
GRADE
****version 1.00****

****Sample input and output data****
In this directory you can find an input file (**test.gro**) and the source codes required to reproduce the output files in directory "TEST-output". Output files are: **test.xvg**, **F4.xvg**, **test_cage512-1.gro**, **test_cage62512-1.gro, test_cage64512-1.gro**
" **test.xvg" and "**F4.xvg**" can be viewed by any text editor program.

Below are the instructions to compile, run and replicate these files from the source code as well as visualizing them:

1. Compile the code in a terminal window using GNU Compiler Collection (version 6.1.0 or newer) and the provided Makefile by typing:
   ```
   $ make
   $ make clean
   ```
2. Give any name to the output files ("test" in this example) and run the code by typing:
   ```
   $ ./GRADE -i test.gro -o test -f4
   ```
3. The "**test_cage512_1.gro**", "**test_cage62512_1.gro**" and "**test_cage64512-1.gro**" files can be visualized in VMD program and applying the following representation settings:
   a. Run the VMD program.
   b. Open an individual output gro file, e.g., File => New Molecule… =>Browse => **test_cage512_1.gro** => Load

   c. Apply following settings:
      Graphics => Representations…
      In 'Selected Atoms' field type "SOL" and press "Enter/Return" on keyboard.
      Choose "Licorice" from "Drawing Method" drop down menu.
      Create a new representation by clicking "Create Rep" button.
      Click on the new representation and in the "Selected Atoms" field type "SOL" press "Enter/Return" on keyboard.
      Choose "HBonds" from "Drawing Method" drop down menu.
      Change "Distance Cutoff" value to 3.5.
      Change "Angle cutoff" value to 30.
      Change "Line Thickness" value to 10.
      Create a new representation by clicking "Create Rep" button.
      Click on the new representation and in the "Selected Atoms" field type "CH3" and press "Enter/Return" on keyboard. This shows methane molecules trapped inside the cages in Cyan wherever they exist.
      Choose "VDW" from "Drawing Method" drop down menu.
      To visualize all 512 and 62512 cages of a frame at the same time, after opening "**test_cage512-1.gro**" open the respective 62512 file (**test_cage62512-1.gro**) and after choosing "**test_cage62512-1.gro**" from "Selected Molecule" drop down menu follow all the procedures in step 'c'.

For clarity, you can change the color of hydrogen bonds in 62512 cages by choosing “HBonds” representation for 62512 “SOL” atoms and choose “ColorID” from “Coloring Method” drop down menu and selecting Number 7 for Green color from the drop down menu beside “ColorID”.
*It should be mentioned that in VMD, any overlapping hydrogen bonds between 512 and 62512 cages, will be shown in the latest applied color (in this case Green).

d. The same procedure can be repeated with a different ColorID for **test_cage64512-1.gro** and 64512 cages.
