GAMESS

Opis

GAMESS (**G**eneral **A**tomic and **M**olecular **E**lectronic **S**tructure **S**ystem) je *ab initio* računalno-kemijska aplikacija opće namjene te posjeduje sve uobičajene QM/MM metode.

GAMESS je otvorenog koda, a koristi MPI paralelizaciju. Određeni izračuni dopuštaju i OpenMP (*threaded*) paralelizaciju.

GAMESS se na računalnom klasteru Supek pokreće prilagođenom **`rungms.mpi`** skriptom.

Pravilno pokretanje GAMESS-a zahtjeva dobro razumijevanje PBS varijabli, odnosno načina kako se dodjeljuju resursi.

GAMESS zahtjeva da prilikom paralelizacije na svakom čvoru ima jednak i paran broj MPI procesa. Naravno, to znači da možete koristiti i samo jedan računalni čvor.

Verzije

Verzija	Modul	Podrška	Paralelizacija	Prevodioc	Knjižnice	Supek	Padobran
September 30, 2022 R2 Public Release	**`scientific/gamess/22.09`**	CPU	MPI + OpenMP	Cray	Cray	✅	❌

Službena dokumentacija

- GAMESS dokumentacija

PBS varijable - resursi

test.pbs

```
#PBS -l select=4:mpiprocs=4:ncpus=4
#PBS -l place=scatter
```

PBS resursi **`mpiprocs`** i **`ncpus`** definirani su po **`select`**-u, odnosno po tzv. *chunku* (komadu čvora).

ncpus predstavlja broj zatraženih **CPU jezgara** po jednom selectu. To znači da je **ukupan broj zatraženih CPU jezgara** jednak **`select×ncpus`**.

Ako nije eksplicitno definiran, podrazumijeva se **`ncpus=1`**.

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mpiprocs predstavlja broj **MPI procesa** po jednom selectu. To znači da je **ukupan broj MPI procesa** jednak **`select×mpiprocs`**.

Za svaki definirani **`select`**, u datoteku **`PBS_NODEFILE`** zapisuje se po **`select×mpiprocs`** *hostname*-ova, odnosno radnih čvorova (čiji je to komad). Koji će to biti čvorovi, ovisi o "raspodjeli" chunkova, odnosno selectova:

- **`place=scatter`** će svaki *chunk* smjestiti na drugi čvor.
- **`place=pack`** će svaki *chunk* smjestiti na isti čvor.
- **`place=free`** će *chunkove* smjestiti na one čvorove koji su slobodni, bez konkretne pravilnosti.

Za svaki zapisani *hostname*, MPI pokretač **`mpiexec`** će pokrenuti će po jedan MPI proces.

Ako nije eksplicitno definiran, podrazmijeva se **`mpiprocs=1`**.

Kako bi se za svaki MPI proces dodijelila po jedna CPU jezgra, nužno je da su vrijednosti ncpus i mpiprocs iste.

OpenMP za svoju varijablu **`OMP_NUM_THREADS`** preuzima (podrazumijeva) vrijednost **`ncpus`**.

Ako ne koristite OpenMP, nužno je u skripti dodatno definirati i **`export OMP_NUM_THREADS=1`**, kako bi se pregazila podrazumijevana vrijednost.

PBS primjeri

U nadolazećim primjerima pokazat će se kako različito definirane **`select`** i **`mpiprocs`** varijable utječu na sadržaj **`PBS_NODEFILE`** datoteke.

Kako je ranije objašnjeno, MPI pokretač **`mpiexec`** čita sadržaj **`PBS_NODEFILE`** datoteke i za svaku liniju (*hostname*) pokreće po jedan MPI proces.

---

1. primjer

test.pbs

```
#PBS -l select=4:mpiprocs=2
#PBS -l place=scatter
```

PBS_NODEFILE

```
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b1n0.hsn.hpc.srce.hr
x8000c0s0b1n0.hsn.hpc.srce.hr
x8000c0s1b0n0.hsn.hpc.srce.hr
x8000c0s1b0n0.hsn.hpc.srce.hr
x8000c0s1b0n1.hsn.hpc.srce.hr
x8000c0s1b0n1.hsn.hpc.srce.hr
```

U gore prikazanoj **`PBS_NODEFILE`** datoteci možemo uočiti 4 jedinstvena *hostname*-a (**`select=4, place=scatter`**) od kojih se svaki ponavlja 2 puta (**`mpiprocs=2`**).

2. primjer

test.pbs

```
#PBS -l select=4:mpiprocs=2
#PBS -l place=pack
```

PBS_NODEFILE

```
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
```

U gore prikazanoj **`PBS_NODEFILE`** datoteci možemo uočiti 8 istih *hostname*-ova, nastalih kao umnožak 4 *chunka* s istog čvora (**`select=4, place=scatter`**) i 2 MPI procesa po chunk-u (**`mpiprocs=2`**).

3. primjer

test.pbs

```
#PBS -l select=1:mpiprocs=8
#PBS -l place=pack
```

PBS_NODEFILE

```
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
```

U gore prikazanoj **`PBS_NODEFILE`** datoteci možemo uočiti isti rezultat kao u **2. primjeru**.

4. primjer

test.pbs

```
#PBS -l select=8
#PBS -l place=pack
```

PBS_NODEFILE

```
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
x8000c0s0b0n1.hsn.hpc.srce.hr
```

U gore prikazanoj **`PBS_NODEFILE`** možemo uočiti isti rezultat kao u prethodna dva primjera, budući da se podrazumijeva **`mpiprocs=1`**.

GAMESS primjeri

U nadolazećim primjerima pokazat će se različiti načini pokretanja GAMESS-a.

Ulaznu datoteku **`input.inp`** možete kopirati iz *code block*-a niže.

input.inp

```
!   File created by the GAMESS Input Deck Generator Plugin for Avogadro
 $BASIS GBASIS=N31 NGAUSS=6 NDFUNC=1 NPFUNC=1 $END
 $CONTRL SCFTYP=RHF RUNTYP=ENERGY DFTTYP=B3LYP $END
 $SYSTEM MWORDS=4000 $END

 $DATA
Title
C1
Br    35,0     3,56792     6,20395     0,27301
O     8,0     5,99385     1,25485     2,14969
O     8,0     4,86398     4,86307     4,91333
O     8,0     9,36952     3,86128     5,45457
O     8,0     1,54687    -0,26364     1,35457
O     8,0    11,23010    -0,35017     7,71431
O     8,0     7,94882    -3,40000     7,34023
O     8,0     7,71226    -3,45738     5,09165
O     8,0     3,54573     4,66607    12,08432
O     8,0     1,06083     5,28575     1,66226
N     7,0     5,86736     3,50561     2,65626
N     7,0     6,76378     4,83325     6,09126
N     7,0     3,13636     1,03709     2,22294
N     7,0     8,95790     1,86028     6,26477
N     7,0     9,37450    -1,11066     6,82270
N     7,0     0,99106     3,20019     2,43191
N     7,0     0,47930     1,60281     6,30486
N     7,0    -4,09822     2,53404     3,48143
N     7,0     0,07650     0,11692     8,10206
N     7,0    -1,61601     1,03380     6,96204
N     7,0    -5,90834     3,08906     2,03608
N     7,0    -6,15293     3,20068     4,22719
C     6,0     6,77054     3,83619     3,77586
C     6,0     7,77853     4,83972     3,18590
C     6,0     7,86928     4,45830     1,73522
```

C	6,0	6,43765	4,05239	1,43978
C	6,0	5,33264	2,21094	2,56285
C	6,0	6,04418	4,51843	4,95775
C	6,0	3,85334	2,06871	3,03035
C	6,0	3,82518	1,69347	4,53030
C	6,0	7,43867	3,82045	6,93742
C	6,0	2,48426	2,08700	5,12569
C	6,0	6,42368	2,85151	7,55072
C	6,0	9,49202	1,34388	7,53402
C	6,0	8,62178	3,18402	6,16079
C	6,0	10,43357	2,39875	8,19614
C	6,0	1,81613	0,80150	1,92414
C	6,0	0,64934	1,77310	2,35908
C	6,0	1,92868	1,40766	6,36426
C	6,0	10,58420	2,18829	9,71051
C	6,0	5,63196	3,34613	8,74061
C	6,0	10,09604	-0,06626	7,32267
C	6,0	-0,77919	1,60233	1,79357
C	6,0	11,77364	2,60004	7,47908
C	6,0	8,04480	-1,29490	6,17027
C	6,0	6,90311	-0,60391	6,92005
C	6,0	-1,81048	1,99183	2,88756
C	6,0	10,80985	3,51979	10,42475
C	6,0	5,42320	-1,01713	6,76441
C	6,0	4,62016	4,30159	8,59811
C	6,0	5,86515	2,79198	10,01310
C	6,0	-3,21452	2,23620	2,34802
C	6,0	7,87635	-2,81520	6,11632
C	6,0	3,91433	4,75877	9,71382
C	6,0	5,13777	3,22430	11,12151
C	6,0	1,30848	4,10447	1,44103
C	6,0	5,04426	-2,41022	7,25155
C	6,0	4,58305	-0,03324	7,59020
C	6,0	4,18971	4,22448	10,96785
C	6,0	-0,27787	0,95739	7,10655
C	6,0	2,08674	3,67797	0,23409
C	6,0	3,21717	4,39098	-0,19055
C	6,0	1,80685	2,46734	-0,40829
C	6,0	-5,29455	2,91008	3,22888
C	6,0	4,15299	3,77527	-1,03839
C	6,0	2,75670	1,83756	-1,21452
C	6,0	3,95783	2,47120	-1,48620
H	1,0	6,20607	5,46475	6,65425
H	1,0	3,74093	0,30166	1,86990
H	1,0	9,63459	1,68432	5,52462
H	1,0	10,01025	-1,89644	6,68656
H	1,0	0,59762	3,67483	3,23782
H	1,0	-0,57546	0,02060	8,86321
H	1,0	1,03955	0,17581	8,39985
H	1,0	-1,88949	1,72173	6,26525
H	1,0	-2,17398	1,09309	7,79882
H	1,0	-6,86736	2,76982	2,04855
H	1,0	-5,40994	2,68962	1,24739
H	1,0	-5,65740	3,26954	5,11098
H	1,0	-6,68607	4,04472	4,04752
H	1,0	8,07045	-2,75206	8,06255
H	1,0	3,09190	5,49713	11,86526
H	1,0	7,24515	2,90504	4,09623
H	1,0	8,77279	4,80883	3,62297
H	1,0	7,41920	5,86992	3,29675
H	1,0	8,54500	3,61423	1,58821
H	1,0	8,20474	5,29051	1,10705
H	1,0	5,87825	4,96011	1,21269
H	1,0	6,37482	3,37867	0,59775
H	1,0	3,38113	3,03839	2,87192
H	1,0	4,62070	2,20001	5,06906
H	1,0	3,99648	0,61838	4,63248
H	1,0	7,90445	4,39567	7,74781
H	1,0	1,80261	1,75289	4,38402
H	1,0	2,36950	3,17263	5,17808
H	1,0	6,91970	1,95570	7,89964

```
H     1,0     5,72799     2,52435     6,78214
H     1,0     8,65416     1,19042     8,21306
H     1,0     9,92936     3,36725     8,11349
H     1,0     0,46571     1,43639     3,37840
H     1,0     2,14881     0,33513     6,30793
H     1,0     2,35175     1,84692     7,26882
H     1,0     9,66694     1,74974    10,12094
H     1,0    11,40373     1,49746     9,93107
H     1,0    -0,96209     0,56666     1,48408
H     1,0    -0,93324     2,24205     0,91930
H     1,0    12,46787     1,77469     7,65101
H     1,0    12,26079     3,51550     7,83202
H     1,0    11,63796     2,71101     6,39850
H     1,0     8,12843    -0,91806     5,14459
H     1,0     7,14143    -0,57307     7,98980
H     1,0     6,93468     0,42482     6,55774
H     1,0    -1,48860     2,90243     3,40933
H     1,0    -1,83994     1,20272     3,65067
H     1,0     9,99350     4,22023    10,20834
H     1,0    11,74724     3,98863    10,11234
H     1,0    10,83987     3,37390    11,50761
H     1,0     5,13946    -0,93789     5,70965
H     1,0     4,35297     4,69340     7,61837
H     1,0     6,60342     2,00600    10,15675
H     1,0    -3,18607     3,08078     1,65166
H     1,0    -3,56863     1,34313     1,82331
H     1,0     3,14195     5,50926     9,57976
H     1,0     5,31545     2,79011    12,10182
H     1,0     5,40037    -2,58094     8,27141
H     1,0     5,42058    -3,19176     6,59269
H     1,0     3,95298    -2,52695     7,25648
H     1,0     5,02155     0,15724     8,57356
H     1,0     3,56567    -0,39229     7,75619
H     1,0     4,50859     0,92190     7,07144
H     1,0     0,87795     1,93984    -0,23697
H     1,0     5,06428     4,29397    -1,32622
H     1,0     2,56523     0,83165    -1,58304
H     1,0     4,72425     1,96229    -2,06482
 $END
```

16 MPI procesa: 16 MPI procesa × 1 čvor

run.sge

```
#PBS -q cpu
#PBS -l select=1:mpiprocs=16:ncpus=16

export OMP_NUM_THREADS=1

cd ${PBS_O_WORKDIR}

module load scientific/gamess/22.09

rungms.mpi input.inp
```

16 MPI procesa: 4 MPI procesa × 4 čvora

run.sge

```
#PBS -q cpu
#PBS -l select=4:mpiprocs=4:ncpus=4
#PBS -l place=scatter

export OMP_NUM_THREADS=1

cd ${PBS_O_WORKDIR}

module load scientific/gamess/22.09

rungms.mpi input.inp
```