

The run keyword

From GPUMD

[Jump to navigation](#)[Jump to search](#)

Contents

- 1 Purpose
- 2 Grammar
- 3 Examples
- 4 Caveats

Purpose

Run a number of steps according to the settings specified for the current run.

Grammar

This keyword only requires a single parameter, which is the number of steps to be run:

```
run number_of_steps
```

Examples

For example, to run one million steps, just write

```
run 1000000
```

Caveats

- The number of steps should be compatible with some parameters in some other keywords.
- We can regard a run as a block of commands from ensemble to run:

```
# the first run
ensemble ...
# other commands
run ...

# the second run
ensemble ...
# other commands
run ...

# the third run
ensemble ...
# other commands
run ...
```

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