This group governs the Localized Molecular Orbital Energy Decomposition Analysis (LMOEDA) and the General Kohn-Sham Energy Decomposition Analysis (GKSEDA). The wave functions of the monomers maybe RHF, ROHF, or UHF, the DFT counterparts of each of these, the MP2 counterparts of each of these, or CCSD and CCSD(T) for RHF and ROHF references. Furthermore, division of the system into "monomers" can involve splitting chemical bond pairs, as the MMULT example below shows.

If one or more monomers are open shell, to be treated by ROHF, use SCFTYP=ROHF in $CONTRL. Whenever a monomer has an even number of electrons, so that its MMULT=1 below, SCFTYP=ROHF (or UHF) automatically reduces to RHF on that monomer. Note that open shell monomers sometimes have more than one possible electron occupancy (for example, oxygen atom can fill 3 p orbitals by 4 electrons in various ways), in which case the energy decomposition isn't unique.

General keywords for LMOEDA, GKSEDA, and XEDA.

➢ MATOM = an array giving the number of atoms in each monomer. Up to ten monomers may be defined. Your input in $DATA must have all the atoms in the first monomer defined before the atoms in the second monomer, before the third monomer etc. The sum of the MATOM array must be equal to the total number in the supermolecule.

➢ MCHARG = an array giving the charge of each monomer. Up to ten monomers may be defined. The sum of the charges in the monomers must be equal to the total charge of the supermolecule.

➤ MMULT = an array giving the multiplicity of each monomer. Up to ten monomers may be defined. A positive integer means alpha spin, a negative integer means beta spin. For example, if an ethane molecule is separated into two neutral CH3 groups, MMULT(1)=2,-2 or MMULT(1)=-2,2.

➤ SUPBAS = a flag to request Boys and Bernardi style counterpoise method for correcting basis set superposition errors. (default is .TRUE.). Usually it works well with Hartree-Fock and MP2 and coupled cluster methods, but less well with DFT methods due to SCF divergent problems.

Keywords for XEDA.

XEDA can do GKSEDA using DFT, do CMOEDA/LMOEDA using Hartree-Fock, MP2, CCSD, CCSD(T), also PCM for all above methods.

➤ EDATYP = NONE, will choose the old version of GKSEDA or LMOEDA.

= GKS, will do the general energy decomposition analysis procedure. (Default).

= BSEDA, will do the GKSEDA(BS) method for open shell singlet.

➤ RDVECM = a flag to request reading vector groups from input file. $VEC0 for supermolecule, $VEC1,2,… for monomers with no BSSE correction, and $VEA1,2,… for monomers with BSSE correction. You can give only the desired vector(s). (Default is .FALSE.)

➤ ITRTN = a flag to request SCF procedure to optimize the wave functions of monomers and supermolecule. If you set this keyword to .FALSE., it will only read the $VEC0,1,2,… from input file and skip SCF procedures. For "ITRTN=FALSE", $VEC0, $VEC1, $VEC2,… must be given, $VEA1,2,… are optional. (Default is .TRUE.)

Additional keywords for GKSEDA(BS)

➢ MULTH = similar to MULT in $CONTRL for high spin state.

➢ MMULTH = similar to MMULT for high spin state.

$VEC0, $VEC1, $VEC2, … are available. $VEC0 and $VEH0 are for the broken symmetry state and the high spin state of supermolecule, respectively. If the Nth monomer is in broken symmetry state, $VECN and $VEHN (N is a number) may be needed for the broken symmetry state and high spin state calculation of this monomer, respectively.

The papers describing this method is

LMOEDA: P. Su, H. Li   J. Chem. Phys. 131, 014102/1-15(2009);

EDAPCM: P. Su, H. Liu, W. Wu   J. Chem. Phys. 137, 034111/1-15(2012);

GKSEDA: P. Su, Z. Jiang, Z. Chen, W. Wu   J. Phys. Chem. A 118, 2531-2542(2014);

        P. Su, Z. Tang, W. Wu   WIREs Comput. Mol. Sci. 10, e1460(2020);

GKSEDA(BS):

Z. Tang, Z. Jiang, H. Chen, P. Su, W. Wu   J. Chem. Phys. 151, 244106(2019);

XEDA program:

Z. Tang, Y. Song, S. Zhang, W. Wang, Y. Xu, D. Wu, W. Wu, P. Su   J. Comput. Chem. 42, 2341-2351(2021).

Notes:

If you choose "EDATYP=NONE", the program will perform EDA with the old EDA version, the result is the same but the consumption may increase.

Scalar relativistic effects can be handled by ECP or MCP, but at present, all electron treatment by RELWFN is not enabled.

Example for XEDA:

```
$contrl scftyp=rhf runtyp=eda dfttyp=b3lyp
         icharg=0 mult=1 maxit=200 $end
$lmoeda matom(1)=3 3 mcharg(1)=0 0 mmult(1)=1 1
         edatyp=gks rdvecm=.t. itrtn=.f. $end          ! itrtn=.f. will skip SCF.
$basis gbasis=acct $end
$scf diis=.t. soscf=.f. dirscf=.t. fdiff=.f. $end
$system memddi=1000 mwords=300 $end
$data
XEDA for water dimer
C1
O               8.0     1.6664883870     0.9195873854     0.1851692504
H               1.0     2.5106282005     0.4594506739     0.2246786378
H               1.0     1.7150338756     1.4448894608    -0.6195549272
O               8.0    -0.5000731323    -1.0068295710    -0.0251256108
H               1.0     0.1805984081    -0.3334561615     0.1212220972
H               1.0    -1.1187977889    -0.8842193875     0.6990610826
$end
$vec0
......       !the wave function of supermolecule.
$end
$vec1
......       !the wave function of monomer 1.
$end
$vec2
......       !the wave function of monomer 2.
$end
$vea1
......       !the wave function of monomer 1 with BSSE correction.
$end
$vea2
......       !the wave function of monomer 2 with BSSE correction.
$end
```

Example: single point energy calculation of one fragment with BSSE correction.

(See GAMESS manual $DATA)

```
$contrl scftyp=rhf runtyp=energy dfttyp=b3lyp
         icharg=0 mult=1 maxit=200 $end
$basis gbasis=acct $end
$scf diis=.t. soscf=.f. dirscf=.t. fdiff=.f. $end
$system memddi=1000 mwords=300 $end
$data
XEDA for water dimer
C1
O              8.0     1.6664883870     0.9195873854     0.1851692504
H              1.0     2.5106282005     0.4594506739     0.2246786378
H              1.0     1.7150338756     1.4448894608    -0.6195549272
O             -8.0    -0.5000731323    -1.0068295710    -0.0251256108
H             -1.0     0.1805984081    -0.3334561615     0.1212220972
H             -1.0    -1.1187977889    -0.8842193875     0.6990610826
$end
```

Note that if ZNUC is negative, the internally stored basis for ABS(ZNUC) is placed on this center, but the calculation uses ZNUC=0 after this. This is useful for basis set superposition error (BSSE) calculations.