The compute sdc keyword

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Purpose

- This keyword computes the self diffusion coefficient (SDC) using the velocity autocorrelation (VAC). If this keyword appears in a run, the VAC will be computed and integrated to compute the SDC.

Grammar

- For this keyword, the command looks like:

```
compute_sdc sample_interval Nc <optional_arg>
```

with parameters defined as:

- `sample_interval`: Sampling interval of the velocity data
- `Nc`: Maximum number of correlation steps

The `optional_arg` allows an additional special keyword. The keyword for this function is `group`. The parameters are:

- `group group_method group`

    group_method: The grouping method to use for computation
    group: The group in the grouping method to use

Examples

Example 1

- An example of this function is:

```
compute_sdc 5 200 group 1 1
```

This means that you (1) want to calculate the SDC; (2) the velocity data will be recorded every 5 steps; (3) the maximum number of correlation steps is 200; (4) You would like to compute only over group 1 in group method 1.

Caveats

- This function cannot be used in the same run with the compute_dos keyword.

Output file

- sdc.out

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