

cp2k

blocked URL

- [Opis](#)
- [Verzije](#)
- [Dokumentacija](#)
- [Primjeri](#)
- [Napomena](#)

Opis

cp2k je aplikacija namijenjena simulaciji fizike čvrstog stanja, tekućina, molekularnih i bioloških sustava korištenjem [ab-inito metoda](#). Osim pružanja [tipičnih mogućnosti](#) kvanto-kemijskog modeliranja [metodama DFT](#) putem [modula QUICKSTEP](#), cp2k pruža i mogućnosti [termodinamičkog simuliranja molekularnih sustava](#), te miješanog [kvantno-kemijskog/termodinamičkog simuliranja](#).

Verzije

verzija	modul	red
2022.1	scientific/cp2k/2022.1-gnu	cpu

Dokumentacija

- Službena stranica - <https://www.cp2k.org>
- Priručnik za korištenje - <https://manual.cp2k.org>

Primjeri

Ispod je opisan primjer podnošenja posla za jedan od [službenih cp2k predložaka \(H2O-64\)](#):

- **H2O-64.inp** - ulazni podaci
- **H2O-64.sh** - skripta sustava PBS

H2O-64.inp

```
&FORCE_EVAL
METHOD QS
&DFT
  BASIS_SET_FILE_NAME GTH_BASIS_SETS
  POTENTIAL_FILE_NAME POTENTIAL
  &MGRID
    CUTOFF 280
    REL_CUTOFF 30
  &END MGRID
  &QS
    EPS_DEFAULT 1.0E-12
    WF_INTERPOLATION PS
    EXTRAPOLATION_ORDER 3
  &END QS
  &SCF
    SCF_GUESS ATOMIC
    &OT ON
    MINIMIZER DIIS
    &END OT
  &PRINT
    &RESTART OFF
```

```

&END
&END

# SCF_GUESS          RESTART
# EPS_SCF            1.0E-7
&END SCF
&XC
  &XC_FUNCTIONAL Pade
&END XC_FUNCTIONAL
&END XC
&END DFT
&SUBSYS
  &CELL
    ABC 12.4138 12.4138 12.4138
  &END CELL
# 64 H2O (TIP5P,1bar,300K) a = 12.4138
&COORD
0      12.235322      1.376642      10.869880
0      6.445390       3.706940      8.650794
0      0.085977       2.181322      8.276663
0      12.052554      2.671366      2.147199
0      12.250036      4.190930      12.092014
0      7.187422       0.959062      4.733469
0      8.346457       7.210040      4.667644
0      12.361546      11.527875     8.106887
0      3.299984       4.440816      9.193275
0      2.855829       3.759909      6.552815
0      1.392494       6.362753      0.586172
0      1.858645       8.694013      2.068738
0      3.770231       12.094519     8.652183
0      6.432508       3.669828      2.772418
0      1.998724       1.820217      4.876440
0      8.248581       2.404730      6.931303
0      5.753814       3.360029     12.461534
0      11.322212      5.649239      2.236798
0      4.277318       2.113956     10.590808
0      5.405015       3.349247      5.484702
0      6.493278       11.869958     0.684912
0      3.275250       2.346576      2.425241
0      7.981003       6.352512      7.507970
0      5.985990       6.512854     12.194648
0      10.636714      11.856872     12.209540
0      9.312283       3.670384      3.508594
0      1.106885       5.830301      6.638695
0      8.008007       3.326363     10.869818
0      12.403000      9.687405     11.761901
0      4.219782       7.085315      8.153470
0      3.781557       8.203821     11.563272
0      11.088898      4.532081      7.809475
0      10.387548      8.408890      1.017882
0      1.979016       6.418091     10.374159
0      4.660547       0.549666      5.617403
0      8.745880       12.256257     8.089383
0      2.662041       10.489890     0.092980
0      7.241661       10.471815     4.226946
0      2.276827       0.276647     10.810417
0      8.887733       0.946877      1.333885
0      1.943554       8.088552      7.567650
0      9.667942       8.056759      9.868847
0      10.905491      8.339638      6.484782
0      3.507733       4.862402      1.557439
0      8.010457       8.642846     12.055969
0      8.374446       10.035932     6.690309
0      5.635247       6.076875      5.563993
0      11.728434      1.601906      5.079475
0      9.771134       9.814114      3.548703
0      3.944355       10.563450     4.687536
0      0.890357       6.382287      4.065806
0      6.862447       6.425182      2.488202
0      3.813963       6.595122      3.762649
0      6.562448       8.295463      8.807182

```

O	9.809455	0.143325	3.886553
O	4.117074	11.661225	2.221679
O	5.295317	8.735561	2.763183
O	9.971999	5.379339	5.340378
O	12.254708	8.643874	3.957116
O	2.344274	10.761274	6.829162
O	7.013416	0.643488	10.518797
O	5.152349	10.233624	10.359388
O	11.184278	5.884064	10.298279
O	12.252335	8.974142	9.070831
H	12.415139	2.233125	11.257611
H	11.922476	1.573799	9.986994
H	5.608192	3.371543	8.971482
H	6.731226	3.060851	8.004962
H	-0.169205	1.565594	7.589645
H	-0.455440	2.954771	8.118939
H	12.125168	2.826463	1.205443
H	12.888828	2.969761	2.504745
H	11.553255	4.386613	11.465566
H	12.818281	4.960808	12.067151
H	7.049495	1.772344	4.247898
H	6.353019	0.798145	5.174047
H	7.781850	7.384852	5.420566
H	9.103203	6.754017	5.035898
H	12.771232	11.788645	8.931744
H	12.018035	10.650652	8.276334
H	3.557245	3.792529	9.848846
H	2.543844	4.884102	9.577958
H	2.320235	4.521250	6.329813
H	2.872128	3.749963	7.509824
H	1.209685	7.121391	1.140501
H	2.238885	6.038801	0.894245
H	2.763109	8.856353	2.336735
H	1.329379	9.047369	2.783755
H	4.315639	11.533388	9.203449
H	3.098742	12.433043	9.244412
H	5.987369	3.448974	3.590530
H	5.813096	3.419344	2.086985
H	1.057126	1.675344	4.969379
H	2.248496	2.292119	5.670892
H	8.508264	1.653337	7.464411
H	8.066015	2.034597	6.067646
H	5.197835	2.915542	11.821572
H	6.630900	3.329981	12.079371
H	10.788986	6.436672	2.127933
H	11.657923	5.463602	1.359832
H	3.544476	1.634958	10.977765
H	4.755770	1.455054	10.087655
H	4.465371	3.375459	5.665294
H	5.682663	4.264430	5.524498
H	6.174815	11.778676	1.582954
H	5.713640	12.089924	0.174999
H	3.476076	1.498708	2.028983
H	2.730229	2.134295	3.182949
H	7.119624	5.936450	7.474030
H	8.536492	5.799405	6.958665
H	5.909499	5.717477	11.667621
H	6.125402	6.196758	13.087330
H	11.203499	12.513536	11.804844
H	10.260930	12.300153	12.970145
H	9.985036	3.927685	2.878172
H	8.545584	3.468329	2.972331
H	1.399882	6.620092	7.093246
H	0.963561	6.112523	5.735345
H	8.067363	3.674002	9.979955
H	8.000737	2.375959	10.756190
H	11.821629	10.402510	12.020482
H	12.206854	8.983242	12.379892
H	3.461473	7.606485	7.889688
H	3.844478	6.304711	8.560946
H	3.179884	7.585614	11.148494

H	4.401957	7.652030	12.039573
H	11.573777	5.053211	7.169515
H	10.342076	4.186083	7.320831
H	10.065640	8.919194	1.760981
H	9.629585	8.322499	0.439729
H	1.396302	6.546079	9.625630
H	1.405516	6.479759	11.138049
H	4.024008	1.232518	5.405828
H	4.736858	0.579881	6.571077
H	9.452293	12.313381	8.732772
H	8.976559	11.502788	7.545965
H	1.834701	10.012311	0.153462
H	3.295197	9.836403	-0.204175
H	7.056724	11.401702	4.095264
H	6.499038	10.020287	3.825865
H	1.365541	0.487338	11.013887
H	2.501591	-0.428131	11.417871
H	8.644279	1.812362	1.005409
H	8.142674	0.388030	1.112955
H	1.272659	8.365063	8.191888
H	2.142485	8.877768	7.063867
H	8.961493	7.826192	9.265523
H	9.227102	8.487654	10.601118
H	10.150144	7.758934	6.392768
H	10.596082	9.187988	6.167290
H	3.463106	4.096188	2.129414
H	3.919461	4.539801	0.755791
H	7.418998	9.394959	12.028876
H	7.430413	7.883095	12.106546
H	7.972905	10.220334	5.841196
H	7.675111	9.631498	7.203725
H	5.332446	6.381336	6.419473
H	5.000025	6.434186	4.943466
H	11.575078	2.271167	4.412540
H	11.219802	0.847030	4.783357
H	8.865342	9.721516	3.843998
H	10.000732	10.719285	3.758898
H	3.186196	10.476397	5.265333
H	4.407331	11.335128	5.013723
H	0.558187	7.255936	3.859331
H	0.341672	5.789383	3.552346
H	7.459933	6.526049	3.229193
H	6.696228	5.483739	2.440372
H	3.864872	6.313007	2.849385
H	2.876419	6.621201	3.953862
H	5.631529	8.079145	8.753997
H	7.003296	7.568245	8.367822
H	9.615413	0.527902	3.031755
H	8.962985	0.109366	4.332162
H	3.825854	11.139182	1.474087
H	4.063988	11.063232	2.967211
H	5.784391	7.914558	2.708486
H	4.780461	8.655167	3.566110
H	10.880659	5.444664	5.046607
H	9.593331	4.687991	4.797350
H	11.562317	8.960134	3.376765
H	11.926084	8.816948	4.839320
H	2.856874	11.297981	7.433660
H	1.492332	11.195517	6.786033
H	7.145820	0.090200	9.749009
H	7.227275	0.077690	11.260665
H	4.662021	9.538430	10.798155
H	5.994537	9.833472	10.142985
H	10.544299	6.595857	10.301445
H	11.281750	5.653082	9.374494
H	12.103020	8.841164	10.006916
H	11.491592	8.576221	8.647557

&END COORD

&KIND H

BASIS_SET TZV2P-GTH

POTENTIAL GTH-PADE-q1

```

&END KIND
&KIND 0
    BASIS_SET TZV2P-GTH
    POTENTIAL GTH-PADE-q6
&END KIND
&END SUBSYS
&END FORCE_EVAL
&GLOBAL
    PROJECT H2O-64
    RUN_TYPE MD
    PRINT_LEVEL LOW
&END GLOBAL
&MOTION
    &MD
        ENSEMBLE NVE
        STEPS 10
        TIMESTEP 0.5
        TEMPERATURE 300.0
    &END MD
&END MOTION

```

H2O-64.sh

```

#!/bin/bash

#PBS -q cray_cpu
#PBS -l select=4:ncpus=8:mem=10GB
#PBS -l place=scatter
#PBS -l walltime=1000

module load cray-pals
module load scientific/cp2k/2022.1-gnu

cd $PBS_O_WORKDIR
mpiexec -n 4 cp2k.psmf -i H2O-64.inp

```

Napomena



cp2k u sebi sadrži dva nivoa paralelizacije:

- **MPI** - broj procesa (ili rangova)
- **OMP** - broj threadova po procesu (ili rangu)

Sintaksa koja će osigurati ispravnu raspodjelu resursa je:

```

...
#PBS -l select=<broj_MPI_procesa>:ncpus=<broj_OMP_niti>
...
mpiexec -np <broj_MPI_procesa> cp2k.psmf ...

```

Jer će ovim načinom sustav PBS automatski definirati varijablu okoliša **OMP_NUM_THREADS**