The compute keyword

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Purpose

This keyword is used to compute and output space and time averaged quantities.

Grammar

- It is used in the following way:

```
compute grouping_method sample_interval output_interval quantity_1 quantity_2 ...
```

- The first parameter `grouping_method` refers to the grouping method defined in xyz.in. This parameter should be an integer and a number m means the m-th grouping method (we count from 0) in xyz.in.
- The second parameter `sample_interval` means sampling the quantities every so many time steps.
- The third parameter `output_interval` means averaging over so many sampled data before giving one output.
- Starting from the fourth parameter, one can list the quantities to be computed.
- The allowed names for the quantities are:
  - `temperature`, which is the temperature
  - `potential`, which is the potential energy
  - `force`, which is the force vector
  - `virial`, which is the diagonal part of the virial
  - `jp`, which is the potential part of the heat current vector
  - `jk`, which is the kinetic part of the heat current vector
- One can write one or more (distinct) names in any order.

Files produced by this keyword

- compute.out

Examples

Example 1

For example,

```
compute 0 100 10 temperature
```

means using the 0-th grouping method defined in xyz.in, sampling `temperature` every 100 time steps and averaging over 10 data points before making an output. That is, there is only one output every $100 \times 10 = 1000$ time steps.

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