# NEB Release 2: Note

M. Haruta, T. Asada, S. Koseki, OPU
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**New features…**
The climbing image method has been installed, so that TSLOCT=.true. is available now. This means that a transition state can be located by using runtyp=nebpath.
Several utility scripts are also prepared for your analyses.

**Modifications…**
1. Most papers use "image" instead of "bead", so that we have replaced the word "bead" by "image". Then, you have to use IMAGES (number of images between reactant and product), instead of NBEADS, in $NEB group. When you restart your job, you have to use $IMAGESX group, instead of $BEADSX group. Or you have to copy and paste $IMAGESX group, instead of $BEADSX group, from your .DAT file.
2. You have to use DELTAT, instead of QUCKDT, in $NEB group. This parameter is a step size for the optimization of reaction path.
3. The whole printings in nebpath routines were cleaned up.
4. A few minor bugs for gradient RMSs were removed.
5. The maximum number of images is set to 200. This affects the record number for the dictionary file.
6. Several options were renamed as shown in the manual, so that the old input files may not be able to be used anymore.
7. Multiple criteria for the convergence of reaction paths are employed: OPTTOL, OPMTOL, CRDTOL, and CRMTOL. See the manual for details. You have to be careful for their units.

**Useful suggestions…**
Many iterations (or optimization cycles) will be needed for good convergence of a reaction path. This means that the energy gradients perpendicular to the reaction path are often large even after many iterations. You many decide to use TSLOCT=.true. or RUNTYP=sadpoint for the next run.

**Source…** nebpath.src

**Manuals…** (see below)

**Test jobs…** "exams" directory
exam01: path for the C–C rotation in ethane at the RHF/6-31++G(d,p) level of theory.
Wall clock time of 27 seconds with Xeon-T5570(2.93GHz)/8 cores of 4 nodes.
Wall clock time of 39 seconds with Core i7-7800X(3.5GHz) 4 cores.
exam02: path for the C–C rotation in ethane at the M06-2X/6-31++G(d,p) level of theory.
Wall clock time of 174 seconds with Xeon-T5570(2.93GHz)/8 cores of 4 nodes.
Wall clock time of 292 seconds with Core i7-7800X(3.5GHz) 4 cores.
exam03: path for the C–C rotation in ethane at the MP2/6-31++G(d,p) level of theory.
Wall clock time of 104 seconds with Xeon-T5570(2.93GHz)/8 cores of 4 nodes.
Wall clock time of 125 seconds with Core i7-7800X(3.5GHz) 4 cores.
exam04: (test for climbing image method) cis-trans isomerization of butadiene at the RHF/6-31+G(d) level of theory.
Wall clock time of 33 seconds with Xeon-T5570(2.93GHz)/8 cores of 4 nodes.
Wall clock time of 32 seconds with Core i7-7800X(3.5GHz) 4 cores.
exam05: 1,5-hydrogen migration in malon-aldehyde within Cs symmetry.
Wall clock time of 165 seconds with Xeon-T5570(2.93GHz)/8 cores of 4 nodes.
Wall clock time of 364 seconds with Core i7-7800X(3.5GHz) 4 cores.
exam06: 1,5-hydrogen migration in malon-aldehyde with MAXCYC=5.

Wall clock time of 77 seconds with Xeon-T5570(2.93GHz)/8 cores of 4 nodes.
Wall clock time of 128 seconds with Core i7-7800X(3.5GHz) 4 cores.

exam07: 1,5-hydrogen migration in malon-aldehyde with restart option.
Wall clock time of 61 seconds with Xeon-T5570(2.93GHz)/8 cores of 4 nodes.
Wall clock time of 147 seconds with Core i7-7800X(3.5GHz) 4 cores.

exam08: (test for MCSCF with MAXCYC=1) cis-trans isomerization of butadiene at the MCSCF(8e,8MOs)/6-31++(d,p) level of theory.
Wall clock time of 23648 seconds with Xeon-T5570(2.93GHz)/8 cores of 4 nodes.
Wall clock time of 9033 seconds with Core i7-7800X(3.5GHz) 4 cores.
MAXCYC=3 ---
Wall clock time of 15589 seconds with Core i7-7800X(3.5GHz) 4 cores.

**Tools** (ba-shell scripts)**…** (This part was modified entirely.)

~~1. tool-exterd.sh: pick up the coordinates in the cc1 format (Chem3D) and the xyz format (ChemCraft).~~

~~2. tool-cc1-xyz.sh: change the cc1 format (Chem3D) into the xyz format (ChemCraft).~~

~~3. tool-exterd-overlap.sh: pickup the coordinates and create an overlap images of all images along your reaction path. This script generates both the cc1 format (Chem3D) and the xyz format (ChemCraft) for the purpose of understanding reaction paths.~~

~~4. tool-forcecsv.sh: pick up the forces (energy gradients) in the CSV format (MS Excel). You can choose the number of the optimization cycles.~~

1. tools/converge-table-csv.sh: pick up the table of forces and displacements at a specific image along the reaction path at any optimization cycles as a CSV file.
2. tools/data-to-csv.sh: pick up the information about the reaction coordinates, the total energies, and forces along the reaction path as a CSV file.
3. tools/extract-coordinates.sh: create a cc1-format file and a xyz-format file for Chem3D and ChemCraft, respectively, by using the “dat” file provided by GAMESS. A movie (.MOV) and a stroboscope can be created by using these data for easily understanding a reaction path.
4. **exams/checktst: can be included into tests/standard/checktst.**

**NEB Release 3** will provide our original free-end TS locator routines (maybe, by the end of this year).

```
C>      @brief      NEBPATH main driver, Release 2
C>
C>      @details    Nudged Elastic Band (NEB) method (Release 2, Sep. 2019)
C>                  find a reaction path for specific reactant and product.
C>                  Multiple transition states can be located along an NEB path.
C>
C>                  PLAN: Release 3 --- Free-end and String method to locate a transition state exactly.
C>                                      (December 2019)
C>
C>      @author     Mamoru Haruta, Nozomi Sawada, Toshio Asada, Shiro Koseki
C>                  Osaka Prefecture University, Japan
```

**Manual**

```
c       **********************
C       Options for $NEB group
c       **********************
C       Caution: The coordinates of the reactant are given by $DATA
c                The coordinates of the product should be given by $DATAPD.
c                The atom order should be same in both reactant and product.
c                The product should be aligned as close to the reactant as possible,
```

```
c                Otherwise, some curious paths could be generated by this routine.
c                The molecular orientation is very important to obtain a reasonable
c                reaction path.                **************
c
c               Basically, molecular symmetry cannot be used.    However, if a reaction
c               path has symmetry on the entire way, you can set MOLSYM=.true.
c
c               MAXCYC is set to 500 as a default, but, generally speaking, the convergence
c               is currently very slow for the optimization of perpendicular gradient.    So,
c               You may need to restart your job several times.    For restart, $NEB and
c               $IMAGES groups in *.DAT file of the previous run need to be pasted into your
c               input file.
c
c               It would be difficult to reach the condition that all energy gradients are smaller
c               than OPTTOL.
c
c               Caution: keywords can have only 6 characters.
c
C       $NEB      IMAGES       = number of images along the NEB path (default=15)
c                                  should not be larger than 200.
c
c               MAXCYC       = maximum number of cycles for geometry optimization
c                              along the path perpendicular to the reaction path.
c                              (default = 500)
c
c               UNTCRD       = unit for the coordinates given by the $DATAPD and $DATAVI
c                              groups; ANGS or BOHR (default = ANGS).    This does not affect
c                              to $DATA.    UNITS in $CONTRL is effective to $DATA but not to
c                              $DATAPD and $DATAVI.
c
c               UNTCNT       = unit for the force constants e.g. SPFORC,OPTTOL
c                              ANGS or BOHR    (default = ANGS)
c                              CAUTION: if you say BOHR, then the following options should be given
c                              in atomic unit.
c
c               RESTRT       = Restart option.    See $IMAGEX.
c                              (default = .false.)
c
c               iSTART       = Number of cycles in the previous calculation
c
c               VIAPNT       = a via-point structure along the reaction path
c                              The coordinates are given in the $DATAVI group.
c                              (default = .false.)
c
c               TSLOCT       = locate a transition state structure
c                              (default = .false.)
c
c               OPTTOL       = tolerance for the root mean square (RMS) for energy gradients
c                              (default = 5.0 [kcal/mol/angs] = 0.00422 [hartree/bohr] )
c
c               OPMTOL       = tolerance for the maximum RMS for energy gradients
c                              (default = 10.0 [kcal/mol/angs] = 0.00843 [Hartree/Bohr])
c
c               CRDTOL       = tolerance for the geometrical displacement of each image
c                              (default = 0.01 [angs] = 0.01890 [bohr])
c
c               CRMTOL       = tolerance for the maximum geometrical displacement of each image
c                              (default = 0.1 [angs] = 0.18897 [bohr])
c
c               DELTAT       = distance multiplier for linear search
c                              (default = 0.01 [angs/sqrt(kcal/mol)] = 0.47338 [bohr/sqrt(Hartree)])
c
C                SPFORC       = force constant for a spring between two adjacent images
```

```
c                               (default = 500.0 [kcal/mol/(angs**2)] = 0.22313 [hartree/(bohr**2)])
c                               (default = 300.9 [kcal/mol/(angs**2)] = 0.13428 [hartree/(bohr**2)])
c
c                 --------- This option should not be listed in the manual...
c                 MORINT      = Caution: Did you examine the geometrical orientation of reactant and product?
c                               (default = .false.)
c                 MOLSYM       = say .true. if your reaction path has molecular symmetry
c                               along the entire way.    Otherwise, only "C1" (no symmetry) can be used
c                               in the $DATA group.
c                               (default = .false.)
c
c                 --------- The followings are unavailable right now
c
c                 METHOD       = method for finding a reaction path (NEB or string)
c
c                 OPTMZR       = method of optimizing a geometrical structure at each image
c                               QUICKMIN (default), BFGS, DIISBFGS,
c                               steepest-descent, and FIRE.
c                              Suggestions: the authors recommend that the users had better use QUICKMIN
c                              in this current version.    BFGS can be used but the several examples indicate
c                              that the current version of BFGS is not so effective.
c
c                 INTERP       = Interpolation method for making initial images
c
c                 FITTNG       = Coordination fitting method in every cycles
c
c                 TANGNT       = Tangent vector definition
c
c                 (more options will be added.)
c
c
c                 --------- The followings are additional options for experts
c                 IPMXCY      = maximum cycles for IDPP interpolation (default = 500)
c                 IPDLTT      = IDPP interpolation NEB DELTAT (default = 0.1)
c                 IPSPFC      = IDPP interpolation NEB SPFORC (default = 0.2)
c                 IPOPTL      = IDPP interpolation NEB OPTTOL (default = 0.01)
c
c
c        ****************
c        Related data groups
c        ****************
c
c        $DATAPD      = the coordinates of a product
c                         atom name, atomic number, x, y, z for each atom
c                         (should be given for all atoms, even if a molecular symmetry is used.)
c
c        $DATAVI       = the coordinates of a via-point structure (optional)
c                         atom name, atomic number, x, y, z for each atom
c                         (should be given for all atoms, even if a molecular symmetry is used.)
c
c        $IMAGESX     = data for a restart job given in *.DAT file.
c
c        ---------------
C         Dictionary file
c        ---------------
c        IREC = 1     Atomic coordinates
c        IREC = 2     Various energy quantities (Common /ENERGYS/)
c        IREC = 3     Gradient vector
c        IREC = 4     Hessian matrix (not use)
c        IREC = 15    Alpha orbitals
c        IREC = 19    Beta    orbitals
c
c        IREC = 701 Number of the image (1), coordinates, energy gradients, VEC at IMAGE #1
```

```
c       IREC = 702 Number of the image (2), coordinates, energy gradients, VEC at IMAGE #2
c       IREC = 703 Number of the image (3), coordinates, energy gradients, VEC at IMAGE #3
c       IREC = 704 Number of the image (4), coordinates, energy gradients, VEC at IMAGE #4
c
c       IREC = 715 Number of the image (15), coordinates, energy gradients, VEC at IMAGE #15 (default)
c
c       IREC = 730 Number of the image (30), coordinates, energy gradients, VEC at IMAGE #30 (if necessary)
c
c       IREC = 900 Number of the image (200), coordinates, energy gradients, VEC at IMAGE #200 (maximum)
c       https://www.msg.chem.iastate.edu/gamess/GAMESS_Manual/prog.pdf
c
```