USING VASP ON ANVIL

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What is VASP?

- The Vienna *Ab initio* Simulation Package (VASP) is a computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, from first principles.
- VASP computes an approximate solution to the **many-body Schrödinger equation**, either within *density functional theory* (DFT), solving the Kohn-Sham equations, or within the *Hartree-Fock* (HF) approximation, solving the Roothaan equations. *Hybrid functionals* that mix the Hartree-Fock approach with density functional theory are implemented as well. Furthermore, *Green's functions methods* (GW quasiparticles, and ACFDT-RPA) and *many-body perturbation theory* (2nd-order Møller-Plesset) are available in VASP.[1]

[1] www.vasp.at

Agenda

- VASP access on Anvil
- Available VASP builds on Anvil
- Compiling VASP on Anvil
- Running VASP on Anvil
- Known errors users run into
- Best practice

VASP on Anvil

VASP ACCESS

VASP Access

- VASP access is controlled by unix groups on Anvil.
- Bring your own VASP license to use VASP on Anvil.
- To request VASP access, please send a ticket to ACCESS Help Desk to request access and provide your ***registered email*** associated with VASP license.
- Prospective users can use the command below to check their unix groups on Anvil.

```
@login02.anvil:[~] $ groups
x-acs00000 vasp6 vasp5
```

VASP on Anvil

Available VASP builds

Available VASP modules on Anvil

Currently, Anvil provides **VASP/5.4.4.pl2** and **VASP/6.3.0** modules with our default environment compiler gcc/11.2.0 and mpi library openmpi/4.0.6.

You can use the **VASP/5.4.4.pl2** module by:

```
$ module load gcc/11.2.0  openmpi/4.0.6
$ module load vasp/5.4.4.pl2
```

You can use the **VASP/6.3.0** module by:

```
$ module load gcc/11.2.0  openmpi/4.0.6
$ module load vasp/6.3.0
```

VASP5 / VASP6 modules on Anvil

- Once a VASP module is loaded, you can choose one of the VASP executables to run your code:

```
vasp_std
vasp_gam
vasp_ncl
```

- The VASP pseudopotential files are not provided on Anvil, you may need to bring your own **POTCAR** files.

Note: only license-approved users can load the VASP module file.

VASP on Anvil

Build your own VASP

Build your own VASP on Anvil

- If you would like to use your own VASP on Anvil, please follow the instructions for Installing VASP.6.X.X and Installing VASP.5.X.X from VASP website:

  www.vasp.at/wiki/index.php/Installing_VASP.6.X.X
  www.vasp.at/wiki/index.php/Installing_VASP.5.X.X

- We also provide instructions about how to install VASP5 and VASP6 with GCC+openmpi or Intel+impi on Anvil and installation scripts:

  VASP 5: www.rcac.purdue.edu/knowledge/anvil/software/installing_applications/vasp/build_your_own_vasp_5
  VASP 6: www.rcac.purdue.edu/knowledge/anvil/software/installing_applications/vasp/build_your_own_vasp_6

VASP on Anvil

Running VASP

VASP input files

VASP requires 4 input files to run a calculation:

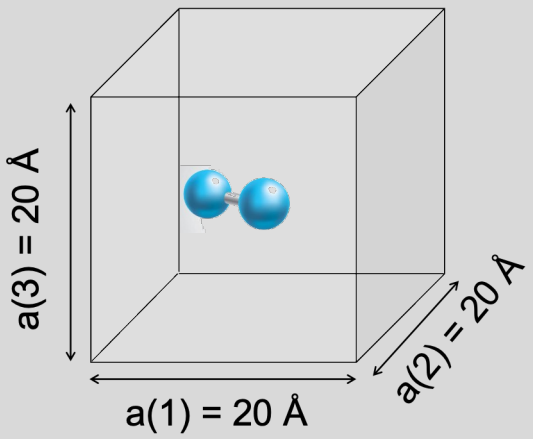
- POSCAR
- INCAR
- KPOINTS
- POTCAR

Example: O_2 molecule in a box

VASP Inputs files – POSCAR

POSCAR is a plain text file and contains at least the lattice geometry and the ionic positions, optionally, also starting velocities for a molecular-dynamics simulation.

```
O2 molecule in a box        ! header (comment)
1.0                         ! scaling parameter
20.0  0.0  0.0              ! Bravais matrix
0.0  20.0  0.0
0.0  0.0  20.0
O                           ! Name(s) of atomic type(s)
2                           ! Number of atoms (of each type)
Selective Dynamics          ! (optional: selective dynamics)
Cartesian                   ! Cartesian or Direct coordinates
10.7 10 11.52  T  T  T      ! positions of each atom
10.7 10 10.28  T  T  T
```



https://www.vasp.at/wiki/index.php/POSCAR

VASP Inputs files – INCAR

INCAR determines what to do and how to do it.

- It contains tags that select the algorithms and set the parameters.
- The settings in the INCAR file are the main source of errors and false results, so carefully checking the meaning of the set INCAR tags.

```
SYSTEM = O2 in a box
GGA = PE
ISMEAR = 0
ISPIN = 2
```

For a list of all INCAR-tags have a look at:
https://www.vasp.at/wiki/index.php/Category:INCAR_tag

VASP Inputs files – KPOINTS

KPOINTS specify the points VASP will use to sample the first Brillouin zone in reciprocal space.

```
Automatic mesh      ! Header (comment)
0                   ! determine number of k points automatically
G or M              ! Γ-centered (G) mesh or Monkhorst-Pack (M) grid
1  1  1             ! subdivisions along the reciprocal lattice vectors
0  0  0             ! optional shift of the mesh
```

https://www.vasp.at/wiki/index.php/KPOINTS

VASP Inputs files – POTCAR

POTCAR contains the pseudopotential for each atomic species used in the calculation. Usually, we will not edit POTCARs. Below shows the beginning lines of POTCAR for O element.

```
PAW_PBE O 08Apr2002
  6.00000000000000
parameters from PSCTR are:
  VRHFIN =O: s2p4
  LEXCH  = PE
  EATOM  =   432.3788 eV,   31.7789 Ry

  TITEL  = PAW_PBE O 08Apr2002
  …
  POMASS =   16.000; ZVAL   =    6.000    mass and valenz
  …
  ENMAX  =  400.000; ENMIN  =  300.000 eV
```

If there are more than one element in your system, use ‘cat’ command to combine POTCARs.

```
$ cat ~/path/C/POTCAR ~/path/H/POTCAR ~/path/O/POTCAR > POTCAR
```

VASP submit script

```
#!/bin/bash

#SBATCH -A myallocation       # Allocation name
#SBATCH --nodes=1             # Total # of nodes
#SBATCH --ntasks=64     # Total # of MPI tasks
#SBATCH --time=00:30:00       # Total run time limit (hh:mm:ss)
#SBATCH -p wholenode           # Queue (partition) name

# Manage processing environment, load compilers and
applications.
module purge
module load gcc/11.2.0  openmpi/4.0.6
module load vasp/6.3.0 # or module load vasp/5.4.4.pl2
module list

# Launch MPI code
mpirun -np $SLURM_NTASKS vasp_std
```

Find allocation name with command, mybalance

```
x-     @login00.anvil:[~] $ mybalance

Allocation      Type    SU Limit    SU Usage   SU Usage  SU Balance
Account                             (account)    (user)
==============  ====  ==========  ========== ==========  ==========
asc170016        CPU    100000.0     54238.7      552.3     45761.3
asc170016-gpu    GPU      5000.0       144.3        0.0      4855.7
```

Find available partitions, showpartitions

```
x-      @login02.anvil:[~] $ showpartitions
Partition statistics for cluster anvil at T
     Partition     #Nodes     #CPU_cores  C
     Name State Total  Idle  Total   Idle F
wholenode    up   750     1  96000   2304
 standard    up   750     1  96000   2304
 shared:*    up   250   176  32000  23139
     wide    up   750     1  96000   2304
  highmem    up    32    28   4096   3633
    debug    up    17     1   2176    314
      gpu    up    16     1   2048   1684
gpu-debug    up    16     1   2048   1684
```

Anvil partitions

All Anvil nodes have 128 processor cores, 256 GB or 1 TB of RAM.

Anvil Production Queues						
Queue Name	**Node Type**	**Max Nodes per Job**	**Max Cores per Job**	**Max Duration**	**Max running Jobs in Queue**	**Max running + submitted Jobs in Queue**
debug	regular	2 nodes	256 cores	2 hrs	1	2
gpu-debug	gpu	1 node	2 gpus	0.5 hrs	1	2
wholenode	regular	16 nodes	2,048 cores	96 hrs	64	2500
wide	regular	56 nodes	7,168 cores	12 hrs	5	10
shared	regular	1 node	128 cores	96 hrs	6400 cores	-
highmem	large-memory	1 node	128 cores	48 hrs	2	4
gpu	gpu	-	-	48 hrs	-	-

https://www.rcac.purdue.edu/knowledge/anvil/run/partitions

How to charge SUs

- The charge unit for Anvil is the Service Unit (SU).
- 1 SU: use of 1 core (≤ 2GB memory) for 1 hour
- Example: a job running with 4 cores for 2 hours:

```
x-     @login00.anvil:[~] $ mybalance

Allocation     Type    SU Limit    SU Usage   SU Usage  SU Balance
Account                            (account)    (user)
=============  ====  ==========  ========== ==========  ==========
asc170016       CPU    100000.0     54238.7      552.3     45761.3
asc170016-gpu   GPU      5000.0       144.3        0.0      4855.7
```

Partitions	Charged SUs
shared, debug	If ~8GB memory, SU = 4 cores x 2 hours = 8
wholenode (standard), wide	SU = 128 cores x 2 hours = 256
highmem	SU = 4 x regular SU amount

- Command to check SU usage for one job

```
@login02.anvil:[~] $ /usr/local/bin/jobsu <jobid>
```

More information about SU charging:
https://www.rcac.purdue.edu/knowledge/anvil/run/accounting

A few useful commands

- sbatch <submit_script>
- scancel <jobid>
- squeue -ul username
- scontrol update job=<jobid> timelimit=03-00:00:00
- jobinfo <jobid>
- mybalance
- myquota

VASP on Anvil

Known errors users run into

Where to find error message?

- OUTCAR (in the end)

  normal termination:

```
          User time (sec):       24.400
        System time (sec):        1.070
       Elapsed time (sec):       26.153

  Maximum memory used (kb):      247100.
  Average memory used (kb):          N/A

        Minor page faults:       162455
        Major page faults:          107
Voluntary context switches:        1806
```

- the .out file (in the end) #SBATCH --output slurm.%N.%j.out

  normal termination:

```
 reached required accuracy - stopping structural energy minimisation
```

- the .err file (in the end) #SBATCH --error=slurm.%N.%j.err

VASP not found

Error:

module: command not found

Root cause:

- No access to VASP modules on Anvil
- check your unix groups with command, groups

```
@login02.anvil:[~] $ groups
x-acs00000 vasp6 vasp5
```

Solution:

send a ticket to ask for VASP access, in the ticket, we need your email address associated with a valid VASP license

https://support.access-ci.org/user/login?destination=/open-a-ticket

Out of memory

Error:

srun: error: axxx: task xx: Out Of Memory

Root cause:

- Not enough cores or space

  check the memory usage with 'jobinfo <jobid>'

  $ jobinfo 6364002
  …
  Mem reserved : xxxxM
  Max Mem used : xxxxM

Solutions:

- reduce the memory demand by reducing ENCUT or KPOINTS
- increase the number of cores
- use wholenode or highmem partition

not divisible by NPAR

Error:

M_divide: can not subdivide

Root cause:

- total number of cores is not divisible by NPAR

Solutions:

- Use default: NPAR default is the same as the total number of cores
- Set NPAR ~ sqrt (total number of cores)

Numa_num

Error:

node_info->numa_num <= ((MPIDI_SHMGR_SYNCPAGE_SIZE / MPIDI_SHMGR_FLAG_SPACE) - 1)

Root cause:

- Unknown
- Good guess: intel mpi on Anvil

Workarounds:

Add '--mpi=pmi2' to your srun or mpirun,

```
srun -n $SLURM_NTASKS --mpi=pmi2 …
```

Segmentation fault

This error may not link to one specific cause, possible reasons can be:

- insufficient memory: not enough cores or space at $HOME or $PROJECT
- POSCAR structure
- MPI abort

  If use intel mpi, try to add '--mpi=pmi2'

VASP on Anvil

Best practice

How many cores/nodes to use?

- VASP in general considered to scale up to 1 core/atom.
  - Conservatively, go with 0.5 core/atom or slightly less
  - If use dense kpoints, use 0.5 core/atom for each kpoint group; the total number of cores = KPAR x 0.5 core/atom x (# of atoms)
  - If there are multiple images, total number of cores = IMAGES x 0.5 core/atom x (# of atoms)
- Using larger number of cores may not reduce the time to solution cost effectively
  - VASP may spend most of the time in the communication even if it does not run into error

Choose right file system

```
x-     @login04.anvil:[~] $ myquota

Type     Location           Size    Limit    Use        Files    Limit     Use
==========================================================================
home     x-               983.5MB   25.0GB     4%            -        -      -
scratch  anvil              512KB  100.0TB  0.00%           0k   1,000k  0.00%
projects x-asc170016     358.0GB    5.0TB     7%          94k   1,048k     9%
```

– Your homes directory, $HOME, is not the right file system to run your VASP jobs – You may exceed your home quota, 25 GB and receive ‘out of memory’ error.

– The scratch directory, $SCRATCH, are recommended file systems to run your jobs both for a larger storage space and a better I/O performance. There are 100TB scratch quota for each user on Anvil.

Important note: your scratch folder will be purged regularly.

– Back up your important files to your project directory, /anvil/projects/x-000000, which has 5TB quota.

Short scaling tests

- Short scaling tests are recommended.
  - starting with 1 core/atom
  - Parameters to consider: NPAR/NCORE, KPAR

    NPAR ~ sqrt (total number of cores) performs better than NPAR=1 or the default NPAR

    KPAR ~ an integer divisor of the total number of cores (e.g. number of nodes)

# of nodes	# of cores	run time (T_r), sec	expected run time (T_{er}), sec	scaling efficiency = T_{er}* 100/T_r , %
0.25	32	228	228	228*100/228=100
0.5	64	125	228/2=114	114*100/125=91
1	128	96	114/2=57	57*100/96=59
2	256	112	57/2=29	29*100/112=26

- Use debug partition to see if your jobs could run to completion before submitting the long jobs

Anvil support

- Anvil user guide

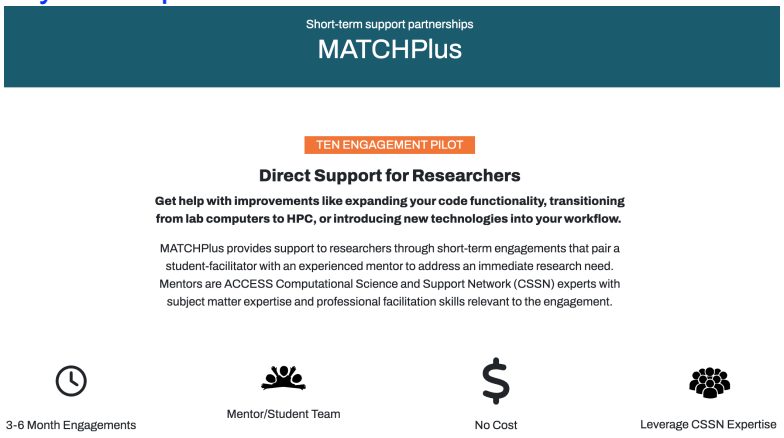
  https://www.rcac.purdue.edu/knowledge/anvil

- For general questions, submit a ticket to ACCESS Help Desk

  https://support.access-ci.org/user/login?destination=/open-a-ticket

- For complex consultation request, submit your request to MATCHPlus

  https://support.access-ci.org/matchplus



THANK YOU!