OrcaLauncher User Guide

Contents

1 What is OrcaLauncher

OrcaLauncher is the program that simplifies your communication with ORCA quantum chemistry package.

- No more need to run ORCA from the command line

- Easy interaction with input and output files

- Controllable queue for executing tasks

- Connectability with third-party programs (Chemcraft, Avogadro)

- It is convenient for small research groups as well as for single researchers

OrcaLauncher is an open-source project. It distributes under the GNU GPL license.

OrcaLauncher is available only for Windows platform to date!

2 Quick start

Download the OrcaLauncher installer (install_orcalauncher_x64.exe) or archive (OrcaLauncher.7z) from the GitHub project page. Install or extract it to your local disc.

Once you run OrcaLauncher.exe, you will see the following window.
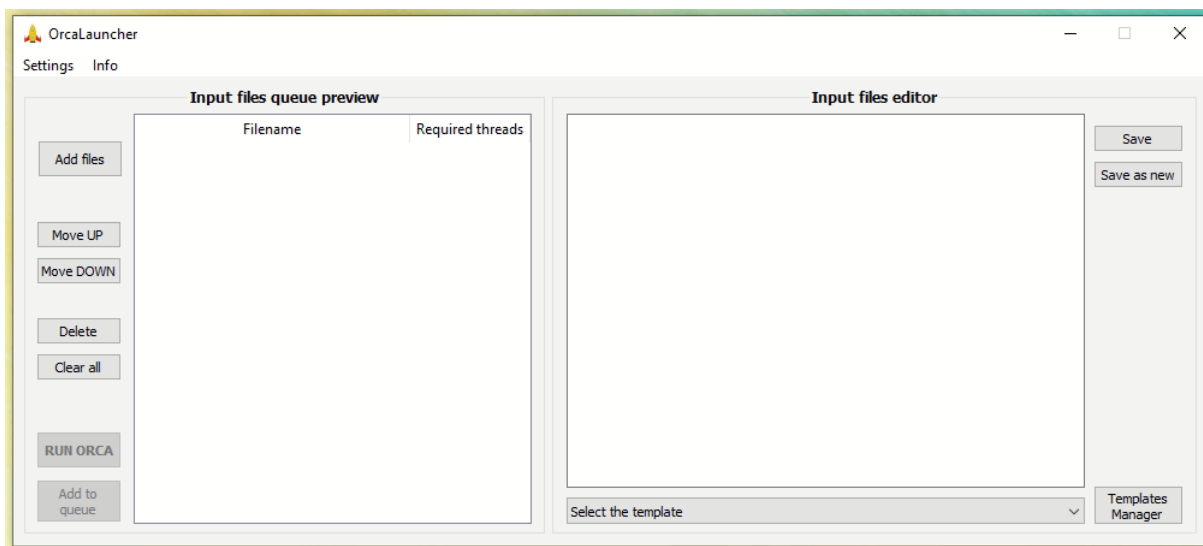
First, you should specify the path to *orca.exe* on your computer (Settings > Set path to orca.exe). Do it only once at first OrcaLauncher run. You can read about other settings in the Section 3.
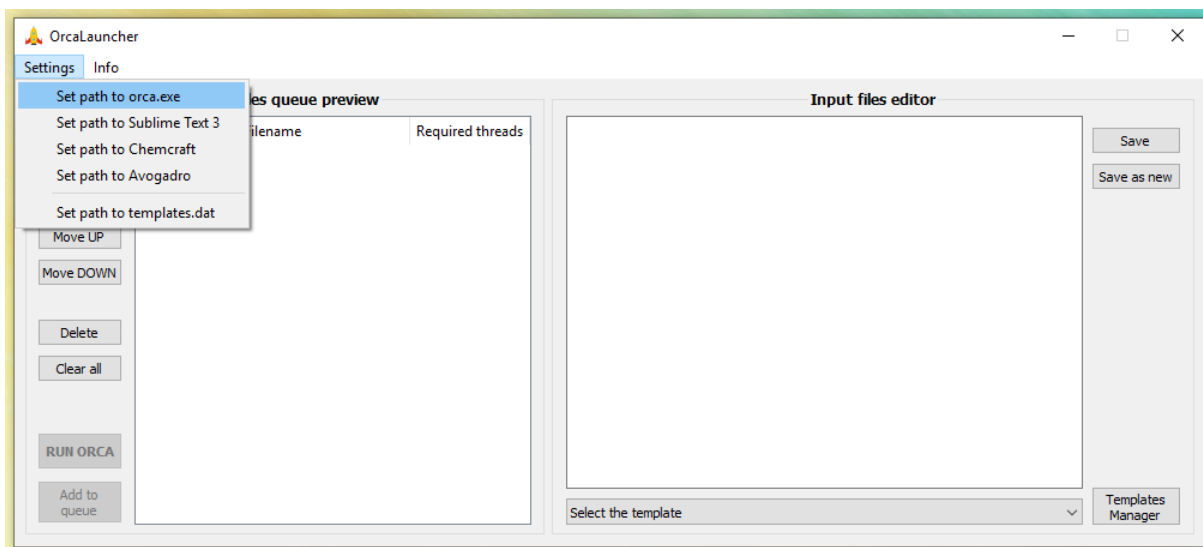
Add your ORCA input files by clicking "Add files". Loaded files appear on the left-hand side of the program (*Input files queue preview*). If you want to correct some input file or just take a look at it, you should left-click on the filename in the table. The content of the input file appears on the right-hand side of the program. If you change an input file, *don't forget to save the updates* ("Save" button)!
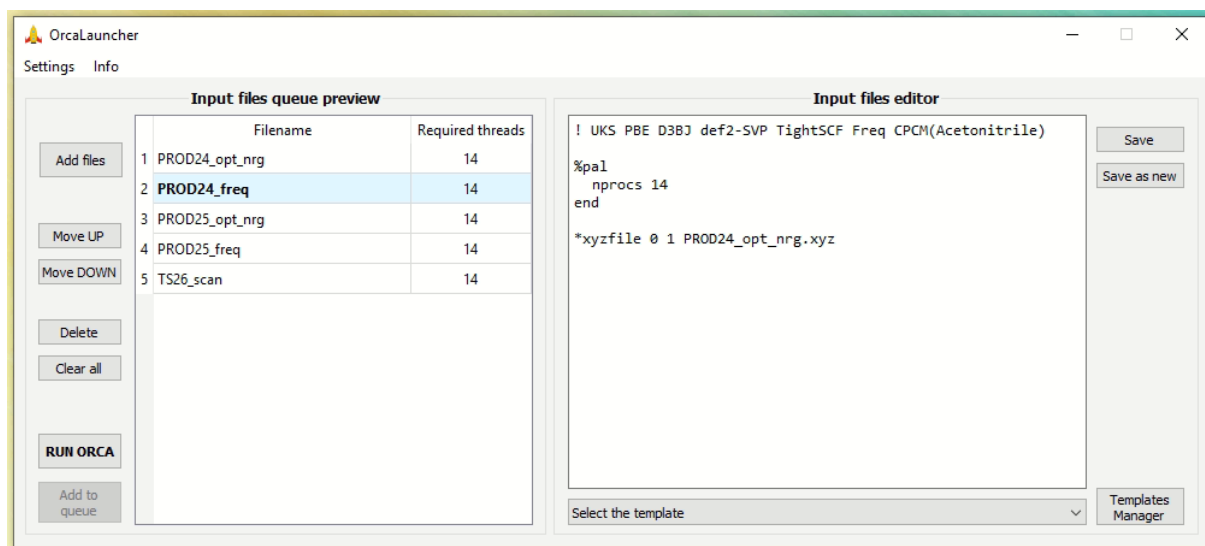
OrcaLauncher is ready to take off! Press "Run orca" button. The main window is hidden and the status window appears in the corner of the screen. Queued tasks will be started one by one following the initial order. Outfiles appear in the same directory as input files located and with the same base names.
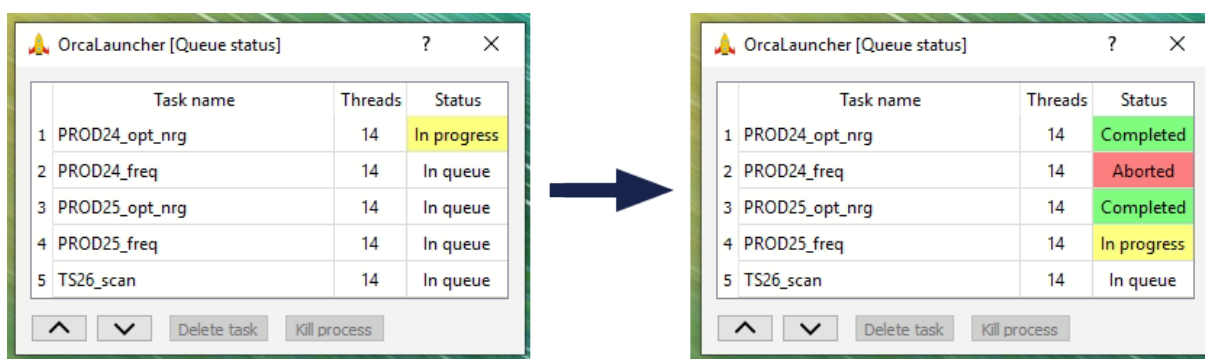
A task may become either "Completed" or "Aborted" depending on the result of ORCA calculations. You can open your outfile in the file explorer by right-click > "Show outfile in explorer". Other options of context menu are discussed in the next section.

3

3   Detailed guide
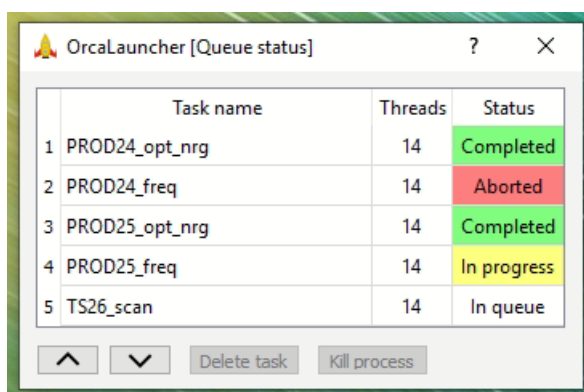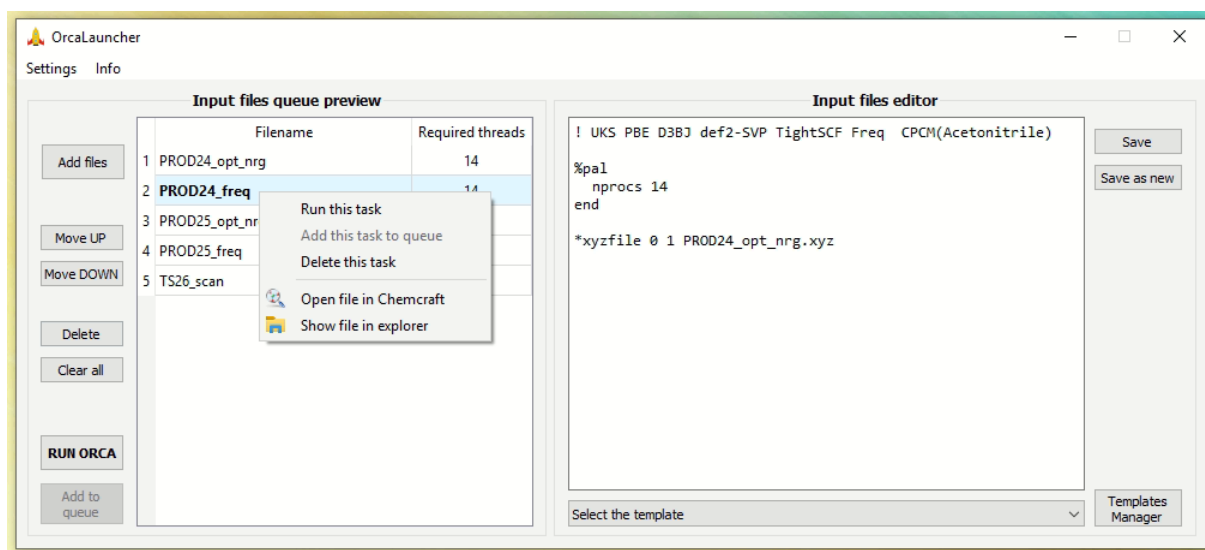
3.1   Queue preview in the main window

Figure 1. OrcaLauncher main window.

On the left-hand side of the main window, you form a queue of tasks by adding input files or creating new files using *Input files editor*. You can change the order of tasks in the queue using "Move UP" and "Move DOWN" buttons. Once the queue is formed, you should press "Run orca". The main window is hidden, and the status window appears in the corner of the screen. After queue launching, the main window remains its functionality and can be used to create a new queue or to edit some input files. Note that you cannot run second queue, but you can add new tasks in executing queue by clicking "Add to queue".

Right-clicking on a filename in the main window opens a context menu, which allows to open the selected file in explorer or in Chemcraft (see also 3.4). It can also be used to run a particular task or add it to an executing queue.

3.2 Queue in the status window

Figure 2. OrcaLauncher status window.

Status window gives information about the executing queue and tasks states and allows to interact with output files. There are four types of task status:

1. In queue means that a task is planned to execute. All queued tasks can be interchanged by clicking △ or ▽ buttons and removed from the queue by "Delete task".

2. In progress means that a task is executing. You can interrupt the execution by clicking "Kill task". This is equal to "End Process" in Windows Task Manager. In this case, the next task starts instantly.

3, 4. Completed or Aborted means that a task is done. The exact status depends on whether the ORCA program has ended without errors or with.

Right-clicking on a filename in the status window opens a context menu, which allows to open the selected file in third-party programs (see also 3.4). It can also be used to make output_filename.wfn using *orca_2aim.exe* and output_filename.gbw for completed tasks.

3.3 Templates

OrcaLauncher provides an opportunity to use templates for input files. They simplify and speed up the creation of input files. You can create a number of templates using the "Templates manager", each one for a particular type of task (e.g. Optimize+Hessian, Scanning bond length, etc.).

All templates are stored in the single file *templates.dat*. You should specify the path to this file if you want to use templates (*note: this file must be named as templates.dat*). The default *templates.dat* file is located in OrcaLauncher directory.
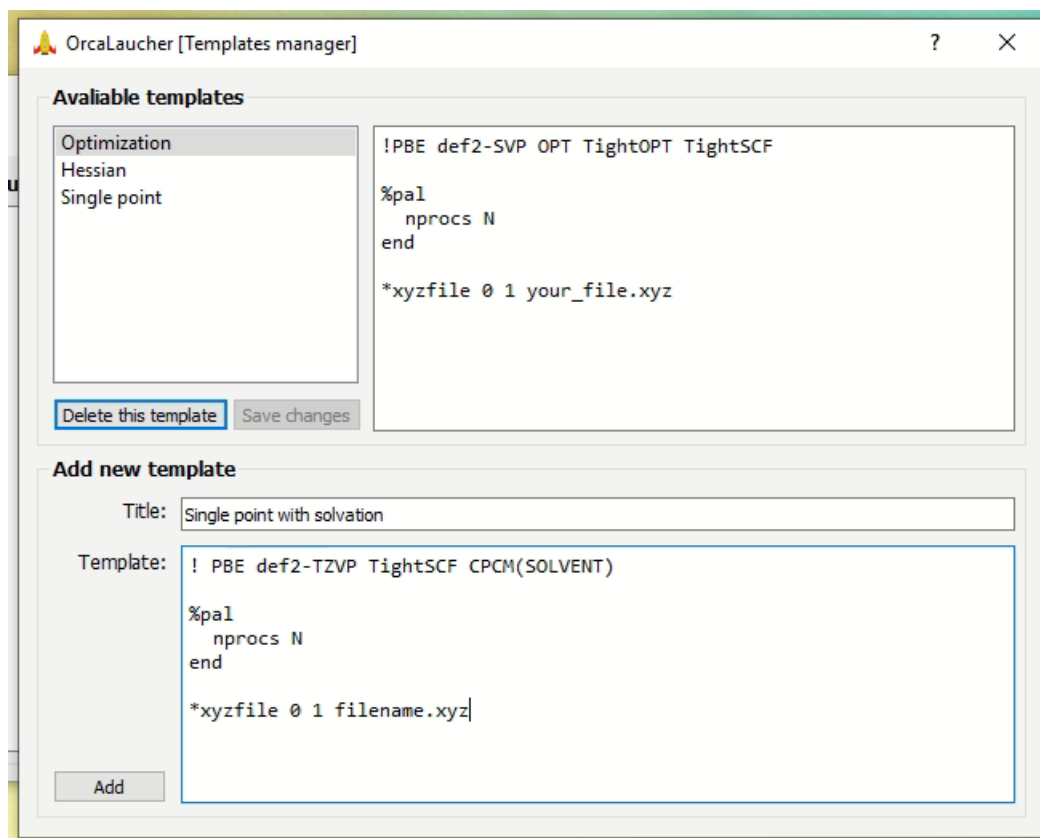
Figure 3. Templates manager.

Since then, creating an input file for a new task, you can choose one form from the drop-down list located at the bottom of *Input files editor*. After a minor revision you should save this file as new input file ("Save as new" button) and it automatically appears in the *Input files queue preview*.
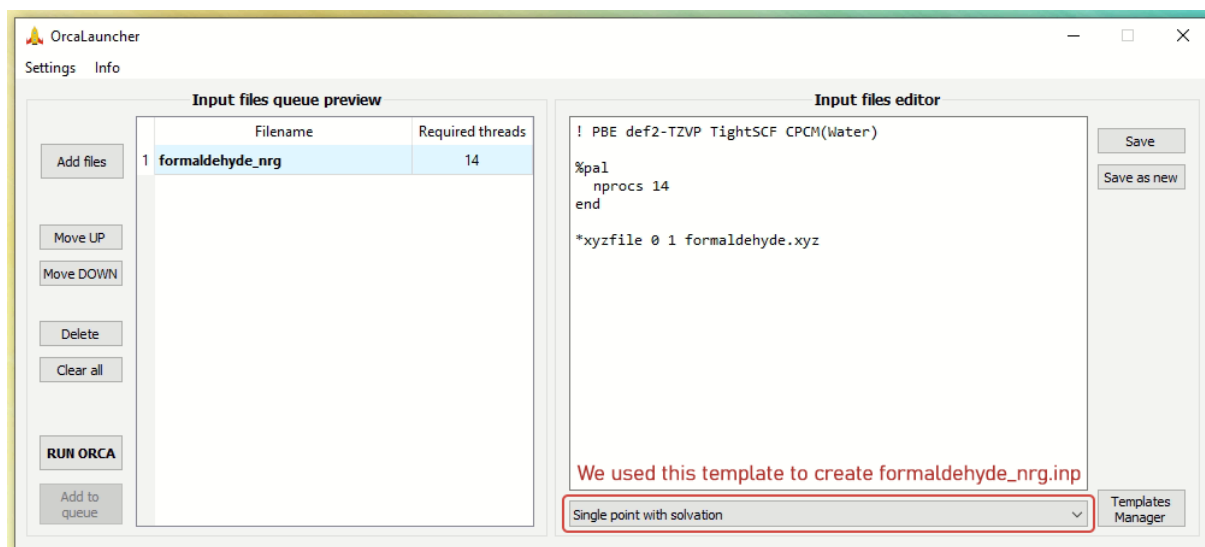

Figure 4. Creation of input file from template.

3.4 Programs-companions

OrcaLauncher can communicate with several programs when it comes to analysis of outfiles. Thus, outfiles that are resulted from queue execution can be easily opened in a third-party program by right-clicking on a filename in the OrcaLauncher status window.
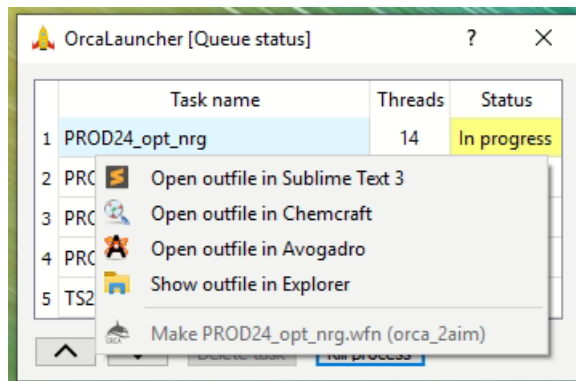

Figure 5. OrcaLauncher status window with opened context menu.

Selected outfile can be opened in Sublime Text by double-clicking as well.

List of the supported programs:

- *Sublime Text* – easy-to-use text editor with simple interface. It is the program of choice for analysis of ORCA output files text. It may be downloaded for free. To use Sublime Text within OrcaLauncher you should specify the path to the *sublime_text.exe* in the Settings.

- *Chemcraft* – the program with user-friendly graphical interface for analysis of different types of ORCA output files. It can visualize optimization steps, animate vibrational modes, render orbitals, etc. More detailed description can be found on `https://www.chemcraftprog.com/index.html`. To use Chemcraft within OrcaLauncher you should specify path to the *Chemcraft.exe* in the Settings.

- *Avogadro* – the open-source molecule editor and visualizer. Similarly to Chemcraft, it can render orbitals and animate vibrational modes. The ORCA enhanced version of Avogadro is available on ORCA Forum. To use Avogadro within OrcaLauncher you should specify path to the *avogadro.exe* in the Settings.