

# Self-diffusion constants along a channel axis

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In this code, an algorithm is implemented which enables one to calculate the self-diffusion constant profile of some selected ion types during their permeation accross a channel.

Run program as: `executable file [input [> output]]`

Below, the data required in the input file is described. It should be noted that a specific format is described between parenthesis, where  $i$  indicates a integer data type,  $r$  indicates a real data type,  $c$  indicates a character data type, and  $b$  indicates a boolean data type. A comment line begins with a symbol `!`, `*` or `#`.

(A) *Initial value and frequency for reading coordinates (.DCD file)*

- Record A1 (i,i):  $N_i, N_f$

$N_i$  and  $N_f$  are the initial value and frequency for reading coordinates from a .DCD file.

(B) *Calculation type*

- Record B1 (b,b):  $\log MSD, \log D$

$\log MSD = .true.$  means that a mean-square displacement (MSD) calculation is activated.  
 $\log D = .true.$  means that the self-diffusion constants are obtained from the MSDs by fitting a straight line.

(C) *MSD calculation (only if  $\log MSD = .true.$ )*

- Record C1 (c,c,b):  $PSF\ filename, DCD\ filename, DCDUnitCell$

Filenames are specified for .PSF and .DCD files.  $DCDUnitCell = .true.$  means that unit cell parameters are included in the .DCD file.

- Record C2 (c):  $\alpha$

$\alpha = x, y, z$  indicates the component along the channel axis.

- Record C3 (b):  $\log PBC$

$\log PBC = .true.$  means that periodic boundary conditions are used.

- Record C3' (r,r,r,r,r,r) (only if  $\log PBC = .true.$ ):  $L_x, L_y, L_z, x_c, y_c, z_c$

$L_x, L_y$  and  $L_z$  are the box legths along  $x, y$  and  $z$  directions, respectively.  $(x_c, y_c, z_c)$  is the position of the box center.

- Record C4 (r,r):  $p_1, p_2$

$p_1$  and  $p_2$  define the region along the channel axis where MSDs will be calculated.

- Record C5 (r,r):  $\Delta t, h$

$\Delta t$  and  $h$  are the time step and grid size used in the MSD calculation.

- Record C6 (i):  $N_t$   
The maximum elapsed time is given by  $N_t N_f \Delta t$ .
  - Record C7 (i):  $N_{types}$   
 $N_{types}$  is the number of selected ion types.
  - Record C8 (c):  $typenam(i), i = 1, N_{types}$   
Ion type names.
  - Record C9 (b):  $outMSD$   
 $outMSD = .true.$  means that MSDs and apparent self-diffusion constants for selected ion types will be printed in an output file. It should be noted that this variable has to be true when  $logD = .false..$
  - Record C9' (c) (only if  $outMSD = .true.$ ):  $MSD filename$   
Output file name of MSDs and apparent self-diffusion constants for selected ion types.
- (D) Self-diffusion constant calculation (only if  $logD = .true.$ )
- Record D1 (c) (only if  $logMSD = .false.$ ):  $MSD filename$   
Input file name of MSDs and apparent self-diffusion constants for selected ion types.
  - Record D2 (i) (only if  $logMSD = .false.$ ):  $N_t$   
Number of snapshots that determine the maximum elapsed time.
  - Record D3 (i) (only if  $logMSD = .false.$ ):  $N_{types}$   
 $N_{types}$  is the number of selected ion types.
  - Record D4 (c) (only if  $logMSD = .false.$ ):  $typenam(i), i = 1, N_{types}$   
Ion type names.
  - Record D5 (i) (only if  $logMSD = .false.$ ):  $N_b(i), i = 1, N_{types}$   
Number of bins for each ion type.
  - Record D6 (i):  $initval(i), endval(i), i = 1, N_{types}$   
Initial and final values for elapsed time for each ion type.
  - Record D7 (c):  $D filename$   
Output file name of self-diffusion constants for each ion type.