

VASP: Introduction

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National Supercomputer Centre (NSC)

@Umeå University, HPC2N, 29th Oct 2019, room UB334



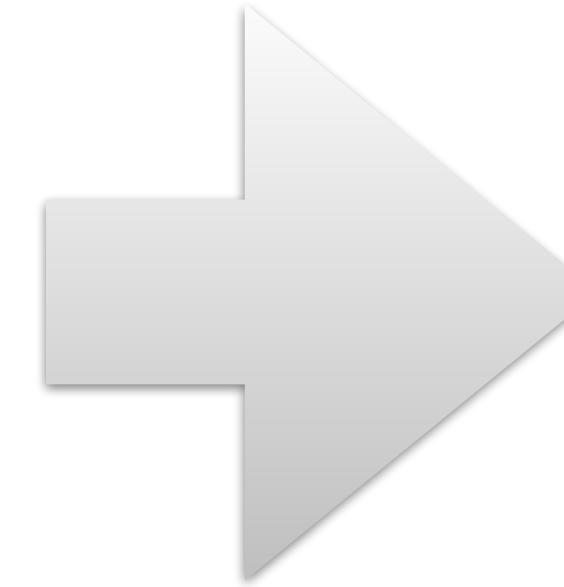
Introduction

- Where to find information
 - VASP at different SNIC HPC centers
- Starting files
- Important parameters
- Input/output
- Examples

... clickable links are underlined

Short background

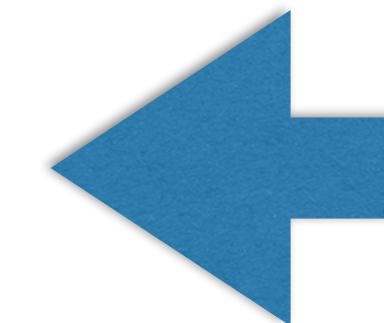
- Software license
- PAW-method
- DFT, post-DFT (HSE06, GW, ...)
- Born-Oppenheimer Molecular Dynamics
- **widely used** in Academia/Industry
 - Efforts from **Intel & Nvidia** for optimization
- 20-25% of Tetralith usage
- next version is **VASP6**



<http://vasp.at/>

Starting advice

- Read the [documentation!](#)
- VASP default settings
- Caution: “inherited” input files
- Avoid overly messy INCAR
- Possible differences in installations & versions
refer to respective webpages / documentation



good starting point

Resources

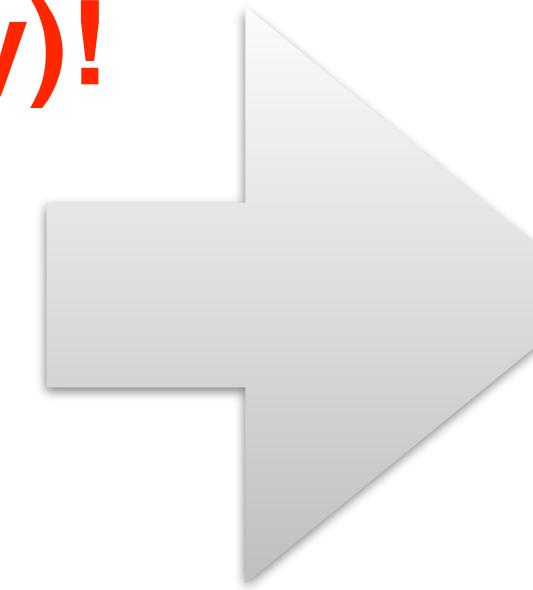
- Manual

Read all (really)!

- Wiki

**examples,
presentations**

- Forum

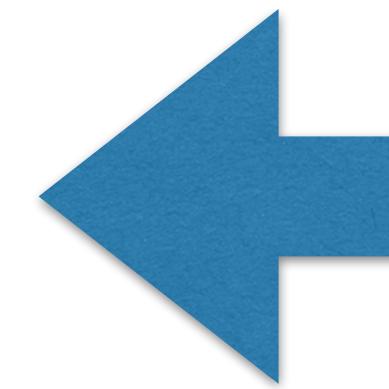


Find the links:

<http://vasp.at/>

- Peter Larsson's old blog at NSC:

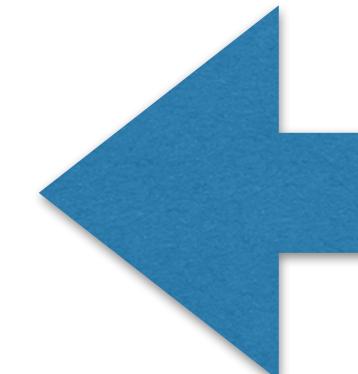
<https://www.nsc.liu.se/~pla/>



**info &
discussion**

Questions/trouble? support@nsc.liu.se, support@hpc2n.umu.se, ...

VASP at SNIC HPC centers

- **Kebnekaise, HPC2N, UmU**  **this course**
- Tetralith / Sigma, NSC, LiU
- Beskow, PDC, KTH
- Also available at other systems/centers
 - On many systems: `$ module avail vasp`
`$ module spider vasp`

VASP versions & utilities

- **Latest:** patch.5.4.4.16052018 for 18Apr17
 - Check centre webpages for details!
- [wannier90](#): maximally localized wannier functions
- [VTST](#): transition state tools for VASP
- [VASPsol](#): solvation model for VASP
- [Beef](#): Bayesian error estimation functionals
- constrained relaxation

The VASP site

https://www.vasp.at

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VASP

Home Documentation News FAQs Resources Contact Impressum



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Impressum



About VASP

What is the Vienna Ab initio Simulation Package and what can it do?



Documentation

Here you'll find the VASP manual, online as well as a pdf copy. We have also started a Wiki, that in future will replace the online manual completely.



Vasp Forum

Subscribe to the VASP forum and post a question!

N.B.: registration is reserved for licensed users!

- You will have to provide a valid license number.
- You may only register with an email address clearly attributable to an academic institution or company. We will not accept addresses from gmail, yahoo, etc.



Related Resources

Links to useful utilities and VASP related third-party resources.



The VASP team

Who we are and how we may be reached.



News

Good news, like highlighted papers about research performed with VASP and interesting new features of VASP, and the bad news, like bug(fixes).

Community Portal

License holders may enter the community portal to access the download area.



Login



FAQs

Frequently asked questions with respect to the administrative side of things, like "how may I obtain a VASP license?".



Important Notice

Beware: Some companies are selling illegal copies of VASP!

Next Up Previous Contents Index

Next: [Introduction](#) [Contents](#) [Index](#)

N.B. This document is no longer maintained, please visit our [wiki](#).



The VASP Manual - Vaspwiki

https://cms.mpi.univie.ac.at/wiki/index.php/The_VASP_Manual

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page discussion view source history

The VASP Manual

All requests for technical support from the VASP group must be addressed to: vasp.materialphysik@univie.ac.at

Contents [hide]

- 1 Getting started
- 2 Input and Output
- 3 Featured topics
- 4 Support

Getting started

How to Install VASP	First install VASP.
Workshops	The collection of workshops is a good place for the introduction to the basics of VASP.
Lectures	The collection of lectures is a good place to start as well.
Tutorials and Examples	The collection of tutorials and examples is a good place to learn the usage of VASP.

Input and Output

INCAR tags	All INCAR tags at a glance.
Input Files	
Output Files	

Category:Examples - Vaspwiki

https://cms.mpi.univie.ac.at/wiki/index.php/Category:Examples

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Category:Examples

All requests for technical support from the VASP group must be addressed to: vasp.materialphysik@univie.ac.at

All articles related to VASP example calculations

Contents

Pages in category "Examples"

The following 81 pages are in this category, out of 81 total.

A

- [Adsorption of H₂O on TiO₂](#)
- [Alpha-AlF₃](#)
- [Alpha-SiO₂](#)
- [At and mol further](#)

B

- [Bandgap of Si in GW](#)
- [Bandgap of Si using different DFT+HF methods](#)
- [Bandstructure and CRPA of SrVO₃](#)
- [Bandstructure of Si in GW \(VASP2WANNIER90\)](#)
- [Bandstructure of SrVO₃ in GW](#)
- [Beta-tin Si](#)

C

- [Calculate U for LSDA+U](#)
- [Cd Si](#)
- [Cd Si relaxation](#)
- [Cd Si volume relaxation](#)
- [CO](#)

E cont.

- [Estimation of J magnetic coupling](#)

F

- [Fcc Ni](#)
- [Fcc Ni \(revisited\)](#)
- [Fcc Ni DOS](#)
- [Fcc Ni DOS with hybrid functional](#)
- [Fcc Si](#)
- [Fcc Si bandstructure](#)
- [Fcc Si DOS](#)

G

- [Graphite interlayer distance](#)
- [Graphite MBD binding energy](#)
- [Graphite TS binding energy](#)

H

- [H₂O](#)
- [H₂O molecular dynamics](#)

N cont.

- [NiO GGA](#)
- [NiO GGA+U](#)
- [NiO HSE06](#)
- [NiO L\(S\)DA+U](#)
- [NiO LSDA](#)
- [NiO LSDA+U](#)
- [Nucleophile Substitution CH₃Cl - Standard MD](#)
- [Nucleophile Substitution CH₃Cl - BM](#)
- [Nucleophile Substitution CH₃Cl - mMD1](#)
- [Nucleophile Substitution CH₃Cl - mMD2](#)
- [Nucleophile Substitution CH₃Cl - mMD3](#)
- [Nucleophile Substitution CH₃Cl - SG](#)

O

- [O atom](#)
- [O atom spinpolarized](#)
- [O atom spinpolarized low symmetry](#)
- [O dimer](#)

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https://www.hpc2n.umu.se

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News and Events

Course: Introduction to GPU programming: When and how to use GPU-acceleration?

Maintenance on cooling system affects Kebnekaise and Abisko, 2019-10-16 - 17

<https://www.hpc2n.umu.se/>

Systems and Support > Software > VASP

<https://www.hpc2n.umu.se/resources/software/vasp>

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Projects and Collaborations

egi

PRACE

EISCAT SCIENTIFIC ASSOCIATION

esfence THE e-SCIENCE COLLABORATION

NÖSEG

Nordic Smart Simulation Energy Group

NLAFET

SNIC Science Cloud

News and Events

Course: Introduction to GPU programming: When and how to use GPU-acceleration?

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		models of macromolecular complexes using Electron Microscopy.	
		External info: External info	
Siesta	Siesta performs electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.	Abisko, Kebnekaise	
	External info: External info		
Turbomole	TURBOMOLE is a quantum chemical program package	Abisko, Kebnekaise	
	Extern info: Extern info		
VASP	Performs ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set.	Abisko, Kebnekaise	
	Extern info: Extern info		
VMD	VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.	Abisko, Kebnekaise	
	Extern info: Extern info		
WRF	Advanced Research WRF (ARW) Modeling System is a flexible, state-of-the-art atmospheric simulation system.	Abisko, Kebnekaise	
	Extern info: Extern info		
Compilers			
GCC	GNU Compiler Collection. Has C, C++, Fortran 77, Fortran 90, and Fortran 95. Available for serial, OpenMP, and MPI code for all languages, with the exception of Fortran 95 MPI programs. Part of several compiler toolchains.	Abisko, Kebnekaise	
	External info: External info		
Intel	Intel Compilers. Has C, C++, Fortran 77, Fortran 90, and Fortran 95. Available for serial, OpenMP, and MPI code for all	Abisko, Kebnekaise	



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freesurfer/5.3.0
fsl/5.0.5
ga/intel-impi-mkl-i8/5.3
gamess-us/20130501-r1
gate/5.0.0_p01
gate/7.1.0
gaussian/09.d.01
geant4/10.01.00
geant4-data/10.01
gmp/gcc/6.1.0
gpaw/0.11.0.13004
gromacs/5.1.1
gurobi/6.5
t-mn01 [~]\$

mpfr/gcc/3.1.3
mumps/gcc/4.10.0
mumps/pgi/4.10.0
mumps/psc/4.10.0
namd/2.9
netcdf/4.1.3
nwchem/6.5
octave/3.6.4
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turbomo
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vasptools/0.2
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voronoi/gcc/0.4.6
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wrf/3.7.1



Home » VASP

VASP

Policy

The Vasp program is not distributed via site licences. However, HPC2N have access to the VASP code to be able to support any research groups that have a valid VASP license.

See the VASP license for information regarding terms for published work.

When you have gotten access to a license, the **license holder** should either add the license info into SUPR (or contact support@hpc2n.umu.se with the following information: license number and list of users who should have access). You will then be given access to using VASP.

Note: only the owner of the license can add/delete users to/from the access list.

General

VASP is a package for performing ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set.

Description

VASP is a complex package for performing ab-initio quantum-mechanical molecular dynamics (MD) simulations using pseudopotentials or the

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https://www.nsc.liu.se

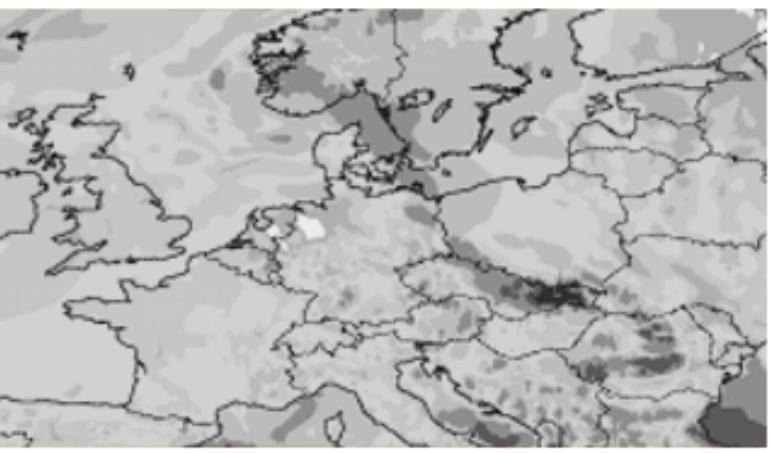
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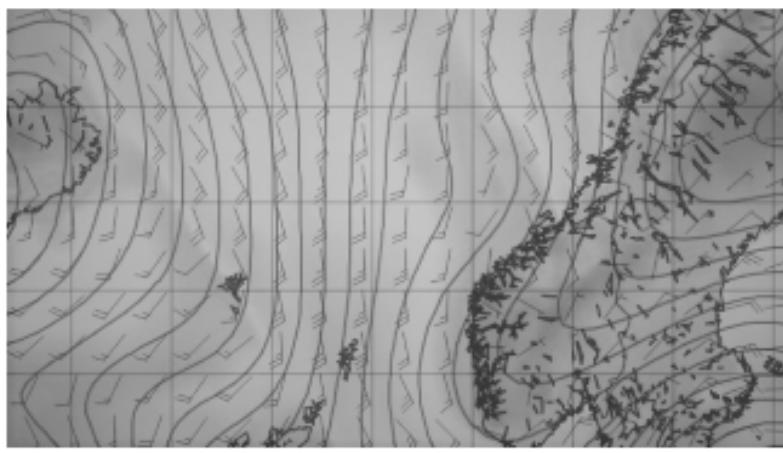
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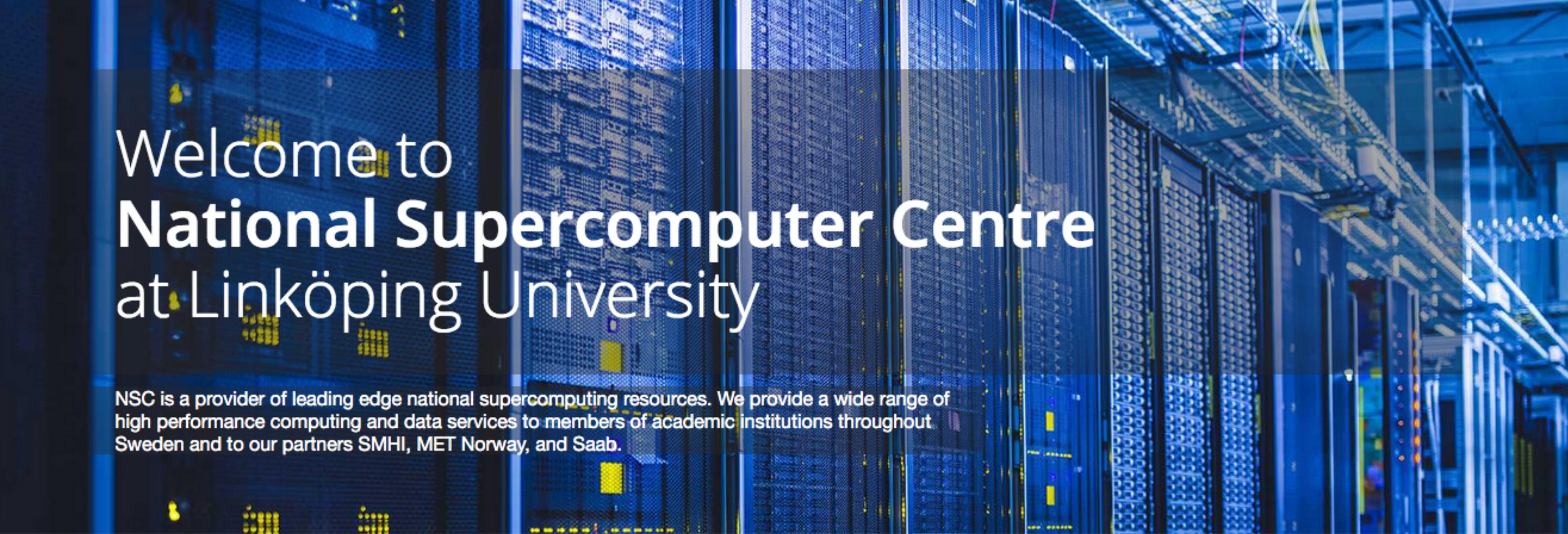
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NSC is a provider of leading edge national supercomputing resources. We provide a wide range of high performance computing and data services to members of academic institutions throughout Sweden and to our partners SMHI, MET Norway, and Saab.

OUR PARTNERS

 SMHI
The Swedish Meteorological and Hydrological Institute (SMHI) is an expert agency under the

 MET Norway
MET Norway is the meteorological service in Norway, serving the public, the civil services



<https://www.nsc.liu.se/> Software > Installed software > Tetralith & Sigma software list > VASP
<https://www.nsc.liu.se/softwareinstalled/tetralith/vasp/>

NSC NSC

https://www.nsc.liu.se

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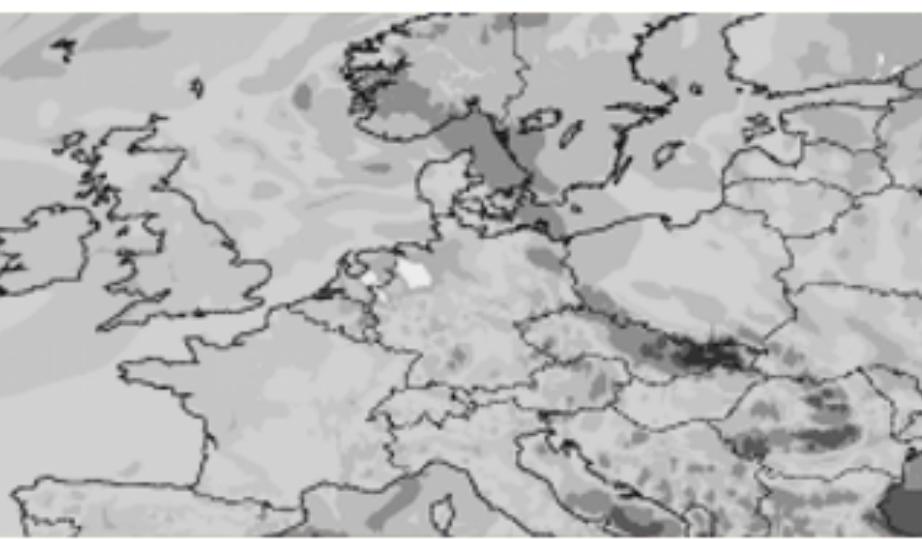
NSC

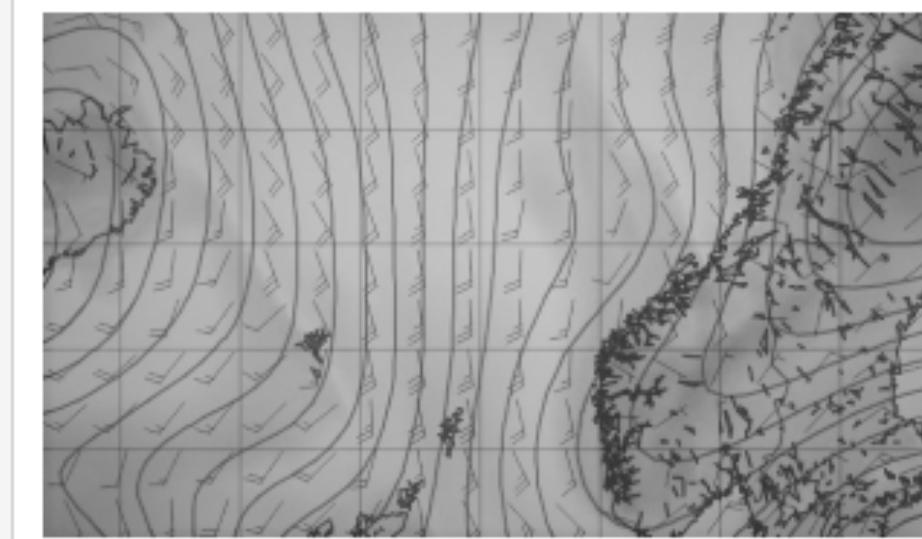
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OUR PARTNERS

 **SMHI**
The Swedish Meteorological and Hydrological Institute (SMHI) is an expert agency under the

 **MET Norway**
MET Norway is the meteorological service in Norway, serving the public, the civil services

NSC Software

https://www.nsc.liu.se/software/

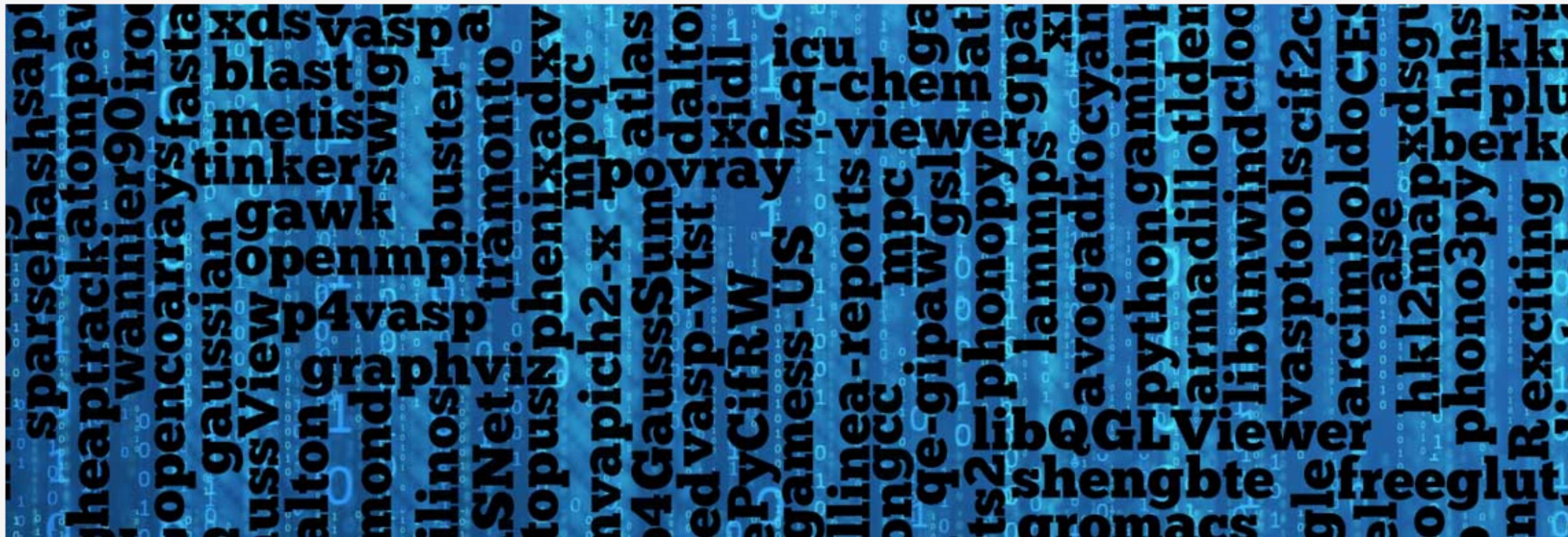
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Search

NSC / Software



Software

Explore this part to find out about all software environment related matters. Please proceed to the [installed software](#) page to find out which scientific software we have on our clusters. If you are going to compile software from source code, we suggest that you read the [NSC build environment](#) introduction and the [compilers](#) section.

Installed software

Which software is available on what systems and how to run it

Software installation policy

What to do if software you need isn't installed

Software licensing

How we handle software licensing of commercial software.

The screenshot shows a web browser window with the title "NSC Installed software". The address bar contains the URL "https://www.nsc.liu.se/software/installed/". The page header includes the NSC logo, a navigation menu with links to "START", "SYSTEMS", "STORAGE", "SOFTWARE", "ABOUT", "USER AREA", and a search bar. Below the header, there is a secondary navigation bar with links to "Installed software", "Software installation policy", "Software licensing", "Compilers", "NSC build environment", "Modules", "MPI libraries", "Math libraries", and "Python at NSC".

NSC / Software / Installed software

Installed software

NSC has a large number of software installations available, often in multiple versions to suit the needs of various user communities. For a list of installed software, please see the corresponding resource page below. If you need software that is presently not installed, please see our [software installation policy](#).

Software portfolios by cluster

- [Tetralith & Sigma Software List](#).
- [Bi Software List](#). This is the main resource for finding out what software is available on Bi.

Module system

You can also query the [module system](#) for available software and recommendations on what versions to use, e.g:

```
module avail  
module add vasp/recommendation
```

SNIC knowledge base

Information on software and availability for all of SNIC is also available in the [SNIC knowledge base software section](#). There is specific information for these NSC resources:

Tetralith & Sigma Software

A list of software installed on Tetralith and Sigma and links to further information

NSC Tetralith & Sigma Software

https://www.nsc.liu.se/software/installed/tetralith/

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Tetralith & Sigma Software

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Tetralith & Sigma Software List

DISCLAIMER: Please note that the software catalogue is a work in progress! If your application is missing, please request it by sending e-mail to [NSC Support](#)

The following scientific applications have been installed centrally under </software/sse/>. This list may not always be 100% up to date. The most reliable source is running the command `module avail` while logged into Tetralith or Sigma, possibly augmented by `ls /software/sse/manual/` to show additional manually performed installations without modules. Please note that some of this software is licensed, and may not be available for everyone. You need ask NSC for access, which is typically granted upon some proof of having a license.

The list was last updated: 2019-02-21

Electronic structure

- Abinit
- ASE
- Elk
- EPW
- exciting
- GPAW
- phonopy
- phono3py
- p4vasp
- Quantum Espresso
- vasptools
- VASP (licensed)
- WIFN2k (licensed)

NSC VASP

https://www.nsc.liu.se/software/installed/tetralith/vasp/

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ABINIT AMBER ANSYS ASE ATAT Allinea Performance Reports Allinea-DDT Allinea-MAP CDO COMSOL

CP2K CPMD DL_POLY Dalton/LSDalton EC-Earth EPW Elk FERRET GPAW Grace Gurobi Optimizer

HDF5 Julia LAMMPS MATLAB MOLDEN Mathematica NAMD NCO NCVIEW Open Babel OpenFOAM

ParaView Quantum ESPRESSO STAR-CCM+ Siesta VMD WEST WIEN2K Yambo ecCodes exciting

grib_api netCDF p4vasp parallel phono3py phonopy vasptools **VASP** Clang Gaussian and GaussView

NSC / Software / Installed software / Tetralith & Sigma Software / VASP

VASP Installations on Tetralith & Sigma

First of all, VASP is licensed software, your name needs to be included on a VASP license in order to use NSC's centrally installed VASP binaries. [Read more about how we handle licensing of VASP at NSC.](#)

Some problems which can be encountered running VASP are described at the end of this page.

How to run: quick start

A minimum batch script for running VASP looks like this:

```
#!/bin/bash
#SBATCH -J jobname
#SBATCH -N 4
#SBATCH --ntasks-per-node=32
#SBATCH -t 4:00:00
#SBATCH -A SNIC-xxx-yyyy

module add VASP/5.4.4.16052018-nsc1-intel-2018b-eb
mpirun vasp_[std/gam/ncl]
```

This script allocates 4 compute nodes with 32 cores each, for a total of 128 cores (or MPI ranks) and runs VASP in parallel using MPI. Note that you should edit the jobname and the account number before submitting.

General information about VASP X +

https://www.pdc.kth.se/software/software/VASP/index.html

PDC Center for High Performance Computing

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KTH / PDC

Software

General information about VASP

Licenses

Available Software - General information about VASP

General information about VASP

System	Available versions
Beskow	5.4.4-wannier90, 5.4.4, 5.4.1.patched, 5.3.5-vtst3.1, 5.3.5-31Mar14
Tegner	5.4.1, 5.3.5

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.

For more information see: <http://vasp.at>

Licenses

VASP is not free software and requires a software license. VASP licenses are managed in [SUPR](#). All people who want to use VASP should have SUPR accounts and be a member of a VASP group in SUPR. VASP groups have owners, typically a principal investigator of a project, and that owner can add and remove people using the SUPR interface. If you are Ph.D student, we suggest that you check with your supervisor.

 SNIC
PDC is a SNIC centre.

Using VASP 5.4.4 on Beskow — +

https://www.pdc.kth.se/software/software/VASP/beskow/5.4.4/ Search

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Software

Using VASP 5.4.4 on Beskow

General observations

NPAR, NCORE and NSIM

How to choose the number of cores

Vasp Filenames

BEEF functionals

VASP TST Tools

VTST Scripts

VASPsol

Using vdW functionals

Running Vasp

Available Software - General information about VASP - Using VASP 5.4.4 on Beskow

Using VASP 5.4.4 on Beskow

General observations

- VASP is not helped by hyper-threading (64 virtual cores per compute node).
- No GPU/OpenMP-support.
- Running on fewer than 32 cores per node allocates more memory to each MPI task. This can in some cases improve performance and is necessary if your job crashes with an OOM error. See the example submit script below on how to do this correctly.

NPAR, NCORE and NSIM

From initial testing, we recommend:

- NPAR = number of compute nodes
- NCORE = cores / node, typically 16,24 or 32.
- NSIM = 2
- KPAR = number of compute nodes (if applicable)

How to choose the number of cores

Rule of thumb:

- 1 atom per core = Good
- 0.5 atom per core = Could work (but bad efficiency and time wasted)

Example of day-to-day tools

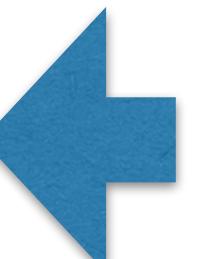
- less / vi reading/editing files
- grace / gnuplot plotting tools
- Bash simple scripts
- cif2cell convert from .cif
- p4vasp analysis of VASP output
- xcrysden / vesta view structure
- Schrödinger create/view structure

@Kebnekaise, Tetralith

Also of interest:

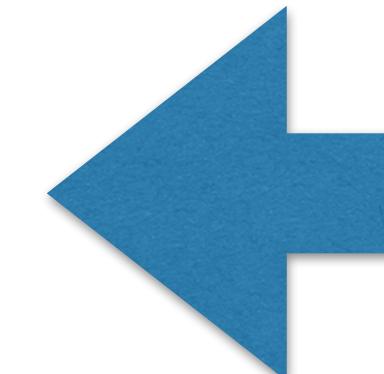
- Python / R analysis etc. (check out e.g. using jupyter)
- ASE different tools and Python modules
- Matlab / Octave analysis etc.

[Check out presentations for Tetralith training](#)



Different types of calculations

- Structural relaxation (different ways)
- Regular E_{tot} scf run using PBE, HSE06, GW, ...
- Density of states, bandstructure, charge density, ...
- Born-Oppenheimer MD
- Used within a special framework (VTST, ...)
- See VASP wiki examples



Input files

- INCAR - input parameters
- POSCAR - structure (generate using e.g. cif2cell)
- POTCAR - PAW potentials (how to select?)
- KPOINTS - k-mesh (or list)
- + job script

SLURM batch queue system &
settings used by SNIC centers

INCAR parameters

- PREC - “precision”, ENCUT and FFT grids
- ENCUT - plane wave energy cutoff
- ALGO - wf optimisation
- NBANDS - if not set, auto-determined
- NSIM - for RMM-DIIS algorithm (ALGO)
- NCORE or NPAR - bands treated in parallel
- KPAR - k-point parallel

INCAR parameters

accuracy /
method

parallel
calcs.

- PREC - “precision”, ENCUT and FFT grids
- ENCUT - plane wave energy cutoff Completeness of basis-set
Recommended to set!
- ALGO - wf optimisation
- NBANDS - if not set, auto-determined
Must be the same for Etot comparison!
- NSIM - for RMM-DIIS algorithm (ALGO)
- NCORE or NPAR - bands treated in parallel
- KPAR - k-point parallel
 - We will get back to the settings in the 2nd part

INCAR defaults

- PREC = Normal Might want “Accurate”
- ENCUT = ? **Always set!** ENMAX $\times 1.0 - \times 1.5$
- ALGO = Normal **good tradeoff**
Can use “Fast” and “VeryFast”
- NBANDS = ? can be **overridden** by VASP
- sometimes extra empty states needed
- NSIM = 4 Typically OK
- NCORE = 1 **Adjust** (if not hybrid-functional, HSE06, etc.)
- KPAR = 1 for k-point parallel calcs.

Will discuss in more detail later on...

INCAR defaults

- NSW = 0 max ionic steps, also MD steps
- NELM = 60 max electronic selfconsistency steps
- NELMIN = 2 min steps. For relaxation/MD set 4-8
- EDIFF = 1E-4 converge to 4 last digits, sometimes higher accuracy is needed
- EDIFFG = EDIFF x10 ionic relaxation break condition, if negative value, break if forces < IEDIFFGI
- ISMEAR = 1 how to treat partial electron occupancy:
1 = metals, 0 = bandgap, -5 = for accurate E_{tot}
- ISPIN = 1 2 = spin-polarized calc.
- IBRION = -1 (NSW=-1,0) or 0 how ions are updated & moved
no update MD =2 ionic relaxation

in very brief,
refer to
VASP wiki
for details

POSCAR

A simple case of fcc Ni, refer to the [VASP wiki example](#)

(hopefully) useful	comment	Ni fcc	
		3.53	lattice constant (\AA)
	lattice vectors	0.5 0.5 0.0 0.0 0.5 0.5 0.5 0.0 0.5	
	number of atoms per type	Ni	element symbols
	position for first atom	1	optional, useful for clarity & plotting
		Cartesian	Cartesian or Direct coordinates
		0 0 0	First letter is sufficient, i.e. “C” for “Cartesian”

Direct coordinates: expressed in terms of the lattice vectors (no lattice constant, scaling)
Cartesian coordinate: expressed as (x,y,z) with the scaling factor included

POSCAR

From the course examples, H and Si on Ag(111) surface:

```
100% H on Si on Ag(111)
10.007900
1.00000000000000 0.00000000000000 0.00000000000000
0.50000000000000 0.866025403784439 0.00000000000000
0.00000000000000 0.00000000000000 4.352531500114909
H Si Ag
14 14 108
Selective dynamics
Direct
```

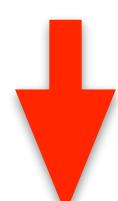
first H atom →

← Note order of atoms

← Relax for different directions

Selective dynamics
always for Direct coord.
T = relax
F = fixed

Rest of H,
Si & Ag atoms
following



0.75833800000000	0.05288160000000	0.60594500000000	T	T	T
0.50524400000000	0.11823100000000	0.60594500000000	T	T	T
0.05078450000000	0.19601700000000	0.60594500000000	T	T	T
0.80035900000000	0.25190300000000	0.60594500000000	T	T	T
0.33333333333333	0.33890200000000	0.60594500000000	T	T	T
0.11419100000000	0.38624400000000	0.60594500000000	T	T	T
0.61847400000000	0.49805800000000	0.60594500000000	T	T	T
0.38126200000000	0.51131300000000	0.60594500000000	T	T	T
0.88307100000000	0.62468400000000	0.60594500000000	T	T	T

POSCAR

Some useful resources:

Crystallography Open Database

Database with published structures
from experiment .cif

The screenshot shows the homepage of the Crystallography Open Database (COD). The page features a large logo 'COD' composed of three colored spheres (blue, green, and red) arranged in a triangular pattern. The title 'Crystallography Open Database' is displayed below the logo. On the left, there is a sidebar with several sections: 'COD Home' (Home, What's new?), 'Accessing COD Data' (Browse, Search, Search by structural formula), 'Add Your Data' (Deposit your data, Manage depositions, Manage/release prepublications), and 'Documentation' (COD Wiki, Obtaining COD, Querying COD, Citing COD, COD Mirrors, Advice to donators, Useful links). The main content area includes a brief description of the database as an open-access collection of crystal structures of organic, inorganic, metal-organics compounds and minerals, excluding biopolymers. It also mentions the software 'CrystalEye' developed by Nick Day at the University of Cambridge under supervision of Peter Murray-Rust. At the bottom, there is a section for 'CIFs Donators' featuring logos of various institutions and a 'Advisory Board' section with logos.

Bilbao Crystallographic Server

Crystallographic tools

The screenshot shows the homepage of the Bilbao Crystallographic Server. The page features a large logo 'bilbao crystallographic server' with 'FCTIZTF' underneath. The top navigation bar includes links for 'Contact us', 'About us', 'Publications', and 'How to cite the server'. The main content area has a sidebar titled 'Quick access to some tables' listing categories: Space Groups, Plane Groups, Layer Groups, Rod Groups, Frieze Groups, 2D Point Groups, 3D Point Groups, and Magnetic Space Groups. The main content area also includes sections for 'Space-group symmetry', 'Magnetic Symmetry and Applications', 'Group-Subgroup Relations of Space Groups', 'Representations and Applications', 'Solid State Theory Applications', 'Structure Utilities', 'Subperiodic Groups: Layer, Rod and Frieze Groups', 'Structure Databases', and 'Raman and Hyper-Raman scattering'. A news section at the bottom left lists two recent articles: one in J. Appl. Cryst. (2019) and another in Acta Cryst. (2019).

POSCAR

A few examples on how to visualize and/or edit POSCAR:

Atomic Simulation Environment (ASE)

Handle structures (and much more) using
python scripts

cif2cell

Versatile script, reads .cif
saves to many formats including
POSCAR

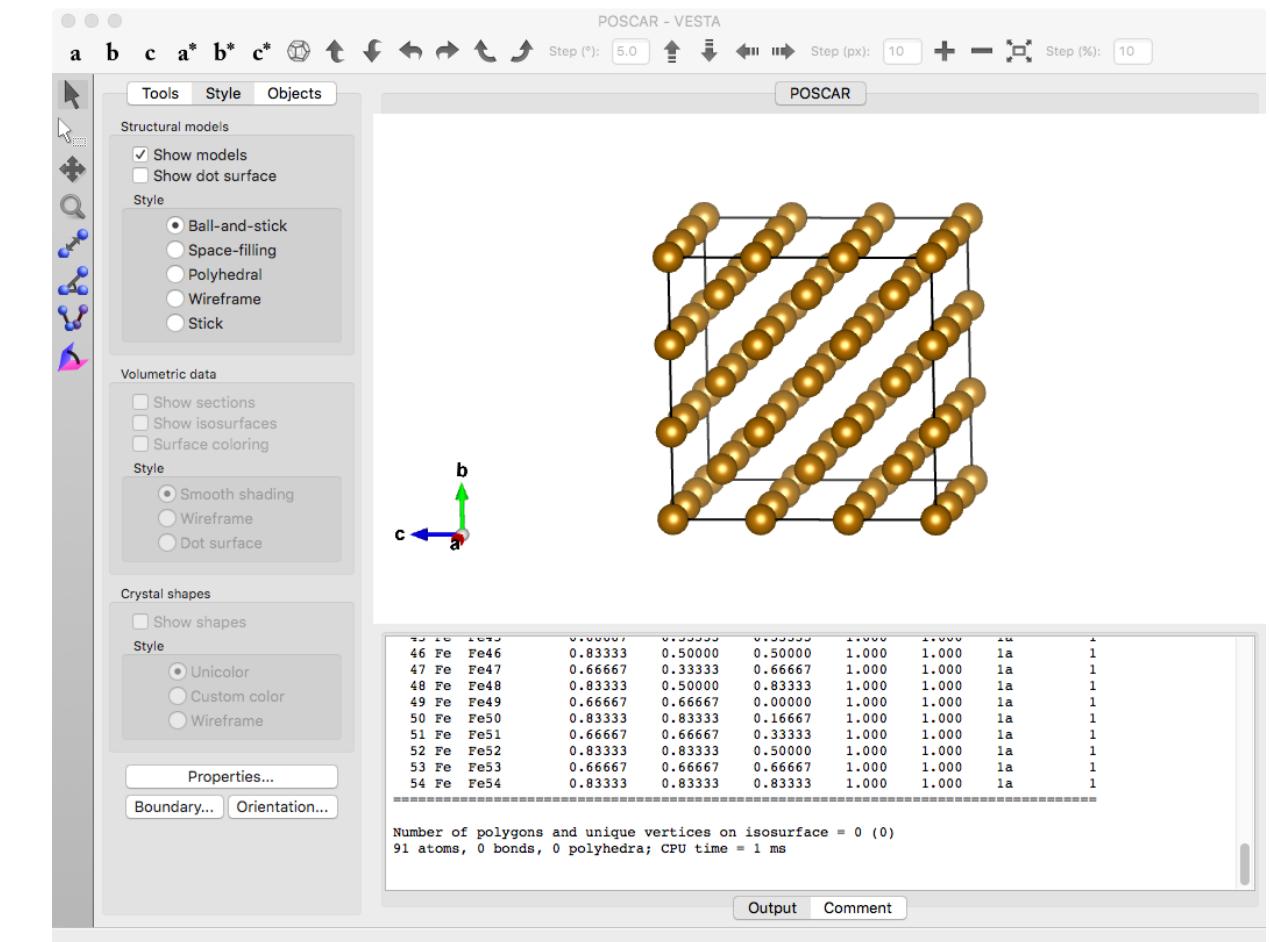
Commercial software:

NanoLab

MedeA

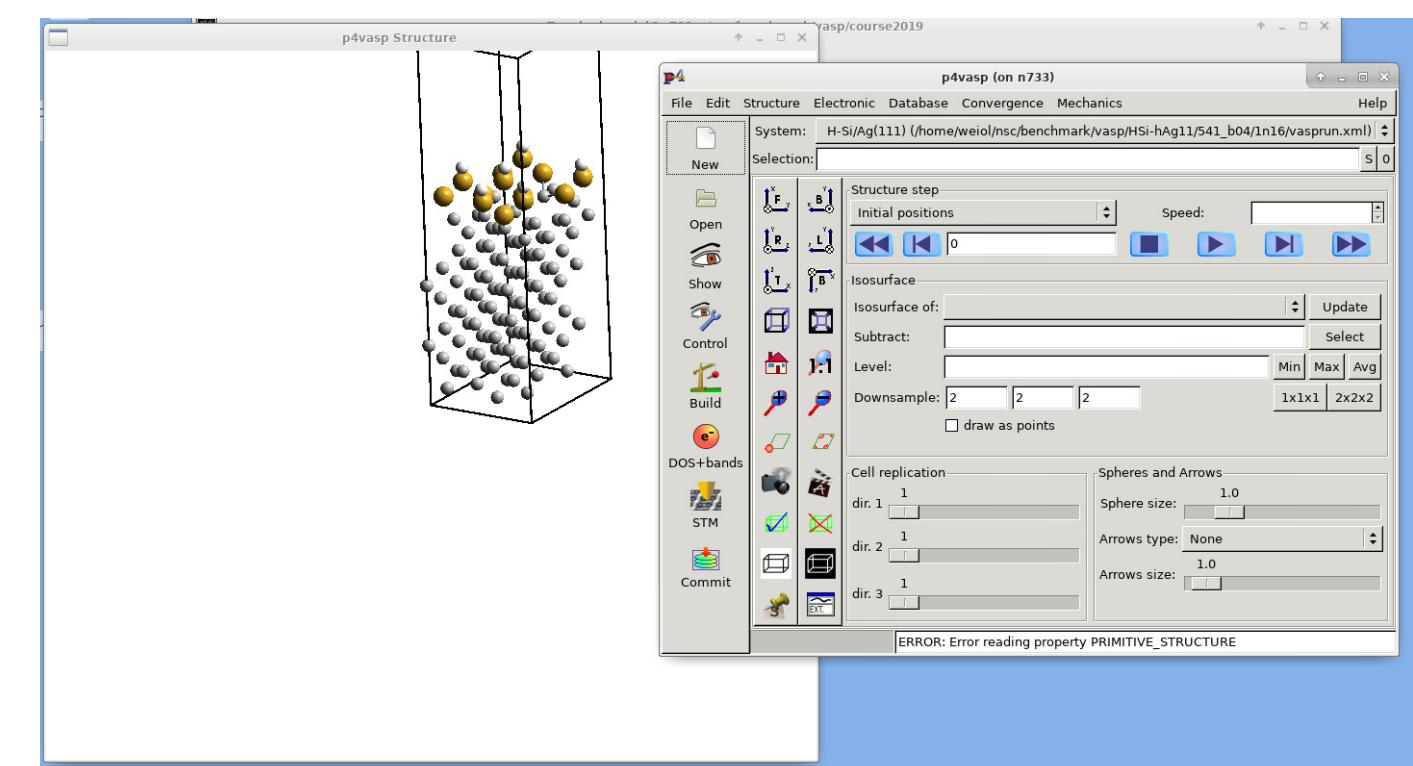
MaterialsStudio

VESTA



Opens .cif displays structure, save as POSCAR

p4vasp



Apart from analysis and visualization, also edit POSCAR

POTCAR

PAW potentials - non-trivial to tailor, select with care

```
-----  
| PAW_PBE Cu 22Jun2005 ← type, element, date  
valence | 11.00000000000000 →  
| parameters from PSCTR are:  
| VRHFIN =Cu: d10 p1 ← atomic configuration  
XC-type | LEXCH = PE  
| EATOM = 1390.9808 eV, 102.2342 Ry  
  
| TITEL = PAW_PBE Cu 22Jun2005  
| LULTRA = F use ultrasoft PP ?  
| IUNSCR = 1 unscreen: 0-lin 1-nonlin 2-no  
| RPACOR = 2.000 partial core radius  
| POMASS = 63.546; ZVAL = 11.000 mass and valenz  
| RCORE = 2.300 outmost cutoff radius  
| RWIGS = 2.200; RWIGS = 1.164 wigner-seitz radius (au A)  
energy cutoff | ENMAX = 295.446; ENMIN = 221.585 eV ← smallest energy cutoff  
| ICORE = 3 local potential  
| LCOR = T correct aug charges  
| LPAW = T paw PP  
| EAUG = 586.980  
| DEXC = 0.000  
| RMAX = 2.344 core radius for proj-oper  
| RAUG = 1.300 factor for augmentation sphere  
| RDEP = 2.302 radius for radial grids  
| RDEPTH = 1.771 core radius for aug-charge
```

POTCAR

- Check [recommendations](#), LDA, PBE

- for short bonds: `_h`
strong pressure

- for GW: `_GW`

- States in valence: `_sv`, `_pv`, `_d`

- “soft” (no short bonds): `_s`

- Where?

@Kebnekaise: \$ echo \$VASP_PP_PATH
/hpc2n/eb/software/Core/VASP-data/5.4/potPP

@Tetralith: /software/sse/manual/vasp/POTCARs

Note several choices, e.g.:
Ga, `Ga_d`, `Ga_d_GW`,
`Ga_GW`, `Ga_h`, `Ga_sv_GW`

Useful commands:

\$ grep PAW POTCAR
\$ grep ENMAX POTCAR

KPOINTS

A simple case of fcc Ni, 1 atom

0 = automatic generation of mesh

k-point mesh

```
|-----|  
| k-points | ← comment  
| 0 |  
|-----|  
| Monkhorst Pack | ← Monkhorst-Pack method (M)  
| 11 11 11 |  
| 0 0 0 | ← optional shift of k-mesh  
|-----|
```

odd kmesh - includes Γ -point

Course example, H and Si on Ag(111) surface, 136 atoms

First letter is sufficient, i.e.
“G” for “Gamma”

```
|-----|  
| Automatic mesh |  
| 0 |  
|-----|  
| Gamma | ← Gamma method (G)  
| 2 2 1 |  
| 0. 0. 0. |  
|-----|
```

- Γ -point included by default
- hexagonal structures only use this!

KPOINTS

For **bandstructure** calculations, provide a list of k-points, [see example](#)

```
'k-points for bandstructure L-G-X-U K-G' <comment>
k-points per line-segment > 10
line <k-points per line-segment>
Reciprocal / Cartesian > Reciprocal
  0.50000  0.50000  0.50000  1 <symmetry point + weight>
  0.00000  0.00000  0.00000  1
  0.00000  0.00000  0.00000  1
  0.00000  0.50000  0.50000  1
  0.00000  0.50000  0.50000  1
  0.25000  0.62500  0.62500  1
  0.37500  0.75000  0.37500  1
  0.00000  0.00000  0.00000  1
```

KPOINTS

- Metal - “many” k-pts
- Band gap materials - “few” k-pts
- Unit cell (few atoms) - more k-pts
real vs. reciprocal space
- Supercell (100s atoms) - few/one, k-pt
- No guarantee for convergence...
- MP method popular, G “safest” to apply
- 1x1x3 cell geometry → 3x3x1 k-mesh
real vs. reciprocal space

VASP binaries

- `vasp_std` - regular version
- `vasp_gam` - one k-point (Gamma), **faster**
- `vasp_ncl` - noncollinear magnetism
- `vasp_gpu`, `vasp_gpu_ncl` - for GPU
- + modifications
 - e.g. constrained relaxation

Job script - Kebnekaise (HPC2N)

```
#!/bin/bash
#SBATCH -A snic2019-3-203
#SBATCH -J test
#SBATCH -t 3:59:00
#SBATCH -n 56

ml icc/2017.4.196-GCC-6.4.0-2.28
ml ifort/2017.4.196-GCC-6.4.0-2.28
ml impi/2017.3.196
ml VASP/5.4.4-18Apr17-hpc2n

mpirun vasp_std
```

#SBATCH -N 2

Example: running on 2 nodes (28x2 cores) @Kebnekaise

Job script - Kebnekaise (HPC2N)

```
#!/bin/bash
#SBATCH -A snic2019-3-203
#SBATCH -J test
#SBATCH -t 3:59:00
#SBATCH -N 2
#SBATCH --ntasks-per-node=14

ml icc/2017.4.196-GCC-6.4.0-2.28
ml ifort/2017.4.196-GCC-6.4.0-2.28
ml impi/2017.3.196
ml VASP/5.4.4-18Apr17-hpc2n

mpirun vasp_std
```

#SBATCH -n 56

Example: running on 2 nodes (28x2 cores), using half the cores
for more memory @Kebnekaise

Job script - Kebnekaise (HPC2N)

GPU calc.

```
#!/bin/bash
#SBATCH -A snic2019-3-203
#SBATCH -J test
#SBATCH -t 3:59:00
#SBATCH -n 28
#SBATCH --gres=gpu:v100:2,gpuexcl

ml icc/2017.4.196-GCC-6.4.0-2.28
ml ifort/2017.4.196-GCC-6.4.0-2.28
ml impi/2017.3.196
ml CUDA/9.1.85
ml VASP/5.4.4-18Apr17-p01-hpc2n

mpirun vasp_gpu
```

Example: running on 1 node (28 cores) with 2xV100 GPUs @Kebnekaise

<https://www.hpc2n.umu.se/resources/software/vasp>

Job script - Tetralith (NSC)

```
#!/bin/bash
#SBATCH -A snic2019-3-203
#SBATCH -J test
#SBATCH -t 3:59:00
#SBATCH -N 2

#SBATCH -n 64
note "mpprun"
module load VASP/5.4.4.16052018-nsc1-intel-2018a-eb
mpprun vasp
```

Example: running on 2 nodes (32x2 cores) @Tetralith

To increase available memory, reduce cores/node, e.g:

```
#SBATCH --ntasks-per-node=16
```

Alternatively, use “fat” memory nodes:

```
#SBATCH -C fat
```

<https://www.nsc.liu.se/software/installed/tetralith/vasp/>

Job script - Beskow (PDC)

```
#!/bin/bash -l
#SBATCH -A 2019-3-203
#SBATCH -J test
#SBATCH -t 3:59:00
#SBATCH --nodes=2

module unload cray-mpich/7.0.4
module load vasp/5.4.4

aprun -n 48 -N 24 vasp
#aprun -n 64 -N 32 vasp
```

Example: running on 2 nodes (24x2 cores) @Beskow
alternatively on 2 nodes (32x2 cores)

<https://www.pdc.kth.se/software/software/VASP/beskow/5.4.4/index.html#running-vasp>

Output files

- OUTCAR - main, detailed output
- OSZICAR - iteration summary
- slurm-**.out - stdout, iteration summary, warnings
- CONTCAR - updated structural data (at finish)
structural relaxation / MD
- XDATCAR - positions at each ionic step
- ...

Output files

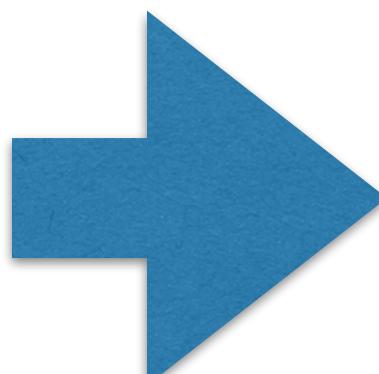
- DOSCAR - total, partial density of states (DOS)
- CHGCAR - charge density
output can also be switched off
- WAVECAR - plane wave coefficients (for restart)
- ...

OSZICAR

Min. algo	Step	Total free Energy	Energy diff.	Eigenvalue diff.				Charge density residual vector
	N	E	dE	d	eps	ncg	rms	rms (c)
DAV:	1	-0.189343666468E+01	-0.18934E+01	-0.20040E+03	904	0.422E+02		
DAV:	2	-0.108926039335E+02	-0.89992E+01	-0.87586E+01	1440	0.554E+01		
DAV:	3	-0.109805531666E+02	-0.87949E-01	-0.87949E-01	1208	0.675E+00		
DAV:	4	-0.109807517982E+02	-0.19863E-03	-0.19863E-03	1368	0.313E-01		
DAV:	5	-0.109807519113E+02	-0.11307E-06	-0.11310E-06	1256	0.684E-03	0.519E+00	
DAV:	6	-0.108723496529E+02	0.10840E+00	-0.69164E-02	1064	0.137E+00	0.317E+00	
DAV:	7	-0.108218097854E+02	0.50540E-01	-0.13575E-01	1120	0.205E+00	0.163E-01	
DAV:	8	-0.108228444695E+02	-0.10347E-02	-0.32972E-03	944	0.419E-01	0.706E-02	
DAV:	9	-0.108230614389E+02	-0.21697E-03	-0.22028E-04	1312	0.111E-01	0.557E-02	
DAV:	10	-0.108230846187E+02	-0.23180E-04	-0.25743E-05	560	0.381E-02		
	1	F= -.10823085E+02 E0= -.10823085E+02	d E =-.431458E-08					

Final total free energy

Total steps: NELMIN to NELM



Need to check if convergence is reached!

In particular if NELM was reached (default = 60 steps)

Stdout (slurm-***.out)

```
running on 2 total cores
distrk: each k-point on 2 cores, 1 groups
distr: one band on 1 cores, 2 groups
using from now: INCAR
vasp.5.4.4.18Apr17-6-g9f103f2a35 (build Sep 13 2019 06:30:52) complex
```

```
POSCAR found type information on POSCAR Si
```

```
POSCAR found : 1 types and 2 ions
```

```
scaLAPACK will be used
```

```
LDA part: xc-table for Pade appr. of Perdew
```

```
POSCAR, INCAR and KPOINTS ok, starting setup
```

- Check for warnings!

```
FFT: planning ...
```

```
WAVECAR not read
```

```
entering main loop
```

	N	E	dE	d eps	ncg	rms	rms(c)
DAV:	1	-0.189343666468E+01	-0.18934E+01	-0.20040E+03	904	0.422E+02	
DAV:	2	-0.108926039335E+02	-0.89992E+01	-0.87586E+01	1440	0.554E+01	
DAV:	3	-0.109805531666E+02	-0.87949E-01	-0.87949E-01	1208	0.675E+00	
DAV:	4	-0.109807517982E+02	-0.19863E-03	-0.19863E-03	1368	0.313E-01	
DAV:	5	-0.109807519113E+02	-0.11307E-06	-0.11310E-06	1256	0.684E-03	0.519E+00
DAV:	6	-0.108723496529E+02	0.10840E+00	-0.69164E-02	1064	0.137E+00	0.317E+00
DAV:	7	-0.108218097854E+02	0.50540E-01	-0.13575E-01	1120	0.205E+00	0.163E-01
DAV:	8	-0.108228444695E+02	-0.10347E-02	-0.32972E-03	944	0.419E-01	0.706E-02
DAV:	9	-0.108230614389E+02	-0.21697E-03	-0.22028E-04	1312	0.111E-01	0.557E-02
DAV:	10	-0.108230846187E+02	-0.23180E-04	-0.25743E-05	560	0.381E-02	

```
1 F= -.10823085E+02 E0= -.10823085E+02 d E =-.431458E-08
```

```
writing wavefunctions
```

Warning/advice output

Check stdout (slurm-*.out)
for warnings!**

Typical warnings:

Reminder to set (if applicable):
[NCORE](#)

typically = used cores/nodes

For high accuracy (default) keep:
[LREAL=.FALSE.](#)

```
|           W   W   AA    RRRRR  N   N  II  N   N   GGGG  !!!
|           W   W   A   A    R   R  NN   N  II  NN   N   G   G  !!!
|           W   W   A   A    R   R  N N   N  II  N N   N   G   !!!
|           W WW W  AAAAAA  RRRRR  N   N N  II  N   N N   G   GGG  !
|           WW  WW  A   A    R   R  N   NN  II  N   NN   G   G
|           W   W   A   A    R   R  N   N  II  N   N   N   GGGG  !!!
```

```
| For optimal performance we recommend to set
| NCORE= 4 - approx SQRT( number of cores)
| NCORE specifies how many cores store one orbital (NPAR=cpu/NCORE).
| This setting can greatly improve the performance of VASP for DFT.
| The default, NCORE=1 might be grossly inefficient
| on modern multi-core architectures or massively parallel machines.
| Do your own testing !!!!
| Unfortunately you need to use the default for GW and RPA calculations.
| (for HF NCORE is supported but not extensively tested yet)
```

```
| ADVICE TO THIS USER RUNNING 'VASP/VAMP' (HEAR YOUR MASTER'S VOICE ...):
```

```
| You have a (more or less) 'large supercell' and for larger cells
| it might be more efficient to use real space projection operators
| So try LREAL= Auto in the INCAR file.
| Mind: If you want to do a very accurate calculations keep the
| reciprocal projection scheme (i.e. LREAL=.FALSE.)
```