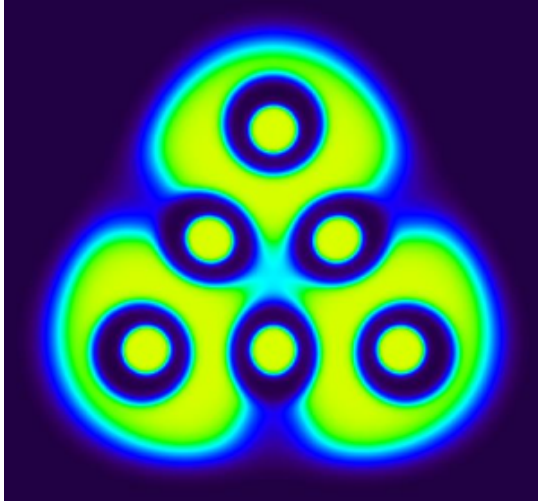


Multiwfn



- Opis
- Službena dokumentacija
- Verzije
- Izvršne datoteke
- Napomena
- Primjer korištenja

Opis

Multiwfn je računalno-kemijska aplikacija za analizu elektronskih valnih funkcija.

Multiwin je otvorenog koda, a posjeduje i mogućnost rada u GUI-ju (grafičkom korisničkom sučelju).

Službena dokumentacija

- Službene stranice
- Manual
- Quick start

Verzije

Verzija	Modul	Kompajler	Podrška	Paralelizacija *	Supek
3.8	scientific/multiwfn/3.8	GNU C kompajler, Intel Fortran kompajler	CPU	SMP	✓

Kod paralelizacije s **dijeljenom memorijom** (engl. *Shared-Memory Parallelism, SMP*) program je podijeljen na više *threadova* i svi imaju pristup istoj, tj. zajedničkoj (dijeljenoj) memoriji.

To znači da se aplikacija mora izvršavati na **jednom radnom čvoru**.

Primjer korištenja

- Za interaktivno pokretanje uz GUI, prvo je potrebno pokrenuti interaktivan posao, uz prosljeđivanje X:

```
$ qsub -I -X -q cpu -l select=1:ncpus=16:mem=32gb
```

- Po pokretanju interaktivno posla, smjestit ćete se u home direktorij. Navigirajte do direktorija u kojem se nalaze Vaša input datoteka, npr.:

```
$ cd multiwfn/
```

- Učitajte modul, a zatim pokrenite aplikaciju.
 - Broj traženih jezgri, odnosno argument **-nt** opcije aplikacije preuzet će se iz Vaše okoline, tj. iz **nproc** opcije.
 - **OMP_STACKSIZE** varijabla automatski će se postaviti po formuli **(0.75*mem) nproc**

```
$ module load scientific/multiwfn/3.8
```

```
$ Multiwfn H2O_m3ub3lyp.wfn
```

- U *promptu* odaberite željene opcije:

```

lsm@kali:~/00000-030d-0x$ cd multi/
lsm@kali:~/00000-030d-0x/multi$ ./multi Load scientific/multi/3.8
lsm@kali:~/00000-030d-0x/multi$ ./multi Load xtd_hubb7d.asf
lsm@kali:~/00000-030d-0x/multi$ ./multi Load MultiFunction NumberFunction Analyzer
lsm@kali:~/00000-030d-0x/multi$ ./multi Load MultiFunction NumberFunction Analyzer
Developer: Team 3 (Building main research Center for Natural Sciences)
Name never used (Please use the name. It will be utilized in your report)
Version 1.0.0.0 (Please release date: Nov-3-2019)
Copyright © 2019 by MultiFunction NumberFunction Analyzer. All rights reserved.
See "How to cite MultiFunc.pdf" in Multi binary package for more information
Multi official website: http://hubb7d.com/030d-0x/
Multi English forum: http://www.030d-0x.com/030d-0x/
Multi Chinese forum: http://www.hubb7d.com/030d-0x/

( Number of parallel threads: 16 Current date: 2024-03-21 Time: 10:53:56 )

Please wait...

Total energy: -76.129638181439 Hartree. Virtual state: 1.9995660
Total Alpha-beta electrons: 16.0000 0.0000 3.40000
Net Charge: -0.0000 Conjugated molecules: 3
The number of substituents: 16 Atoms type: 3, GTT: 36
This is an unsaturated alpha-beta-determinant molecular formula
Orbitals from 1 to 16 are atoms type from 1 to 16 are beta type
1000 line file: alpha-beta-multi.multiplicity/3.8

Loaded xtd_hubb7d.asf successfully!

Formula H2 O1 Total atoms: 3
Molecule weight: 18.01528 Da
Point group: C2v

"q": Exit program gracefully "r": Load a new file
***** Main function menu *****
5 Show molecular structure and site orbitals
3 Output all properties at a point 2 Input/output analysis
1 Output and print specific property in a line

```

```

krembo@krembo005:~/krembo - x      +
Delta= (under Kirschfeld partition): 0.2389876451e-03
User-defined real space constant: 0.3888888888e-01
ESP from nuclear charges: 0.5031777844e-01
ESP from 'electrons': 0.3893853180e-01
Total ESP: 0.141184044e-01 (e.g., 0.38938484e-00 vau, 0.09222844e-01 kcal/mol)

Note: Below information for real electron density

Comments of gradient in x/y/z space
-79.18056228e-03  -0.091324750e-02  -0.665111972e-02
User of gradient: 1.0 0.00000000e-00

Comments of Laplacian in x/y/z space
-0.888936988e-02  -0.3652880455e-01  -0.4387721976e-02
Total: 0.3363377866e-01

Mulliken matrix:
-0.888936988e-02  -0.330494133E-02  -0.159793197E-02
-0.330494133E-02  -0.365288045E-01  -0.368137338E-01
-0.159793197E-02  -0.368137338E-01  -0.438772197E-02
Eigenvalues of matrix: 0.3893853180e-01, 0.3893853180e-01, 0.3893853180e-01
Eigenvectors (columns) of Hessian:
0.9964979782e-01  -0.241833757E-02  -0.979552378E-01
-0.979552378E-01  -0.6328255358e-02  -0.7743991338E-00
-0.6328255358e-02  -0.7743991338E-00  -0.6328255358E-02
Determinant of Hessian: 1.847271756E-08
Elasticity of electron density: 1.392348
eta index: 0.209852

Calculation preparation at a point
user input x,y,z of the point to be studied is now as follows, e.g., 3.1,3.2,8.1
or input "a" to select atomic positions
or input "c" to select nuclei positions
or input "d" to select basis functions
or input "e" to select basis functions and Hessian will be shown
or input "f" can decompose a real space function at specified point to orbital contributions
or input "g" can return

```

Izvršne datoteke

Multiwfn

Multiwfn_noGUI

Napomena

Kako bi se aplikacija uspješno pokrenula uz korištenje grafičkog sučelja, potrebno je spojiti se na pristupni čvor uz prosljeđivanje X11.

U slučaju korištenja **Linuxa** ili **macOS-a**, koristite naredbu:

```
ssh -X -i ~/.ssh/id_rsa username@login-cpu.hpc.  
srce.hr
```

U slučaju korištenja **Windowsa**, potrebno je preuzeti aplikaciju **Xming** te je pokrenuti prije pokretanja **PuTTY**-ja.

Unutar PuTTY-ja, potrebno je uključiti **X11 forwarding** (*Connection* → *SSH* → *X11*, *Enable X11 forwarding*).

