Tutorial 1. Fixed composition of 3D crystals

1. Connect to the account using your login and password.
2. Create the folder for the first example:

$ mkdir EX02

1. Copy files, required for the first example to the folder:

$ cp -r /opt/USPEX/uspex-2022.1-examples/opt/USPEX/uspex-2022.1-examples/EX02-3D\_MgAl2O4\_gulp ./EX02/

1. For now, lets see, what we have in the first example folder:

$ cd EX02/EX02-3D\_MgAl2O4\_gulp

$ ls

you will see the folder content:

*input.uspex jobscript reference Specific*

Here, input.uspex – is the main USPEX file.

*The input.uspex file has json-like syntax and hierarchical structure representing modular nature of USPEX program. It contains the most important parameters of the input. Most of the parameters have reliable default values (this allows you to have extremely short input files!). Those options that have no default should always be specified. Please see the manual* [*https://uspex-team.org/en/uspex/documentation*](https://uspex-team.org/en/uspex/documentation)*.*

jobscript – is a file for the submission of the task to the cluster queue.

*We use slurm task manager (*[*https://slurm.schedmd.com/sbatch.html*](https://slurm.schedmd.com/sbatch.html)*).*

Specific folder consists of executables and enumerated input files for structure relaxation (using external codes, like VASP, SIESTA, GULP.

Reference folder contains final results of the calculation, so you can always compare your results with the reference.

1. Load modules required for the calculations:

$module load module load python/python39 uspex/uspex-2022.1 gulp/gulp

1. Submit the job to the queue:

$ sbatch jobscropt

You will see the following message:

Submitted batch job 11215361

You can check the status of the job:

$ squeue -u userXX