NAME

points.in, — Point specific input file for **surfgen**.

SYNOPSIS

This input file is used by coupled potential surface fitting program **surfgen**. For a detailed description of the program and the evaluation library, see surfgen(1).

Place points.in in the same directory where **surfgen** is being called.

DESCRIPTION

points.in contains input options that will be applied to individual points or set of points during the surface fitting procedure of **surfgen**. **points.in** is a *FORMATTED* input file. Please read **FORMAT** section for details.

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FORMAT

The file consists of two lines of comments followed arbitrary lines of point-specific options. *surfgen* will process options from top down. When conflicting options are given for the same point(s), later options will automatically override earlier ones without warning. Each option consists of a two character keyword and three integers, with the input format
(A2,X,3I5)

The keywords are *case insensitive*. If any state or point specifications exceeds the scope of data, it will be ignored. If a range of states or a range of points exceeds the boundary, it will be rounded to the corresponding boundary. For example, point range -2 to 5 will be automatically changed to 1 to 5, since the lowest allowed point index is 1. Unrecognized keywords will be ignored with warning messages.

The last two integer inputs will often be used to specify a range of states or points. The program will recognize the smaller (larger) number in the pair and use it as the lower (upper) bound of the range.

KEYWORDS

This section contains description of supported keywords and the meaning of the corresponding integer input parameters.

Weight Data Points

WT *$wgt $pt1 $pt2*
: Set the weight for points from *$pt1* to *$pt2*. When *$wgt=0*, the points in the range will be excluded. When *$wgt>0*, the points in the range will be weighed by factor *$wgt*. When *$wgt<0*, the points in the range will be weighed by factor **1/abs($wgt)**.

Exact Equations

LE *$pnt $st1 $st2*
: Fit the energy(energies) of electronic states from *$st1* to *$st2* at point *$pnt* exactly with Lagrange multipliers. Naturally, it is recommended that *1≤$st1,$st2≤$nstates* and *$pnt* specifies a valid point. Note that setting the weight of a point to 0 will override the exact condition and remove the exact equations at the point.

LD *$pnt $st1 $st2*
: Fits the *energy difference* between states *$st1* and *$st2* at point *$pnt* exactly with Lagrange multipliers. They do not have to be adjacent states. Note that setting the weight of a point to 0 will override the exact condition and remove the exact equations at the point.

LG *$pnt $st1 $st2*
: Fit gradient or coupling associated with states *$st1* and *$st2* exactly at point *$pnt*. When *$st1=$st2*, this option specifies the energy gradient vector of a state; otherwise, it specifies the derivative coupling between states *$st1* and *$st2*.

Excluding Equations

EE *$pnt $st1 $st2* Exclude energy of block *$st1*,*$st2* for point *$pnt*. This could specify either a diagonal or off-diagonal block. Note that off-diagonal block may or may not be fit to 0, depending on the value of option `DijScale` in `surfgen.in`.

EG *$pnt $st1 $st2* Exclude gradient or derivative coupling data for point *$pnt*. When *$st1=$st2*, this option specifies the energy gradient vector of a state; otherwise, it specifies the derivative coupling between states *$st1* and *$st2*.

Gradient Ordering

GO *$pnt $st1 $st2* Enforce states from *$st1* to *$st2* to be ordered by gradient matching instead of energy matching at point *$pnt*. Note that this option can be overriden when gradient ordering is turned off altogether by setting *gOrder/[u2264]0* in `surfgen.in`.

SEE ALSO

`surfgen`(1), `surfgen.in`(1)

BUGS

Please send bug reports to Xiaolei Zhu ⟨virtualzx@gmail.com⟩