2 Dimensional Finite Difference Hartree-Fock Program

User's Guide

version 1-2003

Description of the command structure

The input command file consists of separate lines each containing

- a label

- a label followed by a character, integer and/or fix-point or

- a character, integer and/or fix-point constant.

Note that

- labels can be in upper or lower case,

- compulsory labels, i.e. these that must be included in the input command file, are marked "•" and the optional ones "○",

- the compulsory labels must follow the order given below; the optional ones can be inserted anywhere between **title** and **stop** labels,

- optional parameters are enclosed in square brackets,

- r denotes a fix-point constant, i – an integer, c – a string of characters,

- exclamation mark placed anywhere in an input line starts a comment; what follows "!" is ignored.

The following labels can be used:

- **TITLE**

  Format: title
  $$c$$
  c is any string of up to 80 characters describing the current case. This string is used as a header of disk output files containing orbitals and potentials.

- **METHOD**

Format: method c

    Select the type of calculation.

        c: HF – Hartree-Fock method

        c: HFS – Hartree-Fock-Slater method

        c: OED – One Electron Diatomic states

- **NUCLEI**

Format: nuclei Z_A Z_B R [c]

    Set the nuclei charges and the bond length.

    Z_A: nuclear charge of centre A (integer)

    Z_B: nuclear charge of centre B (integer)

    R: bond length (real)

    c: *angstrom* – the internuclear separation can be given in angstrom units if this string is included (the conversion factor 0.529177249 is used)

    If $|Z_A - Z_B| < 10^{-6}$ then the molecule is considered to be a homonuclear one (this threshold can be changed by redefining HOMOLEVL variable in blk_data.inc.raw).

  ◦ **HOMO**

Format: homo

    This label is used to impose explicitly $D_{\infty h}$ symmetry upon orbitals of homonuclear molecules in order to improve scf/sor convergence.

  ◦ **BREAK**

Format: break

    When this label is present homonuclear molecules are calculated in $C_{\infty v}$ symmetry and the $D_{\infty h}$ symmetry labels (u or g) are superfluous (see below).

- **CONFIG**

Format: config i

    i: the total charge of a system

The following cards define molecular orbitals and their occupation. **Note that the last orbital description card must contain an extra label** *end*.

The possible formats are:

Format: $i \quad c$

> i: number of fully occupied orbitals of a given irreducible representation (irrep) of the $C_{\infty v}$ group; 2 electrons make σ orbitals fully occupied and 4 electrons are needed for filling the orbitals belonging to the other irreps
>
> c: symbol of the $C_{\infty v}$ irrep to which the orbitals belong (*sigma, pi, delta* or *phi*)

Format: $i \quad c_1 \quad c_2$

> i: number of fully occupied orbitals of a given irrep of the $D_{\infty h}$ group
>
> c_1: symbol of the $C_{\infty v}$ irrep to which the orbitals belong (*sigma, pi, delta* or *phi*)
>
> c_2: symbol for the inversion symmetry of the $D_{\infty h}$ irreps (u or g)

Use this format for a homonuclear molecule unless **break** command is included.

Format: $i \quad c_1 \quad c_2 \ [c_3 \ [c_4 \ [c_5]]]$

> i: number of orbitals of a given irrep of the $C_{\infty v}$ group
>
> c_1: symbol for the $C_{\infty v}$ irreps to which the orbitals belong (*sigma, pi, delta, phi*)
>
> c_2-c_5: +, − or . (a dot); +/− denotes spin up/down electron and . denotes an unoccupied spin orbital

Format: $i \quad c_1 \quad c_2 \quad c_3 \ [c_4 \ [c_5 \ [c_6]]]$

> i: number of orbitals of a given irrep of the $D_{\infty h}$ group
>
> c_1: symbol for the $C_{\infty v}$ irrep to which the orbitals belong (*sigma, pi, delta, phi*)
>
> c_2: symbol for the inversion symmetry of the $D_{\infty h}$ irrep (u or g)
>
> c_3-c_6: +, − or . (a dot); +/− denotes spin up/down electron and . denotes an unoccupied spin orbital

○ **GRID**

Two possible formats are (the second one is retained for the backward compatibility):

Format: grid $n_\nu \quad R_\infty$

> An integer and a real define a single 2d grid.
>
> n_ν: the number of grid points in ν variable

R_∞: the practical infinity

n_μ is calculated so as to make the step size in μ variable equal to the stepsize in ν variable. n_ν and n_μ have to meet special conditions. If the conditions are not fulfilled the nearest (but smaller) appropriate values are used.

Format: grid n_ν n_μ R_∞
Two integers and one real define a single 2d grid.

n_ν: the number of grid points in ν variable

n_μ: the number of grid points in μ variable

R_∞: the practical infinity

n_ν and n_μ have to meet special conditions. If the conditions are not fulfilled the nearest (but smaller) appropriate values are used.

○ **SUBGRID**

Format: subgrid n_{grids}
$$n_\nu \; n_\mu^{(1)} \; [\; n_\mu^{(2)} \; [\; n_\mu^{(3)} \;]\;]$$
$$h_\mu^{(1)} \; [\; s^{(2)} [\; s^{(3)}]\;]$$
Define up to 3 subgrids.

n_{grids}: number of subgrids (integer)

n_ν: the number of grid points in ν variable (integer)

$n_\mu^{(1)} \ldots n_\mu^{(3)}$: number of points in the μ direction for each of the subgrids (integers)

$h_\mu^{(1)}$: the step size in μ variable for the first subgrid (real)

$s^{(2)} \; s^{(3)}$: step sizes (reals) for other subgrids are defined as $h_\mu^{(2)} = s^{(2)} h_\mu^{(1)}$, $h_\mu^{(3)} = s^{(3)} h_\mu^{(1)}$

Note that either GRID of SUBGRID label must be included in the input command file.

○ **INTERP**

Format: interp
Use this label to change the grid between separate runs of the program. The restriction is that only the number of grid points in one of the variables or R_∞ can be changed at a time.

● **INITIAL**

Format: initial i_1 i_2 [i_3]

i_1: determine the initial source of orbitals and potentials:

* $i_1 = 1$ – molecular orbitals are formed as a linear combination of hydrogenic functions on centres A and B; in the case of HF or HFS calculations Coulomb (exchange) potentials are approximated as a linear combination of Thomas-Fermi $(1/r)$ potentials at the two centres; if method OED is chosen the potential function is approximated as a linear combination of Z_A/r_1 and Z_B/r_2 terms and the exchange potentials are set to zero

* $i_1 = 2$ – GAUSSIAN94 output is used to retrieve exponents and expansion coefficients of (uncontracted) molecular orbitals (it is assumed that the output is contained in gauss94.out and gauss94.pun files) and Coulomb and exchange potentials are initialized as in $i_1 = 1$ case; see routine PREPG94 for more details

* $i_1 = 3$ – GAUSSIAN94 modified output is used to retrieve exponents and expansion coefficients of molecular orbitals (it is assumed that the output is contained in gauss94l.out file) and Coulomb and exchange potentials are initialized as in $i_1 = 1$ case; see routine PREPG94L for details

* $i_1 = 5$ – initial orbitals and potentials are retrieved from disk files created in a previous run

* $i_1 = 6$ – orbitals and Coulomb potentials are retrieved from disk files and exchange potentials are initialized as in $i_1 = 1$ case (convenient when going from HFS to HF calculations)

i_2: specifies how exchange potentials will be read/written and manipulated (stored in memory). The program always keeps all orbitals and Coulomb potentials in core. The exchange potentials can also be all kept in core (if there is enough memory). However, during a relaxation of a particular orbital only a fraction of them is in fact needed. Thus all exchange potentials can be kept on disk as separate files (named fort.31, fort.32, ... during a run) and only relevant ones are being retrieved when necessary.[1]

* $i_2 = 0$ – read exchange potentials as separate files and write them back as separate files

---

[1]A note of warning for the users of the g77 compiler. You might encounter an I/O error when trying to run cases requiring more than 70 exchange potentials. By default g77 accepts file unit numbers in the range 0-99. If you need more files to be opened you have to edit f/runtime/libI77/fio.h in the g77 source tree, changing the line: #define MXUNIT 100. Change the line so that the value of MXUNIT is defined to be at least one greater than the maximum unit number needed.

* $i_2 = 1$ – read all exchange potentials in a file but write them out as separate files
* $i_2 = 2$ – read all exchange potentials separately but write them out as a single file
* $i_2 = 3$ – read and write exchange potentials in the form of a single file

i_3: if $i_1 = 1$ then this parameter must be set to 1 or 2. In such a case the initialization of each of the orbitals has to be defined in terms of the linear combination of atom centered hydrogen-like functions. For each orbital include a card of the following format (the order of orbitals should match the order specified under the **config** label):

Format: c_A n_A l_A ζ_A $\quad c_B$ n_B l_B ζ_B $\quad i_1$ $\quad [\, i_2 \,]$
where

c_A – mixing coefficient for a hydrogenic orbital on the Z_A centre (real),

n_A – its principle quantum number (integer)

l_A – its orbital quantum number (integer)

ζ_A – the effective nuclear charge if $i_3 = 1$ or a screening parameter if $i_3 = 2$ (real)

c_B – mixing coefficient for a hydrogenic orbital on the Z_B centre (real),

n_B – its principle quantum number (integer)

l_B – its orbital quantum number (integer)

ζ_B – the effective nuclear charge if $i_3 = 1$ or a screening parameter if $i_3 = 2$ (real)

i_1 – set to 1 to freeze the orbital during scf; otherwise set to 0 (integer)

i_2 – a number of successive over-relaxations for a given orbital (integer); if omitted is set to 10

○ **FEFIELD**

Format: fefield r

r: a strength of an external static electric field directed along the internuclear axis (in atomic units)

○ **MULTIPOL**

Format: multipol r

r: if $r > 0$ multipole moment expansion coefficients are recalculated when the maximum error in orbital energy is reduced by r (the default value is 1.15). To suppress recalculation of the coefficients set r to a negative real number. This is useful when generating potentials from a set of fixed orbitals, e.g from GAUSSIAN94 orbitals.

○ **SCF**

Format: scf $[\ i_1\ [\ i_2\ [\ i_3\ [\ i_4\ [i_5]\ ]\ ]\ ]\ ]$

i_1: maximum number of scf iterations (default 1000); to skip the scf step set i_1 to a negative integer,

i_2: every i_2 scf iterations orbitals and potentials are saved on disk (default 100). If $i_2 = 0$ functions are saved on disk upon completion of the scf process. If $i_2 < 0$ functions are never written to disk,

i_3: if the maximum error in orbital energy is less than 10^{-i_3} than the scf process is terminated (the default value is 10),

i_4: if the maximum error in orbital norm is less than 10^{-i_4} than scf process is terminated (the default is 10),

i_5: the level of output during scf process

* $i_5 = 1$ – the orbital convergence rate, orbital energy and normalization of every orbital is printed in every scf iteration

* $i_5 = 2$ – the orbital convergence rate, orbital energy and normalization of the worst converged orbital is printed in every scf iteration (default)

* $i_5 = 3$ – the orbital convergence rate, orbital energy and normalization of the worst converged orbital is printed every i_2 iterations. Printing of "... multipole moment expansion coefficients (re)calculated ..." communique is suppressed

Total energy is printed every i_2 iterations.

○ **FIX**

Format: fix $[\ i_1\ [\ i_2\ [\ i_3\ ]\ ]\ ]$

If i_1, i_2 or i_3 are set to 1 then orbitals, Coulomb potentials or exchange potentials, respectively, are kept frozen during the scf/sor process (the respective default values are 0, 0 and 2). If $i_3 = 2$ then exchange potentials are relaxed only once during an scf cycle. i_2 and i_3 cannot be set to 1 if hydrogenic orbitals are used to initiate the orbitals.

○ **XALPHA**

Format: xalpha *alpha*

If this label is present the Slater exchange approximation, i.e. $V_x = -\frac{3}{2}\alpha(\frac{3}{\pi}\rho)^{1/3}$, is used and the parameter α can be modified. This approximation is useful to quickly improve the initial HF orbitals. α is a real number and 0.7 is its default value.

○ **SOR**

Format: sor $[\, i_1 \, [\, i_2 \, [\, i_3 \,] \,] \,]$

Change default values of sor parameters.

i_1: the number of (MC)SOR iterations (over each subgrid) for a given function being relaxed in a single SCF cycle (the default value is 10)

i_2: a scaling factor used to change i_1 when relaxing potentials (see RELCOUL1/2 and RELEXCH1/2). The new value of (MC)SOR iterations is calculalated as i_1/i_2; the default value of i_2 is 1.

i_3: if $i_1 = 1(2)$ SOR (MCSOR) method is used to solve Poisson equations for orbitals and potentials (the default value is 1); if $i_1 = 3$ SOR method is used to solve Poisson equations for orbitals and MCSOR – for potentials

• **OMEGA**

Format: omega
$$\omega_{orb}^{(1)} \, [\, \omega_{orb}^{(2)} \, [\, \omega_{orb}^{(3)} \,] \,]$$
$$\omega_{pot}^{(1)} \, [\, \omega_{pot}^{(2)} \, [\, \omega_{pot}^{(3)} \,] \,]$$

Up to three real numbers in each line setting over-relaxation parameter ω for relaxation of orbitals and potentials for each subgrid. If the second or the third parameter is omitted, the value for the first subgrid is used.

Note that a semiempirical formula can be used to calculate a near-optimal value of ω_{pot} by specifying $\omega_{pot}^{(1)}$ as a negative real number.

○ **ORDER**

Format: order $[\, i_1 \, [\, i_2 \, [\, i_3 \,] \,] \,]$

Up to three integers defining the ordering of mesh points on subgrids.

$i_k = 1$: natural ordering

$i_k = 2$: 'middle' type of sweep (the default)

○ **FERMI**

    Format: fermi r_A r_B
        When this label is present, the Fermi nuclear charge distribution is used. r_A and r_B define the atomic masses (in amu) of nuclei A and B.

○ **GAUSS**

    Format: gauss r_A r_B
        When this label is present, the Gauss nuclear charge distribution is used. r_A and r_B define the atomic masses (in amu) of nuclei A and B.

○ **DEBUG**

    Format: debug $i_1 \dots i_{20}$
        Up to 20 different debug flags can be set at a time. If the integer i_k is encountered the debug flag i_k is set, i.e. idbg$(i_k) = 1$ $(1 \leq i_k < 600)$.

• **STOP**

    Format: stop
        This label indicates the end of input data.

Examples of input command cards

1. ^{2}S ground state of the Th^{+89} one-electron system.

```
TITLE
     Th+89  point/finite  nucleus R = 2.5
METHOD OED
NUCLEI  90.0 0.0  2.0
CONFIG 89
  1 sigma +  end
GRID 169 193  2.5
INITIAL  1 3 1
 1.0 1 0 90.0   0.0   1 0  1.0  0
SCF  30 10 8
omega
 1.80
 1.80
! fermi 232.0 0.0
STOP
```

2. First excited ^{2}S state of the Th^{+89} one-electron system.

```
TITLE
     Th+89  point/finite  nucleus R = 2.5
METHOD OED
NUCLEI  90.0 0.0  2.0
CONFIG 88
  1 sigma +
  1 sigma +  end
GRID 169 193  2.5
INITIAL  5 3 1
 1.0 2 0 90.0   0.0   1 0  1.0  0
 1.0 1 0 90.0   0.0   1 0  1.0  1 ! 1s orbital must be kept frozen
SCF  30 10 8
omega
 1.80
 1.80
!fermi 232.0 0.0
STOP
```

3. Hartree-Fock ground state of the beryllium atom.

```
TITLE
   Be R_inf=35.0 bohr  R = 2.3860 bohr
METHOD  hf ! or METHOD HFS
NUCLEI  4.0  0.0  2.386
CONFIG  0
        2 sigma  end
GRID    91 35.0
grid 169 35.0
INITIAL  1 3 1
 1.0   2 0 4.0     0.0   1 0 9.0   0 0
 1.0   1 0 4.0     0.0   1 0 9.0   0 0
SCF 300 10 8 12 1
! note that omega for potentials is set automatically
omega
  1.80
 -1.87
stop
```

4. Hartree-Fock ground state energy of the hydrogen molecule.

```
title
   H2: [169x193;35]  R = 1.4au
method hf
nuclei  1.0 1.0  1.4
!homo
!break
config 0
  1 sigma g end
!grid 169 193  35.0
grid 169  35.0
initial  1 3 1
 1.0 1 0 1.0   1.0   1 0  1.0  0
scf  2000 50 10
omega
 1.85
 1.87
stop
```

5. Hartree-Fock ground state of the BF molecule.

```
TITLE
   BF: R = 2.386 bohr
```

```
METHOD HF
NUCLEI  5.0  9.0  2.386
CONFIG  0
 1 pi
 5 sigma     end
! initial orbitals are taken from GAUSSIAN94 output (see bf.inp)
! bf_g94.out and bf_g94.pun files must be copied into a working
! directory as gauss94.out and gauss94.pun files, respectively
INITIAL  2 3
GRID 169 35.0
SCF 200 20 8
omega
 1.85
 1.97
multipol -1
fix 1 0 2        ! orbitals are not relaxed
STOP
```

6. HF calculations for the lowest ^3P state of the carbon atom.

```
TITLE
 3P C   R = 2.386
METHOD HF
NUCLEI  6.0  0.0  2.386
CONFIG  0
 1 pi   + . +
 1 sigma
 1 sigma    end
GRID    169 30.0
INITIAL   1 3 1
 1.0   2 1 5.0    0.0   1 0 9.0   0
 1.0   2 0 6.0    0.0   1 0 9.0   0
 1.0   1 0 6.0    0.0   1 0 9.0   0
SCF 400 20 12 12
omega
 1.80
 1.87
STOP
```

7. HF calculations for the lowest ^2P state of the C^+ ion.

```
TITLE
```

```
   1P C+   R = 2.386
METHOD HF
NUCLEI  6.0  0.0  2.386
CONFIG  1
 1 pi    +
 1 sigma
 1 sigma    end
GRID   169 30.0
INITIAL   1 3 1 ! or INITIAL  5 3 1 and using 3P results
 1.0   2 1 5.0     0.0   1 0 9.0   0
 1.0   2 0 6.0     0.0   1 0 9.0   0
 1.0   1 0 6.0     0.0   1 0 9.0   0
SCF 500 20 7
omega
 1.82
 1.87
STOP
```

8. HF calculations for the lowest state of the C_2 molecule.

```
TITLE
   C2      R = 2.358
METHOD HF
NUCLEI  6.0 6.0 2.358
homo
!break
CONFIG  0
 1 pi     u
 1 sigma u
 1 sigma g
 1 sigma u
 1 sigma g end
GRID   169 193 40.0
INITIAL   2 3 0
! just a couple of dozen iterations to start with
SCF 50 10 10 10 1
! note the small value of overrelaxation parameter for orbitals
! often initial scf/sor iterations have to be require slower
! convergence rates
omega
 1.25
 1.85
STOP
```

```
TITLE
   C2      R = 2.358
METHOD HF
NUCLEI  6.0 6.0 2.358
homo
!break
CONFIG  0
 1 pi     u
 1 sigma u
 1 sigma g
 1 sigma u
 1 sigma g end
GRID  169 193 40.0
INITIAL   5 3 0
SCF 500 10 10 10 1
! the overrelaxation parameter for potentials is at its more or less
! optimal value
omega
 1.75
 1.85
STOP
```

9. HF calculations for the lowest state of the N_2 molecule.

```
TITLE
    N2      R = 2.068
METHOD HF
NUCLEI  7.0 7.0 2.068
homo
CONFIG  0
 1 pi     u
 1 sigma g
 1 sigma u
 2 sigma g
 1 sigma u end
GRID  169 193 40.0
INITIAL   1 3 1
 0.5   2 1 5.0     0.5   2 1 5.0   0
 1.5   2 1 5.0     0.0   2 1 5.0   0
 0.5   2 0 7.0    -0.5   2 0 7.0   0
 0.5   2 0 7.0     0.5   2 0 7.0   0
 0.5   1 0 7.0     0.5   1 0 7.0   0
```

```
    0.5    1 0 7.0    -0.5    1 0 7.0    0
   SCF 2000 10 10 10 2
   omega
    1.65
    1.85
   STOP
```

10. HF calculations for the lowest state of the F_2 molecule.

```
   TITLE
    F2      R = 2.668   (1.4118449A)
   METHOD HF
   NUCLEI  7.0 7.0 2.668
   homo
   !break
   CONFIG  0
    1 pi     u
    1 sigma g
    1 sigma u
    1 sigma g
    1 sigma u
    1 sigma g end
   GRID   169 193 40.0
   INITIAL   2 3
   SCF 100 10 10 10
   omega
    1.75
    1.75
   STOP
```

Description of the data file structure of the program

There are several standard names used by the program to keep track of its input and output disk files. Normally the program writes out the data in the course of computations and upon the completion into the following disk files:

2dhf_output.orb containing molecular orbitals (in the order specified by the input data following **config** label) followed by their normalization factors, orbital energies, Lagrange multipliers and multipole moment expansion coefficients (see WTDISK for more details),

2dhf_output.coul containing corresponding Coulomb potentials and

2dhf_output.exch containing all exchange potentials if i_2 parameter on **initial** card is 2 or 3 or

fort.31, fort.32, ... if i_2 is 0 or 1 where each file contains the exchange potential for a particular pair of orbitals.

If i_1 parameter on **initial** card is 5 the orbitals are retrieved from **2dhf_input.orb** file, Coulomb potentials from **2dhf_input.coul** and exchange potentials from **2dhf_input.exch** file (or **fort.31**, **fort 32**, ... files). Note that there is only one set of **fort**.i files.

How to run the program?

In order to simplify the usage of the program, the xhf script is provided which facilitates handling of the disk files. The command xhf requires one, two or three parameters:

xhf c_1 [c_2 [c_3]]

where

- c_1 is either

  - the prefix of a command data file which name is of the form c_1.data,

  - *rename* to change the names of temporary files with 2dhf_input-/2dhf_output prefixes into the corresponding names with prefixes specified by c_2 and/or c_3 strings. This is useful when the command xhf is aborted and files with 2dhf_input/2dhf_output prefixes are left. It is thus recommended that the process x2dhf itself should be killed, if necessary, not xhf itself.

  - *remove* to remove all temporary files.

- c_2 is either

  - the prefix of names of output files produced by the program if c_2 is the last command argument, i.e. the output files 2dhf_output.orb, 2dhf_output.coul and 2dhf_output.exch (fort.31, ...) are renamed as c_2.orb, c_2.coul, c_2.exch (c_2.fort.31, ...), respectively,

  - the prefix of names of input files required by the program to continue calculations, i.e. the input files c_2.orb, c_2.coul, c_2.exch (c_2.fort.31, ...) are moved into 2dhf_input.orb, 2dhf_input.coul, and 2dhf_input.exch (fort.31, ...).

- c_3 is the prefix of names of output files generated by the program.

If, for example, `be.data` file contains input data cards for the beryllium atom (see Example 3) then

xhf be be-1

starts and performs the first 300 scf iterations. Type

xhf be be-1 be-2

to continue calculations. In order to converge the scf process increase the maximum value of the scf iterations and use the following command

xhf be be-2 be-1

How to stop the program?

How to abort the program during a lengthy calculation without killing the process and interrupting the disk read/write operations which can well happen when separate files for the exchange potentials are being used? All you have to do is to create a (zero length) file named **stop_x2dhf** in a working directory (the Unix **touch** command will do the job). The program aborts gracefully whenever this file is detected upon the completion of a current orbital/potential relaxation.

Useful hints

- The program should be easy to use provided you can start a calculation for a specific system. You should not encounter any serious problems when the system contains atoms from the first two rows of the Periodic Table. Then even the rough hydrogenic estimates of the orbitals should prove adequate and after the initial couple of dozen of iterations a smooth convergence should set in.

  If, however, a system contains more than 15-20 electrons the initial estimates of the orbitals have to be good enough to avoid divergences. Then, you have to choose the parameters of the hydrogenic orbitals carefully or perform the finite basis set calculations using the Gaussian94 to provide the initialization data for orbitals.

- Do not start calculations on too dense a grid. For example, the 61×61 grid is sufficient to check the quality of the initial data for the Ne_2 system.

- At the very beginning set the maximum number of scf iterations to something between 20 and 50 and/or impose crude convergence criteria for the orbital energy and normalization.

- Choose small values of the relaxation parameters ($1 < \omega < 1.2$) to avoid divergence in the first few dozens of iterations. Later on the parameters should be increased to a desired (optimum) values (see the Ne_2 example).

The dependence of the optimum value of the relaxation parameter ω_{pot} on the grid size is illustrated by the following table:

$n_\nu \times n_\mu$	ω_{pot}
50×50	1.89
100×100	1.94
159×100	1.96
300×300	1.98

Now it is possible to set ω_{pot} to its near-optimal value by using a semiempirical formula (B.Sobczak MSc Thesis, Torun 2002); see the description of the $OMEGA$ label above.

Optimum values of the orbital relaxation parameter are somewhat smaller and are not directly related to the grid size. In most cases choosing $1.75 \leq \omega_{orb} \leq 1.85$ should lead to fairly good convergence rates.