# HP-SEE

## Firefly Scientific Software

www.hp-see.eu

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HP-SEE

High-Performance Computing Infrastructure
for South East Europe's Research Communities

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# Firefly

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- *ab initio* and DFT software
  - SCF
  - DFT
  - CI, CIS
  - MP2, MP3, MP4
  - TDDFT
  - solvation models
- **no support for CC (coupled cluster) and FMO methods**
- 32 bit mpich/openmpi libraries needed to run Firefly on 64 bit systems
- Obtainable at:

  http://classic.chem.msu.su/gran/gamess/index.html

# Example PBS submission script

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```
#!/bin/bash
#PBS -q hpsee
#PBS -l nodes=2:ppn=8
#PBS -l walltime=200:00:00
#PBS -e ${PBS_JOBID}.err
#PBS -o ${PBS_JOBID}.out

cd $PBS_O_WORKDIR
cat $PBS_NODEFILE
${MPI_MPICH_MPIEXEC} /opt/exp_soft/hpsee/firefly/firefly -ex /
opt/exp_soft/hpsee/firefly/
```

# Some Command Line Options

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- -ex
  - specifies path from which to duplicate run time extension files
  - -ex /opt/exp_soft/hpsee/firefly/
- -b
  - specifies external basis set lib file
- -i, -o
  - overwrite default input/output
  - default input is a file named “input”

# Example Input File

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```
 $contrl scftyp=RHF runtyp=ENERGY mplevl=2 units=ANGS icharg=0 mult=1 $end
-$contrl exetyp=check $end
 $system MWORDS=256 $end
 $basis gbasis=N31 ngauss=6 ndfunc=1 nffunc=0 npfunc=1 diffsp=.TRUE. $end
 $guess guess=huckel $end
 $data
Water MP2/6-31+G(d,p) single point energy calculation
CNv 2

O  8.0  0.00000000      0.00000000      0.11761300
H  1.0  0.00000000      0.75734800     -0.47045000
 $end
```

# More Examples

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```
 $contrl scftyp=rhf runtyp=optimize coord=zmt $end
 $system memory=4000000 $end
 $basis  gbasis=sto ngauss=3 $end
 $guess  guess=huckel $end
 $pcm    solvnt=water $end
 $data
a water molecule solvated by PCM water
Cnv 2

O
H 1 rOH
H 1 rOH 2 aHOH

rOH=0.95
aHOH=104.5
 $end
```

# More Examples

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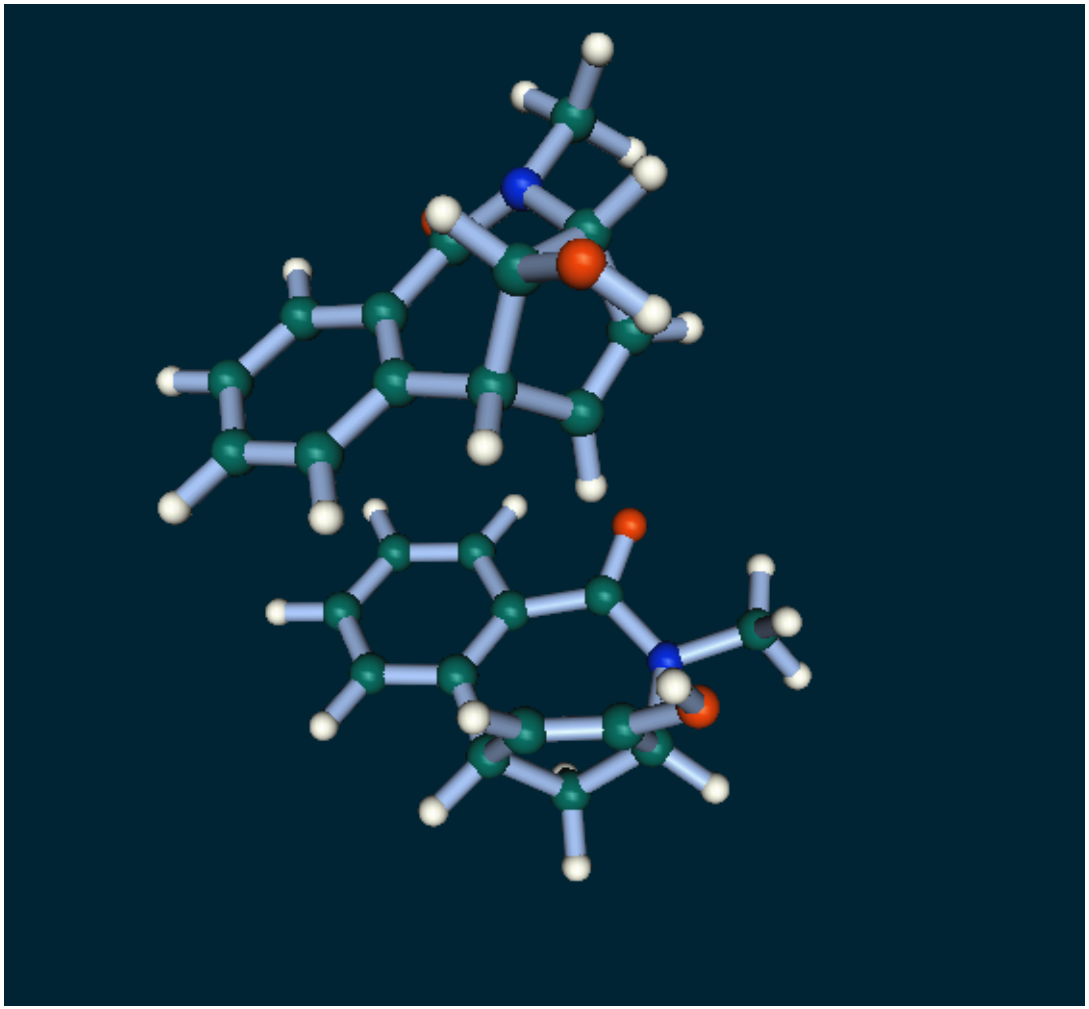
```
! HESSIAN JOB TRIAL
 $CONTRL SCFTYP=RHF DFTTYP=B3LYP1 runtyp=hessian $END
 $CONTRL COORD=CART UNITS=ANGS $END
 $SYSTEM MEMORY=30000000 $END
 $BASIS extfil=.t. GBASIS=SVP $END
 $DATA
cisOH_closeTS
C1
C      6.0     3.9612000000   -0.3934000000   -1.1776000000
N      7.0     2.6357000000   -1.0468000000   -1.4065000000
C      6.0     1.9496000000   -1.4506000000   -0.2384000000
O      8.0     2.4644000000   -1.2190000000    0.8570000000
Pd    46.0    -0.4181000000    0.1491000000   -0.4819000000
O      8.0    -0.1361000000    2.2197000000    0.0109000000
P     15.0    -0.5688000000    0.5140000000    1.6771000000
. . .
H      1.0    -1.2760000000    4.4789000000    1.1412000000
H      1.0    -1.3087000000    5.2574000000   -0.4557000000
 $END
```

# More Examples



**Final energies (Eh):**
**(DFT def2-SVP)**

**-707.927233962**
**-707.917050837**

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**diff. 26.74 kJ/mol**

# More Examples