2. VASP - Basics

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National Supercomputer Centre (NSC), Linköping University
NAISS-ENCCS training, online 17-18th Apr 2024

LINKÖPINGS UNIVERSITET

VASP - Best Practices Workshop

NAISS

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

https://www.naiss.se/

https://enccs.se/

https://www.vasp.at/

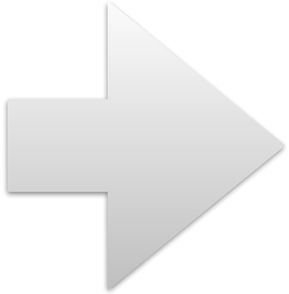
Introduction

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

… clickable links are underlined

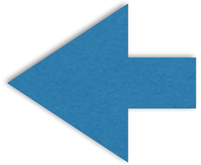
Short background

- 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  good starting point
- Caution: “inherited” input files
- Avoid overly messy INCAR…
- Possible differences in installations & versions

refer to respective center webpages / documentation

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

VASP & HPC centers

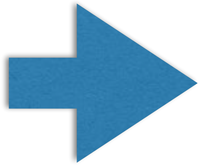
- **Tetralith (NAISS)** / Sigma, NSC, LiU  this course
  Installed!
- Dardel (NAISS), PDC, KTH
  Installed!
- Other systems/centers (e.g. Kebnekaise, HPC2N)
  Installed!
- LEONARDO (EuroHPC) - workshop  this course
- LUMI (EuroHPC & NAISS)

- Check for modules:

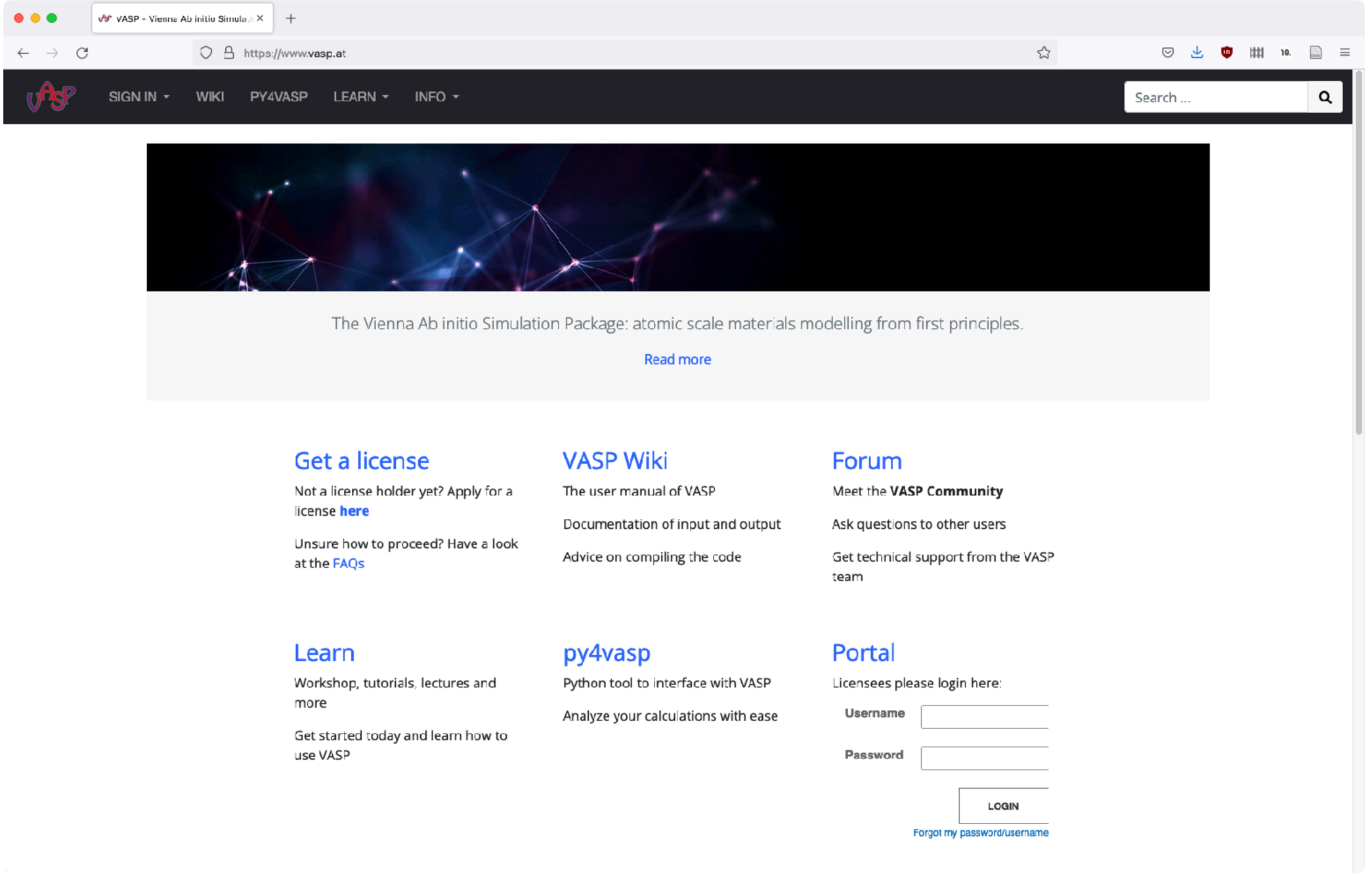
```
$ module avail vasp
$ module spider vasp
```

VASP versions & utilities

- **Latest:** 6.4.3 (from March -24)
  - 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

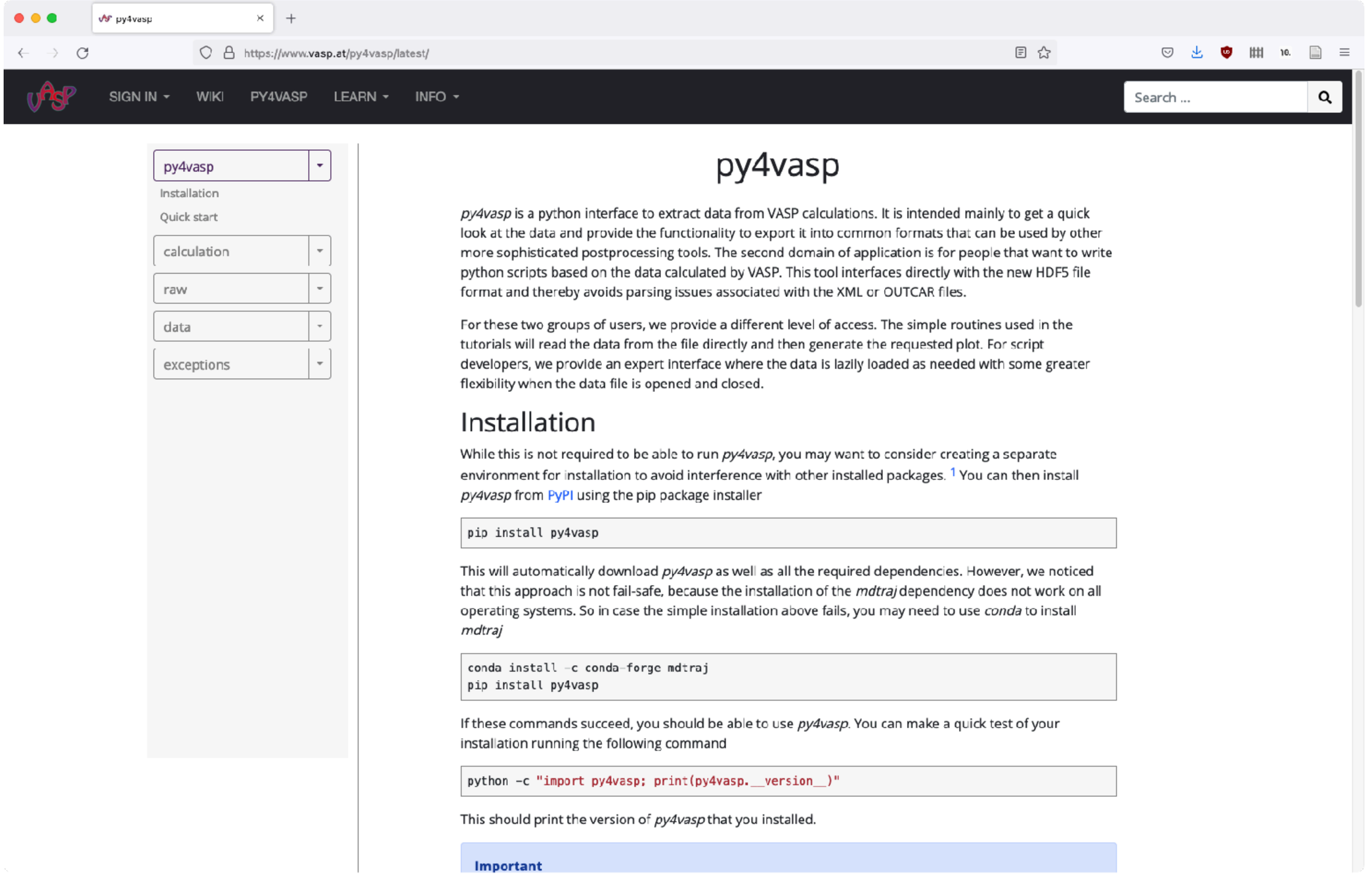


…more about utilities tomorrow



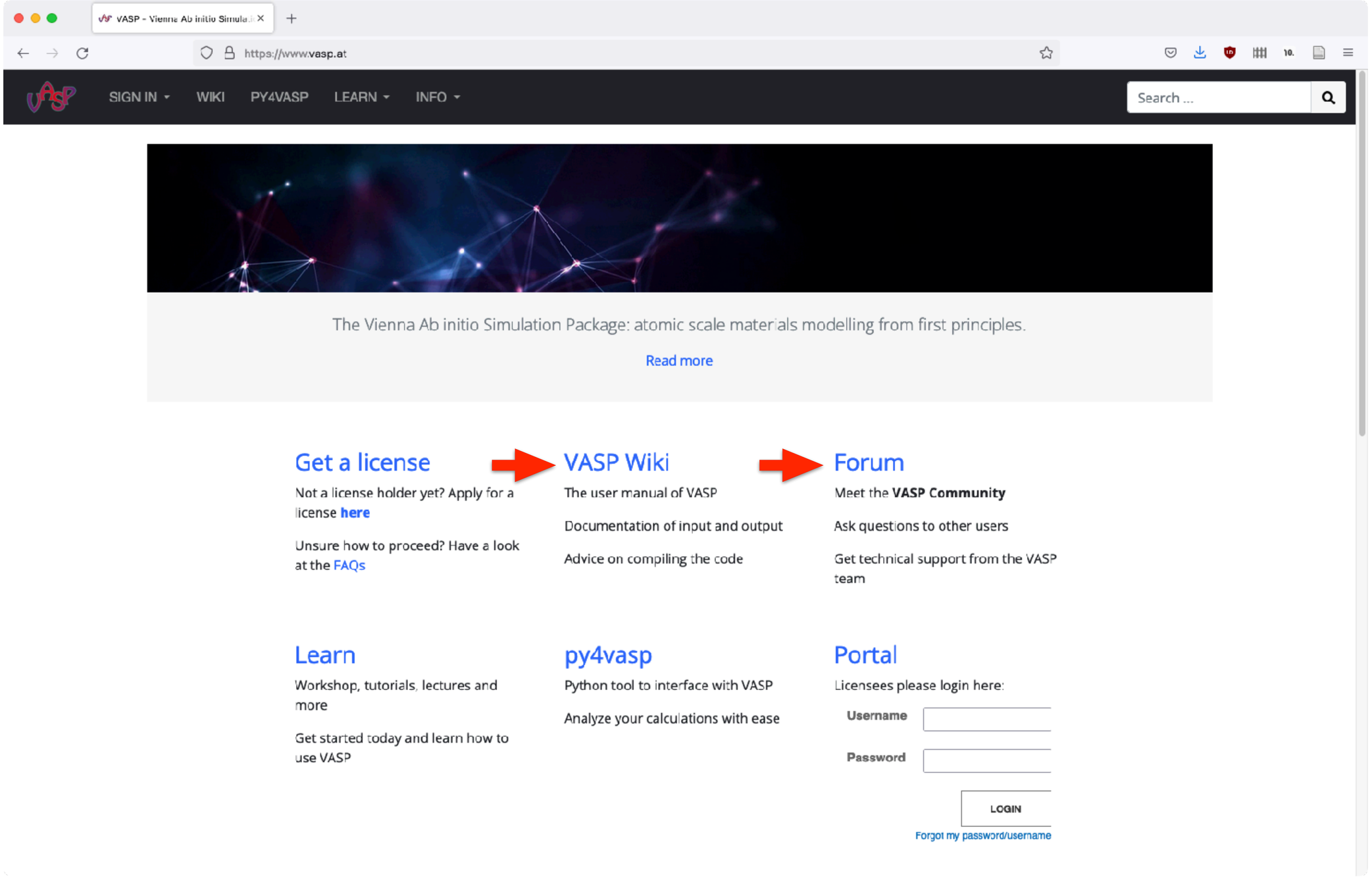
https://www.vasp.at/

…the official VASP webpage



https://www.vasp.at/

…py4vasp useful tool for quick analysis!



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	*subtopics (amongst others)*
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 mimimization	Structure optimization, ionic-mimimization methods, forces, etc.

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Page information

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 mimimization	Structure optimization, ionic-mimimization methods, forces, etc.
Molecular dynamics	Barostats, thermostats, ensembles, etc.
Ensemble properties	Monitoring geometric parameters, pair-correlation function, etc.
Advanced molecular-dynamics sampling	Interface pinning, constrained molecular dynamics, metadynamics, thermodynamic integration, etc.
Machine-learned force fields	Training and application of force fields.
Phonons	Lattice vibrations, electron-phonon interactions.
Response theory	Static and frequency-dependent dielectric properties, Berry phases, spectroscopy (UV, VIS, X-ray), phonons, etc.
Many-body perturbation theory	ACFDT, BSE, GW, MP2, CRPA.
Localized basis and projection	Obtaining Wannier functions, SCDM, etc.
Performance	Parallelization, memory management, 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.

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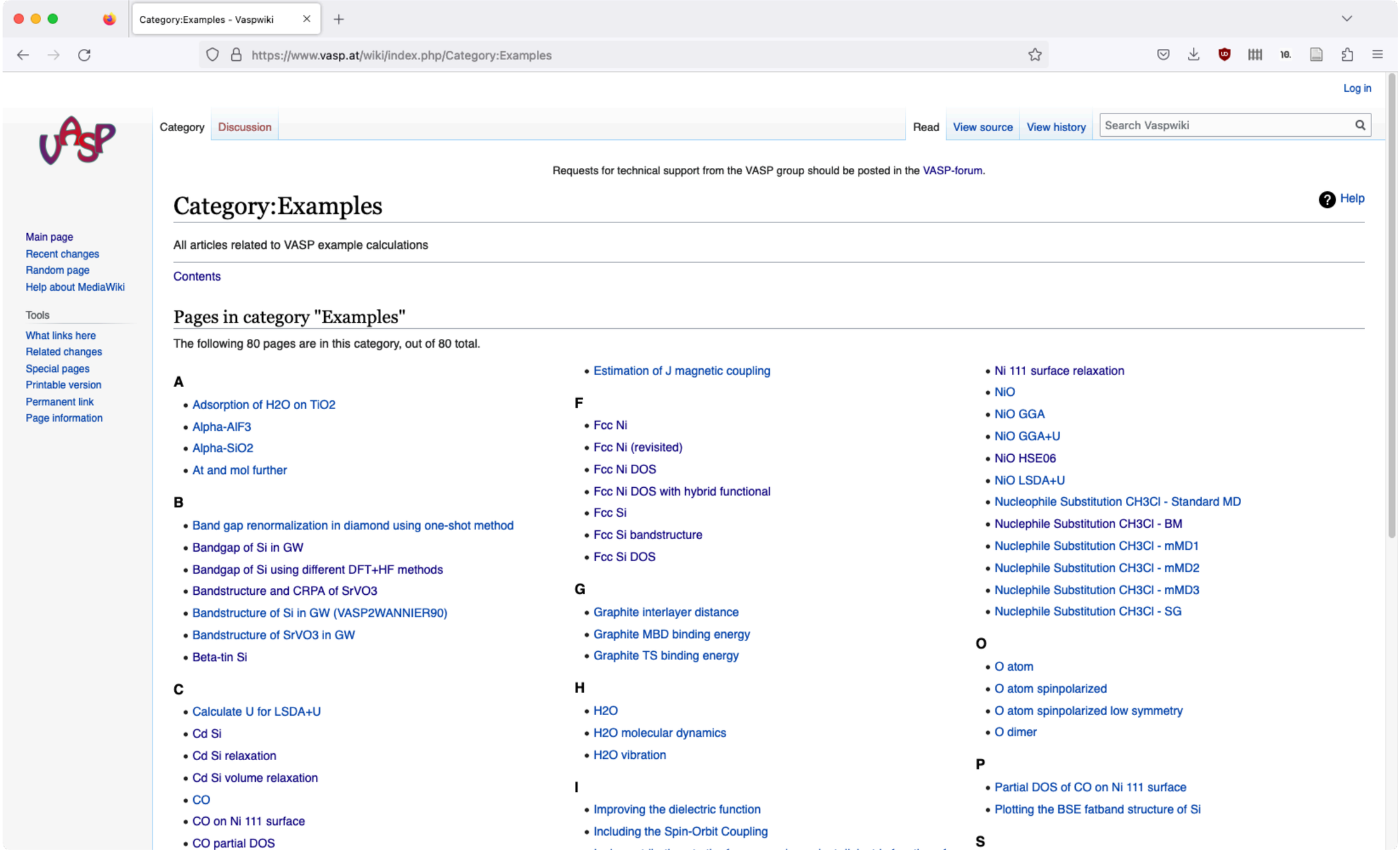
https://www.vasp.at/wiki/index.php/The_VASP_Manual



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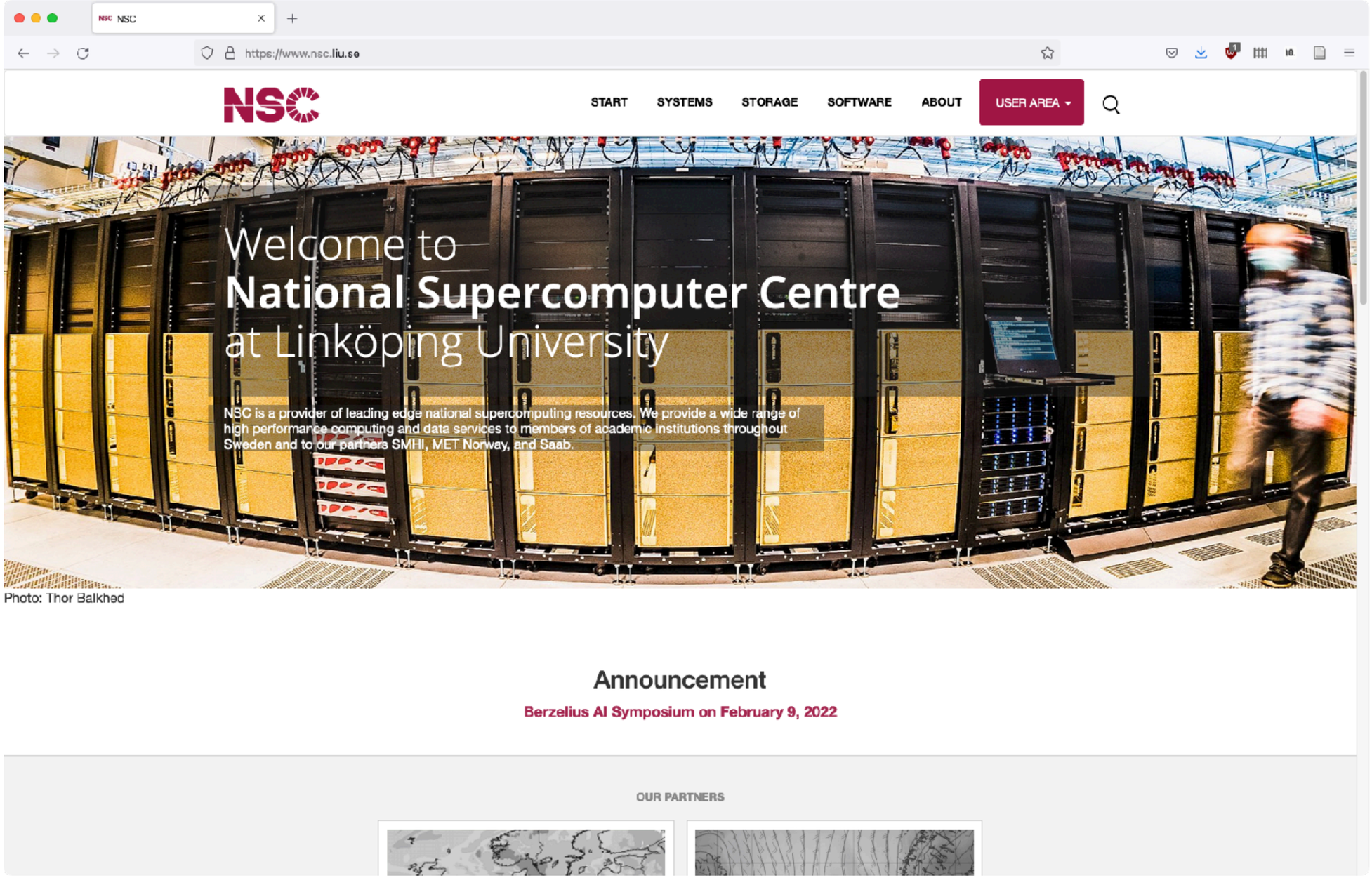


https://www.nsc.liu.se/ Software > Installed software > Tetralith & Sigma software list > VASP

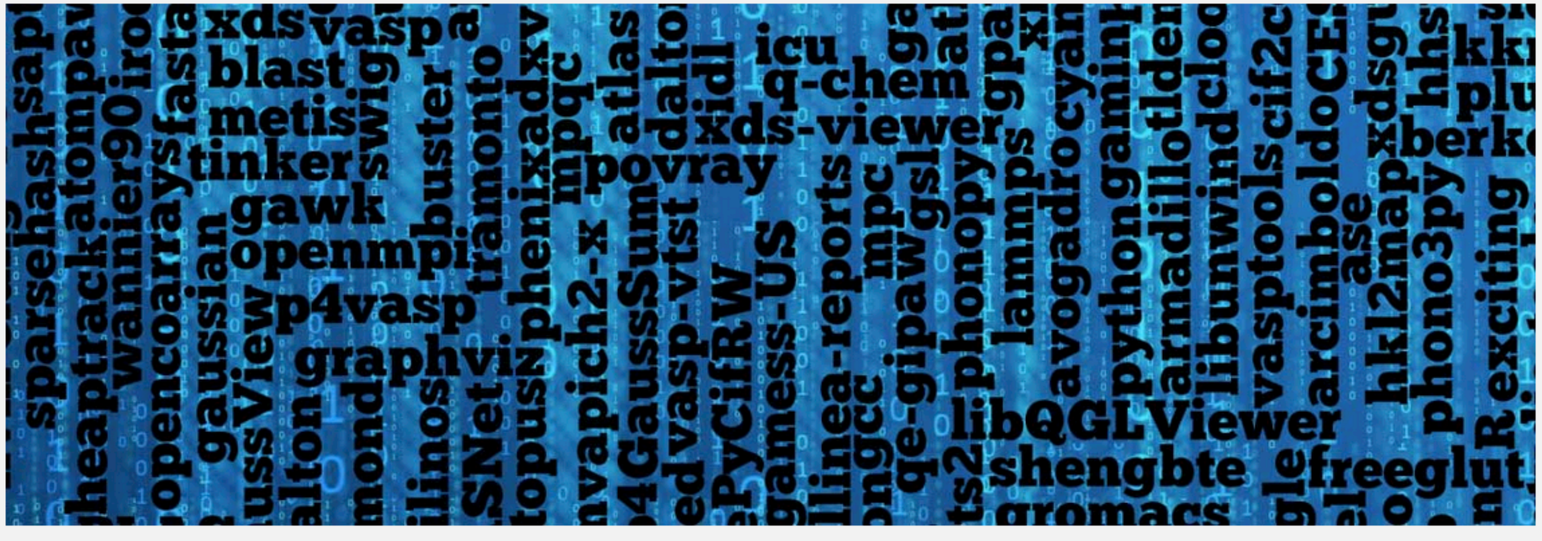
https://www.nsc.liu.se/software/installed/tetralith/vasp/

Photo: Thor Balkhed

Announcement

Berzelius AI Symposium on February 9, 2022

OUR PARTNERS



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

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.
- For Bi and Nebula, please look at the list above (software present there that is not already on Bi/Nebula can be requested).

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.

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

Software on Tetralith and Sigma

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

Search: vasp

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)

National Supercomputer Centre
Linköping University
581 83 LINKÖPING
SWEDEN

E-mail: support@nsc.liu.se
Tel.: 013-281000 (switchboard)
Fax.: 013-149403
Further address information

Org.nr: 202100-3096
VAT.nr: SE202100309601

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VASP

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/

Homepage: vasp.at/

NSC documentation

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

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

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.

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VASP Installations on Tetralith & Sigma

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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

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.

Disclaimer

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.

Installed software

Cluster	How to use	How to build
Tegner	5.3.5 5.4.1	5.3.5 5.4.1

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 uner 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

Explanation of above:

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

Quick guide to Tetralith for the workshop
(Presentations from NSC 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 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

- 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!**

parallel calcs.

- 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 x1.0 - x1.5
- 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…

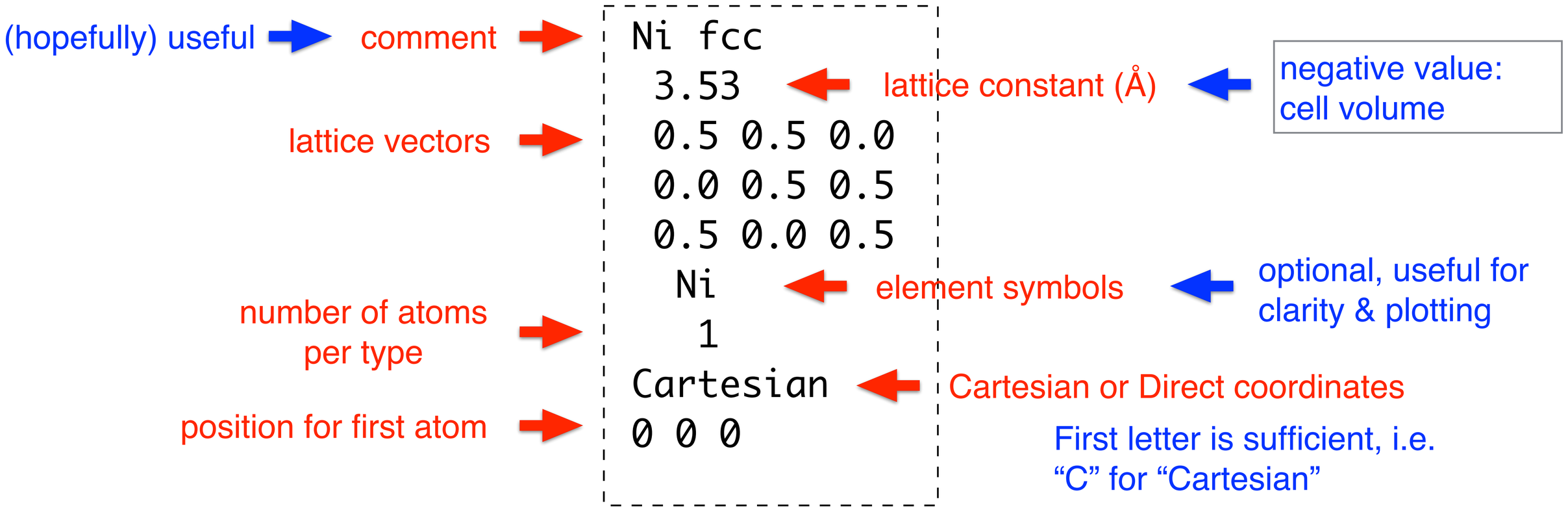
INCAR defaults

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 < |EDIFFG|
- 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 & movded: no update; MD; =2 ionic relaxation

POSCAR

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



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
  1.000000000000000   0.000000000000000   0.000000000000000
  0.500000000000000   0.866025403784439   0.000000000000000
  0.000000000000000   0.000000000000000   4.352531500114909
  H    Si   Ag
  14   14 108
Selective dynamics
Direct
  0.758338000000000   0.052881600000000   0.605945000000000  T   T   T
  0.505244000000000   0.118231000000000   0.605945000000000  T   T   T
  0.050784500000000   0.196017000000000   0.605945000000000  T   T   T
  0.800359000000000   0.251903000000000   0.605945000000000  T   T   T
  0.333333333333333   0.338902000000000   0.605945000000000  T   T   T
  0.114191000000000   0.386244000000000   0.605945000000000  T   T   T
  0.618474000000000   0.498058000000000   0.605945000000000  T   T   T
  0.381262000000000   0.511313000000000   0.605945000000000  T   T   T
  0.883071000000000   0.624684000000000   0.605945000000000  T   T   T
```

Note order of atoms

Relax for different directions

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

first H atom

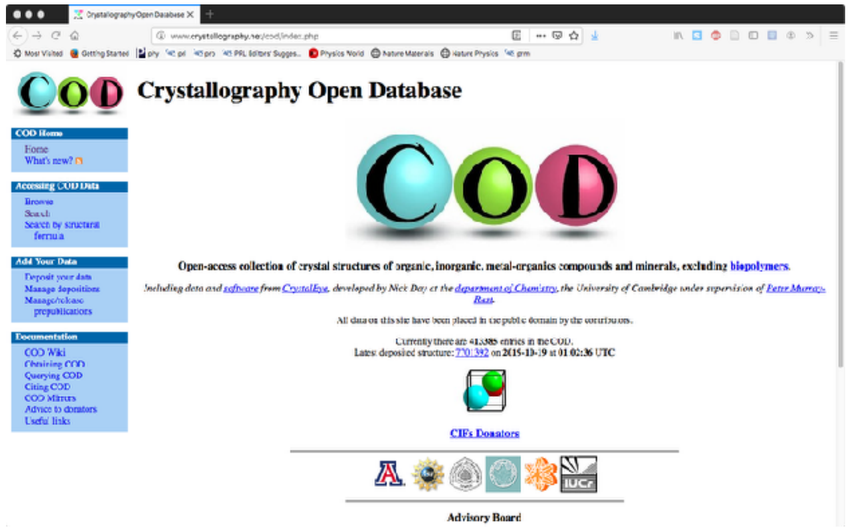
Rest of H, Si & Ag atoms following

POSCAR

Some useful resources:

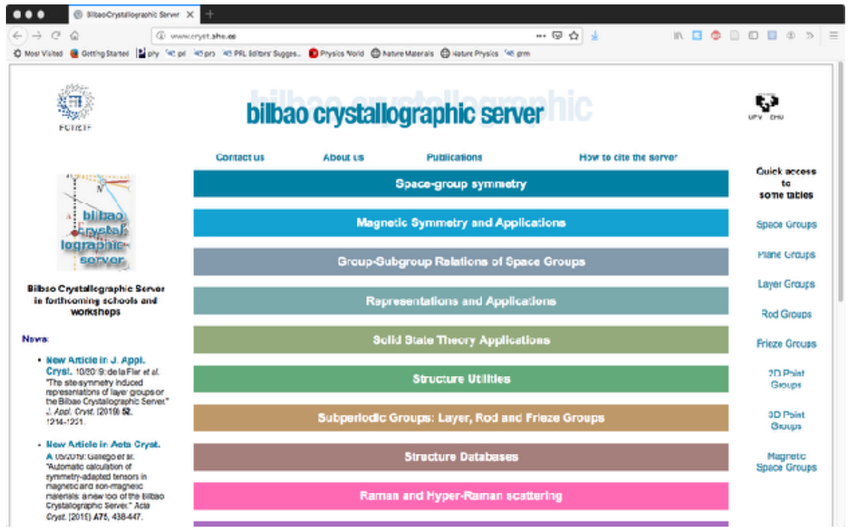
[Crystallography Open Database](#)

Database with published structures from experiment `.cif`



[Bilbao Crystallographic Server](#)

Many Crystallographic tools, e.g. check [BZ of fcc cell](#)



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

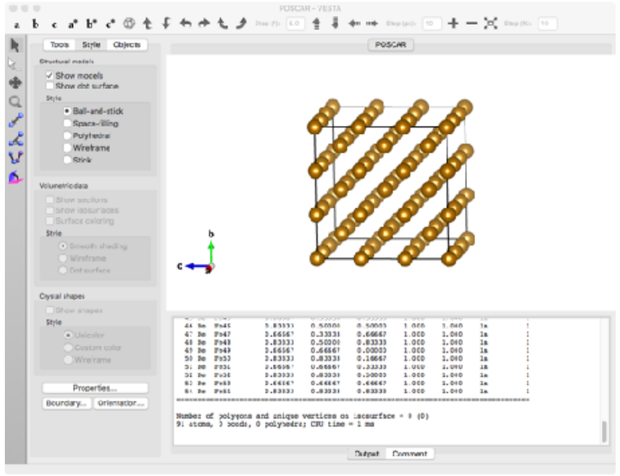
Commercial software:

[NanoLab]

[MedeA]

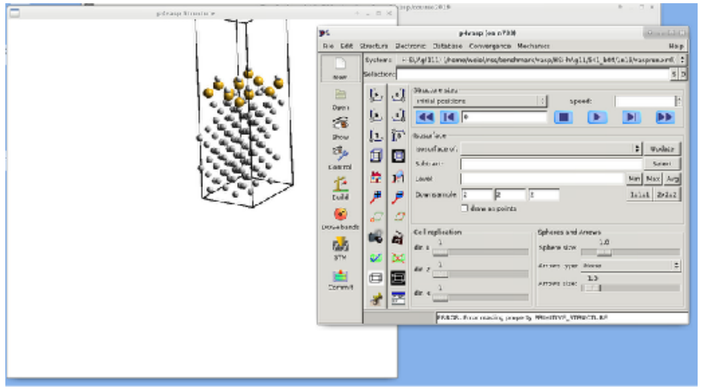
[MaterialsStudio]

[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
   11.0000000000000
 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
    RDEPT  =    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

```
k-points
 0
Monkhorst Pack
 11 11 11
 0  0  0
```

comment

0 = automatic generation of mesh

Monkhorst-Pack method (M)

k-point mesh

odd kmesh - includes Γ-point

optional shift of k-mesh

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

```
Automatic mesh
0
Gamma
2  2  1
0. 0. 0.
```

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

Gamma method (G)

- 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
 10
line
Reciprocal
  0.50000  0.50000  0.50000    1
  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
```

comment

k-points per line-segment

k-points per line-segment

Reciprocal / Cartesian

symmetry point + weight

KPOINTS

- Metal - “many” k-pts
- Band gap materials - “few” k-pts
- Unit cell (few atoms) - more k-pts
- 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

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

module load VASP/5.4.4.16052018-nsc1-intel-2018a-eb
mpprun vasp
```

`#SBATCH -n 64`

note “mpprun”

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

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
- WAVECAR - plane wave coefficients (for restart)
- …

output can also be switched off

OSZICAR

Min. algo

Step

Total free Energy

Energy diff.

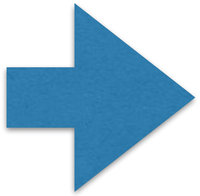
Eigenvalue diff.

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
 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
```

- Check for warnings!

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.

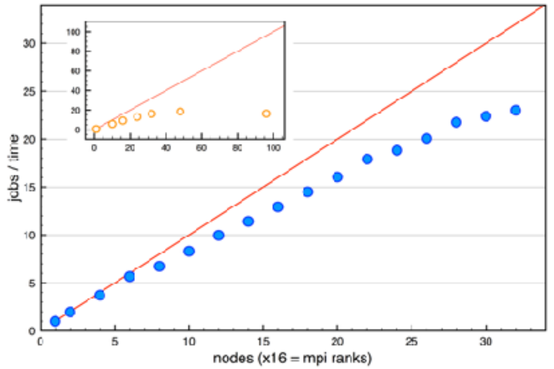
```
 -----------------------------------------------------------------------------
|                                                                             |
|           W    W    AA    RRRRR   N    N  II  N    N   GGGG   !!!          |
|           W    W   A  A   R    R  NN   N  II  NN   N  G    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   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.)             |
|                                                                             |
 -----------------------------------------------------------------------------
```

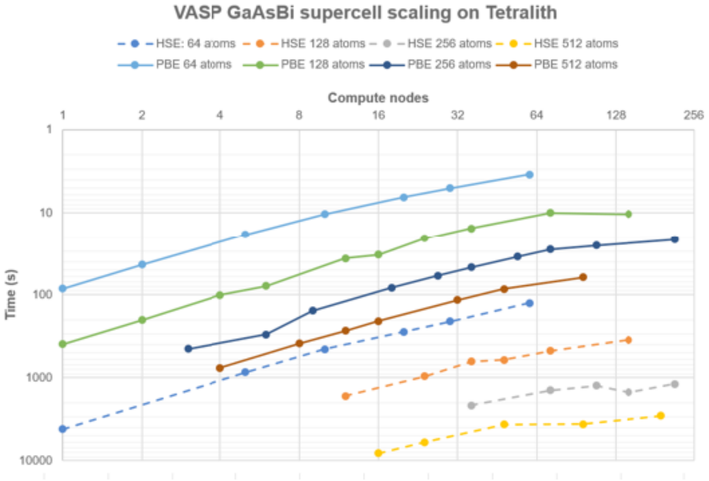
VASP6

- 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)

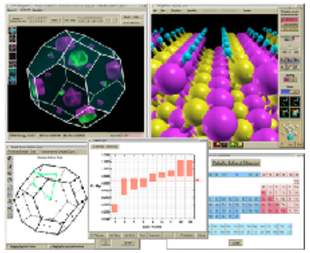
Tomorrow:

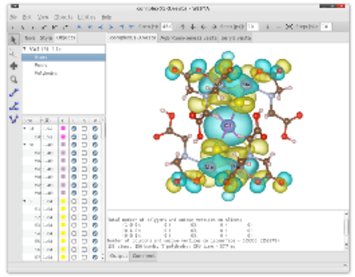
- Running & Performance
  - Parallelization
  - Efficient settings
  - Problems

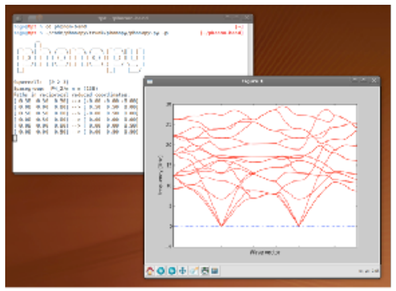




- Utilities & Summary







USPEX Computational Materials Discovery

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