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-----------------------------------------------------------------------
      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 to 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.......... KOOPMANS            Calculate IPs using Koopmans' Theorem
C                     = 0       (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
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
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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)
```

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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- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
```