native text files under control of the `native_files` protocol. GAMESS users are strongly advised to at least set `protocols.native_files = "input"` so that the job is reproducible. @loriab
- (GH#325) Torsiondrive - learned to use multiple molecules as input to torsiondrives. @jthorton
- (GH#327) TorchANI - learned to use GPUs if available. @kexul
- (GH#330, GH#332) NWChem - learned to restart from existing scratch if QCEngine is killed. @WardLT

5.9.4 v0.20.1 / 2021-10-08

Bug Fixes

- (GH#322) Psi4 - allowed more test cases with gradients and Hessians after a compatibility PR started saving them. @loriab
- (GH#323) Turbomole - learned to store calcinfo_natom so that gradients and Hessians can be computed after QCElemental started using that quantity for shape checking in [v0.22.0](https://github.com/MolSSI/QCElemental/blob/master/docs/source/changelog.rst#0220–2021-08-26) @eljost

5.9.5 v0.20.0 / 2021-10-01

New Features

- (GH#305) TorsionDrive - new procedure to automate constrained optimizations along a geometry grid. Akin to the longstanding QCFractal TorsionDrive service. @SimonBoothroyd

Enhancements

- (GH#307) NWChem - learns to automatically increase the number of iterations when SCF, CC, etc. fails to converge. @WardLT
- (GH#309) `qcengine info` learned to print the location of found CMS programs, and geometric, OpenMM, and RDKit learned to return their versions. @loriab
- (GH#311) CFOUR, GAMESS, NWChem harnesses learned to notice which internal module performs a calc (e.g., tce/cc for NWChem) and to store it in `AtomicResult.provenance.module`. Psi4 already does this. @loriab
- (GH#312) CFOUR, GAMESS, NWChem harnesses learned to run and harvest several new methods in the MP, CC, CI, DFT families. @loriab
- (GH#316) Config - `TaskConfig` learned a new field `scratch_messy` to instruct a `qcng.compute()` run to not clean up the scratch directory at the end. @loriab
- (GH#316) GAMESS - harness learned to obey ncores and scratch_messy local_config options. When `ncores > 1`, the memory option is partitioned into replicated and non after exetyp=check trials. @loriab
- (GH#316) Psi4 - harness learned to obey scratch_messy and memory local_config options. Memory was previously off by a little (GB vs GiB). @loriab

- (GH#316) CFOUR - harness learned to obey scratch_messy and memory local_config options. Memory was previously off by a little. @loriab
- (GH#316) NWChem - harness learned to obey scratch_messy and memory local_config options. Memory was previously very off for v7. @loriab
- (GH#315) CFOUR, GAMESS, NWChem – learned to return in AtomicInput or program native orientation depending on fix_com & fix_orientation= T or F. Psi4 already did this. Previously these three always returned AtomicInput orientation. Note that when returning program native orientation, the molecule is overwritten, so AtomicResult is not a superset of AtomicInput. @loriab
- (GH#315) CFOUR, GAMESS, NWChem – learned to harvest gradients and Hessians. @loriab
- (GH#317) Docs - start "new harness" docs, so contributors have a coarse roadmap. @loriab
- (GH#318) Docs - documentation is now served from https://molssi.github.io/QCEngine/ and built by https://github.com/MolSSI/QCEngine/blob/master/.github/workflows/CI.yml . https://qcengine.readthedocs.io/en/latest/ will soon be retired. @loriab
- (GH#320) CFOUR, NWChem – learned to run with ghost atoms, tentatively. @loriab

Bug Fixes

- (GH#313, GH#319) OpenMM - accommocate both old and new simtk/openmm import patterns. @dotsdl

5.9.6 v0.19.0 / 2021-05-16

New Features

- (GH#290) MCTC-GCP - harness for new implementation of gCP, *mctc-gcp*, whose cmdline interface is drop-in replacement. @loriab
- (GH#291) DFTD4 - new harness for standalone DFT-D4 executable. @awvwgk
- (GH#289) TeraChem - new harness for TeraChem Protocol Buffer Server mode. @coltonbh

Enhancements

- (GH#288) GAMESS, Cfour, NWChem - add calcinfo harvesting, HF and MP2 gradient harvesting. @loriab

Bug Fixes

- (GH#288) Avert running model.basis = BasisSet schema even though they validate. @loriab
- (GH#294) NWChem - fixed bug where was retrieving only the first step in a geometry relaxation with line-search off. @WardLT
- (GH#297) MDI - Update interface for v1.2. @loriab

5.9.7 v0.18.0 / 2021-02-16

New Features

- (GH#206) OptKing - new procedure harness for OptKing optimizer. @AlexHeide
- (GH#269) MRChem - new multiresolution chemistry program harness. @robertodr
- (GH#277) ADCC - new program harness for ADC-connect. (Requires Psi4 for SCF.) @maxscheurer
- (GH#278) gCP - new program harness for geometric counterpoise. @hokru
- (GH#280) Add framework to register identifying known outfile errors, modify input schema, and rerun. @WardLT
- (GH#281) NWChem - new procedure harness to use NWChem's DRIVER geometry optimizer with NWChem's program harness gradients. @WardLT
- (GH#282) DFTD3 - added D3m and D3m(bj) parameters for SAPT0/HF. Allow pairwise analysis to be returned. @jeffschriber

Enhancements

- (GH#274) Entos/Qcore - renamed harness and updated to new Python bindings. @dgasmith
- (GH#283) OpenMM - transition harness from *openforcefield* packages on omnia channel to *openff.toolkit* packages on conda-forge channel. @SimonBoothroyd
- (GH#286, GH#287) CI - moves from Travis-CI to GHA for open-source testing. @loriab

Bug Fixes

- (GH#273) TeraChem - fixed bug of missing method field. @stvogt

5.9.8 v0.17.0 / 2020-10-02

New Features

- (GH#262) Add project authors information. @loriab

Enhancements

- (GH#264) Turbomole - add analytic and finite difference Hessians. @eljost
- (GH#266) Psi4- error messages from Psi4Harness no longer swallowed by *KeyError*. @dotsdl

Bug Fixes

- (GH#264) Turbomole - fix output properties handling. @eljost
- (GH#265) xtb - ensure extra tags are preserved in XTB harness. @WardLT
- (GH#270) TorchANI - now lazily loads models as requested for compute. @dotsdl

5.9.9 v0.16.0 / 2020-08-19

New Features

Enhancements

- (GH#241) NWChem - improved performance by turning on `atoms_map=True`, which does seem to be true. @WardLT
- (GH#257) TorchANI - learned the ANI2x model and to work with v2. @farhadrgh
- (GH#259) Added MP2.5 & MP3 energies and HF, MP2.5, MP3, LCCD gradients reference data to stdsuite. @loriab
- (GH#261) Q-Chem - learned to return more informative Provenance, learned to work with v5.1. @loriab
- (GH#263) NWChem - learned how to turn off automatic Z-Matrix coordinates with `geometry__noautoz = True`. @WardLT

Bug Fixes

- (GH#261) Molpro - learned to error cleanly if version too old for XML parsing. @loriab
- (GH#261) Q-Chem - learned to extract version from output file instead of `qchem -h` since command isn't available from a source install. @loriab

5.9.10 v0.15.0 / 2020-06-26

New Features

- (GH#232) PyBerny - new geometry optimizer procedure harness. @jhrmnn
- (GH#238) Set up testing infrastructure, "stdsuite", where method reference values and expected results names (e.g., total energy and correlation energy from MP2) are stored here in QCEngine but may be used from anywhere (presently, Psi4). Earlier MP2 and CCSD tests here converted to new scheme, removing `test_standard_suite_mp2.py` and `ccsd`.
- (GH#249, GH#254) XTB - new harness for xtb-python that natively speaks QCSchema. @awvwgk

Enhancements

- (GH#230) NWChem - improved dipole, HOMO, LUMO harvesting.
- (GH#233) `qcng.util.execute` learned argument `exit_code` above which to fail, rather than just `!= 0`.
- (GH#234) MDI - harness updated to support release verion v1.0.0 .
- (GH#238) Cfour, GAMESS, NWChem – harnesses updated to collect available spin components for MP2 and CCSD. Also updated to set appropriate `qcel.models.AtomicProperties` from collected QCVariables.
- (GH#239) OpenMM - OpenMM harness now looks for cmiles information in the molecule extras field when typing. Also we allow for the use of gaff forcefields. @jthorton
- (GH#243) NWChem - more useful stdout error return.
- (GH#244) Added CCSD(T), LCCD, and LCCSD reference data to stdsuite. @loriab
- (GH#246) TorchANI - harness does not support v2 releases.
- (GH#251) DFTD3 - added D3(0) and D3(BJ) parameters for PBE0-DH functional.

Bug Fixes

- (GH#244) Psi4 - fixed bug in `extras["psiapi"] == True` mode where if calc failed, error not handled by QCEngine. @loriab
- (GH#245) Added missing import to sys for `test_standard_suite.py`. @sjrl
- (GH#248) NWChem - fix HFexch specification bug.
- Psi4 – QCFractal INCOMPLETE state bug https://github.com/MolSSI/QCEngine/issues/250 fixed by https://github.com/psi4/psi4/pull/1933 .
- (GH#253) Make compatible with both py-cpuinfo 5 & 6, fixing issue 252.

5.9.11 v0.14.0 / 2020-02-06

New Features

- (GH#212) NWChem - Adds CI for the NWChem harness.
- (GH#226) OpenMM - Moves the OpenMM harness to a canonical forcefield based method/basis language combination.
- (GH#228) RDKit - Adds MMFF94 force field capabilities.

Enhancements

- (GH#201) Psi4 - `psi4 --version` collection to only grab the last line.
- (GH#202) Entos - Adds wavefunction parsing.
- (GH#203) NWChem - Parses DFT empirical dispersion energy.
- (GH#204) NWChem - Allows custom DFT functionals to be run.
- (GH#205) NWChem - Improved gradient output and added Hessian support for NWChem.
- (GH#215) Psi4 - if Psi4 location can be found by either PATH or PYTHONPATH, harness sets up both subprocesses and API execution.

- (GH#215) `get_program` shows the helpful "install this" messages from `found()` rather than just saying "cannot be found".

Bug Fixes

- (GH#199) Fix typo breaking NWChem property parsing.
- (GH#215) NWChem complains *before* a calculation if the necessary `networkx` package not available.
- (GH#207) NWChem - Minor bug fixes for NWChem when more than core per MPI rank is used.
- (GH#209) NWChem - Fixed missing extras tags in NWChem harness.

5.9.12 v0.13.0 / 2019-12-10

New Features

- (GH#151) Adds a OpenMM Harness for evaluation of SMIRNOFF force fields.
- (GH#189) General MPI support and MPI CLI generator.

Enhancements

- (GH#175) Allows specifications for `nnodes` to begin MPI support.
- (GH#177) NWChem - Parsing updates including Hessian abilities.
- (GH#180) GAMESS - Output properties improvements.
- (GH#181) NWChem - Output properties improvements.
- (GH#183) Entos - Hessian and XTB support.
- (GH#185) Entos - Improved subcommand support.
- (GH#187) QChem - Support for raw log files without the binary file requirements and improved output properties support.
- (GH#188) Automatic buffer reads to prevent deadlocking of process for very large outputs.
- (GH#194) DFTD3 - Improved error message on failed evaluations.
- (GH#195) Blackens the code base add GHA-based lint checks.

Bug Fixes

- (GH#179) QChem - fixes print issue when driver is of an incorrect value.
- (GH#190) Psi4 - fixes issues for methods without basis sets such as HF-3c.

5.9.13 v0.12.0 / 2019-11-13

New Features

- (GH#159) Adds MolSSI Driver Interface support.
- (GH#160) Adds Turbomole support.
- (GH#164) Adds Q-Chem support.

Enhancements

- (GH#155) Support for Psi4 Wavefunctions using v1.4a2 or greater.
- (GH#162) Adds test for geometry optimization with trajectory protocol truncation.
- (GH#167) CFOUR and NWChem parsing improvements for CCSD(T) properties.
- (GH#168) Standardizes on `dispatch.out` for the common output files.
- (GH#170) Increases coverage and begins a common documentation page.
- (GH#171) Add Molpro to the standard suite.
- (GH#172) Models renamed according to https://github.com/MolSSI/QCElemental/issues/155, particularly `ResultInput -> AtomicInput`, `Result -> AtomicResult`, `Optimization -> OptimizationResult`.

Bug Fixes

5.9.14 v0.11.0 / 2019-10-01

New Features

- (GH#162) Adds a test to take advantage of Elemental's Protocols. Although this PR does not technically change anything in Engine, bumping the minor version here allows upstream programs to note when this feature was available because the minimum version dependency on Elemental has been bumped as well.

Enhancements

- (GH#143) Updates to Entos and Molpro to allow Entos to execute functions from the Molpro Harness. Also helps the two drivers to conform to GH#86.
- (GH#145, GH#148) Initial CLI tests have been added to help further ensure Engine is running proper.
- (GH#149) The GAMESS Harness has been improved by adding testing.
- (GH#150, GH#153) TorchANI has been improved by adding a Hessian driver to it and additional information is returned in the `extra` field when `energy` is the driver. This also bumped the minimum version of TorchANI Engine supports from 0.5 to 0.9.
- (GH#154) Molpro's harness has been improved to support `callinfo_X` properties, unrestricted HF and DFT calculations, and the initial support for parsing local correlation calculations.
- (GH#158) Entos' output parsing has been improved to read the json dictionary produced by the program directly. Also updates the input file generation.
- (GH#161) Updates MOPAC to have more sensible quantum-chemistry like keywords by default.

Bug Fixes

- (GH#156) Fixed a compatibility bug in specific version of Intel-OpenMP by skipping version 2019.5-281.
- (GH#161) Improved error handling in MOPAC if the execution was incorrect.

5.9.15 v0.10.0 / 2019-08-25

New Features

- (GH#132) Expands CLI for `info`, `run`, and `run-procedure` options.
- (GH#137) A new CI pipeline through Azure has been developed which uses custom, private Docker images to house non-public code which will enable us to test Engine through integrated CI on these codes securely.
- (GH#140) GAMESS, CFOUR, NWChem preliminary implementations.

Enhancements

- (GH#138) Documentation on Azure triggers.
- (GH#139) Overhauls install documentation and clearly defines dev install vs production installs.

5.9.16 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.

5.9.17 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

5.9.18 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.

5.9.19 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`.

5.9.20 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.

5.9.21 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.

5.9.22 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`.

5.9.23 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.

5.9.24 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.

5.9.25 v0.6.1 / 2019-02-20

Bug Fixes

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

5.9.26 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.

5.9.27 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.

5.9.28 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.

5.9.29 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.

5.10 Adding a New Program Harness

Program harnesses are for community CMS codes that can independently (or with a SCF bootstrap) compute single-point energies, derivatives, or properties or components thereof (e.g., dispersion corrections).

A single CMS code generally has one program harness. However, if there are drastically different ways of running a code (e.g., TeraChem text input file and TeraChem PBS), separate harnesses may be created. Also, if there are specialty capabilites not fitting into "single-point energies . . . " (e.g., GAMESS makefp task), an additional *procedure* harness may be created.

This guide is a coarse path through adding a new program harness.

1. Open up communication with the QCEngine maintainers. Post an issue to GitHub and join the Slack channel (link off GH README) so you can get advice.

1. Copy a similar harness. Choose a program that your code behaves roughly like (mostly consider parsed vs. API access) and copy that harness, renaming it as your own and commenting out all but the structure. Search for the (copied) harness name to register it.

1. Fill in the `_defaults` section with program name and characteristics.

1. Fill in the `def found` function using `which` and `which_import` from QCElemental. See NWChem and OpenMM for examples of handling additional dependencies.

1. If your code's version can be extracted short of parsing an output file, fill in `def get_version` next. After this, `> qcengine info` should show your code (provided it's in path).

1. To get a string output of QCSchema Molecule in your code's format, you may need to add a `dtype` at `qcelemental/molparse/to_string.py`.

1. If your code's of the common translate-QCSchema-to-input, run, translate-output-to-QCSchema variety, next work on the `def execute` function. This is fairly simple because it calls the powerful qcengine.util.execute to handle scratch, timeout, file writing and collection, etc. The harness function needs the names of input files (hard-code a string for now), the execution command, and the names of any scratch files to return for processing. Once ready, fill in `def get_version` if not done above.

1. Now fill in the short `def compute` entirely and `def build_input` and `def parse_output` skeletally. Set up a simple molecule-and-model `AtomicInput` dictionary and run it with `qcng.compute(atomicinput, "yourcode")` to get something to iterate on.

1. Fill in `def build_input` to form your code's usual input format from the fields of `AtomicInput`.

1. Fill in `def parse_output` to take results and put them into `AtomicResult`. Most important is the `return_result` field. `AtomicResultProperties` can be populated when convenient. `WavefunctionProperties` is great but save for a later pass.

1. At this point your harness can correctly run one or more QCSchema inputs of your devising. Time to put it through paces. Register your code in `_programs` in `testing.py`. Most tests will then need a `@using("yourcode")` decorator so that they don't run (and fail the test suite) when your code isn't available.

1. Add basic tests to qcengine/tests/test_harness_canonical.py * def test_compute_energy(program, model, keywords): * def test_compute_gradient(program, model, keywords): * def test_compute_energy_qcsk_basis(program, model, keywords):

1. Add basic failure tests to qcengine/tests/test_harness_canonical.py * def test_compute_bad_models(program, model):

1. Add tests for the runtime config and to qcengine/programs/tests/test_canonical_config.py

1. For QM codes, consider adding lines to the qcengine/programs/tests/test_standard_suite.py to check energies, gradients, and Hessians against other codes.

1. For codes that can produce a Hartree–Fock, add lines to the qcengine/program/tests/test_alignment.py to check molecular and properties orientation handling.

1. If your code is available as a visible binary (e.g., pip, conda, docker download with no or trivial build), create a testing lane by adding to `devtools/conda-envs/` and `.github/workflows/CI.yml`. This will check your code for every PR. We're looking into private testing for codes that aren't available.

1. Throughout, talk with the maintainers with questions. Error handling, especially, is intricate.

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