FALDI Advanced Options

FALDI TYPE [X]

Default option **A**

Available options: A, B, C, D

*Controls the base algorithm used by FALDI, ranging from **A** to **D** (and as detailed by Cooper et al 2022)*.

Syntax:

FALDI TYPE D

Isopycnic Transformations

Default option: On

Available Options: ON, OFF, FINAL

Controls whether or not to perform Isopycnic Transformations on the various FALDI fields. 'ON' will apply isopycnic transformations on all FALDI fields throughout the Orthodox, LO and LDO processes. 'FINAL' will only apply isopycnic transformations on the final produced density matrices

Syntax:

ISOPYCNIC OFF

Selection of overlap algorithm

Default option: Orthodox

Available options: NONE, ORTHODOX, LO, LDO

Controls the overlap algorithm used during calculation of density matrices. 'Orthodox' will calculate the QTAIM delocalization and localization indices, 'None' will calculate the QTAIM delocalization indices but without performing diagonalization of the matrices, 'LO' uses the Localized-Overlap algorithm and 'LDO' uses the Localized-Delocalized-Overlap algorithm

Syntax:

OVERLAP LDO

NDF Cutoff numbers

Default option: 1×10^{-7}

Available options: LNDF, DNDF

Controls the minimum eigenvalue of NDFs saved, and printed, in all FALDI calculations. All NDFs with eigenvalues lower than the cutoff will be discarded after initial diagonalization. 'LNDF' controls localized NDF's cutoffs, and 'DNDF' controls delocalized NDF's cutoffs.

Syntax:

CUTOFF LNDF 0.00000001

CUTOFF DNDF 1E-08

Printing Atomic Overlap Matrices

Default option: off

If present, all atomic overlap matrices will be saved to a text file

Syntax:

PRINT AOM