Submit ORCA jobs (osub)

Overview

osub is a command-line tool that simplifies job submission for the quantum chemistry software ORCA.
You can submit a job by simply providing an input file.

Supported ORCA Versions

4.2.1, 5.0.3, 5.0.4, 6.0.1, 6.1.0, 6.1.1 (Default: 6.1.0)

- Version 6.1.1 is the latest version
- You can automatically select the latest version with the `--latest` or `-l` option

Basic Usage

Simplest Execution Example

```
$ osub input.inp
```

This runs the calculation with the following default settings:

- ORCA 6.1.0
- 8 CPU cores
- 1200 MB/core memory
- 72-hour time limit

Commonly Used Option Examples

```
# Specify CPU count and memory
$ osub -np 16 -m 1500 input.inp

# Use the latest version
$ osub --latest input.inp
$ osub -l input.inp  # Short form

# Specify a version
$ osub -v 5.0.4 -np 4 input.inp
$ osub --version 6.1.1 -np 8 input.inp

# Multi-node execution (4 nodes × 64 cores = 256 core parallel)
$ osub -np 64 --nodes 4 input.inp


# Allocate more resources to increase memory per core (8 cores in parallel, 2400 MB/core)
$ osub -np 16 -mp 8 -m 2400 input.inp
```

```
# Large memory (largemem)
$ osub -np 64 -m 6000 -j largemem input.inp

# Do not use the compute node's local scratch (intermediate calculation results can be seen in the working directory)
$ osub -N input.inp

# Submit multiple files at once (sequential execution)
$ osub -np 8 *.inp
```

Main Options

Resource Specification

Option	Description	Default
`-np`, `--ncpus`	Number of CPUs to allocate	8
`-m`, `--maxcore`	Memory per core (MB)	1200
`--nodes`	Number of nodes	1
`-mp`, `--mpiprocs`	MPI processes/node	Same as ncpus
`-t`, `--walltime`	Walltime (hh:mm:ss)	72:00:00

ORCA Configuration

Option	Description	Default
`-v`, `--version`	ORCA version	6.1.0
`-l`, `--latest`	Use the latest version (currently: 6.1.1)	False
`--noedit`	Skip editing the input file	False
`-N`, `--no-local-scratch`	Disable local scratch usage	False
`-ng`, `--nprocs-group`	Number of parallel processes for subtasks (ORCA 6.0 and later only)	-

Notes:

- When both `--version` and `--latest` are specified, the `--version` value takes precedence
- `--nprocs-group` is only valid for ORCA 6.0 and later (ignored in version 5.x and earlier)

Job Control

Option	Description	Default
`-j`, `--jobtype`	Specify job type	Auto-detect
`-g`, `--group`	User group specification	Primary group
`-P`, `--prep-only`	Generate script only	False

Other Options

Option	Description	Default
`-O, --overwrite`	Overwrite existing files	False
`--mail`	Email notification	False
`--name`	Specify job name	-
`--autoname`	Auto-generate job name from filename	False

Version Management

Checking Available Versions

```
$ osub
```

When run without arguments, a list of available versions is displayed:

```
Supported ORCA versions:
 4.2.1 [ORCA4]
 5.0.3 [ORCA5]
 5.0.4 [ORCA5]
 6.0.1 [ORCA6]
 6.1.0 [ORCA6] (default)
 6.1.1 [ORCA6] (latest)
```

How to Select Versions

```
# Use default version (6.1.0)
$ osub input.inp

# Use latest version (6.1.1)
$ osub --latest input.inp

# Specify a version
$ osub --version 5.0.4 input.inp
```

Input File Processing

Automatic Handling of External File References

osub automatically detects external file references in input files and converts relative paths to absolute paths to ensure proper execution in scratch directories.

? Files Automatically Detected as External

Strings containing periods (excluding decimal numbers)

? Processing Behavior

- Relative paths → Automatically converted to absolute paths (reflected in `<original_filename>.ap`)
- Absolute paths → Left unchanged

- Non-existent files → A warning is displayed during job submission

? Explicit Specification of External Files

To manually specify files that are not automatically detected:

```
# Explicitly specify files without periods
# (The entries 'basis' and 'coord' in the input file will be converted to absolute paths)

$ osub --external-files basis --external-files coord input.inp
```

Troubleshooting

Common Errors and Solutions

? 1. ERROR: invalid ncpus value

```
 # Cause: 65–127 cores are not available on the system

? $ osub -np 100 input.inp

? $ osub -np 64 input.inp

? $ osub -np 128 input.inp
```

? 2. Memory Shortage

```
# Allocate more resources to increase memory per core
$ osub -np 16 -mp 8 -m 2400 input.inp

# Or use large memory job type
$ osub -np 64 -j largemem input.inp
```

Display Debug Information

```
# Generate the job script without submitting it
$ osub -P -np 8 input.inp
```

Generated Files

Job Script

- `H-<PID>.sh`: PBS job script

Edited Input File

- `<original_filename>.ap`: Modified input file with resource settings appended

Output Files

- `<input_filename>.out`: ORCA calculation log

Support & Contact

For questions or bug reports, please contact your system administrator.