DoNOF is a computational chemistry software program that stands for
Donostia Natural Orbital Functional. The original code started on
January 21, 2009 as PNOFID. It will run on essentially any machine
with a FORTRAN 90 compiler for 64 bit processing.

DoNOF can perform computational chemistry calculations based on the
Natural Orbital Functional Theory (NOFT), including PNOF5, PNOF6 and
PNOF7. Correlation corrections after PNOF calculations can be
estimated by second order perturbation theories. The total spin is
conserved, not just the spin projection.

The solution is established optimizing the energy functional with
respect to the occupation numbers (ONs) and to the natural orbitals
(NOs), separately. The constrained nonlinear programming problem for
the ONs is treated under pairing restrictions as an unconstrained
minization, while the orbital optimization is carried out by a
self-consistent procedure which yields the NOs automatically
orthogonal. To achieve convergence, the direct inversion of the
iterative subspace (DIIS) extrapolation technique is used, and a
variable scale factor balances the symmetric matrix subject to the
iterative diagonalizations.

The &INPRUN and &NOFINP namelists specify the input and output, and
the fundamental job options. These options are controlled by the
following keywords:

```
C------------------------------------------------------------------------
C                      --- NAMELIST VARIABLES ---
C------------------------------------------------------------------------
C
C RUNTYP             specifies the run calculation
C      = ENERGY      1) single-point energy calculation (Default)
C      = GRAD        2) energy + gradients with respect to nuclear coord.
C      = OPTGEO      3) optimize the molecular geometry
C
C MULT               Multiplicity of the electronic state
C      = 1           singlet (Default)
C      = 2,3,...     doublet, triplet, and so on
C
C ICHARG             Molecular charge
C      = 0           Neutral Molecule (Default)
C
C IECP               Effective Core Potentials (to be implemented)
C      = 0           (Default) All electron calculation
C      = 1           Read ECP potentials in the $ECP group
C
C IEMOM              Electrostatic moments calculation
C      = 1           calculate dipole moments (Default)
C        2           also calculate quadrupole moments
C        3           also calculate octopole moments
C
C UNITS              Distance units (any angles must be in degrees)
C      = ANGS        Angstroms (Default)
C      = BOHR        Bohr atomic units
C
C EVEC               An array of the three x,y,z components of
C                    the applied electric field, in a.u.
C                    (1 a.u. = 1 Hartree/e*bohr = 5.1422082(15)d+11 V/m)
C      = 0.0D0       (Default)
C
C DONTW              Do not write 2e- integrals on the disk (Unit=1)
C      = T           (Default)
C
C------------------------------------------------------------------------
C     NAMELIST/INPRUN/RUNTYP,MULT,ICHARG,IECP,IEMOM,UNITS,EVEC,DONTW
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C     Initial Values for the namelist variables
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
      RUNTYP = ENERGY
      MULT   = 1
      ICHARG = 0
      IECP   = 0
      IEMOM  = 1
```

```
      UNITS  = ANGS
      EVEC   = 0.0D0      ! EVEC(1,2,3)=0
      DONTW  = .TRUE.


***********************************************************************

C-----------------------------------------------------------------------
C                       --- NAMELIST VARIABLES ---
C-----------------------------------------------------------------------
C
C.......... MAXIT              Maximum number of OCC-SCF iterations
C                     = 1000   (DEFAULT)
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C Type of Calculation
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C.......... ICOEF              Energy Optimization with respect NOs
C                     = 0      Optimize only with respect to ONs
C                     = 1      Optimize by the ONs and NOs (DEFAULT)
C                     = 2      Optimize only by NOs keeping fixed ONs
C                     = 3      Optimize by all ONs and core-fragment
C                              orbitals. The rest of fragment orbitals
C                              remain frozen
C
C.......... IEINI              Calculate only the initial energy
C                     = 0      (DEFAULT)
C
C.......... NO1                Max. index of NOs with Occupation = 1
C                     = -1     Consider Core NOs (DEFAULT)
C                     = 0      All NOs are considered
C                     = Value  User specifies how many NOs have OCC.=1
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C Hartree-Fock
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C.......... HFID               Use the Iterative Diagonalization Method
C                              to generate the HF Orbitals
C                     = T      (DEFAULT)
C
C.......... NTHRESHEID         Convergence of the TOTAL ENERGY
C                              THRESHEID=10.0**(-NTHRESHEID)
C                     = 8      (DEFAULT)
C
C.......... MAXITID            Maximum number of external iterations
C                     = 30     (DEFAULT)
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C PNOF Selection
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C.......... IPNOF              Type of Natural Orbital Functional (NOF)
C                     = 5      PNOF5
C                     = 6      PNOF6
C                     = 7      PNOF7 (DEFAULT)
C
C.......... Ista               Use Static version of PNOF7
C                     = 0      PNOF7 (DEFAULT)
C                     = 1      PNOF7s
C
C.......... HighSpin           Spin-uncompensated calculation type
C                     = F      (DEFAULT) Multiplet state (Ms=0)
C                     = T      High-spin uncompensated state (Ms=S)
C
C.......... NCWO               Number of coupled weakly occupied MOs
C                              per strongly occupied = Nc -> PNOFi(Nc)
C                     = 1      NCWO = 1 (DEFAULT)
C                     = 2,3,...
C                     =-1      NCWO = NVIR/NDOC
C                              NVIR: Number of HF virtual  MOs (OCC=0)
C                              NDOC: Number of strongly occupied MOs
C
```

```
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C Convergence Criteria in NOF calculation
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C.......... NTHRESHL              Convergence of the Lagrange Multipliers
C                                 THRESHL=10.0**(-NTHRESHL)
C                     = 4         (DEFAULT)
C
C.......... NTHRESHE              Convergence of the total energy
C                                 THRESHE=10.0**(-NTHRESHE)
C                     = 8         (DEFAULT)
C
C.......... NTHRESHEC             Convergence of the total energy (ORBOPT)
C                                 THRESHEC=10.0**(-NTHRESHEC)
C                     = 10        (DEFAULT)
C
C.......... NTHRESHEN             Convergence of the total energy (OCCOPT)
C                                 THRESHEN=10.0**(-NTHRESHEN)
C                     = 10        (DEFAULT)
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C Options for the Orbital Optimization Program (ID Method)
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C.......... NOPTORB               Number of the optimized orbitals
C                     = NBF       (DEFAULT)
C
C.......... MAXLOOP               Maximum Iteration Number for the SCF-
C                                 iteration cycle in each ITCALLs
C                     = 30        (DEFAULT)
C
C     The straightforward iterative scheme fails to converge very
C     often due to the values of some off-diagonal elements Fki. The
C     latters must be suffciently small and of the same order of
C     magnitude. A variable factor scales Fki. We establish an upper
C     bound B, in such a way that when the absolute value of the
C     matrix element Fki is greater than B, it is scaled by a factor
C     Cki (F'ki = Cki*Fki ), as to satisfy ABS(Fki) <= B.
C
C.......... SCALING               A variable factor scales Fki
C                     = T         (DEFAULT)
C
C.......... NZEROS                B = 10.0**(1-NZEROS).
C                                 Initial number of ZEROS in Fij. The
C                                 scaling factor varies until the number
C                                 of ZEROS (.000##) is equal for all
C                                 elements Fij.
C                     = 0         B = 10.0 (DEFAULT)
C
C.......... NZEROSm               B = 10.0**(1-NZEROSm)
C                                 Maximum number of zeros in Fij.
C                     = 4         B = 10.0 (DEFAULT)
C
C.......... NZEROSr               B = 10.0**(1-NZEROSr)
C                                 Number of zeros in Fij to restart
C                                 automatically the calculation.
C                     = 0         B = 10.0 (DEFAULT)
C
C.......... ITZITER               Number of Iterations for constant scaling
C                     = 10        (DEFAULT)
C
C.......... DIIS                  Direct Inversion in the Iterative
C                                 Subspace in the orbital optimization if
C                                 DUMEL < THDIIS every NDIIS loops
C                     = T         (DEFAULT)
C
C.......... NTHDIIS               Energy threshold to begin DIIS
C                     = 3         THDIIS = 10.0**(-NTHDIIS) (DEFAULT)
C
C.......... NDIIS                 Number of considered loops to interpolate
C                                 the generalized Fock matrix in the DIIS
C                     = 5         (DEFAULT)
C
```

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C.......... PERDIIS         Periodic DIIS
C                  = T       Apply DIIS every NDIIS (DEFAULT)
C                  = F       DIIS is always applied after NDIIS
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C Options for pertubative calculations
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C.......... OIMP2           NOF - Orbital Invariant MP2
C                  = F       (DEFAULT)
C
C.......... NO1PT2          Frozen MOs in perturbative calculations
C                           Maximum index of NOs with Occupation = 1
C                  = -1      = NO1 (DEFAULT)
C                  = 0       All NOs are considered
C                  = Value   User specifies how many NOs are frozen
C
C.......... SC2MCPT         SC2-MCPT perturbation theory is used to
C                           correct the PNOF5 Energy.
C                           2 outputs: PNOF5-SC2-MCPT and PNOF5-PT2
C                  = F       (DEFAULT)
C
C.......... NEX             Number of excluded coupled orbitals
C                           in the PNOF5-PT2 calculation
C                  = 0       All NOs are included (DEFAULT)
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C Input Options for Gamma (Occ), C and Diagonal F
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C                  --- Restart Options ---
C
C.......... RESTART         Restart from GCF file (DEFAULT=F)
C                  = F       INPUTGAMMA=0,INPUTC=0,INPUTFMIUG=0
C                  = T       INPUTGAMMA=1,INPUTC=1,INPUTFMIUG=1
C
C.......... INPUTGAMMA      Guess for GAMMA variables (ONs)
C                  = 0       Close Fermi-Dirac Distribution (DEFAULT)
C                  = 1       Input from file GCF
C
C.......... INPUTC          Guess for Coefficient matrix (NOs)
C                  = 0       Use HCORE or HF Eigenvectors (DEFAULT)
C                  = 1       Input from file GCF
C
C.......... INPUTFMIUG      Guess for Diagonal elements (FMIUG0)
C                  = 0       Use single diag. of Lagragian (DEFAULT)
C                  = 1       Input from file GCF
C
C.......... INPUTCXYZ       Nuclear Coordinates (CXYZ)
C                  = 0       Input from input file (*.inp) (DEFAULT)
C                  = 1       Input from file GCF
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C Output Options
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C.......... NPRINT          Output Option (DEFAULT VALUE: 0)
C                  = 0       Short Printing (Occ,Emom,Energies)
C                  = 1       Output at initial and final iterations
C                  = 2       Output everything in each iteration
C
C.......... IWRITEC         Output Option for the Coefficient matrix
C                  = 0       No output (DEFAULT)
C                  = 1       Output the Coefficient Matrix (NOs)
C
C.......... IMULPOP         Mulliken Population Analysis
C                  = 0       Not do it (DEFAULT)
C                  = 1       Do it
C
C.......... PRINTLAG        Output Option for Lagrange Multipliers
C                  = F       No Output (DEFAULT)
C
C.......... DIAGLAG         Diagonalize Lagrange Multipliers
```

```
C                                    Print new 1e- Energies, Canonical MOs,
C                                    and new diagonal elements of the 1RDM
C                      = F           Not do it (DEFAULT)
C
C.......... IEKT                     IPs by Ext. Koopmans' Theorem (EKT)
C                      = 0           Not calculate the IPs
C                      = 1           Calculate ionization potentials (IPs)
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C.......... IAIMPAC                  Write information into WFN file (UNIT 7)
C                                    for THE AIMPAC PROGRAM
C                      = 0           DO NOT DO
C                      = 1           Write INTO WFN file (DEFAULT)
C
C.......... NOUTRDM                  Print OPTION for ATOMIC RDMs
C                      = 0           NO Output (DEFAULT)
C                      = 1           Print ATOMIC RDMs IN 1DM and 2DM files
C
C.......... NTHRESHDM                THRESHDM=10.0**(-NTHRESHDM)
C                      = 6           (DEFAULT)
C
C.......... NSQT                     Print OPTION for 2DM file
C                      = 1           UNforMATTED (DEFAULT)
C                      = 0           forMATTED (SEE SUBROUTINE OUTPUTRDMrc)
C
C.......... NOUTCJK                  Print OPTION for CJ12 and CK12
C                      = 0           NO Output (DEFAULT)
C                      = 1           Print CJ12 and CK12 in file 'CJK'
C
C.......... NTHRESHCJK               THRESHCJK=10.0**(-NTHRESHCJK)
C                      = 6           (DEFAULT)
C
C.......... NOUTTijab                Print OPTION for Tijab
C                      = 0           NO Output (DEFAULT)
C                      = 1           Print Tijab in file 'Tijab'
C
C.......... NTHRESHTijab             THRESHTijab=10.0**(-NTHRESHTijab)
C                      = 6           (DEFAULT)
C
C.......... APSG                     Open an APSG file for printing the
C                                    coefficient matrix ($VEC-$END) and the
C                                    expansion coefficients of the APSG
C                                    generating wavefunction.
C                      = F           No Output (DEFAULT)
C
C.......... NTHAPSG                  Threshold for APSG expansion coefficient
C                                    THAPSG = 10.0**(-NTHAPSG)
C                      = 10          (DEFAULT)
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C Optional Options
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C.......... ORTHO                    Orthogonalize the initial orbitals
C                      = F           No
C                      = T           Yes (DEFAULT)
C
C.......... CHKORTHO                 Check the Orthonormality of the MOs
C                      = F           No (DEFAULT)
C                      = T           Yes
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C Options related to Frozen coordinates in gradient computation
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C.......... FROZEN                   Is there any fixed coordinate
C                      = F           (DEFAULT)
C
C.......... IFROZEN                  By pairs, what coordinate of which atom,
C                                    e.g. 2,5,1,1 means "y" coordinate of
C                                    atom 5 and "x" coor of atom 1 to freeze.
C                                    MAXIMUM of frozen coordinates = 10
```

```
C                                = 0        (DEFAULT)
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
C
C.......... ICGMETHOD             Define the Conjugate Gradient Method in
C                                 OCCOPTr, CALTijabIsym and OPTIMIZE
C                       = 1       (DEFAULT)
C                                 SUMSL: CGOCUPSUMSLr,OPTSUMSL
C                                 SparseSymLinearSystem_CG
C                       = 2       Use NAG subroutines:
C                                 E04DGF: OPTCGNAG,CGOCUPNAGr
C                                 F11JEF: SparseSymLinearSystem_NAG
C                       = 3       LBFGS: OPTLBFGS, LBFGSOCUPr
C
C-----------------------------------------------------------------------------
      NAMELIST/NOFINP/MAXIT,ICOEF,IEINI,NO1,HFID,NTHRESHEID,MAXITID,
     &                IPNOF,Ista,HighSpin,NCWO,NTHRESHL,NTHRESHE,
     &                NTHRESHEC,NTHRESHEN,NOPTORB,MAXLOOP,SCALING,
     &                NZEROS,NZEROSm,NZEROSr,ITZITER,DIIS,NTHDIIS,
     &                NDIIS,PERDIIS,SC2MCPT,NO1PT2,NEX,OIMP2,
     &                RESTART,INPUTGAMMA,INPUTC,INPUTFMIUG,INPUTCXYZ,
     &                NPRINT,IWRITEC,IMULPOP,APSG,NTHAPSG,PRINTLAG,
     &                DIAGLAG,IAIMPAC,IEKT,NOUTRDM,NTHRESHDM,NSQT,
     &                NOUTCJK,NTHRESHCJK,NOUTTijab,NTHRESHTijab,
     &                ORTHO,CHKORTHO,FROZEN,IFROZEN,ICGMETHOD
C-----------------------------------------------------------------------------
C     Preset values to namelist variables
C-----------------------------------------------------------------------------
      MAXIT=1000

C     Type of Calculation
      ICOEF=1
      IEINI=0
      NO1=-1

C     Hartree-Fock
      HFID=.TRUE.
      NTHRESHEID=8
      MAXITID=30

C     PNOF Selection
      IPNOF=7
      Ista=0                                   ! PNOF7n
      HighSpin=.FALSE.                         ! Multiplet
      NCWO=1                                   ! Perfect Pairing

C     Convergence Criteria in NOF calculation
      NTHRESHL=4
      NTHRESHE=8
      NTHRESHEC=10
      NTHRESHEN=10

C     Options for the Orbital Optimization Program (ID Method)
      NOPTORB=-1                               ! NOPTORB=NBF
      MAXLOOP=30
      SCALING=.TRUE.
      NZEROS=0
      NZEROSr=0
      NZEROSm=NTHRESHL                         ! NTHRESHL
      ITZITER=10
      DIIS=.TRUE.
      NTHDIIS=3
      NDIIS=5
      PERDIIS=.TRUE.

C     Options for pertubative calculations
      SC2MCPT=.FALSE.
      NEX=0
      NO1PT2=-1
      OIMP2=.FALSE.

C     Input Options for Gamma (Occ), C and Diagonal F
      RESTART=.FALSE.
```

```
        INPUTGAMMA=0
        INPUTC=0
        INPUTFMIUG=0
        INPUTCXYZ=0

C       Output Options
        NPRINT=0

C       for NPRINT>0
        IWRITEC=0
        IMULPOP=0
        APSG=.FALSE.
        NTHAPSG=10
        PRINTLAG=.FALSE.
        DIAGLAG=.FALSE.   ! Only in the final Output
        IAIMPAC=1
        IEKT=0            ! Only in the final Output
C
        NOUTRDM=0
        NTHRESHDM=6
        NSQT=1
C
        NOUTCJK=0
        NTHRESHCJK=6
        NOUTTijab=0
        NTHRESHTijab=6

C       Optional Options
        ORTHO=.TRUE.
        CHKORTHO=.FALSE.

C       Frozen coordinates
        FROZEN=.FALSE.
        IFROZEN=0

C       Options for the Conjugate Gradient Method
        ICGMETHOD=1
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```