

# The dump position keyword

From GPUMD

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## Purpose

Dump the atom positions (coordinates) to a text file named movie.xyz.

## Grammar

```
dump_position interval <options>
```

- The interval parameter is the output interval (number of steps) of the atom positions.
- The <options> can be group or precision, which can be in any order.
- The option group should have two parameters:

```
group grouping_method group_id
```

which means only dumping positions of atoms in group `group_id` within the grouping method `grouping_method`. If this option is not used, positions will be dumped for all the atoms.

- The option precision should have one parameter which can only be single or double

```
precision single # output data with %0.9f format  
precision double # output data with %0.17f format
```

If this option is not used, data will be output with the %g format.

## Examples

### Example 1

To dump all the positions every 1000 steps for a run, one can add

```
dump_position 1000
```

before the run keyword.

## Example 2

Similar to the above example, but only for atoms in group 1 within grouping method 2

```
dump_position 1000 group 2 1
```

## Example 3

Similar to the above example, but using double precision

```
dump_position 1000 group 2 1 precision double  
# or equivalently:  
dump_position 1000 precision double group 2 1
```

## Caveats

- This keyword is not propagating. That is, its effect will not be passed from one run to the next.
- The output file has an appending behavior and will result in a single movie.xyz file no matter how many times the simulation is run.

## Output file

- movie.xyz

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