

Chemistry at the speed of graphics...

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Opis

TeraChem je računalni programski paket za kemijske simulacije. Omogućuje simuliranje svojstava molekula, kao što su geometrija, energija, spektroskopija i reaktivnost, koristeći metode kvantne kemije i molekularne mehanike.

GPU (Grafička procesorska jedinica) podrška omogućuje TeraChemu da koristi snagu grafičkih kartica kako bi ubrzao izvođenje računalnih simulacija.

Verzije

Verzija	Modul	Red	Supek	Padobran
1.96	scientific/terachem/1.96	gpu	✓	✗

Službena dokumentacija

- <http://www.petachem.com/doc/userguide.pdf>

Primjer

Postavke simulacije, kao što su tip posla, DFT funkcional, osnovni skup, naboj molekule te ime datoteke u kojoj se nalaze koordinate, definirane su u `.sp` datoteci (`start.sp`). Primjer je dan niže:

start.sp

```
# Job: minimize

# SCF method (rhf/blyp/b3lyp/etc...)
method      b3lyp

# basis set
basis       def2-svp

# coordinates file
coordinates  molecule.xyz

# molecule charge
charge      0

# add dispersion correction (DFT-D)
dftd        yes

# type of the job (energy/gradient/md/minimize/ts)
run          minimize

end
```

Koordinate atoma molekule nalaze se u **molecule.xyz** datoteci. Primjer je dan niže:

molecule.xyz

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N	11.6312087516194644	18.5712818987571495	5.4905821448133807
C	10.2318126720333478	18.5712818987571495	5.4905821448133807
C	9.5876915784923433	17.2153785305662126	5.5096080438463382
C	10.3945049832847349	16.0290934656690354	5.5275827408182341
C	11.8237433842737740	16.1265858360994869	5.5401985630719253
C	12.4934396107196726	17.4694910128286693	5.4859112144712032
C	8.1953385452329748	17.1123895696302668	5.4982449714725004
C	7.5731551972501006	15.8439889650339154	5.4833934715330539
C	8.3191491563154614	14.6490541494093289	5.4868301803081305
C	9.7632753843514219	14.7298407588396305	5.5245096420666417
C	12.6025620551488160	14.9670669009358601	5.5762435811528626
C	11.9906100294747997	13.6944701474983646	5.5876129589202179
C	10.5890961111393498	13.5441041624243290	5.5566713827362921
C	9.9395162537441148	12.2078154908889580	5.5483255717149973
C	8.4966881716416136	12.1270288814586600	5.4764407343974337
C	7.6708052491384873	13.3127654778739544	5.4459178139415396
C	10.6836248483065432	11.0128806752643680	5.6014405171404533
C	10.0621055533559343	9.7444800706680184	5.5690916135773136
C	8.6728963618024153	9.6414911097320672	5.4748901765206277
C	7.8670413778113790	10.8277761746292445	5.4316616597670127
C	6.2709775931689471	13.1623994927999188	5.3705442243524857
C	5.6616475719806676	11.8898027393624215	5.3128253387426447
C	6.4409579682478544	10.7302838041988000	5.3359136843287320
C	5.7773027661090275	9.3873786274696140	5.2310236247041679
N	6.6366993968075256	8.2855877415411356	5.3010329320783161
C	8.0320701241976700	8.2855877415411339	5.4070985754492860
O	8.6590004912903584	7.2322510850242878	5.4259269632705358
O	9.6052585890175397	19.6246185552739831	5.4618388946989072
O	4.5695409037684733	9.2322833057320963	5.0872737912405732
O	13.7086227113054200	17.6245863345661888	5.4341158208927993
H	6.2014363558304861	7.3741469483238262	5.1852346190386704
H	12.0739965639529583	19.4827226919744483	5.4081071947234935
H	11.7671541439977574	11.0423815130944032	5.6666644377234512
H	6.4877990920463340	15.8144881272038909	5.4663048983260172
H	5.6257379184858110	14.0359401282361578	5.3522758732650555
H	12.6353783061458671	12.8209295120621238	5.6183023680911717
H	10.6574037146316023	8.8341078658810623	5.6083660833147064

H	7.5987759905766037	18.0227617744172193	5.4922865175440041
H	4.5797007311464419	11.7927943609273118	5.2460693293634861
N	13.6864563803527304	15.0640752793709769	5.5916845322291255
N	8.8659732180638144	19.1329933820270597	2.1715591085968633
C	7.6539245673596898	18.4342294394891404	2.1629539226503933
C	7.7722533189872944	16.9391789922589950	2.0877413412880443
C	9.0609882708612428	16.3134829777864283	2.0950248443339134
C	10.2532239219725696	17.1110132112079967	2.1276269007059767
C	10.1635739546973305	18.6090403394207087	2.1676958207849815
C	6.6160474910636324	16.1562402133379166	2.0373739076437118
C	6.7070384430610464	14.7473867971010932	2.0062332662014004
C	7.9502184595082337	14.0827888826899432	2.0311658304243654
C	9.1598342755455651	14.8724924087487764	2.0778931774130296
C	11.5057020937517631	16.4940492044448384	2.1336815097270616
C	11.6076788257897778	15.0848829253070047	2.1287903788079010
C	10.4685597519058042	14.2563548391947457	2.1104339750785126
C	10.5693038958287318	12.7740807576083402	2.1305640990575299
C	9.3596258840762125	11.9843772315495141	2.0854755722826201
C	8.0521985536494185	12.6005148011035448	2.0187293990580901
C	11.8107976499100076	12.1094828431971973	2.1999286766856248
C	11.8991665974216900	10.7006294269603686	2.2378762986205061
C	10.7424690441058743	9.9176906480392955	2.2004655374710200
C	9.4568890836574564	10.5433866625118604	2.1100498812405668
C	6.9149648442683826	11.7719867149912876	1.9506947586783223
C	7.0162775232741179	10.3628204358534468	1.9633010313828514
C	8.2656118533474743	9.7458564290902956	2.0521940050867844
C	8.3519669646864525	8.2478293008775783	2.0989425851120753
N	9.6455423491239891	7.7238762582712237	2.2011449406711705
C	10.8547567714264090	8.4226402008091377	2.2844303643339732
O	11.9161965533588567	7.8245979328828970	2.4226270526982567
O	6.5850635471820524	19.0322717074153900	2.2203024613281013
O	7.3763092987375742	7.5062240280700010	2.0668794668575465
O	11.1388553365693230	19.3506456122282771	2.2096738013327286
H	9.7075677505769349	6.7142174100745713	2.3027783186373192
H	8.7964230452544268	20.1426522302237139	2.2681989937602474
H	12.7361162169278455	12.6775424180662917	2.2288264469560630
H	5.7821912740552737	14.1793272222319953	1.9649144378474368
H	5.9214795830075477	12.2059535019062881	1.8888881459078171
H	12.6029908965631527	14.6509161383920024	2.1424616442024469
H	12.8659045386542523	10.2046435511325360	2.3002599553483449
H	5.6473620654613850	16.6522260891657403	2.0263053092187722
H	6.1235353548242184	9.7422120668383112	1.9127381099903769
H	12.3997086555823675	17.1146575734599757	2.1509284153106378



Korištenje aplikacije TeraChem ograničeno je na **gpu red čekanja**, tj. na GPU poslužitelje.



TeraChem aplikacija nema mogućnost širenja posla van **jednog čvora**!

U primjeru niže, aplikacija će se pokrenuti na **jednom GPU** čvoru, **2 GPU-a** i **32 CPU** jezgre.

terachem_test.pbs

```
#PBS -q gpu
#PBS -l select=1:ngpus=2:ncpus=32

module load scientific/terachem/1.96

cd $PBS_O_WORKDIR

terachem start.sp
```