

Critic2

Verzija	Moduli
1.1	critic2/1.1

GIT: <https://github.com/aoterodelaroza/critic2>

Pages: <https://aoterodelaroza.github.io/critic2/>

libxc: <https://tddft.org/programs/libxc/download/>

qhull: <http://www.qhull.org/download/qhull-2020-src-8.0.2.tgz>

Upute za korištenje: <https://aoterodelaroza.github.io/critic2/manual/inputoutput/>

Primjer korištenja

```
#!/bin/bash

#$ -N critic2-tst
#$ -pe *mpisingle 2
#$ -cwd

OMP_NUM_THREADS=$NSLOTS

module load critic2/1.1

critic2 benzene.cri > benzene.out
```



Critic2 je više ineraktivne narav, stoga se zadaje OMP_NUM_THREADS kod zadavanja posla za željeni broj korištenih dretvi.

Instalacija

Instalirani su libovi: libxc(6.1.0) i qhull(8.0.2)

```
wget https://github.com/aoterodelaroza/critic2/archive/refs/tags/1.1stable.tar.gz
cd 1.1stable.tar.gz
module load openmpi21-intel-x86_64
./configure --prefix=/apps/critic2/1.1 LDFLAGS="-L/apps/critic2/deps/libxc-6.1.0/lib -L/apps/critic2/deps/qhull-2020.2/lib" --with-libxc-include=/apps/critic2/deps/libxc-6.1.0/include --with-qhull-inc=/apps/critic2/deps/qhull-2020.2/include/libqhull CC=icc CXX=icpc
make
make install
```