

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 (default)

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

# 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

# Specify ORCA version
$ osub -v 5.0.4 -np 4 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
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Option	Description	Default
-v, --version	ORCA version	6.1.0
--noedit	Skip input file editing	False
-ng, --nprocs-group	Subtask parallelism (ORCA6 only)	-

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

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.