

# 2. VASP - Basics

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National Supercomputer Centre (NSC), Linköping University

NAIIS-ENCCS training, online 4-5<sup>th</sup> Apr 2023

# VASP - Best Practices Workshop



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

**NAISS**

<https://www.naiss.se/>



EuroCC National Competence Centre Sweden

<https://enccs.se/>



<https://www.vasp.at/>

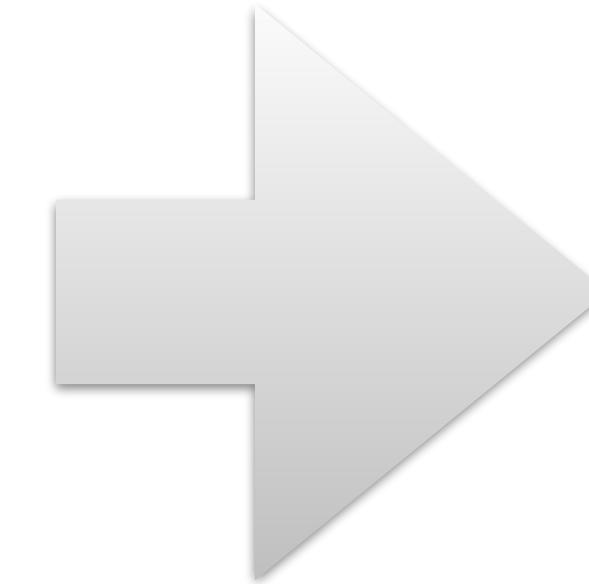
# Introduction

- Where to find information
  - VASP at different NAISS HPC centers (examples)
- Starting files
- Important parameters
- Input/output
- Examples

... clickable links are underlined

# Short background

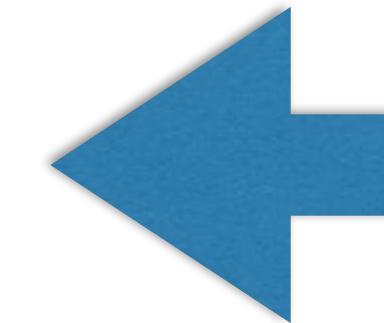
- Software license
- PAW-method
- DFT, post-DFT (HSE06, GW, ...)
- Born-Oppenheimer Molecular Dynamics
- **widely used** in Academia/Industry
  - Efforts from **Intel & Nvidia** for optimization
- 20-25% of Tetralith usage
- **VASP6** is available since 2020



<https://vasp.at/>

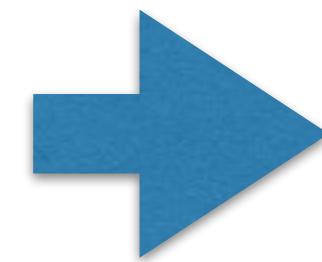
# Starting advice

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

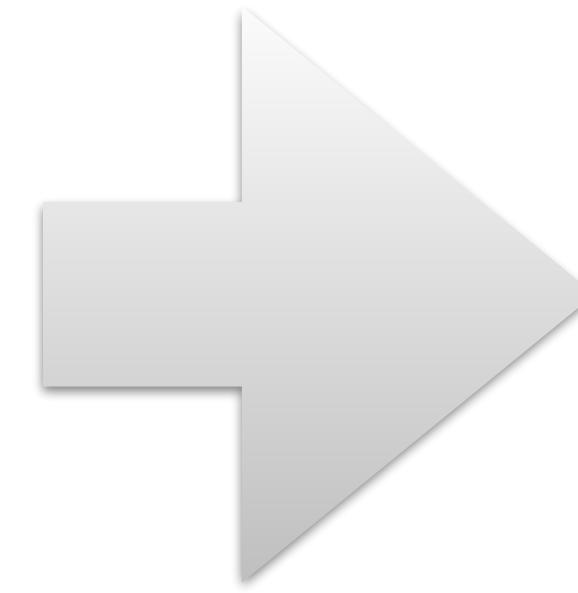


good starting point

# Resources



- Wiki and Manual  
**Check in detail!**
- Examples, tutorials
- Presentations
- Forum

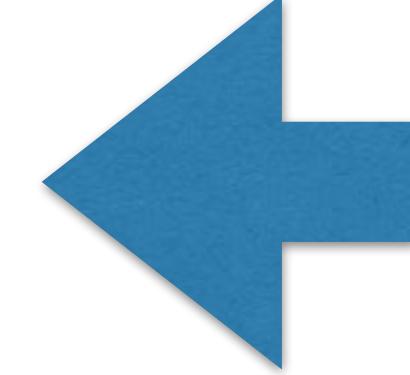
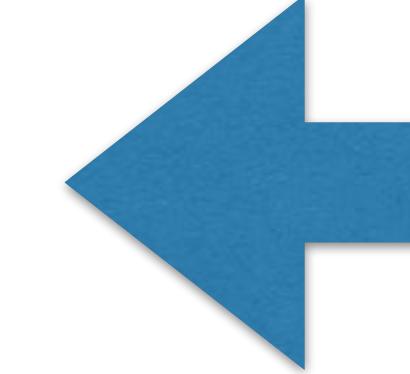


Find all the links:  
<https://vasp.at/>

- Also other resources, materials and tools for VASP (see presentation 4.)
- Peter Larsson's old blog at NSC: <https://www.nsc.liu.se/~pla/>
- NSC VASP installations: <https://www.nsc.liu.se/software/installed/tetralith/vasp/>

Questions / trouble @NSC clusters? [support@nsc.liu.se](mailto:support@nsc.liu.se)

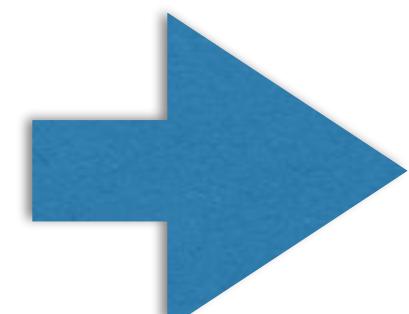
# VASP & HPC centers

- Tetralith (NAISS) / Sigma, NSC, LiU  **this course**  
**Installed!**
- Dardel (NAISS), PDC, KTH  
**Installed!**
- Other systems/centers (e.g. Kebnekaise, HPC2N)  
**Installed!**
- MeluXina (EuroHPC) - workshop  **this course**
- LUMI (EuroHPC & NAISS)

- Check for modules: \$ module avail vasp  
\$ module spider vasp

# VASP versions & utilities

- **Latest:** 6.4.0 (from Feb -23)  
- Check center [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



...more about utilities tomorrow

VASP - Vienna Ab initio Simulation Package



The Vienna Ab initio Simulation Package: atomic scale materials modelling from first principles.

[Read more](#)

### Get a license

Not a license holder yet? Apply for a license [here](#)

Unsure how to proceed? Have a look at the [FAQs](#)

### VASP Wiki

The user manual of VASP  
Documentation of input and output  
Advice on compiling the code

### Forum

Meet the **VASP Community**  
Ask questions to other users  
Get technical support from the VASP team

### Learn

Workshop, tutorials, lectures and more  
Get started today and learn how to use VASP

### py4vasp

Python tool to interface with VASP  
Analyze your calculations with ease

### Portal

Licensees please login here:

Username

Password

[Forgot my password/username](#)

The screenshot shows a web browser window with the URL <https://www.vasp.at/py4vasp/latest/>. The page title is "py4vasp". The left sidebar contains a navigation menu with sections: "py4vasp" (selected), "Installation", "Quick start", "calculation" (selected), "raw", "data", and "exceptions". The main content area starts with a section titled "py4vasp" which describes the tool as a Python interface for VASP calculations. It highlights two main domains of application: extracting data from VASP calculations and writing Python scripts based on VASP data. Below this, a section titled "Installation" provides instructions for installing py4vasp. It suggests creating a separate environment for installation to avoid interference with other packages. It includes two command-line examples: one for pip install (`pip install py4vasp`) and another for conda install (`conda install -c conda-forge mdtraj` followed by `pip install py4vasp`). Finally, it provides a test command (`python -c "import py4vasp; print(py4vasp.__version__)"`) to check if the installation was successful.

# py4vasp

*py4vasp* is a python interface to extract data from VASP calculations. It is intended mainly to get a quick look at the data and provide the functionality to export it into common formats that can be used by other more sophisticated postprocessing tools. The second domain of application is for people that want to write python scripts based on the data calculated by VASP. This tool interfaces directly with the new HDF5 file format and thereby avoids parsing issues associated with the XML or OUTCAR files.

For these two groups of users, we provide a different level of access. The simple routines used in the tutorials will read the data from the file directly and then generate the requested plot. For script developers, we provide an expert interface where the data is lazily loaded as needed with some greater flexibility when the data file is opened and closed.

## Installation

While this is not required to be able to run *py4vasp*, you may want to consider creating a separate environment for installation to avoid interference with other installed packages.<sup>1</sup> You can then install *py4vasp* from [PyPI](#) using the pip package installer

```
pip install py4vasp
```

This will automatically download *py4vasp* as well as all the required dependencies. However, we noticed that this approach is not fail-safe, because the installation of the *mdtraj* dependency does not work on all operating systems. So in case the simple installation above fails, you may need to use *conda* to install *mdtraj*

```
conda install -c conda-forge mdtraj  
pip install py4vasp
```

If these commands succeed, you should be able to use *py4vasp*. You can make a quick test of your installation running the following command

```
python -c "import py4vasp; print(py4vasp.__version__)"
```

This should print the version of *py4vasp* that you installed.

**Important**

<https://www.vasp.at/>

...py4vasp useful tool for quick analysis!

VASP - Vienna Ab initio Simulation Package

SIGN IN WIKI PY4VASP LEARN INFO Search ...



The Vienna Ab initio Simulation Package: atomic scale materials modelling from first principles.

[Read more](#)

**Get a license** → **VASP Wiki** → **Forum**

**Get a license**  
Not a license holder yet? Apply for a license [here](#)  
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**VASP Wiki**  
The user manual of VASP  
Documentation of input and output  
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**py4vasp**  
Python tool to interface with VASP  
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**Username**   
**Password**   
**LOGIN**  
[Forgot my password/username](#)

<https://www.vasp.at/>

...wiki important resource & also check forum

The VASP Manual - Vaspwiki

https://www.vasp.at/wiki/index.php/The\_VASP\_Manual

Log in

Page Discussion Read View source View history Search Vaspwiki

Requests for technical support from the VASP group should be posted in the [VASP-forum](#).

# The VASP Manual

## Getting started

How to Install VASP	First install VASP.
Learn ↗	Tutorials using notebooks ↗, video lectures ↗, etc.
More	How to's, examples and tutorials on the Wiki, some lectures and schedules from previous workshops, etc.
VASP6	Features that will only be available in VASP.6.X.

## Featured topics

Category	<i>subtopics (amongst others)</i>
Theoretical background	Density-functional theory, projector-augmented-wave method, molecular dynamics, GW approximation, etc.
Calculation setup	Installation, input files, output files, INCAR tags, How to's, etc.
Electronic minimization	Davidson, RMM-DIIS, Conjugate-gradient, preconditioning, density mixing, etc.
Electronic ground-state properties	Band structure, density of states, etc.
Spin degree of freedom	Spin-orbit coupling, noncollinear magnetism, spin spirals, constrained magnetism, etc.
Exchange-correlation functionals	LDA, GGA, meta-GGA, DFT+U, hybrid functionals, van der Waals functionals.
Symmetry and structure	Crystal symmetry, reciprocal space, surfaces, pair-correlation function for liquids, etc.
Ionic minimization	Structure optimization, ionic-mimimization methods, forces, etc.

[https://www.vasp.at/wiki/index.php/The\\_VASP\\_Manual](https://www.vasp.at/wiki/index.php/The_VASP_Manual)

The VASP Manual - Vaspwiki

https://www.vasp.at/wiki/index.php/The\_VASP\_Manual

Symmetry and structure	Crystal symmetry, reciprocal space, surfaces, pair-correlation function for liquids, etc.
Ionic minimization	Structure optimization, ionic-mimimization methods, <a href="#">forces</a> , etc.
Molecular dynamics	Barostats, <a href="#">thermostats</a> , <a href="#">ensembles</a> , etc.
Ensemble properties	Monitoring geometric parameters, pair-correlation function, etc.
Advanced molecular-dynamics sampling	<a href="#">Interface pinning</a> , constrained molecular dynamics, metadynamics, thermodynamic integration, etc.
Machine-learned force fields	Training and application of force fields.
Phonons	Lattice vibrations, <a href="#">electron-phonon interactions</a> .
Response theory	Static and frequency-dependent <a href="#">dielectric properties</a> , Berry phases, spectroscopy (UV, VIS, X-ray), <a href="#">phonons</a> , etc.
Many-body perturbation theory	ACFDT, BSE, GW, MP2, CRPA.
Localized basis and projection	Obtaining Wannier functions, SCDM, etc.
Performance	<a href="#">Parallelization</a> , <a href="#">memory management</a> , profiling, etc.
Outlook	Features that will only be available in VASP.6.X.

## Support

If you have questions or run into trouble, please have a look at the [known issues](#) and/or post a question at the [VASP forum](#).

**Mind:** We offer support on a courtesy base only, not as a contractual service.

[Back to the top](#)

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Category:Examples - Vaspwiki

https://www.vasp.at/wiki/index.php/Category:Examples

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VASP

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Requests for technical support from the VASP group should be posted in the [VASP-forum](#).

## Category:Examples

All articles related to VASP example calculations

Contents

### Pages in category "Examples"

The following 80 pages are in this category, out of 80 total.

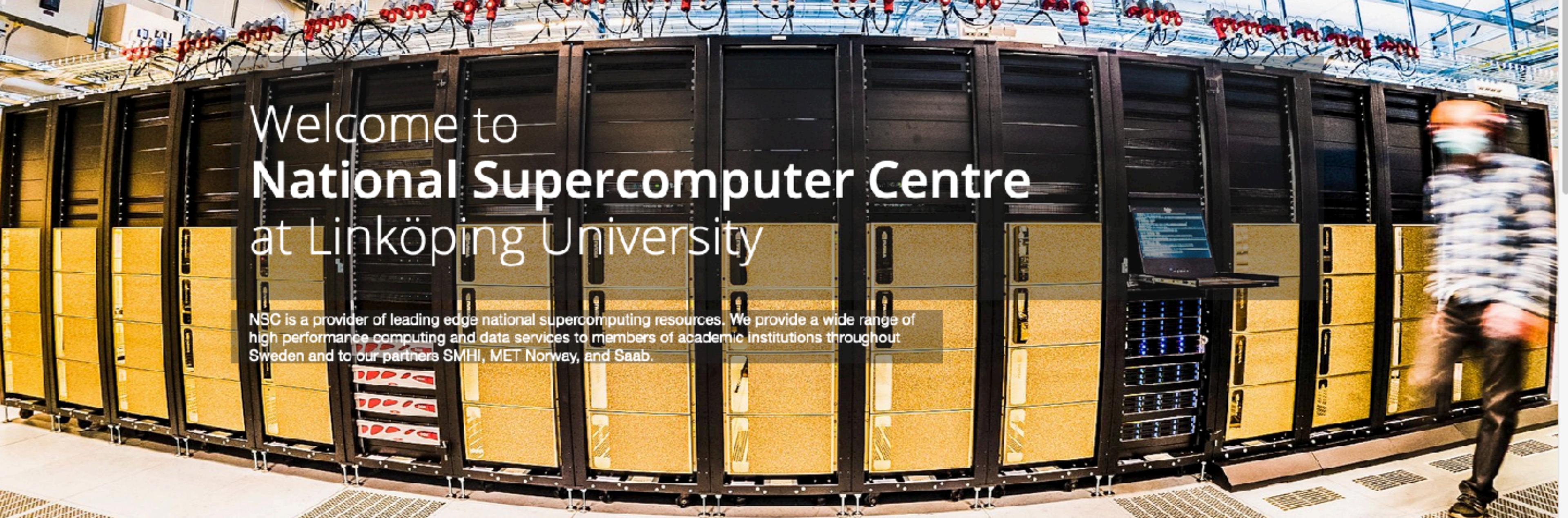
- A**
  - Adsorption of H<sub>2</sub>O on TiO<sub>2</sub>
  - Alpha-AlF<sub>3</sub>
  - Alpha-SiO<sub>2</sub>
  - At and mol further
- B**
  - Band gap renormalization in diamond using one-shot method
  - Bandgap of Si in GW
  - Bandgap of Si using different DFT+HF methods
  - Bandstructure and CRPA of SrVO<sub>3</sub>
  - Bandstructure of Si in GW (VASP2WANNIER90)
  - Bandstructure of SrVO<sub>3</sub> in GW
  - Beta-tin Si
- C**
  - Calculate U for LSDA+U
  - Cd Si
  - Cd Si relaxation
  - Cd Si volume relaxation
  - CO
  - CO on Ni 111 surface
  - CO partial DOS
- 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**
  - H<sub>2</sub>O
  - H<sub>2</sub>O molecular dynamics
  - H<sub>2</sub>O vibration
- I**
  - Improving the dielectric function
  - Including the Spin-Orbit Coupling
- N**
  - Ni 111 surface relaxation
  - NiO
  - NiO GGA
  - NiO GGA+U
  - NiO HSE06
  - NiO LSDA+U
  - Nucleophile Substitution CH<sub>3</sub>Cl - Standard MD
  - Nucleophile Substitution CH<sub>3</sub>Cl - BM
  - Nucleophile Substitution CH<sub>3</sub>Cl - mMD1
  - Nucleophile Substitution CH<sub>3</sub>Cl - mMD2
  - Nucleophile Substitution CH<sub>3</sub>Cl - mMD3
  - Nucleophile Substitution CH<sub>3</sub>Cl - SG
- O**
  - O atom
  - O atom spinpolarized
  - O atom spinpolarized low symmetry
  - O dimer
- P**
  - Partial DOS of CO on Ni 111 surface
  - Plotting the BSE fatband structure of Si
- S**
  - Spin-orbit coupling

NSC NSC

https://www.nsc.liu.se

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Welcome to  
**National Supercomputer Centre**  
at Linköping University

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.

Photo: Thor Balkhed

## Announcement

Berzelius AI Symposium on February 9, 2022

### OUR PARTNERS



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

NSC NSC

https://www.nsc.liu.se

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SEARCH



# Welcome to National Supercomputer Centre at Linköping University

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Photo: Thor Balkhed

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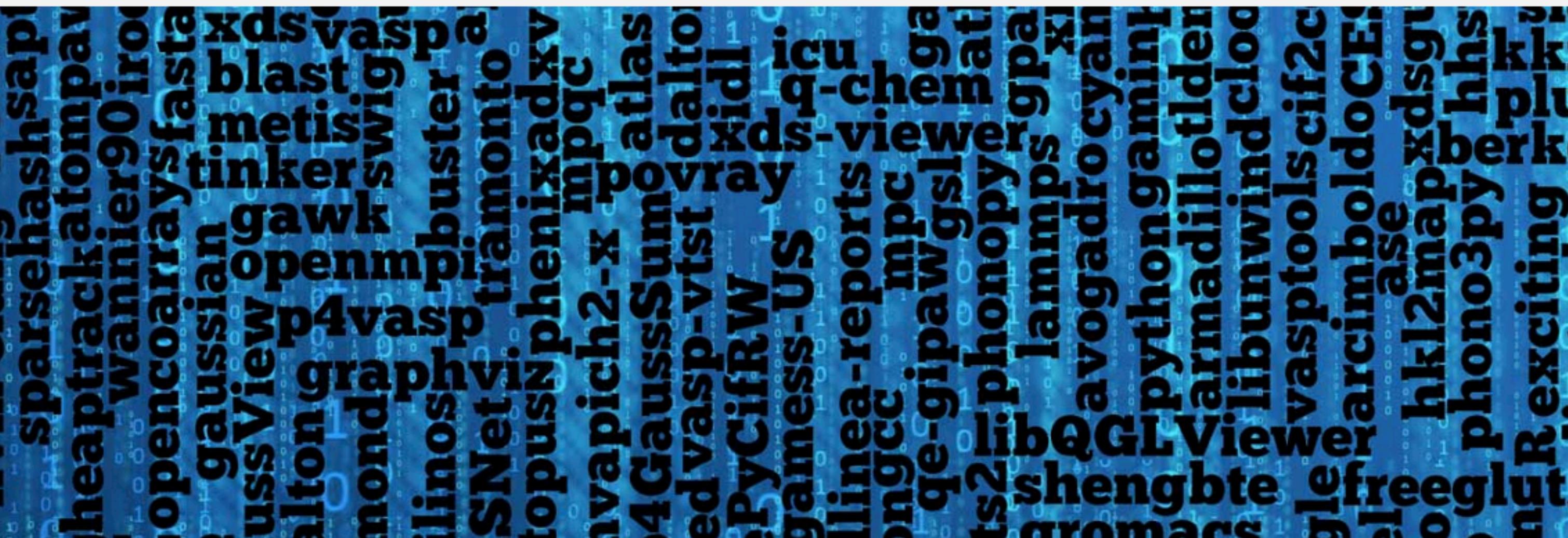
NSC Software

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

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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.

### Compilers

Available compilers and recommendations.

### NSC build environment

Our recommended way to compile and run your own programs.

### Modules

Module system integration at NSC



NSC Installed Software | Tetralith Soft X +

NSC Software Installations

Tetralith Sigma Nebula Bi Berzelius

## Software on Tetralith and Sigma

The scientific applications listed in the table below have been installed centrally under [/software/sse/](#). Each software installation is categorized into one of three [software support tiers](#), depending on the level of help we can provide for that particular software.

Some useful software and tools, such as a few editors are installed as part of the operating system and are not listed here.

This list was last updated on: 2023-03-20

All Chem Phys Bio CAE Geo Math Devel Data Tools Vis Misc

Search:

Software ↑↓	Description	Support ↑↓
<a href="#">ABAQUS</a>	The Abaqus FEA software suite offers various tools for stress analysis, heat transfer, fluid mechanics etc.	tier3
<a href="#">ABINIT</a>	ABINIT calculates the total energy and properties of materials and molecules using, primarily, DFT.	tier2
<a href="#">allinea-DDT</a>	ARM/Allinea DDT is a debugging tool for scalar, multi-threaded and large-scale parallel applications.	tier2
<a href="#">allinea-forge</a>	ARM/Allinea DDT is a debugging tool for scalar, multi-threaded and large-scale parallel applications.	tier2
<a href="#">allinea-MAP</a>	ARM/Allinea MAP is a profiler for scalar, multi-threaded and large-scale parallel applications.	tier2
<a href="#">AlphaFold</a>	Implementation of the inference pipeline of AlphaFold v2.0.	tier3
<a href="#">Amber</a>	Amber is a suite of biomolecular simulation programs.	tier3
<a href="#">Anaconda</a>	The Anaconda Python distribution platform for Python and R scientific computing.	tier2
<a href="#">ANSYS</a>	Software suite for computational fluid dynamics, stress analysis and many more CAE tasks.	tier2
<a href="#">ANSYS-EM</a>	Software suite for Electromagnetics simulations.	tier3

NSC Installed Software | Tetralith Soft X

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

Tetralith Sigma Nebula Bi Berzelius



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This list was last updated on: 2023-03-20

All

Chem

Phys

Bio

CAE

Geo

Math

Devel

Data

Tools

Vis

Misc

Search:

Software	Description	Support
p4vasp	p4vasp is a popular tool for VASP visualization.	tier3
VASP	Electronic structure calculations using PAW-method DFT	tier1
VASP-OMC	Modified VASP for occupation matrix control	tier3
VASP-VTST	Utility version of VASP including: VTST 3.2, VASPsol, BEEF	tier3
vasptools	A collection of useful VASP scripts.	tier3

Showing 5 entries (filtered from 163 total entries)



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Linköping University  
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SWEDEN

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Fax.: 013-149403  
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NSC VASP | Tetralith Software Module X +

NSC Software Installations

Tetralith Sigma Nebula Bi Berzelius

# VASP

**i** This software is under support tier 1!

## Software description

VASP - Vienna ab initio simulation package, "a computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum mechanical molecular dynamics, from first principles."

## License

Note: VASP is a licensed software. Please check further information on the licensing page: [www.nsc.liu.se/software/software-licensing/vasp/](https://www.nsc.liu.se/software/software-licensing/vasp/)

Homepage: [vasp.at/](http://vasp.at/)

## NSC documentation

**i** Please make sure to read our documentation: [VASP](#)

## Available Modules

- [6.3.2.27062022-omp-nsc1-intel-2018a-eb](#)
- [6.3.1.04052022-omp-nsc1-intel-2018a-eb](#)
- [6.3.0.20012022-omp-nsc1-intel-2018a-eb](#)
- [6.2.1.29042021-omp-nsc1-intel-2018a-eb](#)
- [6.2.0.14012021-omp-nsc1-intel-2018a-eb](#)
- [6.1.2.25082020-omp-nsc1-intel-2018a-eb](#)
- [6.1.2.25082020-nsc1-intel-2018a-eb](#)
- [6.1.0.28012020-nsc1-intel-2018a-eb](#)
- [5.4.4.16052018-wannier90-nsc2-intel-2018a-eb](#)
- [5.4.4.16052018-wannier90-nsc1-intel-2018a-eb](#)
- [5.4.4.16052018-vanilla-nsc1-intel-2018a-eb](#)
- [5.4.4.16052018-nsc2-intel-2018a-eb](#)
- [5.4.4.16052018-nsc1-intel-2018b-eb](#)

NSC VASP

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

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ABAQUS ABINIT AMBER ANSYS ANSYS-EM ASE ATAT Allinea Performance Reports Allinea-DDT

Allinea/ARM-MAP CASTEP CDO CESM COMSOL CP2K CPMD DL\_POLY Dalton/LSDalton EC-Earth

EPW Elk FERRET GPAW GROMACS Grace Gurobi Optimizer HDF5 Julia LAMMPS MATLAB

MOLDEN Mathematica NAMD NCO NCVIEW NorESM Open Babel OpenFOAM ParaView Pymatgen

Quantum ESPRESSO STAR-CCM+ Siesta USPEX UppASD VMD VisIt WEST WIEN2K Yambo ecCodes

exciting grib\_api netCDF p4vasp parallel phono3py phonopy vasptools Schrödinger suite VASP

Clang Gaussian and GaussView

NSC / Software / Installed software / VASP

## VASP Installations on Tetralith & Sigma

First of all, **VASP** is a 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.

### VASP6

VASP6 was released in beginning of 2020. This means e.g. that VASP5 license holders will need to update their license in order to access VASP6 installations at NSC. If you have a VASP 5.4.4 license, you are typically covered for updates of VASP 6.X.X for three years, check your license for the exact details.

### Documentation

For using VASP, refer to [the extensive VASP wiki](#) which includes many examples and topics on how to run VASP. It can also be very useful to check the forum and other resources available at [the VASP webpage](#).

The new features of VASP6 are described in [the VASP wiki](#).

From time to time NSC will arrange seminars or brief workshops on VASP, with focus typically on how to get started using

NSC VASP

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

# NSC

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ABAQUS ABINIT AMBER ANSYS ANSYS-EM ASE ATAT Allinea Performance Reports Allinea-DDT

Allinea/ARM-MAP CASTEP CDO CESM COMSOL CP2K CPMD DL\_POLY Dalton/LSDalton EC-Earth

EPW Elk FERRET GPAW GROMACS Grace Gurobi Optimizer HDF5 Julia LAMMPS MATLAB

MOLDEN Mathematica NAMD NCO NCVIEW NorESM Open Babel OpenFOAM ParaView Pymatgen

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

grib\_api netCDF p4vasp parallel phono3py phonopy vasptools Schrödinger suite VASP Clang

Gaussian and GaussView

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

## VASP6 is available

VASP6 was released in beginning of 2020. This means e.g. that VASP5 license holders will need to update their license in order to access VASP6 installations at NSC. If you have a VASP license 5.4.4, you are probably covered for version up to 6.X.X already, check your license details.

The new features are described in [the VASP wiki](#).

## 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
```

General information about VASP X +

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

PDC Center for High Performance Computing PDC svensk webbplats

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KTH / PDC / Software

**Software**

General information about VASP  
Licenses  
Disclaimer  
Installed software

The Vienna Ab initio Simulation Package (VASP) is a computer program for atomic scale materials modeling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, from first principles.

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

# General information about VASP

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.

## Licenses

PDC takes no responsibility for the correctness of results produced with the binaries. Always evaluate the binaries against known results for the systems and properties you are investigating before using the binaries for production jobs.

## Disclaimer

## Installed software

Cluster	How to use	How to build
Tegner	<a href="#">5.3.5</a> <a href="#">5.4.1</a>	<a href="#">5.3.5</a> <a href="#">5.4.1</a>

How to use VASP — PDC software

https://www.pdc.kth.se/software/software/VASP/cpe21.11/6.2.1-vanilla/index\_using.html

PDC Center for High Performance Computing

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# How to use VASP

Software	Version	Cluster
VASP	6.2.1-vanilla	Dardel

This is a *vanilla* version of VASP 6.2.1, i.e. no extensions have been added to the VASP source code.

For a list of new features in VASP6, see the [VASP wiki](#).

## General observations

- VASP is not helped by hyperthreading.
- Running on fewer than 128 tasks 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 out-of-memory (OOM) error. Further information from the VASP wiki can be found [here](#) and [here](#). You can check the example job script for using 64 MPI tasks x 2 OpenMP threads per node under [Running Vasp](#).

## How to choose the number of cores

Rule of thumb:

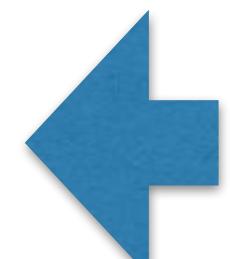
- 1 atom per core = Good
- 0.5 atom per core = Could work (but bad efficiency and time wasted)
- < 0.5 atom per core = Don't do it

# Example of day-to-day tools

- less / gedit / vi / nano      reading/editing files
- grace / gnuplot                plotting tools
- Bash                            simple scripts
- cif2cell                      convert from .cif, create structures
- p4vasp                    analysis of VASP output
- xcrysden / vesta        view structure
- ASE                        different tools (Python), create structures

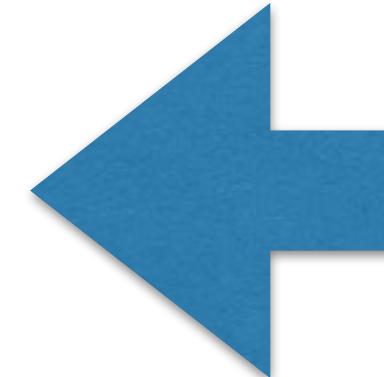
## Also of interest:

- Python / R                    analysis etc. (check out e.g. using jupyter)
- Matlab / Octave             analysis etc.
- Schrödinger                  create/view structure                @Tetralith



# Different types of calculations

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



# 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 NAISS 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 part 3!

# 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

in very brief,  
refer to  
VASP wiki  
for details

- 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

# POSCAR

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

(hopefully) useful	comment	Ni fcc	
		3.53	lattice constant ( $\text{\AA}$ )
	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 1	element symbols
	position for first atom	Cartesian 0 0 0	optional, useful for clarity & plotting
			Cartesian or Direct coordinates
			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 one of my own 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
```

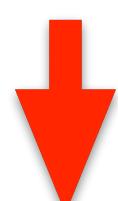
first H atom →

← 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 main title 'Crystallography Open Database' is displayed below the logo. On the left, there is a sidebar with links for 'COD Home', 'Accessing COD Data', 'Add Your Data', and 'Documentation'. The main content area includes a brief description of the database, a statistics section showing 41385 entries, and a 'CIFs Dossiers' section. At the bottom, there is an 'Advisory Board' section with logos of various organizations.

### Bilbao Crystallographic Server

Many Crystallographic tools, e.g. check BZ of fcc cell

The screenshot shows the homepage of the Bilbao Crystallographic Server. The header features the server's name and logos for UPV/EHU and IUPAC. The main menu includes 'Contact us', 'About us', 'Publications', and 'How to cite the server'. Below the menu, there is a sidebar titled 'Quick access to some tables' listing 'Space Groups', 'Plane Groups', 'Layer Groups', 'Rod Groups', 'Frieze Groups', '2D Point Groups', '3D Point Groups', and 'Magnetic Space Groups'. The central content area contains several sections with links: '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 provides updates on recent publications.

# POSCAR

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

## Atomic Simulation Environment (ASE)

Handle structures (and much more) using  
python scripts, also GUI

## cif2cell

Versatile script, reads .cif  
saves to many formats including  
POSCAR - also build supercells

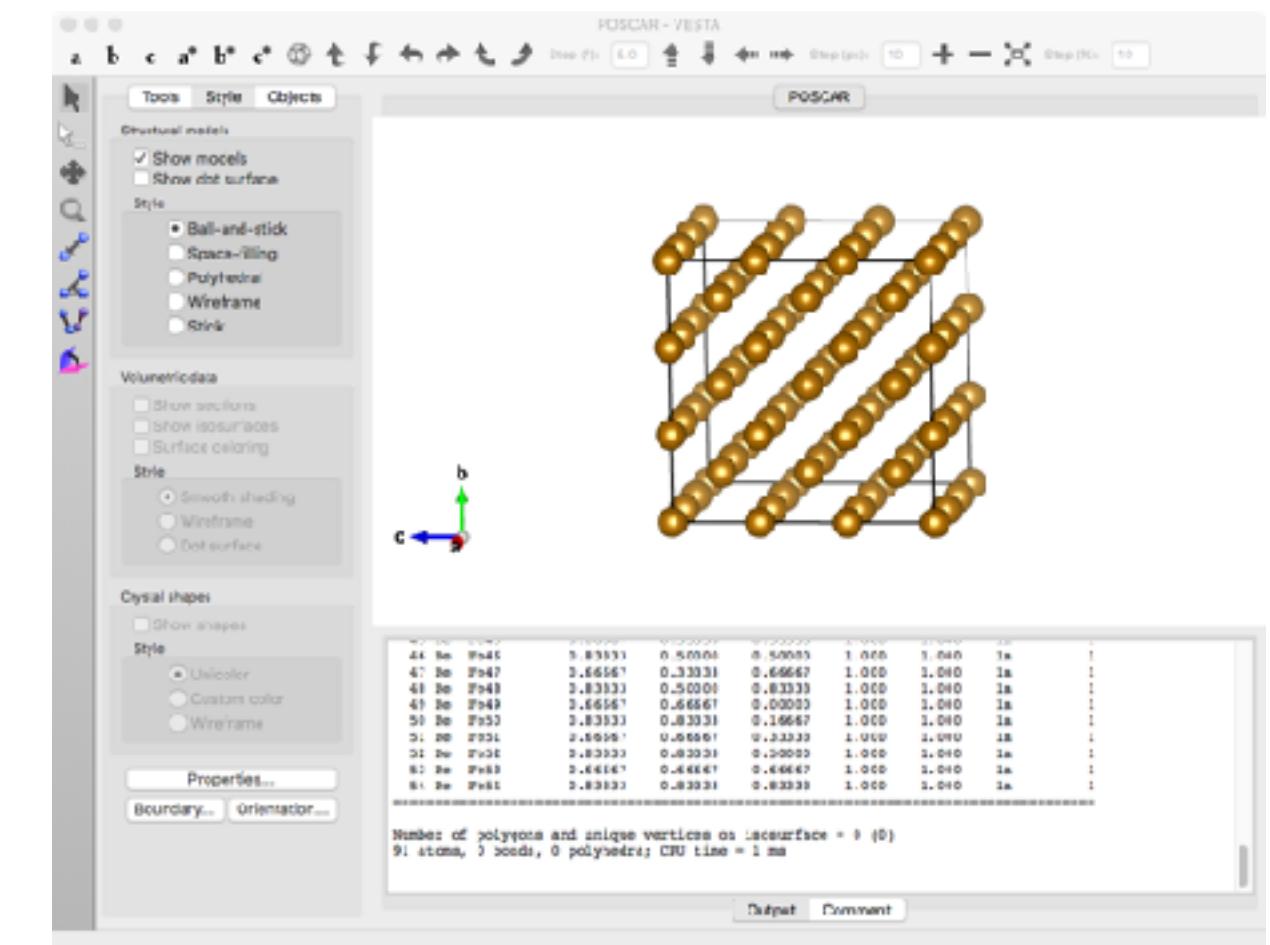
## Commercial software:

NanoLab

MedeA

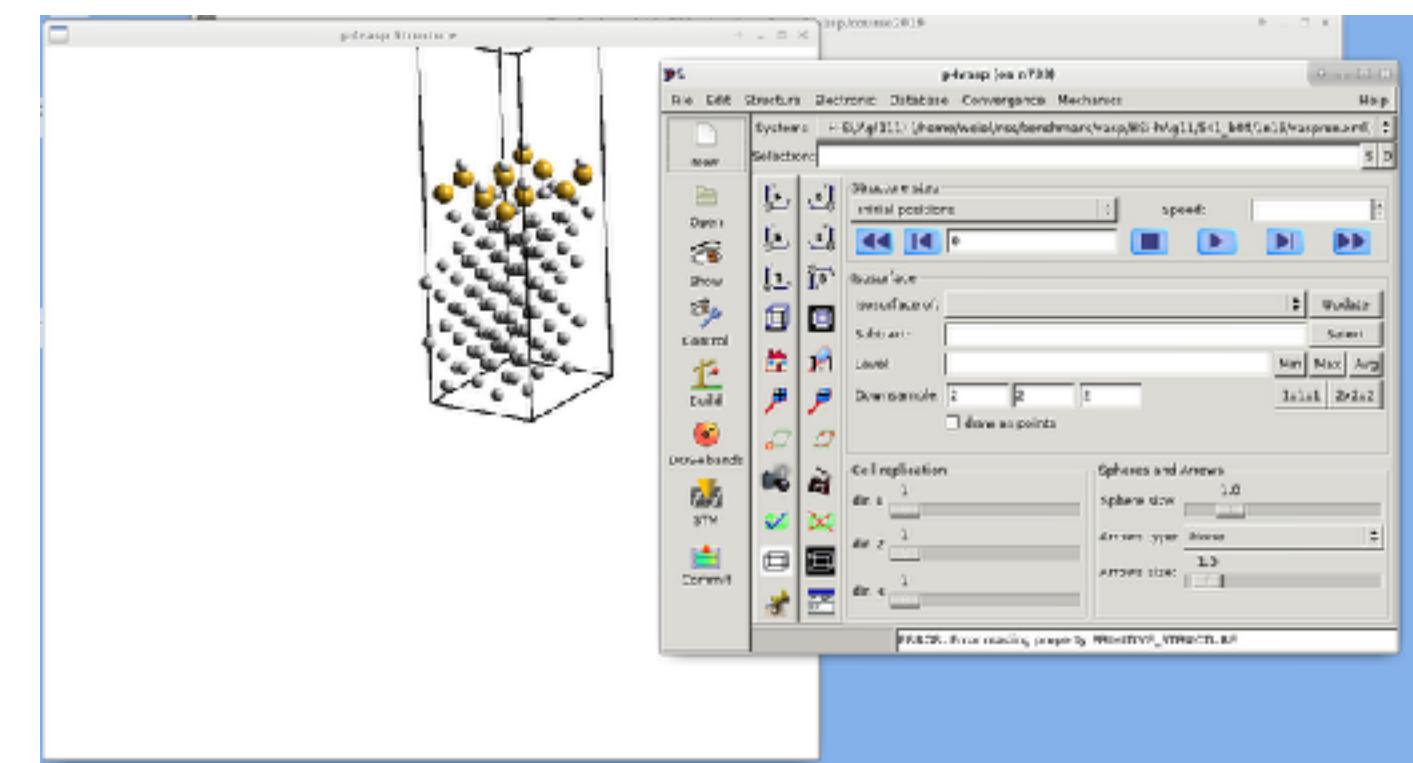
MaterialsStudio

## 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?

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`

@Tetralith: [/software/sse/manual/vasp/POTCARs](#)

# 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	odd kmesh - includes $\Gamma$ -point
0 0 0	optional shift of k-mesh

My 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	- $\Gamma$ -point included by default
0. 0. 0.	- 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				
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	0.7500	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
- OpenACC GPU binaries, same names
- + modifications
  - e.g. constrained relaxation

# 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 - Dardel (PDC)

Example might be outdated!

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

module load PDC/21.11
module load vasp/6.2.1-vanilla

export OMP_NUM_THREADS=1

srun vasp
```

Example: running on 2 nodes (128x2 cores) @Dardel

[https://www.pdc.kth.se/software/software/VASP/cpe21.11/6.2.1-vanilla/index\\_using.html](https://www.pdc.kth.se/software/software/VASP/cpe21.11/6.2.1-vanilla/index_using.html)

# 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

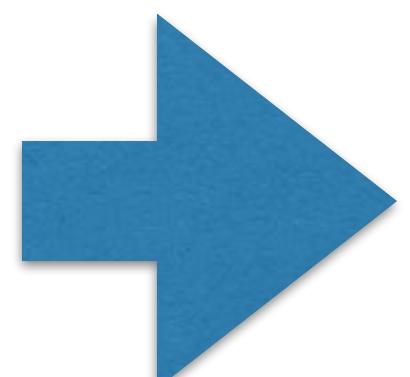
- DOSCAR - total, partial density of states (DOS)
- CHGCAR - charge density  
output can also be switched off
- WAVECAR - plane wave coefficients (for restart)
- ...

# 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   R   N   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 ...):

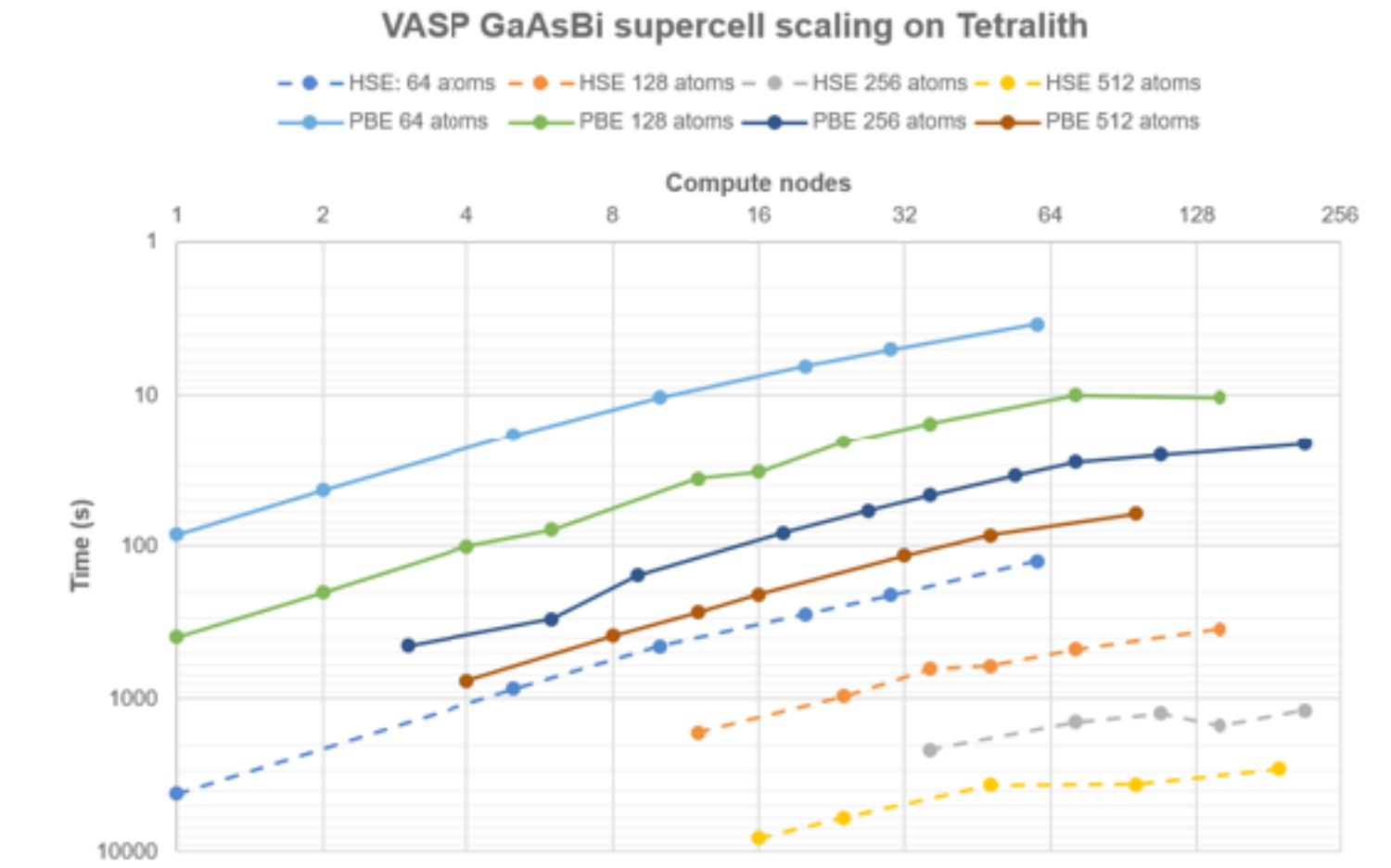
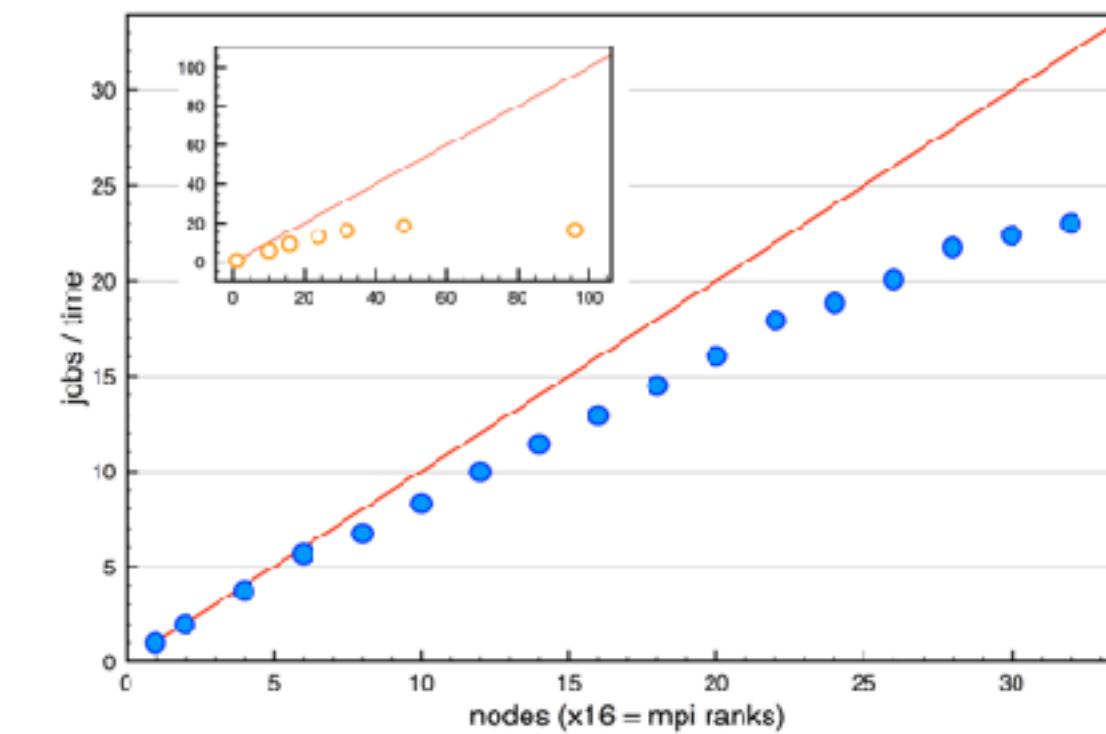
| You have a (more or less) 'large supercell' and for larger cells  
| it might be more efficient to use real space projection operators  
| So try LREAL= Auto in the INCAR file.  
| Mind: If you want to do a very accurate calculations keep the  
| reciprocal projection scheme (i.e. LREAL=.FALSE.)

# VASP6

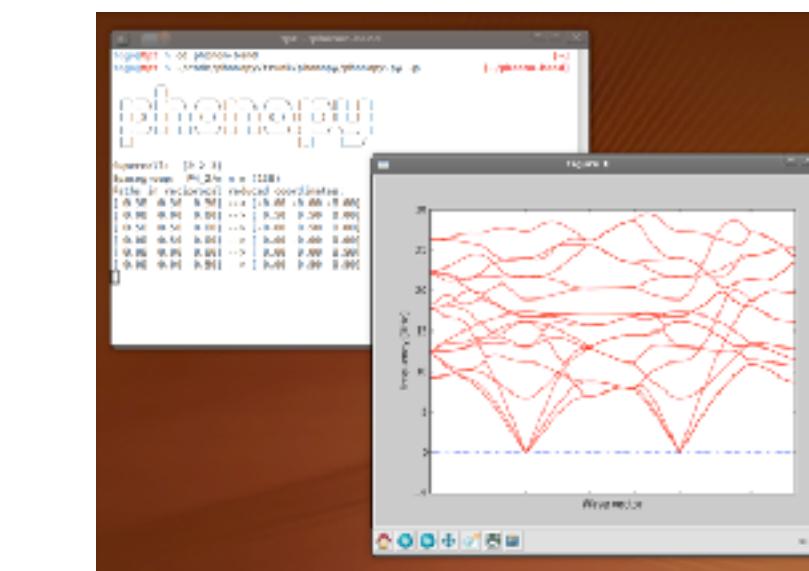
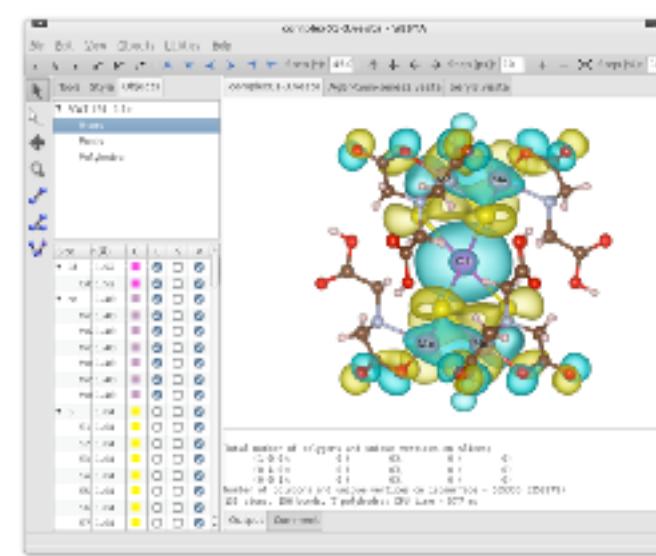
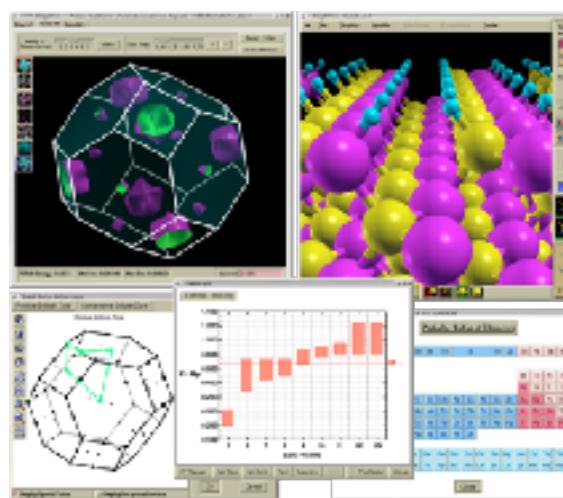
- Link to features in VASP6.X
- Hybrid OpenMP & MPI parallelization
- OpenACC for GPU
- Cubic scaling RPA and GW
- Electron-phonon coupling using stochastic displacements of atoms
- 6.3: Machine learning force-fields for MD, 6.4 updates -> increased speed (at least 10x noticed)

# Tomorrow:

- Running & Performance
  - Parallelization
  - Efficient settings
  - Problems



- Utilities & Summary



VTST•Tools

**USPEX** Computational Materials Discovery