2. VASP - Basics

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SNIC-PRACE training, online @NSC 22-23rd Feb 2022

LINKÖPINGS UNIVERSITET

VASP - Best Practices Workshop

https://www.nsc.liu.se/ https://www.snic.se/ https://training.prace-ri.eu/

https://www.vasp.at/

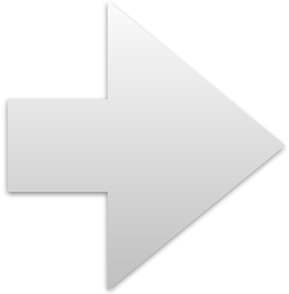
Introduction

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

… clickable links are underlined

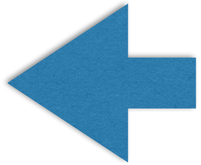
Short background

- 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

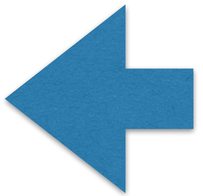
refer to respective center webpages / documentation

Resources

- Wiki / Manual
  Check in detail!
- Wiki
  examples, presentations
- Forum

Find the links:
https://vasp.at/

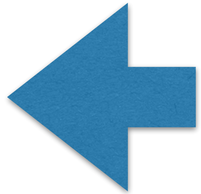
- Peter Larsson's (old) blog at NSC:
  https://www.nsc.liu.se/~pla/



info & discussion

Questions / trouble? support@nsc.liu.se, …

VASP at SNIC HPC centers

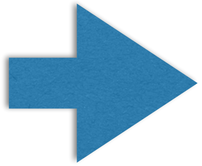
- **Tetralith** / Sigma, NSC, LiU  this course
- Kebnekaise, HPC2N, UmU
- Dardel, PDC, KTH
- Also available at other systems/centers

- On many systems:

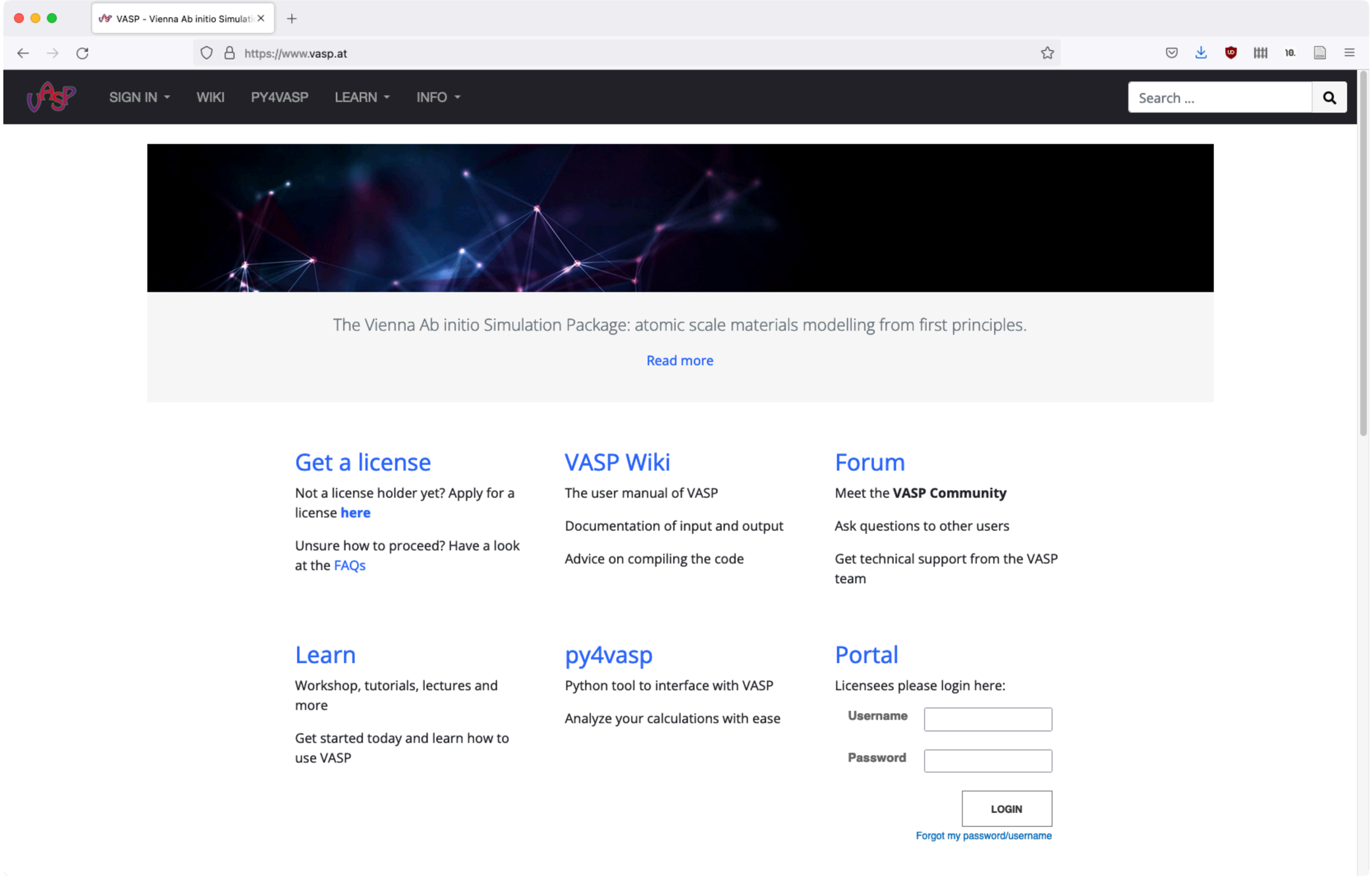
```
$ module avail vasp
$ module spider vasp
```

VASP versions & utilities

- **Latest:** 6.3.0 (from Jan -22)
  - 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

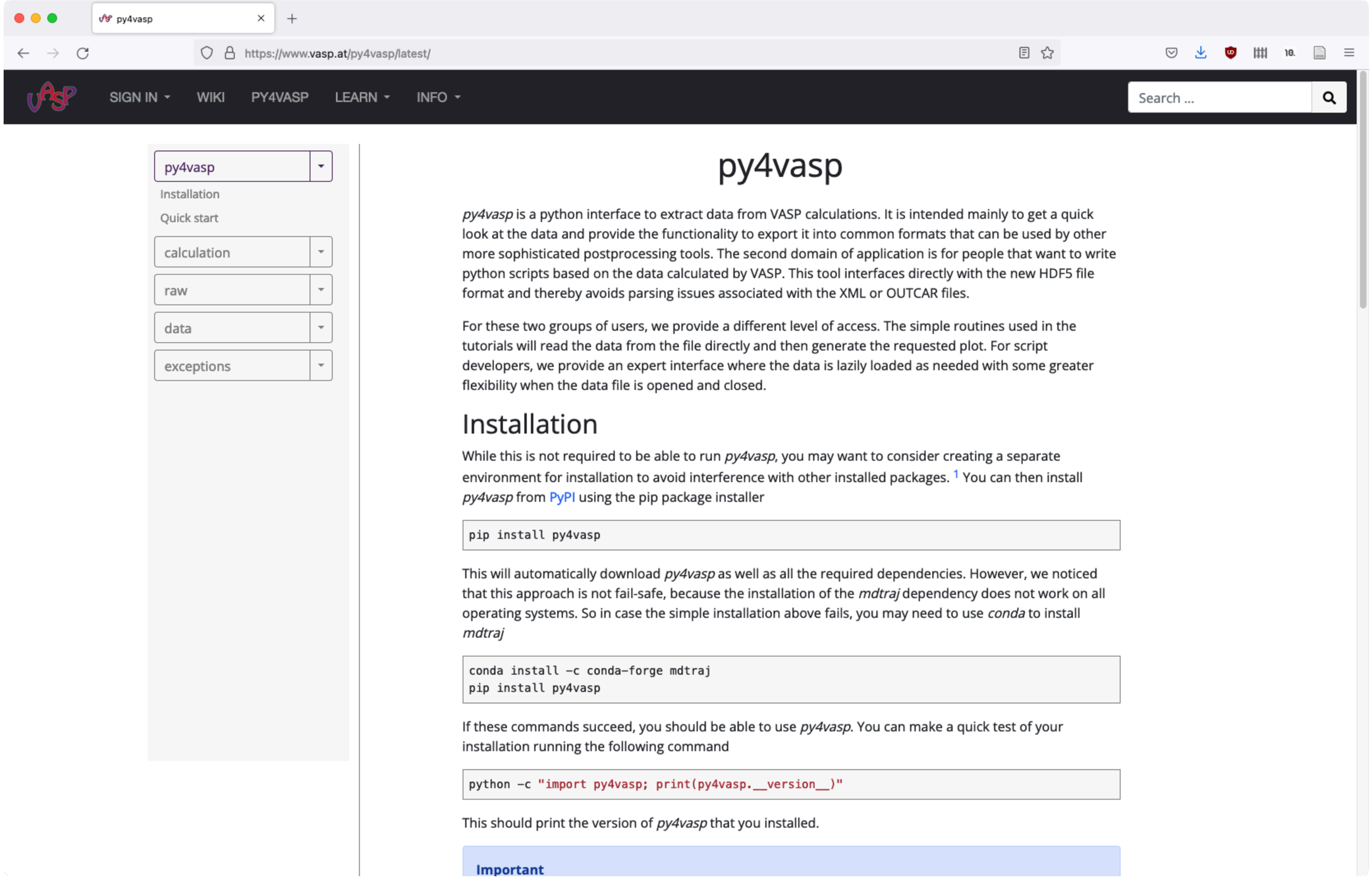


…more about utilities tomorrow



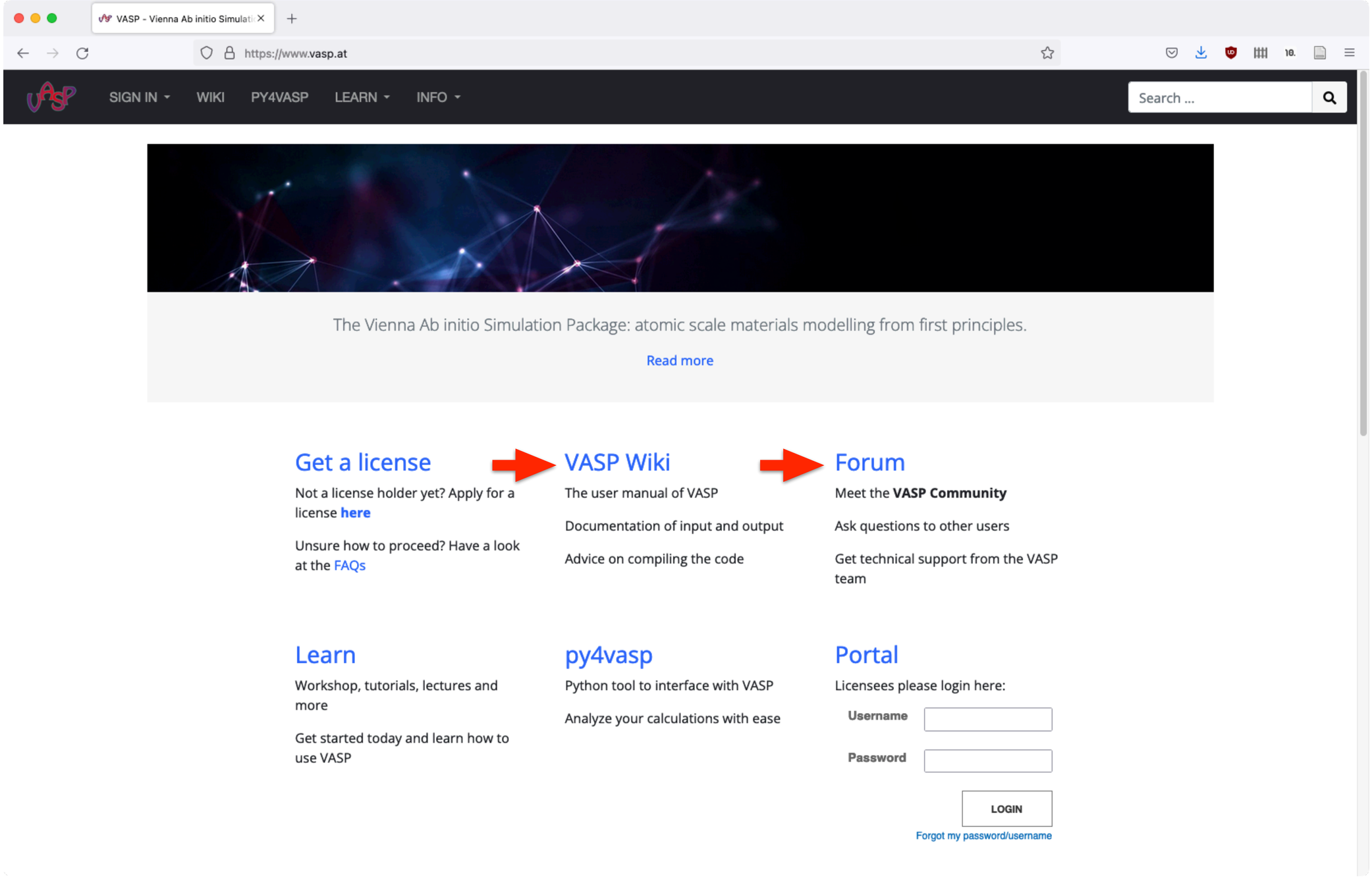
https://www.vasp.at/

…was updated just before this workshop!



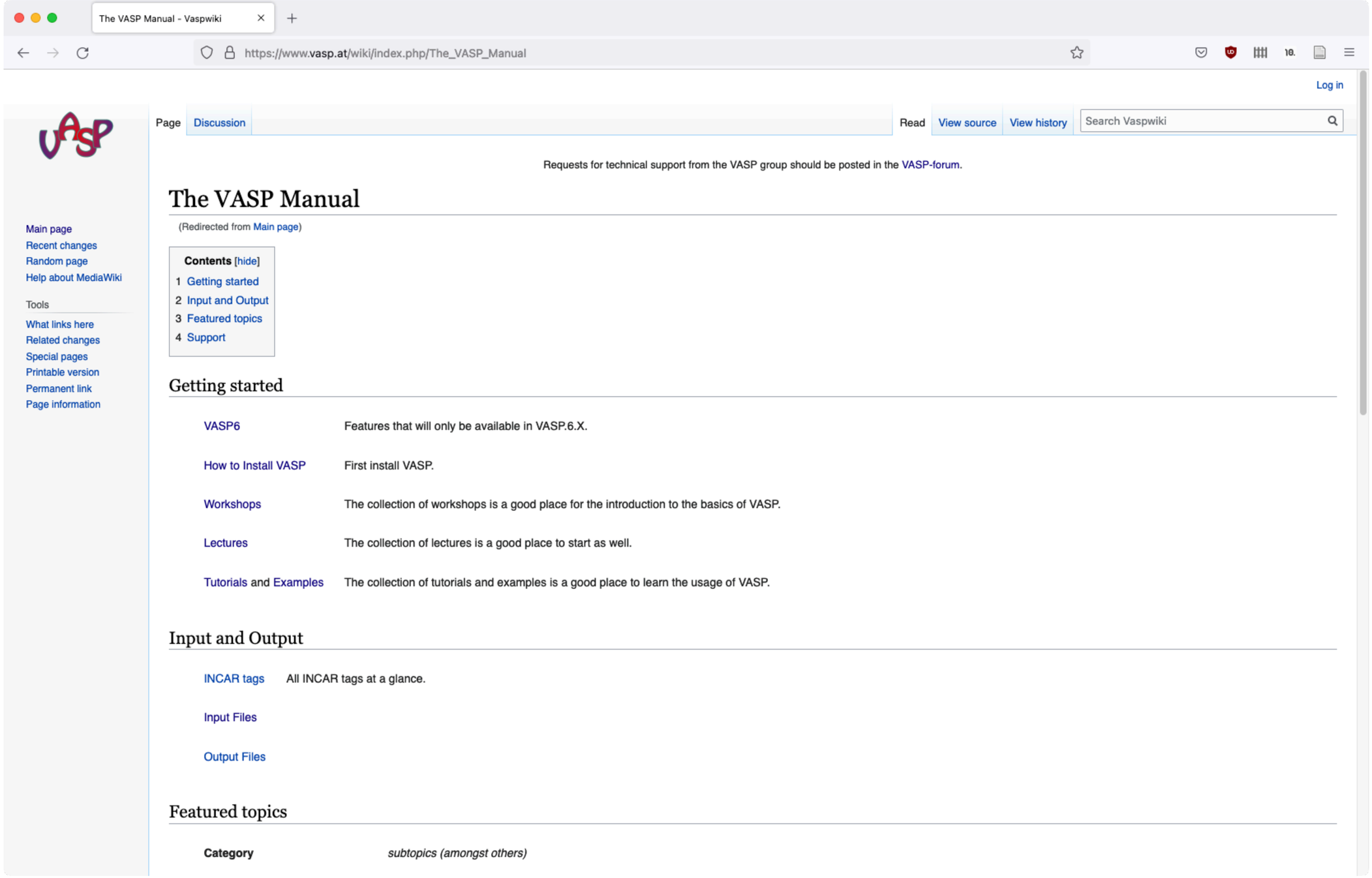
https://www.vasp.at/

…py4vasp new useful tool!

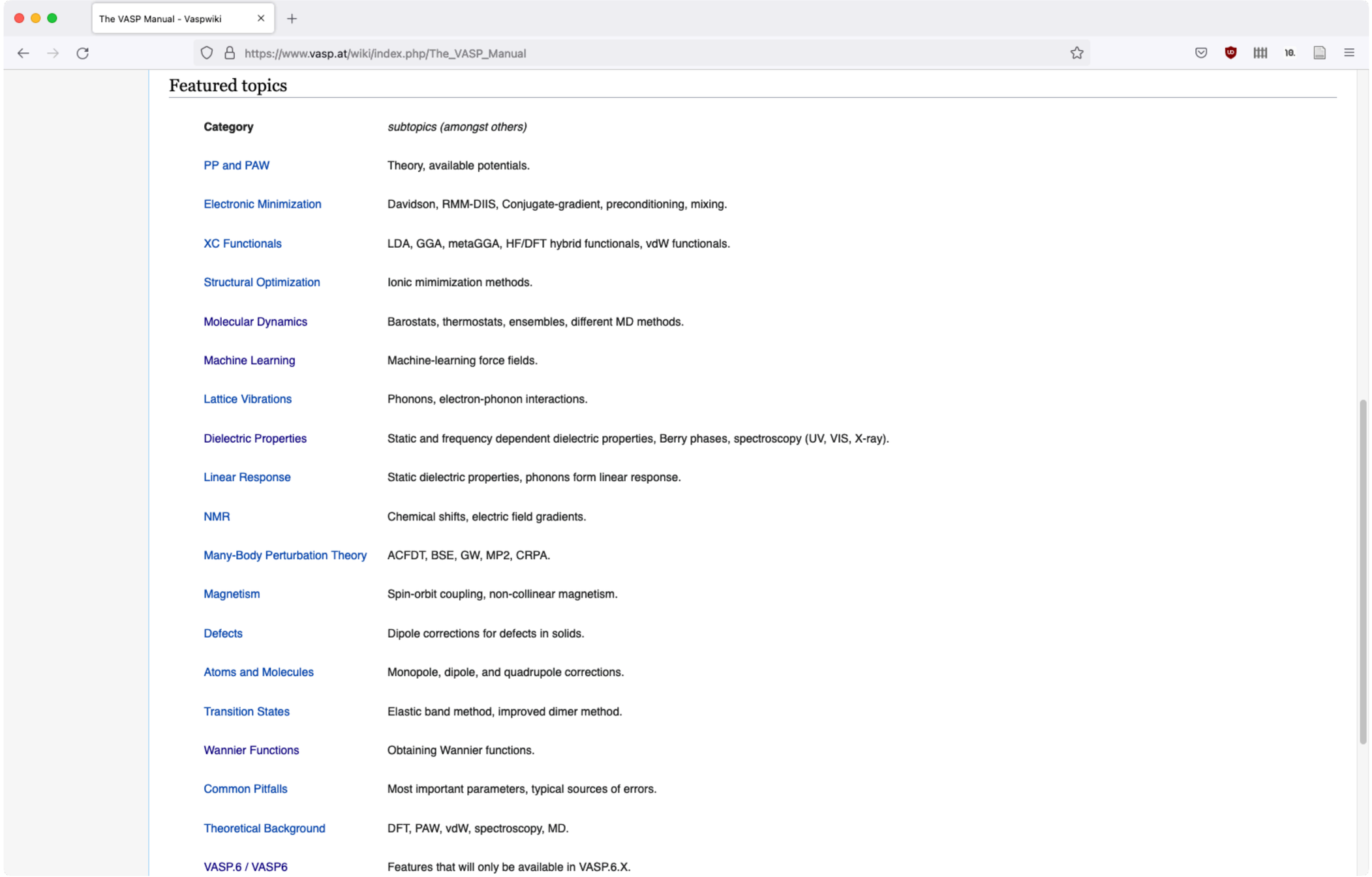


https://www.vasp.at/

…wiki important resource & also check forum



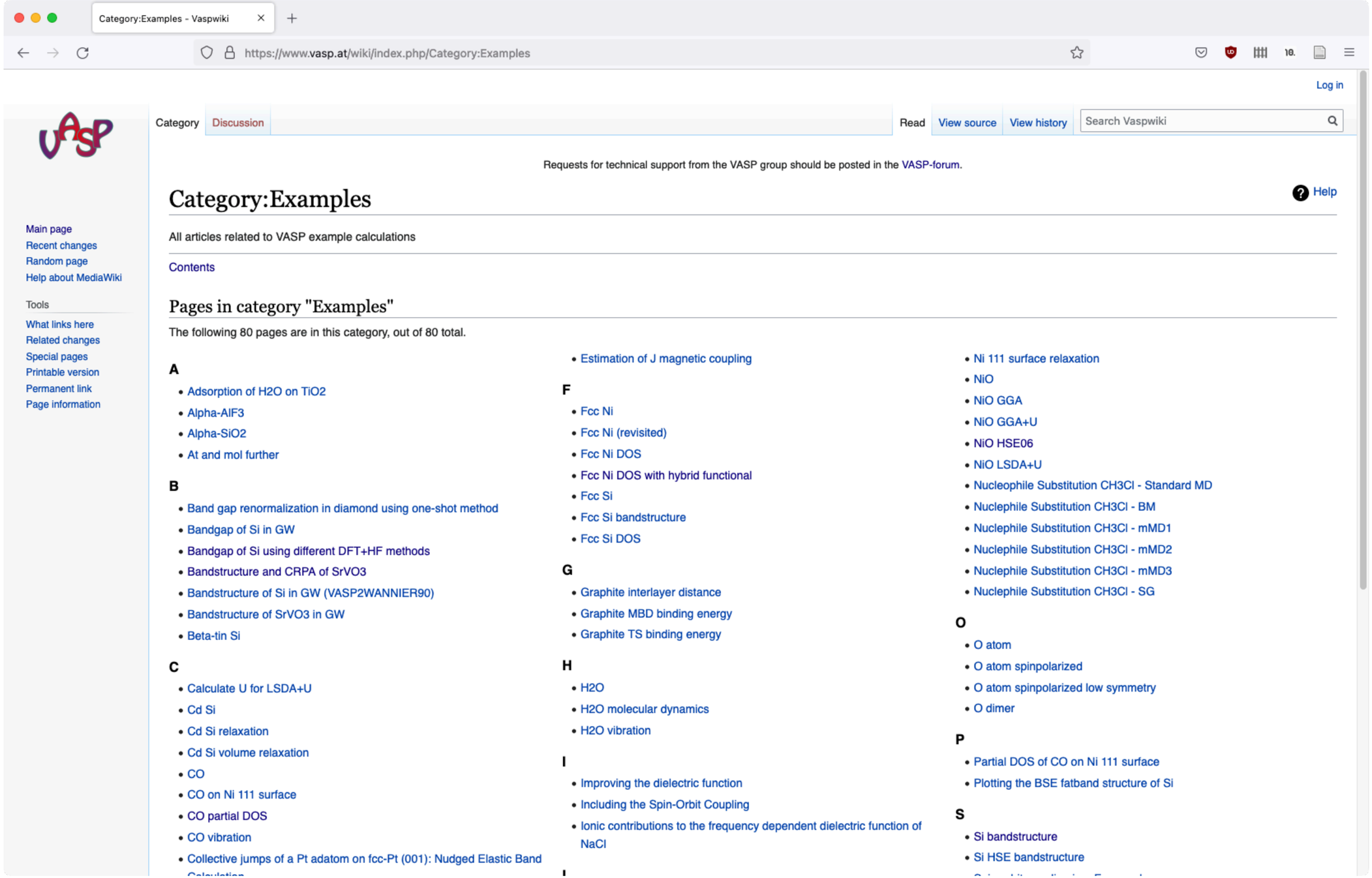
https://www.vasp.at/wiki/index.php/The_VASP_Manual



Featured topics

Category	*subtopics (amongst others)*
PP and PAW	Theory, available potentials.
Electronic Minimization	Davidson, RMM-DIIS, Conjugate-gradient, preconditioning, mixing.
XC Functionals	LDA, GGA, metaGGA, HF/DFT hybrid functionals, vdW functionals.
Structural Optimization	Ionic mimimization methods.
Molecular Dynamics	Barostats, thermostats, ensembles, different MD methods.
Machine Learning	Machine-learning force fields.
Lattice Vibrations	Phonons, electron-phonon interactions.
Dielectric Properties	Static and frequency dependent dielectric properties, Berry phases, spectroscopy (UV, VIS, X-ray).
Linear Response	Static dielectric properties, phonons form linear response.
NMR	Chemical shifts, electric field gradients.
Many-Body Perturbation Theory	ACFDT, BSE, GW, MP2, CRPA.
Magnetism	Spin-orbit coupling, non-collinear magnetism.
Defects	Dipole corrections for defects in solids.
Atoms and Molecules	Monopole, dipole, and quadrupole corrections.
Transition States	Elastic band method, improved dimer method.
Wannier Functions	Obtaining Wannier functions.
Common Pitfalls	Most important parameters, typical sources of errors.
Theoretical Background	DFT, PAW, vdW, spectroscopy, MD.
VASP.6 / VASP6	Features that will only be available in VASP.6.X.

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



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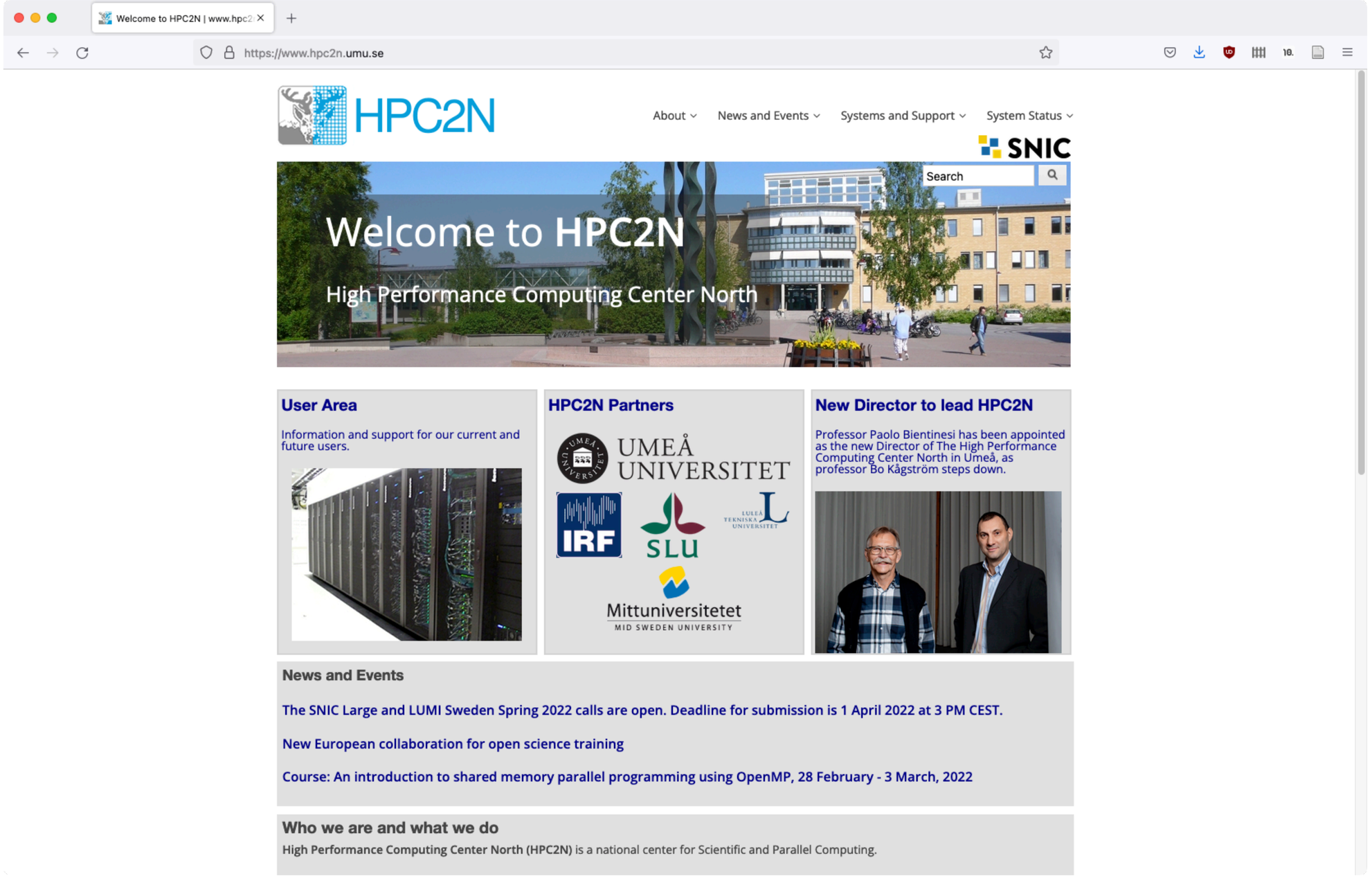

https://www.hpc2n.umu.se/ Systems and Support > Software > VASP

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

Welcome to HPC2N | www.hpc2n

https://www.hpc2n.umu.se

HPC2N

About | News and Events | Systems and Support | System Status

SNIC

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Welcome to HPC2N

High Performance Computing Center North

User Area

Information and support for our current and future users.

HPC2N Partners

UMEÅ UNIVERSITET

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LULEÅ TEKNISKA UNIVERSITET

Mittuniversitetet
MID SWEDEN UNIVERSITY

New Director to lead HPC2N

Professor Paolo Bientinesi has been appointed as the new Director of The High Performance Computing Center North in Umeå, as professor Bo Kågström steps down.

News and Events

The SNIC Large and LUMI Sweden Spring 2022 calls are open. Deadline for submission is 1 April 2022 at 3 PM CEST.

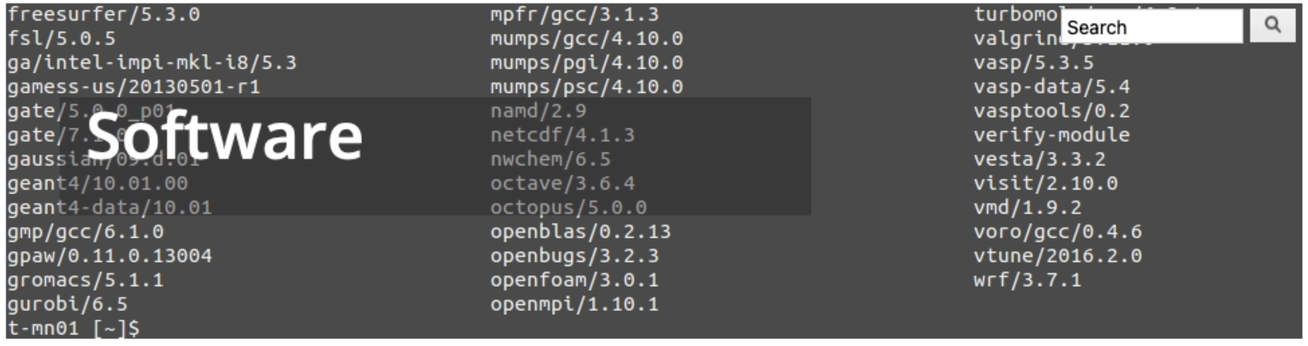
New European collaboration for open science training

Course: An introduction to shared memory parallel programming using OpenMP, 28 February - 3 March, 2022

Who we are and what we do

High Performance Computing Center North (HPC2N) is a national center for Scientific and Parallel Computing.

	External info:
Siesta	Siesta performs electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids. External info:
Singularity	Singularity is a is a free, cross-platform and open-source computer program that performs operating-system-level virtualization also known as containerization. Extern info:
Turbomole	TURBOMOLE is a quantum chemical program package Extern info:
VASP	Performs ab-initio quantum-mechanical molecular dynamics (MD) using pseudopotentials and a plane wave basis set. 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. Extern info:
WRF	Advanced Research WRF (ARW) Modeling System is a flexible, state-of-the-art atmospheric simulation system. 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. External info:
Intel	Intel Compilers. Has C, C++, Fortran 77, Fortran 90, and Fortran 95. Available for serial, OpenMP, and MPI code for all languages. Part of several compiler toolchains. External info:
PGI	Portland Group Compilers. Has C, C++, Fortran 77, Fortran 90, and Fortran 95. Avaliable for serial, OpenMP, and MPI code for all languages, with the exception of Fortran 96 MPI programs.



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.

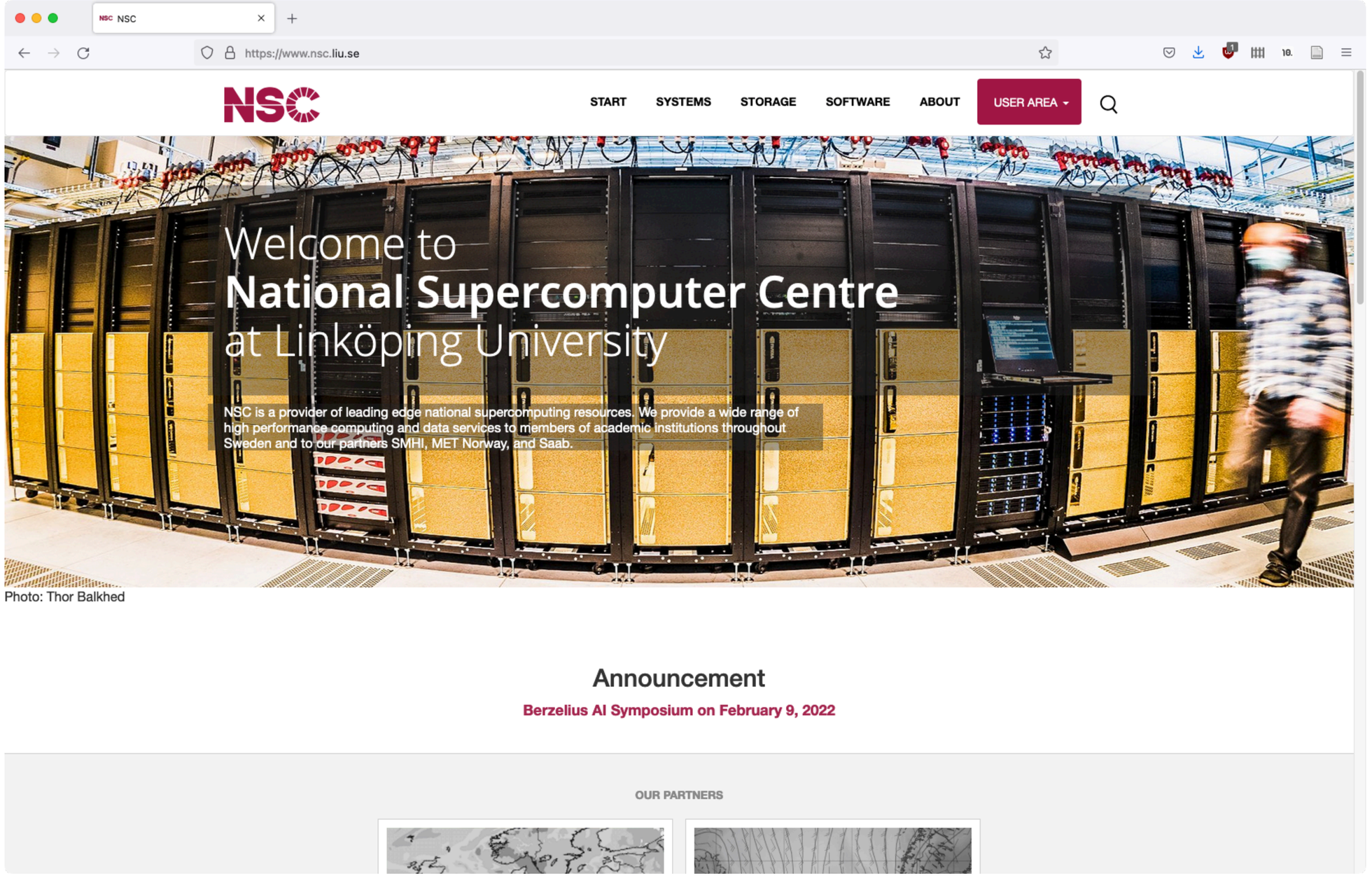
General

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 projector-augmented wave method and a plane wave basis set. The approach implemented in VASP is based on the (finite-temperature) local-density approximation with the free energy as variational quantity and an exact evaluation of the instantaneous electronic ground state at each MD time step.

VASP uses efficient matrix diagonalisation schemes and an efficient Pulay/Broyden charge density mixing. These techniques avoid all problems possibly occurring in the original Car-Parrinello method, which is based on the simultaneous integration of electronic and ionic equations of motion.



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

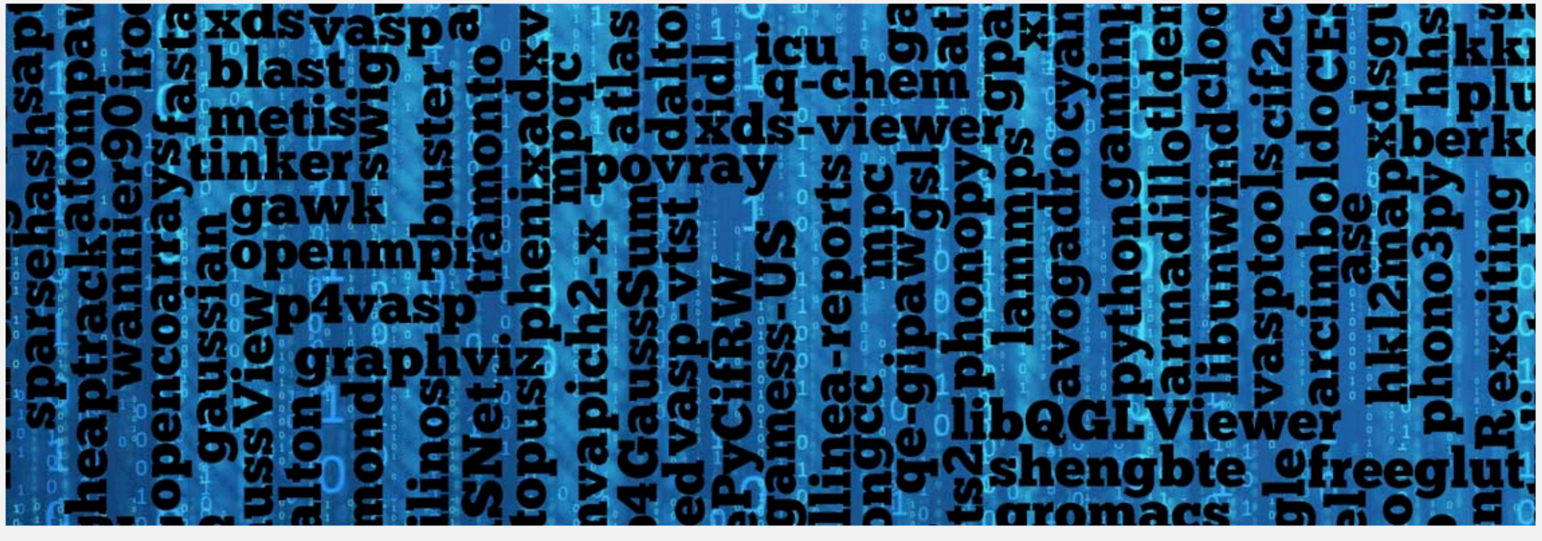
https://www.nsc.liu.se/software/installed/tetralith/vasp/

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.

Tetralith & Sigma Software

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: 2020-03-16

Electronic structure

- Abinit
- ASE
- CASTEP
- Elk
- EPW
- exciting
- GPAW
- phonopy
- phono3py
- p4vasp
- Quantum Espresso
- USPEX (licensed)
- vasptools
- VASP (licensed)
- WIEN2k (licensed)
- Yambo

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

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

@Kebnekaise, Tetralith

Quick guide to Tetralith for the workshop
(Presentations from old 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 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

- 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…

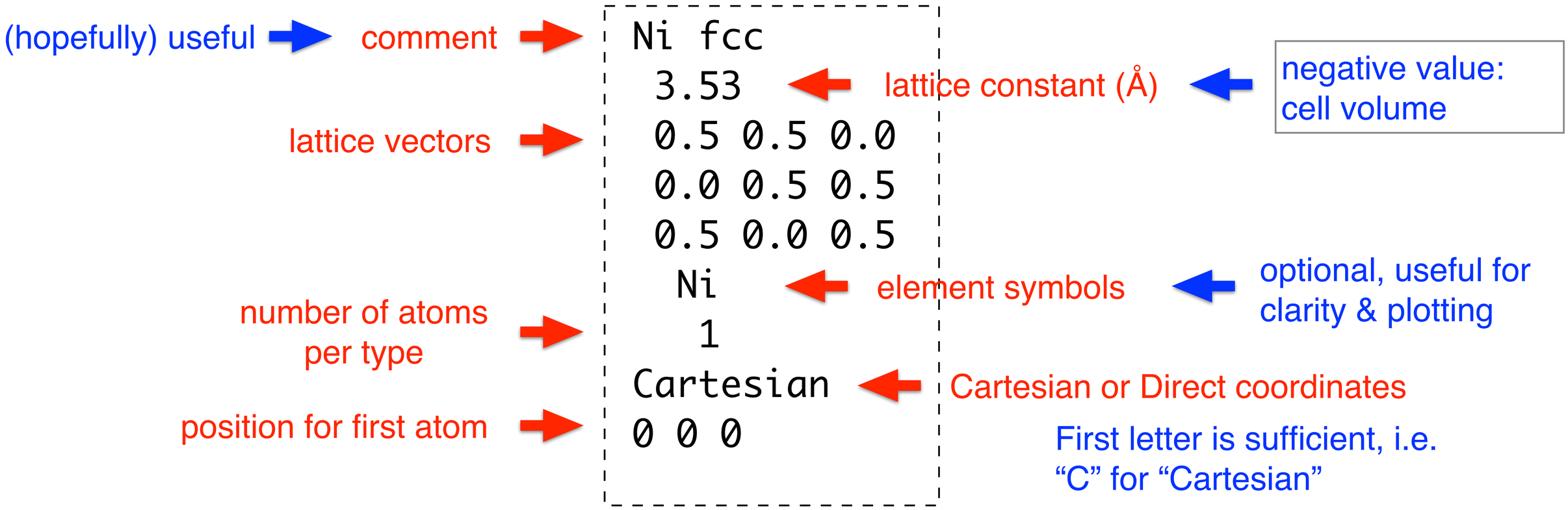
INCAR defaults

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

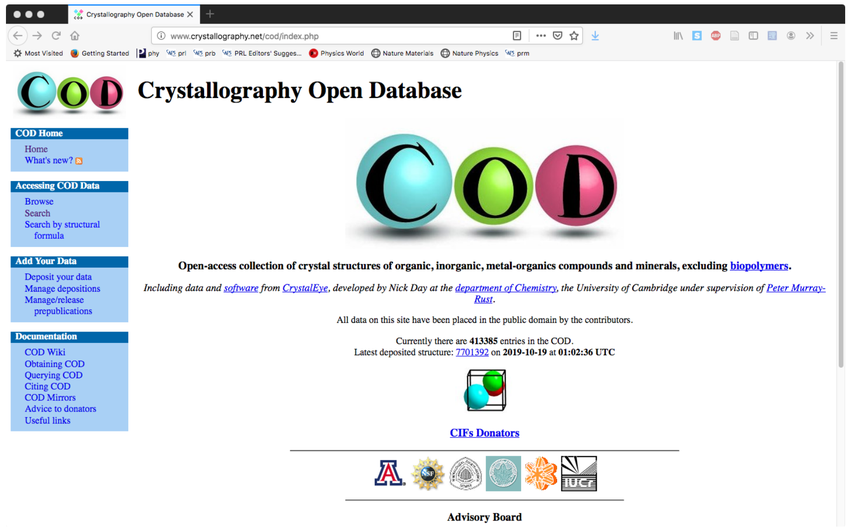
Rest of H, Si & Ag atoms following

POSCAR

Some useful resources:

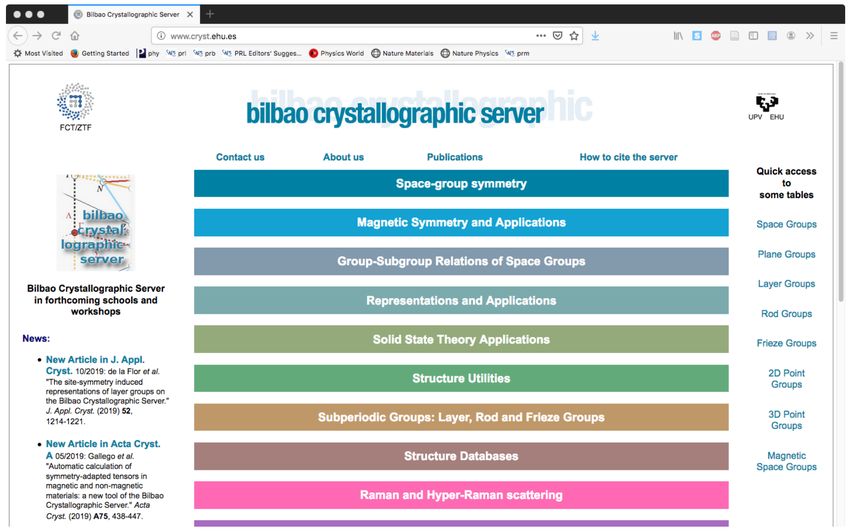
[Crystallography Open Database](#)

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

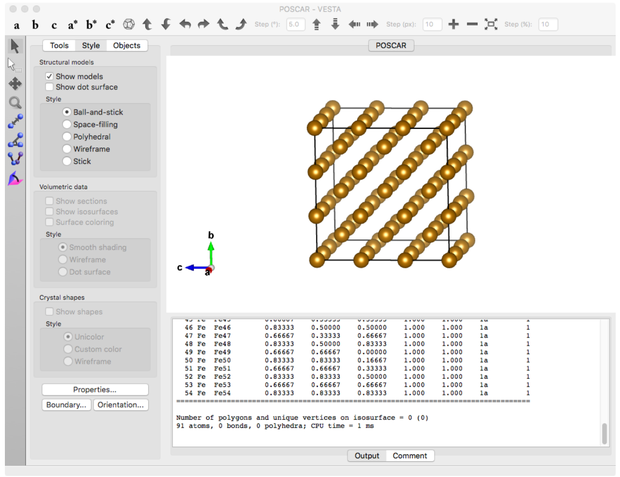
Commercial software:

[NanoLab]

[MedeA]

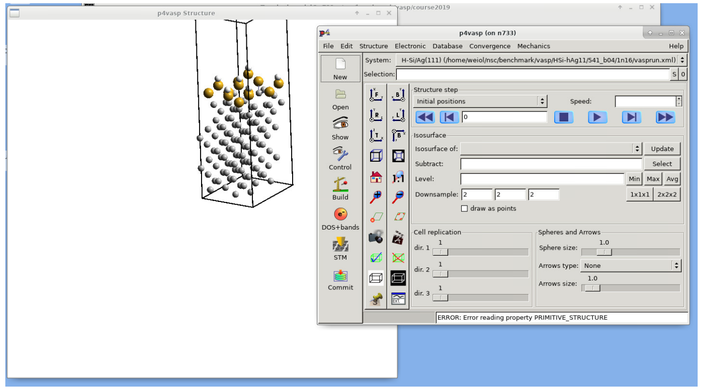
[MaterialsStudio]

[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
  11.0000000000000
 parameters from PSCTR are:
   VRHFIN =Cu: d10 p1
   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)
   ENMAX  =  295.446; ENMIN  =  221.585 eV
   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
```

type, element, date

valence

atomic configuration

XC-type

energy cutoff

smallest energy cutoff

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
```

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

@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
- 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

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

running @Abisko: note differences

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

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

running @Abisko: note differences

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

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 - Beskow (PDC)

Note:
Beskow is now retired!

```
#!/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

Job script - Dardel (PDC)

- I'll test running VASP @Dardel in near future

```
#!/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.

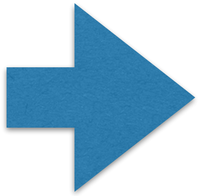
Eigenvalue diff.

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.

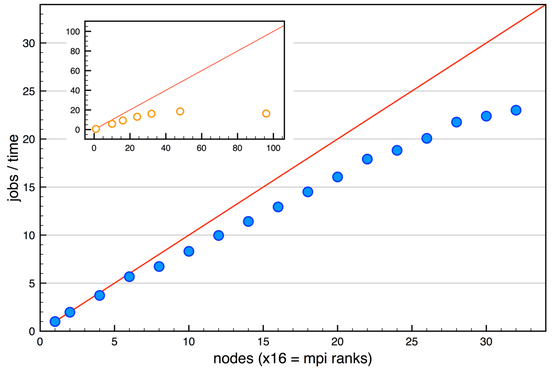
```
 -----------------------------------------------------------------------------
|                                                                             |
|           W    W    AA    RRRRR   N    N  II  N    N   GGGG   !!!          |
|           W    W   A  A   R    R  NN   N  II  NN   N  G 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

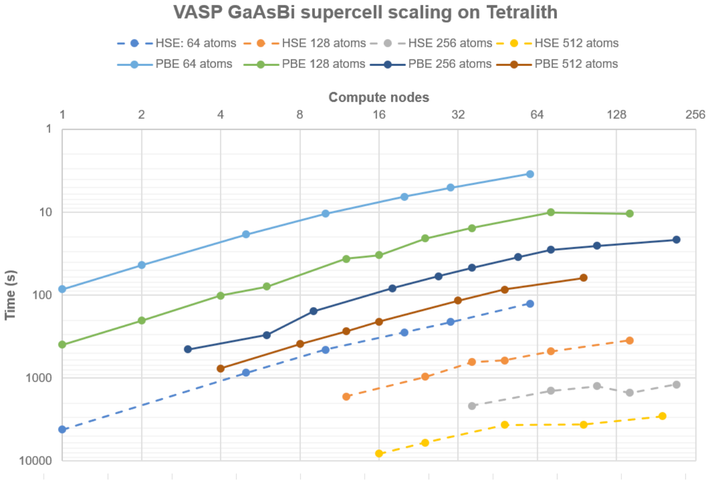
VASP6

- 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

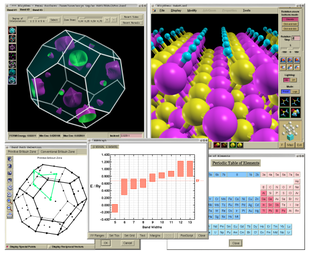
Tomorrow:

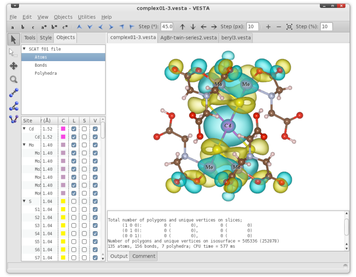
- Running & Performance
  - Parallelization
  - Efficient settings
  - Problems

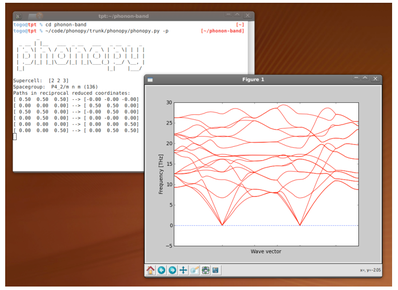




- Utilities & Summary







USPEX Computational Materials Discovery

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