Collective diffusion model for ion conduction through channels

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A collective diffusion model based on the linear response theory has been defined that enables one to determine the ion channel conductance from equilibrium simulations [1]. In this code, this model is implemented in an efficient algorithm. It should be noted that periodic boundary conditions need to be used in the simulations.

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): $logQ$, $logMSD$

  $logQ = .true.$ means that amount of charge transfer calculation is activated. $logMSD = .true.$ means that a mean-square displacement (MSD) calculation is activated.

(C) Amount of charge transfer calculation (only if logQ = .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 (r): δt

  Time step size.

- Record C3 (c): α

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

- Record C4 (r,r,r,r,r,r): x_c, y_c, z_c, L_x, L_y, L_z

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

- Record C5 (r,r,r,r,r,r): x_1, x_2, y_1, y_2, z_1, z_2

  The channel region is defined by $[x_1, x_2] \times [y_1, y_2] \times [z_1, z_2]$.

- Record C6 (b): Q_{at}

  $Q_{at} = .true.$ means that all atoms are considered in the calculation. $Q_{at} = .false.$ means that only ions are considered in the calculation.

- Record C6′ (i) (only if $Q_{at} = .false.$): N

  Number of ion types

- Record C6″ (c) (only if $Q_{at} = .false.$): $ion_name(i)$, $i = 1, N$

  Ion type names

- Record C7 (b): $outQ$

  $outQ = .true.$ means that the amount of charge transfer through the channel at several time steps will be printed in an ouput file. It should be noted that this variable has to be true when $logMSD = .false.$.

- Record C9′ (c) (only if $outQ = .true.$): Q filename

  Ouput file name for the amount of charge transfer through the channel at several time steps.

(D) Mean-square displacement calculation (only if logMSD = .true.)

- Record D1 (c) (only if $logQ = .false.$): Q filename

  Input file name for the amount of charge transfer through the channel at several time steps.

- Record D2 (i,i): M_i, M_f

  Initial and final values for elapsed time.

- Record D3 (c): *D MSD filename*

  Output file name for mean-square-displacement of the amount of charge transfer.

- Record D4 (b): Q_{regr}

  $Q_{regr} = .true.$ means that a linear regression fitting is applied to calculate the diffusion coefficient of the amount of charge transfer.

- Record D4′ (c) (only if $Q_{regr} = .true.$): *D filename*

  Ouput file name for the diffusion coefficient of the amount of charge transfer.

References

[1] Y. Liu and F. Zhu, *Biophys. J.* **104**, 368 (2013).