

# An Update on ADF/AMS software on Graham

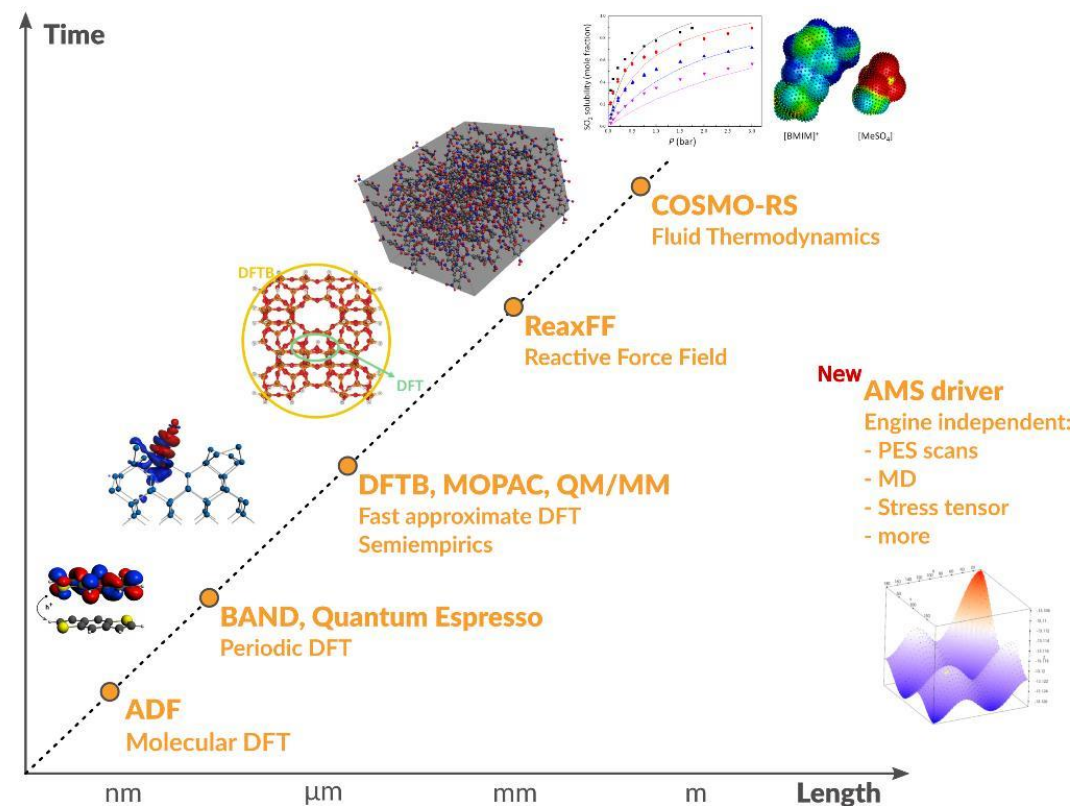
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- Interface with and binaries for QE
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- ReaxFF: Reactive MD
  - Dynamics of large complicated systems
- COSMO-RS: fluid thermodynamics
  - VLE, LLE, logP, solubility
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# ADF, AMS on Graham

```
[jemmyhu@gra-login3 ~]$ module spider adf
```

---

```
adf:
```

---

```
Versions:
```

```
  adf/2016.106
```

```
  adf/2017.207
```

```
  adf/2018.104
```

```
  adf/2019.305
```

```
module unload openmpi  
module load adf/2019.305
```

```
[jemmyhu@gra-login3 ~]$ module spider ams
```

---

```
ams: ams/2020.102
```

---

```
module unload openmpi  
module load ams/2020.102
```

# What's new in AMS 2020

## ADF is an AMS Engine

The most important change in AMS2020 is that

- ADF is only accessible via the AMS driver program.
- The standalone program 'adf' does not exist anymore.
- The job of the AMS driver is to handle all changes in the geometry, e.g. during a geometry optimization, using so-called engines like ADF for the calculation of energies and forces.

## Some of the changes:

- environment variables AMSHOME, AMSBIN (instead of ADFHOME, ADFBIN)
- ams (instead of adf)
- major restructuring of input and input keys
- output files in separate directory
- ams.rkf new binary output file, contains mainly geometry related data
- adf.rkf binary output file (instead of TAPE21), contains mainly single point related data
- AMS does not symmetrize coordinates by default, which ADF used to do.

## Restructuring of input keys

ADF2019 key / feature	ADF2020 key / AMS2020 key / comments
\$ADFBIN	\$AMSBIN
\$ADFHOMES	\$AMSHOMES
\$ADFRESOURCES	\$AMSRESOURCES=\$AMSHOMES/atomicdata
\$ADFHOMES/atomicdata	\$AMSHOMES/atomicdata/ADF. Directory with ADF basis sets.
\$ADFHOMES/atomicdata/ZORA	\$AMSHOMES/atomicdata/ADF/ZORA. Directory with ADF ZORA basis sets.
'ANALYTICALFREQ'	subkey 'NormalModes' of key 'Properties' in <a href="#">AMS driver</a> .
'AORESPONSE'	subkey 'FreqRange' and 'Frequency' removed. Use new subkey 'Frequencies'.

[https://www.scm.com/doc/ADF/General/AMSification\\_of\\_ADF.html](https://www.scm.com/doc/ADF/General/AMSification_of_ADF.html)

# ADF input and run (with ADF script)

Title WATER Geometry Optimization with Delocalized Coordinates

Atoms

O	0.000000	0.000000	0.000000
H	0.000000	-0.689440	-0.578509
H	0.000000	0.689440	-0.578509

End

Basis

Type TZP  
Core Small

End

Geometry

Optim Deloc  
Converge grad=1e-07

End

End Input

```
#!/bin/bash
#SBATCH --account=def-jemmyhu
#SBATCH --nodes=1 --ntasks-per-node=8
#SBATCH --mem-per-cpu=2G
#SBATCH --time=00-01:00
#SBATCH --output=adf_test.log
```

```
module unload openmpi
module load adf/2019.305
ADF adf_test.inp
```

```
[jemmyhu@gra-login1 adf_test]$ sbatch adf_test.sh
Submitted batch job 46326722
```

# Output

```
[jemmyhu@gra-login1 adf_test]$ ls  
adf_test.inp  adf_test.sh
```

```
[jemmyhu@gra-login1 adf_test]$ sbatch adf_test.sh  
Submitted batch job 46326722
```

```
[jemmyhu@gra-login1 scratch]$ pwd  
/home/jemmyhu/scratch  
[jemmyhu@gra-login1 scratch]$ ls  
46326722  
[jemmyhu@gra-login1 scratch]$ cd 46326722/  
[jemmyhu@gra-login1 46326722]$ ls  
[jemmyhu@gra-login1 46326722]$
```

```
[jemmyhu@gra-login1 adf_test]$ ls  
adf_test.inp  adf_test.log  adf_test.sh  logfile  t21.H  t21.O  TAPE21
```



# ADF input (ADF script is not a must)

```
#!/bin/bash

$ADFBIN/adf << eor
Title WATER Geometry Optimization with Delocalized Coordinates
Atoms
  O      0.000000   0.000000   0.000000
  H      0.000000  -0.689440  -0.578509
  H      0.000000   0.689440  -0.578509
End

Basis
Type TZP
Core Small
End

Geometry
Optim Deloc
Converge grad=1e-07
End

End Input
eor
```

```
#!/bin/bash
#SBATCH --account=def-jemmyhu
#SBATCH --nodes=1 --ntasks-per-node=8
#SBATCH --mem-per-cpu=2G
#SBATCH --time=00-01:00
#SBATCH --output=adf_test.log

module unload openmpi
module load adf/2019.305
bash adf_test.run
```

Both the input .run file and the script .sh file have to be executable

Same output result.

```
SCM_TMPDIR = /scratch/$env(USER)
```

Runtime temp files stay in /scratch/username,  
no /scratch/username/jobid

# ADF -> AMS input

```
#!/bin/bash

$ADFBIN/adf << eor
Title WATER Geometry Optimization with Delocalized Coordinates
Atoms
  O      0.000000  0.000000  0.000000
  H      0.000000 -0.689440 -0.578509
  H      0.000000  0.689440 -0.578509
End

Basis
  Type TZP
  Core Small
End
Geometry
  Optim Deloc
  Converge grad=1e-07
End

End Input
eor
```



```
#!/bin/sh
$AMSBIN/ams <<eor
System
  Atoms
    O      0.000000  0.000000  0.000000
    H      0.000000 -0.689440 -0.578509
    H      0.000000  0.689440 -0.578509
  End
End
Task GeometryOptimization
  GeometryOptimization
    Convergence gradients=1e-7
  End
# should be specified in the 'Engine ADF' block:
Engine ADF
  Basis
    Type TZP
  End
  XC
    GGA PBE
  End
EndEngine
eor
```

Note: In ams/2020.102, `$AMSBIN/adf` exists, it's not to run adf job, but its supposed to convert ADF input to AMS input

# AMS run and output

```
#!/bin/bash
#SBATCH --account=def-jemmyhu
#SBATCH --nodes=1 --ntasks-per-node=8
#SBATCH --mem-per-cpu=2G
#SBATCH --time=00-01:00
#SBATCH --output=ams_adf.log
```

```
module unload openmpi
module load ams/2020.102
bash ams_adf.run
```

```
[jemmyhu@gra-login1 scratch]$ ls
46326722
amstmp_ams_test_kid4.270101662
amstmp_ams_test_kid0.270101662
amstmp_ams_test_kid5.270101662
amstmp_ams_test_kid1.270101662
amstmp_ams_test_kid6.270101662
amstmp_ams_test_kid2.270101662
amstmp_ams_test_kid7.270101662
amstmp_ams_test_kid3.270101662
```

```
[jemmyhu@gra-login1 ams_test]$ ls
ams_test.run ams_test.sh
```

```
[jemmyhu@gra-login1 ams_test]$ ls
ams.results ams_test.log ams_test.run ams_test.sh
[jemmyhu@gra-login1 ams_test]$ cd ams.results
[jemmyhu@gra-login1 ams.results]$ ls
adf.rkf ams.log ams.rkf CreateAtoms.out t12.rel
t21.584EDA59.H t21.5E11565E.O
```

adf.rkf: single point related data (replace TAPE21)

ams.log: logfile

Optional: SAVE TAPE13 or TAPE21

```
[jemmyhu@gra-login1 adf_test]$ ls
adf_test.inp adf_test.log adf_test.sh logfile t21.H t21.O TAPE21
```

# AMS named job

```
#!/bin/sh
```

```
AMS_JOBNAME=ams_named $AMSBIN/ams <<eor
```

```
System
```

```
Atoms
```

O	0.000000	0.000000	0.000000
H	0.000000	-0.689440	-0.578509
H	0.000000	0.689440	-0.578509

```
End
```

```
End
```

```
Task GeometryOptimization
```

```
GeometryOptimization
```

```
Convergence gradients=1e-4
```

```
End
```

```
Engine ADF
```

```
Basis
```

```
Type TZP
```

```
End
```

```
XC
```

```
GGA PBE
```

```
End
```

```
EndEngine
```

```
eor
```

```
[jemmyhu@gra-login1 ams_test]$ ls  
ams_named.log ams_named.sh ams_test.log ams_test.run  
ams_named.run ams.results ams_named.results ams_test.sh
```

```
[jemmyhu@gra-login1 ams_test]$ cd ams_named.results  
[jemmyhu@gra-login1 ams_test.results]$ ls  
adf.rkf ams.log ams.rkf CreateAtoms.out t12.rel  
t21.1A3C2F76.O t21.2A82192B.H
```

For whatever reason you have to re-run the same job, you need to rename or remove the previous **###.results** ahead of time.

```
[jemmyhu@gra-login1 ams_test]$ ls  
ams.results ams_test.log ams_test.run ams_test.sh  
[jemmyhu@gra-login1 ams_test]$ rm -rf ams.results  
ams_test.log  
[jemmyhu@gra-login1 ams_test]$ vi ams_test.run  
[jemmyhu@gra-login1 ams_test]$ ls  
ams_test.run ams_test.sh  
[jemmyhu@gra-login1 ams_test]$ sbatch ams_test.sh
```

# ADF/AMS GUI on Graham's vdi nodes

Use TigerVNC client to connect to

[gra-vdi.computecanada.ca](https://gra-vdi.computecanada.ca)

<https://docs.computecanada.ca/wiki/VNC>

```
[jemmyhu@gra-vdi3 ~]$ module load clumod  
[jemmyhu@gra-vdi3 ~]$ module avail
```

```
----- Cluster specific modules -----  
adf/2016.106 (chem)  adf/2018.104 (chem)  ams/2020.102  
adf/2017.207 (chem)  adf/2019.305 (chem,D)  ftdt/2020a
```

**adfjobs**  
**adfinput**  
**adfview**  
.....

**amsjobs**  
**amsinput**  
**amsview**  
.....

## Compute Canada wiki docs

<https://docs.computecanada.ca/wiki/ADF>

<https://docs.computecanada.ca/wiki/AMS>

## Examples

/opt/software/ams/2020.102/examples

## Demos?

**ADF/AMS slurm jobs on Graham's compute nodes**

**ADF/AMS GUI on Graham's vdi nodes**