

PARCAS example

1 PARCAS

The MD code PARCAS can be downloaded from the web-page

<https://gitlab.com/acclab/parcas>

and compiled with the instructions given there.

2 Example input

The input files and the input folder (in.tar.gz) can be downloaded at

<https://github.com/shortlab/2021-Ti-Wigner/>

under the folder: 3_SIM/0_PKA/

This input folder should be unpacked, for instance with the command

```
tar -xvf in.tar.gz
```

and contains everything for a single 5 keV cascade in Ti at 570K. The included input cell is thermalized at 570K. In this example every 100th frame is printed out to the movie file and the interval can be modified by changing the "nmovie" parameter. Note the time between frames is not constant due to the adaptive timestep used to capture the correct trajectories at high energies. Full detailed list and description of the parameters is found with the source code.

3 Running the simulation

The program should be executed in the folder where the "in" folder exists. The code can be executed serially or parallel, with the command

```
mpirun -np X parcas
```

where X is the number of cores/threads to be used. Note that the produced output will be around 4Gb with the current nmovie parameter.

After the simulation, a folder called "out" is generated, where some restart files and the movie file are found. Please refer to the manual of PARCAS to see the details. The movie (out/md.movie file) will contain every frame saved and can be visualized with different software. The format of the movie is the xyz-format, with the columns "Atom type", "Position x", "Position y", "Position z", "Atom type identifier", "Atom index" after the two comment lines, with "Number of atoms" on the first line and the "Box size" on the second.