

# The compute hac keyword

From GPUMD

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

## Contents

- 1 Purpose
- 2 Grammar
- 3 Examples
  - 3.1 Example 1
  - 3.2 Example 2
- 4 Output file
- 5 Related tutorial

## Purpose

This keyword is used to calculate the HAC (heat current autocorrelation) and RTC (running thermal conductivity) using the Green-Kubo method.

## Grammar

- This keyword has 3 parameters:

```
compute_hac sampling_interval correlation_steps output_interval
```

- The first parameter is the sampling interval for the heat current data.
- The second parameter is the maximum correlations steps.
- The third parameter for is the output interval of the HAC and RTC data.

## Examples

### Example 1

```
time_step 1
compute_hac 10 100000 1
run 1000000
```

- This means that:
  - You want to calculate the thermal conductivity using the Green-Kubo method (the EMD method) in this run, which has 10 milillion steps with a time step of 1 fs.
  - The heat current data will be recorded every 10 steps. Therefore, there will be 1 million heat current data in each direction.
  - The maximum number of correlation steps is  $10^5$ , which is one tenth of the number of heat current data. This is a very good choice. The maximum correlation time will be  $10^5 \times 10 = 10^6$  time steps, i.e., 1 ns.
  - (4) the HAC/RTC data will not be averaged before outputting, generating  $10^5$  rows of data in the output file.

## Example 2

```
compute_hac 10 100000 10
```

- This is similar to the above example, but with one exception: The HAC/RTC data will be averaged for every 10 data before outputting, generating  $10^4$  rows of data in the output file.

## Output file

- hac.out

## Related tutorial

- Tutorial: Thermal conductivity from EMD

Retrieved from "[https://gpumd.zheyongfan.org/index.php?title=The\\_compute\\_hac\\_keyword&oldid=21530](https://gpumd.zheyongfan.org/index.php?title=The_compute_hac_keyword&oldid=21530)"

- 
- This page was last edited on 30 August 2020, at 07:25.