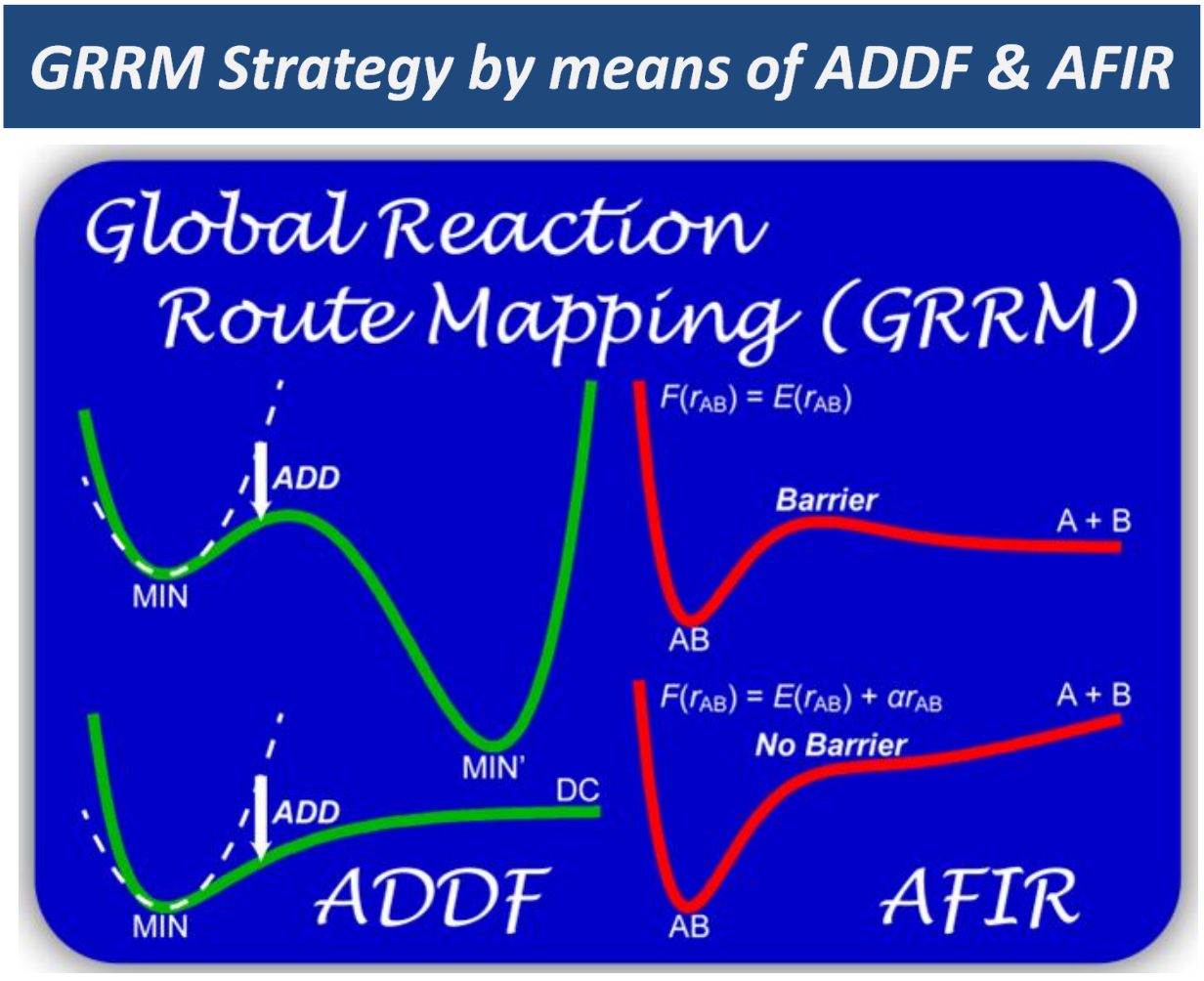
GRRM NEWS No. 007

GRRM NEWS reports recent developments of GRRM programs searching chemical structures and reaction pathways.

The most basic versions of GRRM programs are GRRM1.xx (1.00-1.22), which have been released for many users. In the **GRRM1.xx**, the ADD following (ADDf) algorithm is applied to only one equilibrium structure (EQ) at one time, and after having completed the ADDf procedures around one EQ then the next ADDf around an 'undone' EQ is started consecutively until there becomes no 'undone' EQ. Parallel treatments of ADDf around many EQs at the same time become possible in the **GRRM11.xx** (11.00-11.03). The parallel GRRM has considerably accelerated global reaction route mapping of the entire reaction pathways.



A new approach finding reaction pathways efficiently is the AFIR technique. In AFIR, artificial forces are applied between A and B, and then a product of AB can be obtained quickly without barrier, but the real reaction route with a barrier can easily be retained automatically by removing the artificial forces.

A combined approach finding reaction pathways by using ADDf and AFIR (Artificial Force Induced Reaction) methods is now called GRRM strategy (S. Maeda, K. Ohno, and K. Morokuma, *Phys. Chem. Chem. Phys.*, 15, 3683-3701 (2013)).

(1) A renewed **Web page of GRRM** can be seen at the following URL.
http://grrm.chem.tohoku.ac.jp/GRRM/index_e.html
The main contents are as follows.
GRRM guide.
GRRM & Problems in Chemistry.
GRRM-Strategy.
GRRM-References.
GRRM-GDSP DEMO.
GRRM_Animation.
GRRM_Animation_2.

(2) Trouble handlings for g09 users.
Because of changes in default treatments of Gaussian programs, some troubles happen during some GRRM operations with g09.

(a) Memory sized requirement has been enlarged.
(GRRM1.xx) Add a line for the dynamical memory of %mem=30000000 or more at the Options section in the input data.

```
Options
GauMEM = 30000000
```

(GRRM11.xx) Add a line for the dynamical memory %mem=30 MW or more at the Options section in the input data

```
Options
GauMEM = 30
```

(b) Due to changed treatments during force calculations by g09, 'Segmentation Violation' or large amount of error messages happen to appear just after having started a GRRM job.
In such a case, once close the linux window, and then open the linux window again if necessary.
Or, error messages may be discarded by using /dev/null as follows.

GRRMp [xxx] –p[n] –h[m] >& /dev/null &

(3) A new GRRM version of **GRRM14** will be released in this year (October 1, 2014). GRRM14 includes AFIR together with some new functions. Application form will become available at the **Web page of GRRM**
GRRM14 can only be used with a USB controller that handles the security of the GRRM program. This USB controller named as GRRM controller needs to be purchased at the application to GRRM14. The detailed information will also be available at the Web page of GRRM.

(4) An institute related to GRRM has been opened as **Institute for Quantum Chemical Exploration (IQCE)** in Tokyo. For the moment, a Web page in Japanese is only available; http://icqc.jp/
Also, annual symposium for reaction path search and some other events are held in Japan, which are supported by IQCE.

(5) The GRRM programs (GRRM1.xx, GRRM11.xx, and GRRM14) can only be used in a computer or one node. New versions using many cores over many nodes and computers are developing.