# The dump netcdf keyword

From GPUMD
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## Purpose

Dump the atom positions (coordinates) in the NetCDF format.

## Grammar

- This keyword's usage will have the following format:

```
dump_netcdf interval <optional_args>
```

- The `interval` parameter is the output interval (number of steps) of the atom positions.
- The `optional_args` provide additional functionality. Currently, the following optional argument is accepted:
- - `precision`: *single* or *double*. If `precision` is *single*, the output data are 32-bit floating point numbers. If `precision` is *double*, the output data are 64-bit floating point numbers. The default value is *double*.

## Requirements and specifications

- This keyword requires an external package to operate. The binary format NetCDF (https://www.unidata.ucar.edu/software/netcdf/) package instructions can be found here.
- The NetCDF format follows the AMBER conventions (http://ambermd.org/netcdf/nctraj.pdf).
- The *single* option is good for saving space, but does not follow the official AMBER 1.0 conventions.
- All NetCDF output files can be read by VMD (https://www.ks.uiuc.edu/Research/vmd/) and OVITO (https://ovito.org/) for visualization.
- The NetCDF files also stores cell lengths and angles which can be used in the visualization software to illustrate boundaries and show periodic copies of the structure.

# Examples

## Single precision example

To dump the positions every 1000 steps to a NetCDF file with 32-bit floating point values, one can add

```
dump_netcdf 1000 precision single
```

before the run.

## Double precision example

To dump the positions every 1000 steps to a NetCDF file with 64-bit floating point values, one can add

```
dump_netcdf 1000
```

before the run.

# Caveats

- This keyword is not propagating. That is, its effect will not be passed from one run to the next.
- The outputs append to the same file for different runs in the same simulation. Re-running the simulation will create a new output file.
- If the `precision` changes between different runs, the first defined precision will still be used (i.e. changes in precision are ignored during a simulation).

# Output file

- movie.nc (http://ambermd.org/netcdf/nctraj.pdf)