

Error estimate code

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This code implement error estimates on averages of correlated data [1,2].

Run program as: executable file *input* [$>$ *output*]

1 Commands

Some conventions are used in the description on the different commands. On the one hand, keywords are written in bold characters. On the other hand, data provided by the user are written in italic characters. Optional data are encapsulated between square brackets: [*option*].

1.1 General commands

- **INPUT unit** *iwinp* **name** *inputfile*: Open an *inputfile* file linked to an *iwinp* integer unit. This file contains a column with a set of correlated data.
- **OUTPUT unit** *iuwt* **name** *outputfile*: Open an *outputfile* file linked to an *iuwt* integer unit. In this file, the code stores some relevant information for extracting an error estimate from either blocking method [1] or statistical inefficiency [2].
- **CLOSE unit** *iunit*: Close a file linked to an *iunit* integer unit (*iunit* = *iwinp* or *iuwt*).
- **READ npoints** *npoints* **init** *init* [**ntot** *ntot*] [**nsave** *nsave*]: Read data from *inputfile*, where *npoints* is the number of data to be considered, *init* is the number of initial data to be skipped, *ntot* is the total number of data (default value = *npoints* + *init*), and *nsave* is the frequency for data collection (default = 1).
- **CALC type** *itype*: Calculate some relevant information which enables one to obtain an error estimate using blocking method [1] (*itype* = 1) or statistical inefficiency [2] (*itype* = 2).

References

- [1] H. Flyvbjerg and H. G. Petersen, *J. Chem. Phys.* **91**, 461–466 (1989).
- [2] M. P. Allen and D. J. Tildesley, *Computer simulation of liquids*. Oxford: Clarendon Press (1987).