

The minimize keyword

From GPUMD

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Purpose

- This keyword is used to minimize the energy of the system. Currently, only the **steepest descent** method has been implemented.

Grammar

- This keyword is used as follows:

```
minimize sd force_tolerance maximal_number_of_steps
```

- sd means using the **steepest descent** method.
- force_tolerance is in units of eV/Å. When the largest absolute force component among the $3N$ force components in the system is smaller than force_tolerance, the energy minimization process will stop even though the number of steps (iterations) performed is smaller than maximal_number_of_steps
- maximal_number_of_steps is the maximal number of steps (iterations) to be performed for the energy minimization process.

Examples

Example 1

- For example, the command

```
minimize sd 1.0e-6 10000
```

means that one wants to do an energy minimization using the **steepest descent** method, with a force tolerance of 1.0e-6 eV/Å for maximally 10000 steps.

Example 2

- If you have no idea how small force_tolerance should be, you can simply assign a negative number to it:

```
minimize sd -1 10000
```

In this case, the energy minimization process will definitely run 10000 steps.

Caveats

- This keyword should occur after all the potential keywords.
- Currently, the simulation box is fixed during the energy minimization.

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