

The sdc.out output file

From GPUMD

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Brief Description

This file contains the data of the velocity autocorrelation (VAC) and self diffusion coefficient (SDC).

The keyword which produces the current file

- `compute_sdc` in `run.in`.

File format

- The data in this file are organized as follows:
 - column 1: correlation time (in units of ps)
 - column 2: VAC (in units of $\text{\AA}^2/\text{ps}^2$) in the x direction
 - column 3: VAC (in units of $\text{\AA}^2/\text{ps}^2$) in the y direction
 - column 4: VAC (in units of $\text{\AA}^2/\text{ps}^2$) in the z direction
 - column 5: SDC (in units of $\text{\AA}^2/\text{ps}$) in the x direction
 - column 6: SDC (in units of $\text{\AA}^2/\text{ps}$) in the y direction
 - column 7: SDC (in units of $\text{\AA}^2/\text{ps}$) in the z direction

Tips

- Only the selected group in the `compute_sdc` keyword is included in this output.

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