Introduction to WIEN2k

Weine Olovsson
National Supercomputer Centre (NSC), Linköping University
SNIC training, online mini workshop @NSC 18th Nov 2021

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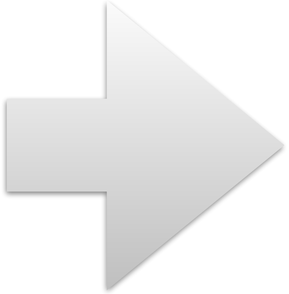
Schedule



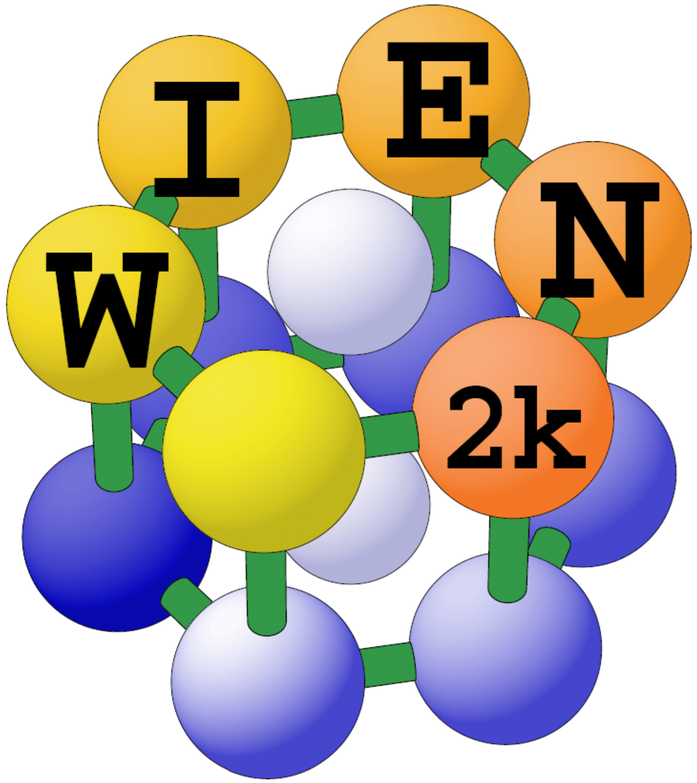
https://www.nsc.liu.se/support/Events/WIEN2k_intro_Nov2021/

Tentative Schedule

Tentative schedule, times might differ. It will end at latest 17:00, probably earlier. There will also be some breaks.

13:00 -14:30 Theory and basics
14:30 -15:30 Practical examples
15:30 -17:00 Hands-on and questions

Let’s take breaks at times!



WIEN2k

An Augmented Plane Wave Plus Local Orbitals Program
for Calculating Crystal Properties

http://wien2k.at/

Introduction to WIEN2k

- Basic theory (very brief) *- see resources for refs.*
- Focus on practical aspects of running WIEN2k at NSC
- Setting up a job: `init_lapw` (script) & w2web (GUI)
- Running efficiently, benchmarks
- Examples
- Check out resources!
  - examples, hints, etc.

… clickable links are underlined

1. Theory & Resources

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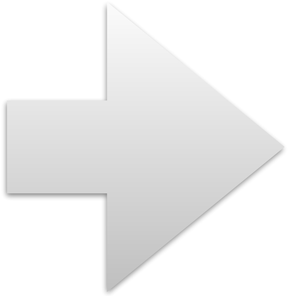
Short background

- Software license (group)
- DFT, FPLAPW-method, (L)APW+lo
- Beyond DFT (GW, BSE, DMFT, …)
- widely used for high accuracy
- Specialized programs (NMR, TELNES, …)



http://wien2k.at/

APW methods

- Augmented Plane Waves (APW), *J.C. Slater*

  Phys. Rev. 51, 846 (1937)

- Linear APW (LAPW), *O.K. Andersen*

  Phys. Rev. B 12, 3060 (1975)

- Local orbitals, *D.J. Singh*

  Phys. Rev. B 43, 6388 (1991)

- APW+lo, *E. Sjöstedt, L. Nordström, D.J. Singh*

  Sol. Stat. Com. 114, 15 (2000)

FPLAPW & WIEN2k

- All electron method
- Full-potential (no shape approx.)
- Core, semi-core & valence states
- WIEN2k, mixed basis set: APW+lo & LAPW+LO
- P. Blaha *et al.* J. Chem. Phys. **152**, 074101 (2020)

  https://doi.org/10.1063/1.5143061

Accuracy: WIEN2k as reference

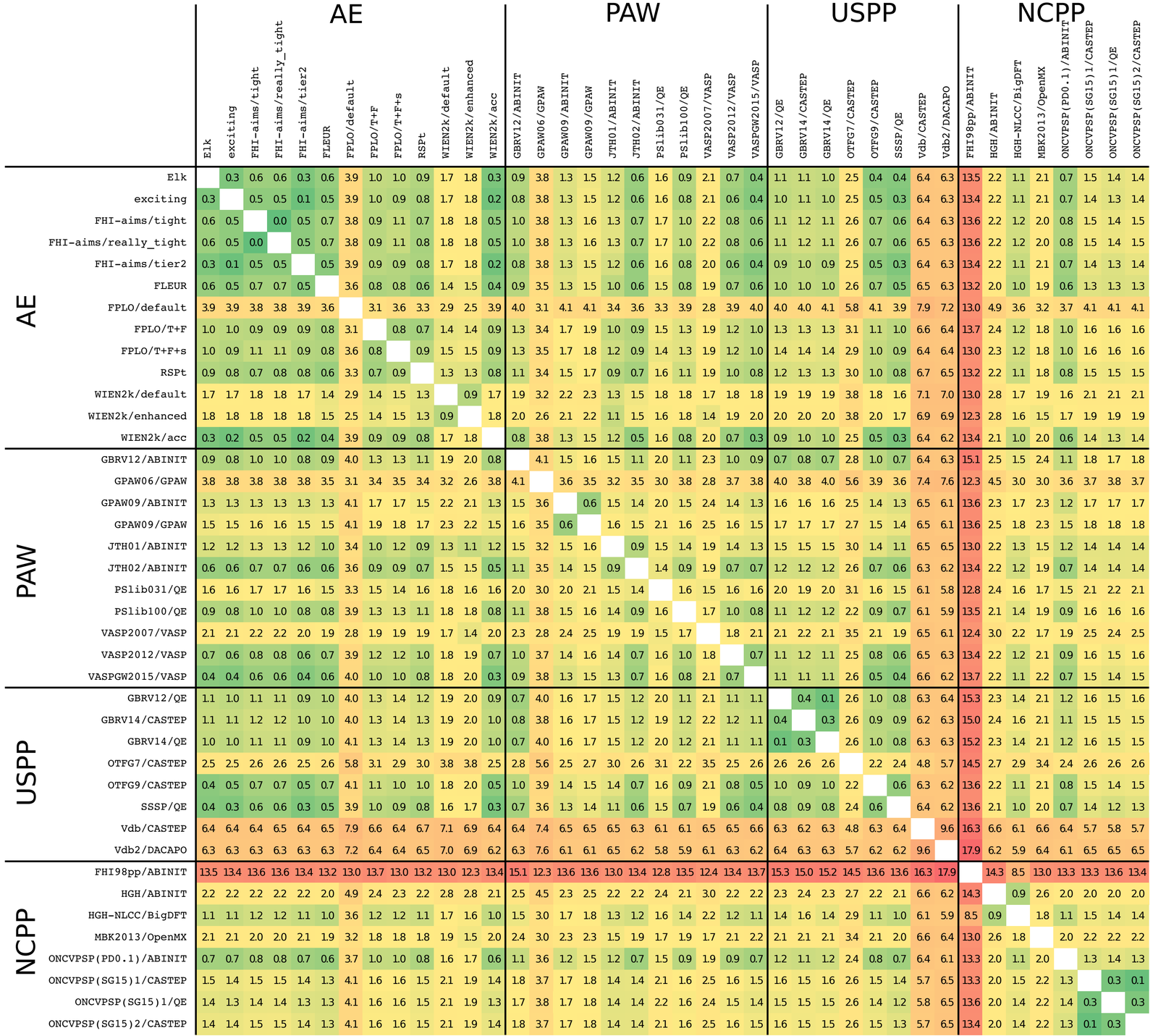
PAW (VASP) compared with FPLAPW (WIEN2k):

$\Delta(\text{PAW})_{(\text{VASP})} = 1.9$ meV/atom

H																	He
0.1																	0.0
Li	Be											B	C	N	O	F	Ne
0.2	0.1											0.3	0.3	10.6	8.3	1.5	0.1
Na	Mg											Al	Si	P	S	Cl	Ar
0.0	0.7											0.3	2.0	3.8	3.3	4.0	0.1
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
0.1	0.2	0.4	0.9	1.3	3.1	1.4	3.4	3.4	2.0	0.4	0.3	0.2	2.4	1.7	1.5	1.5	0.1
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
0.1	0.1	0.5	2.7	7.3	5.5	8.3	2.3	5.4	4.4	4.1	1.4	0.4	0.2	0.1	0.5	0.9	0.1
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
0.3	0.7	4.3	1.2	1.0	3.5	4.3	3.8	1.9	2.5	5.9	0.5	0.4	0.6	0.4	0.4		0.0

Lejaeghere et al. Crit. Rev. Solid State Mat. Sci. 39, 1 (2014)

Lejaeghere et al. Science 351, 1415 (2016)



Other FPLAPW software

- Free to use, available at NSC

```
$ module avail name
```

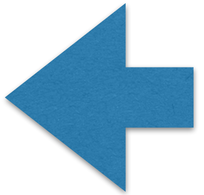
- Different specialities, check websites

http://exciting.wikidot.com/

https://elk.sourceforge.io/

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

WIEN2k @SNIC HPC centers

- **Tetralith** / Sigma, NSC, LiU  this mini workshop
- Kebnekaise, HPC2N, UmU
- Dardel, PDC, KTH *to be installed*
- …

- On many systems:

```
$ module avail wien2k
$ module spider wien2k
```

WIEN2k @NSC

- Only load WIEN2k module (not compilers etc.)
- Use latest version

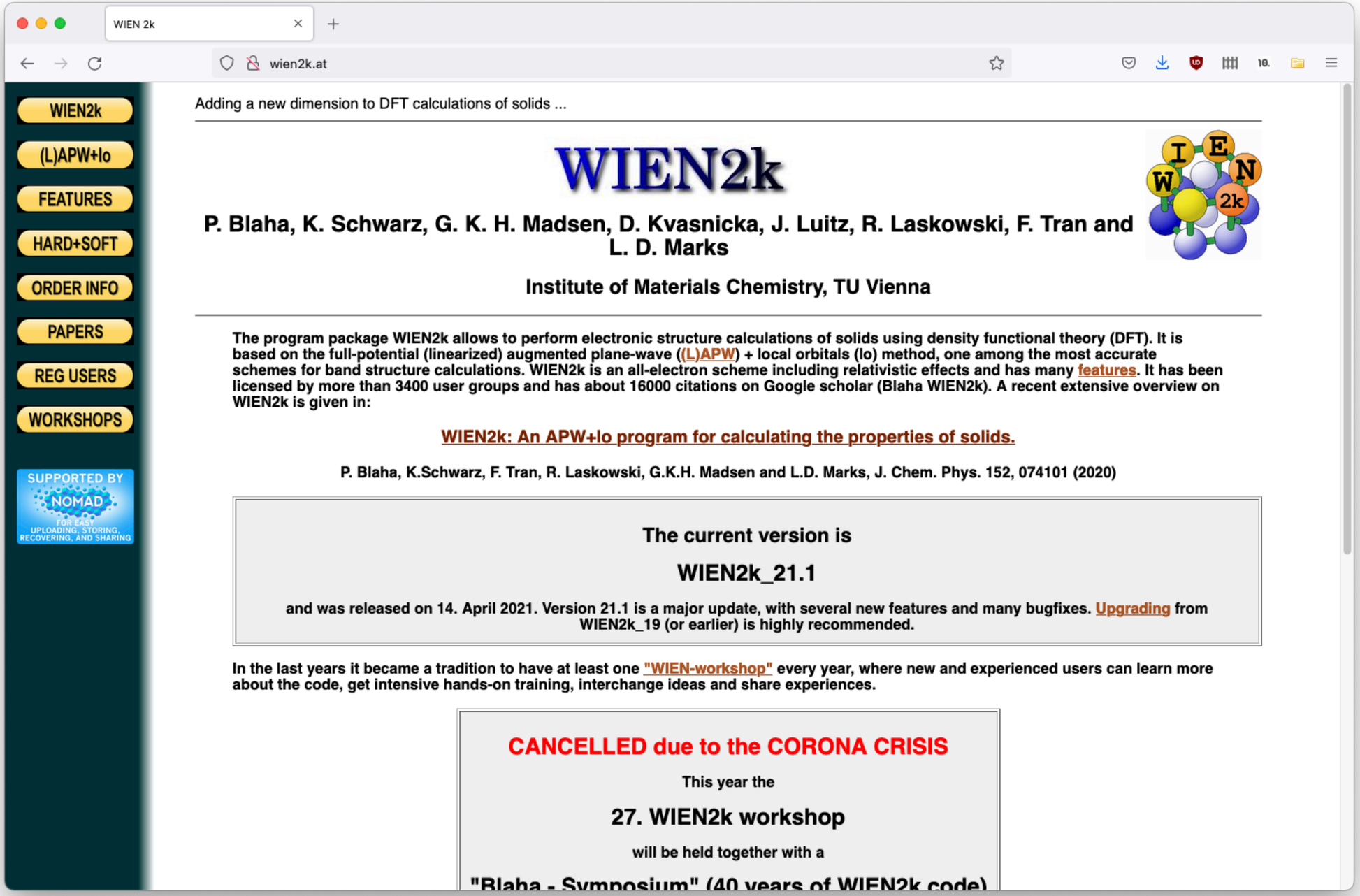
```
[weiol@tetralith2 ~]$ module avail wien2k

------------------------------------ /software/sse/modules -------------------------------------
   WIEN2k/recommendation            (D)    WIEN2k/19.1-nsc1-intel-2018b-eb
   WIEN2k/18.2-nsc1-intel-2018a-eb         WIEN2k/21.1-nsc1-intel-2018b-eb
   WIEN2k/18.2-nsc2-intel-2018a-eb

  Where:
   D:  Default Module

Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the “keys".

[weiol@tetralith2 ~]$ module add WIEN2k/21.1-nsc1-intel-2018b-eb
```

Resources

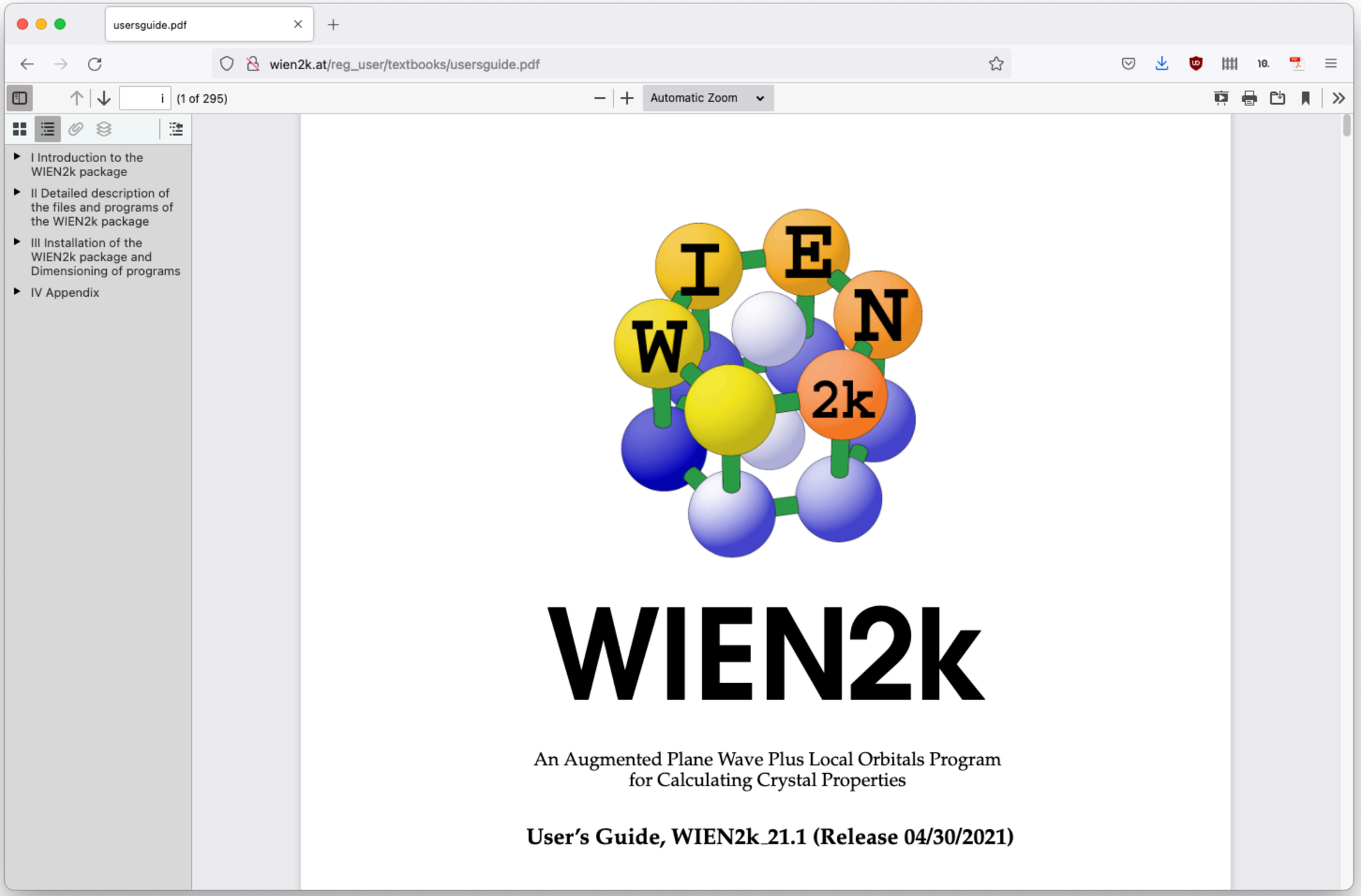
- The WIEN2k user guide - Start here! Check carefully!
- Presentations (.pdf, video) - Very useful!
- The email list (search it!) - Similar problem was solved?
- Check around the website (useful links, FAQ, …)
- P. Blaha et al., WIEN2k paper (2020)

Questions/trouble running at NSC? support@nsc.liu.se

http://wien2k.at/



http://wien2k.at/



http://wien2k.at/reg_user/textbooks/usersguide.pdf

The Journal of Chemical Physics ARTICLE scitation.org/journal/jcp

WIEN2k: An APW+lo program for calculating the properties of solids

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Note: This paper is part of the JCP Special Topic on Electronic Structure Software.
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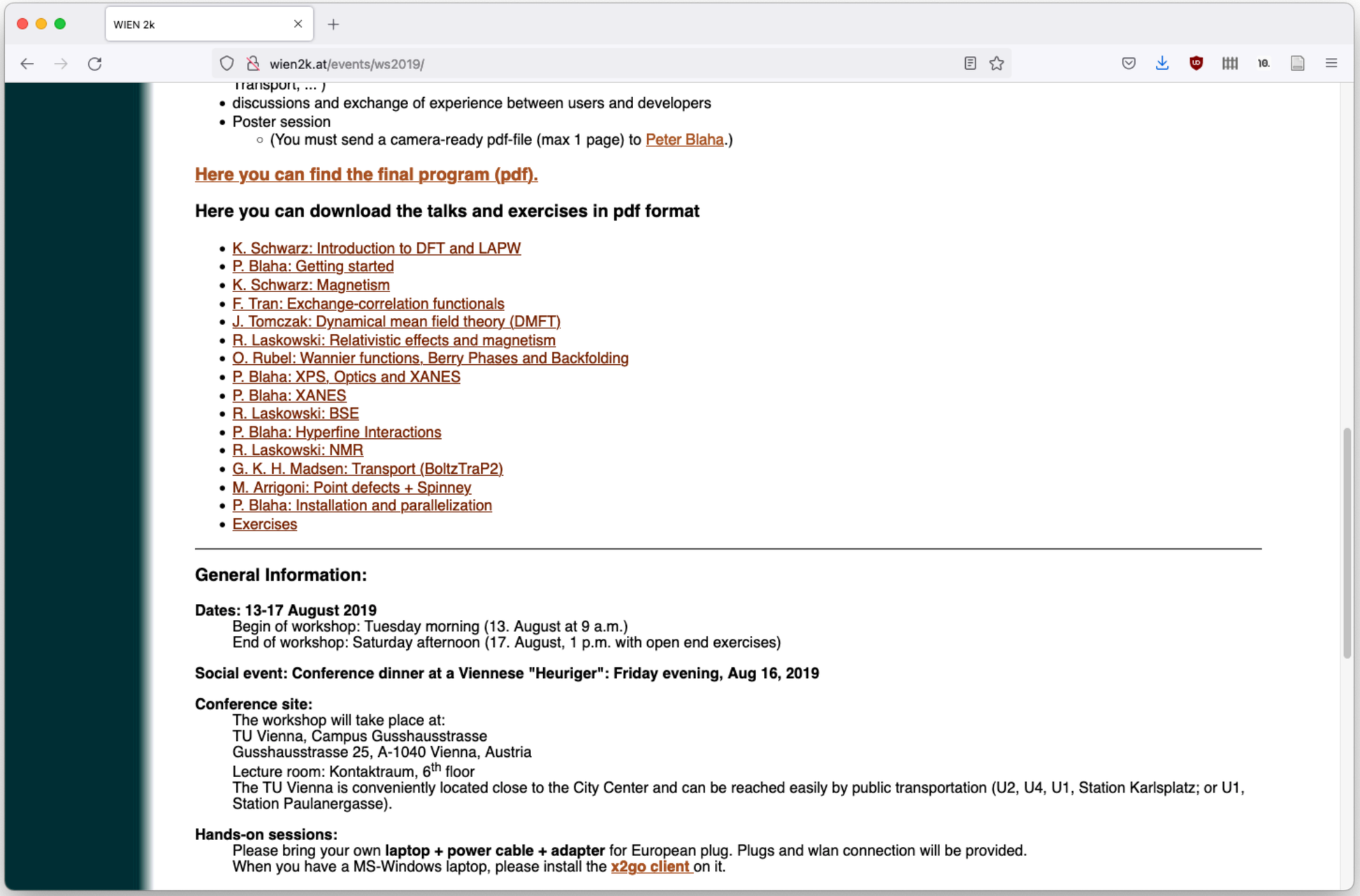
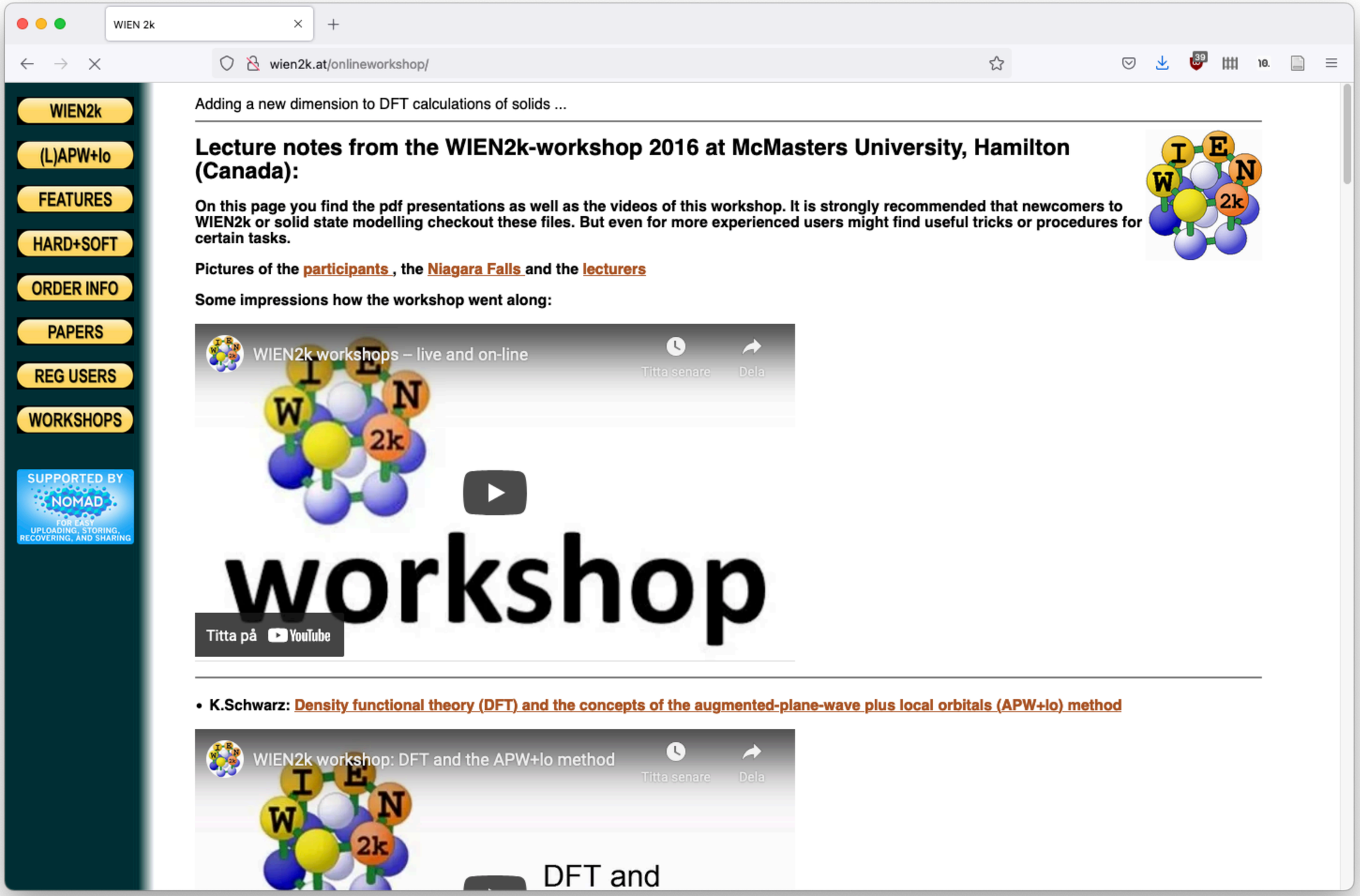
ABSTRACT

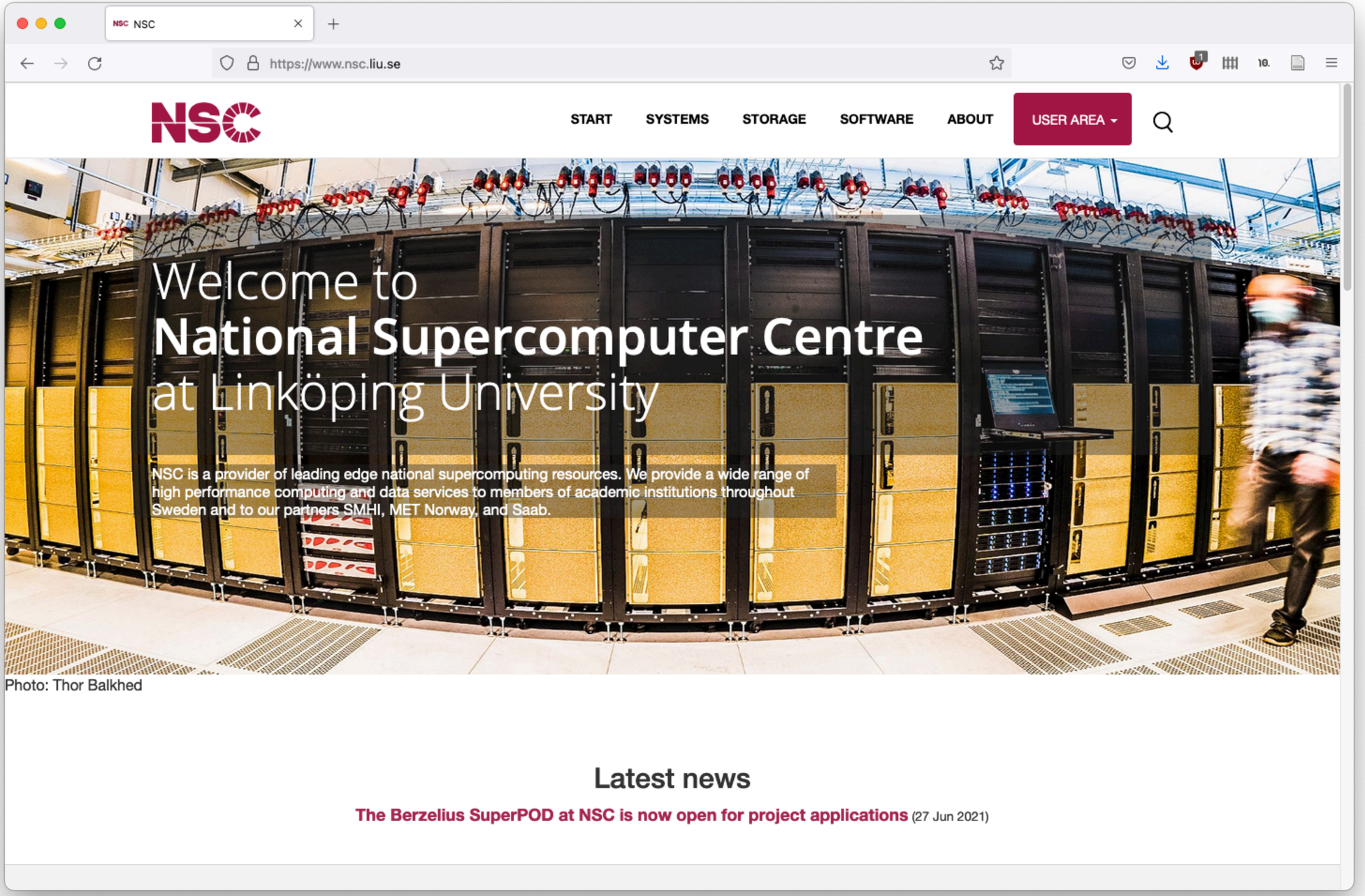
The WIEN2k program is based on the augmented plane wave plus local orbitals (APW+lo) method to solve the Kohn–Sham equations of density functional theory. The APW+lo method, which considers all electrons (core and valence) self-consistently in a full-potential treatment, is implemented very efficiently in WIEN2k, since various types of parallelization are available and many optimized numerical libraries can be used. Many properties can be calculated, ranging from the basic ones, such as the electronic band structure or



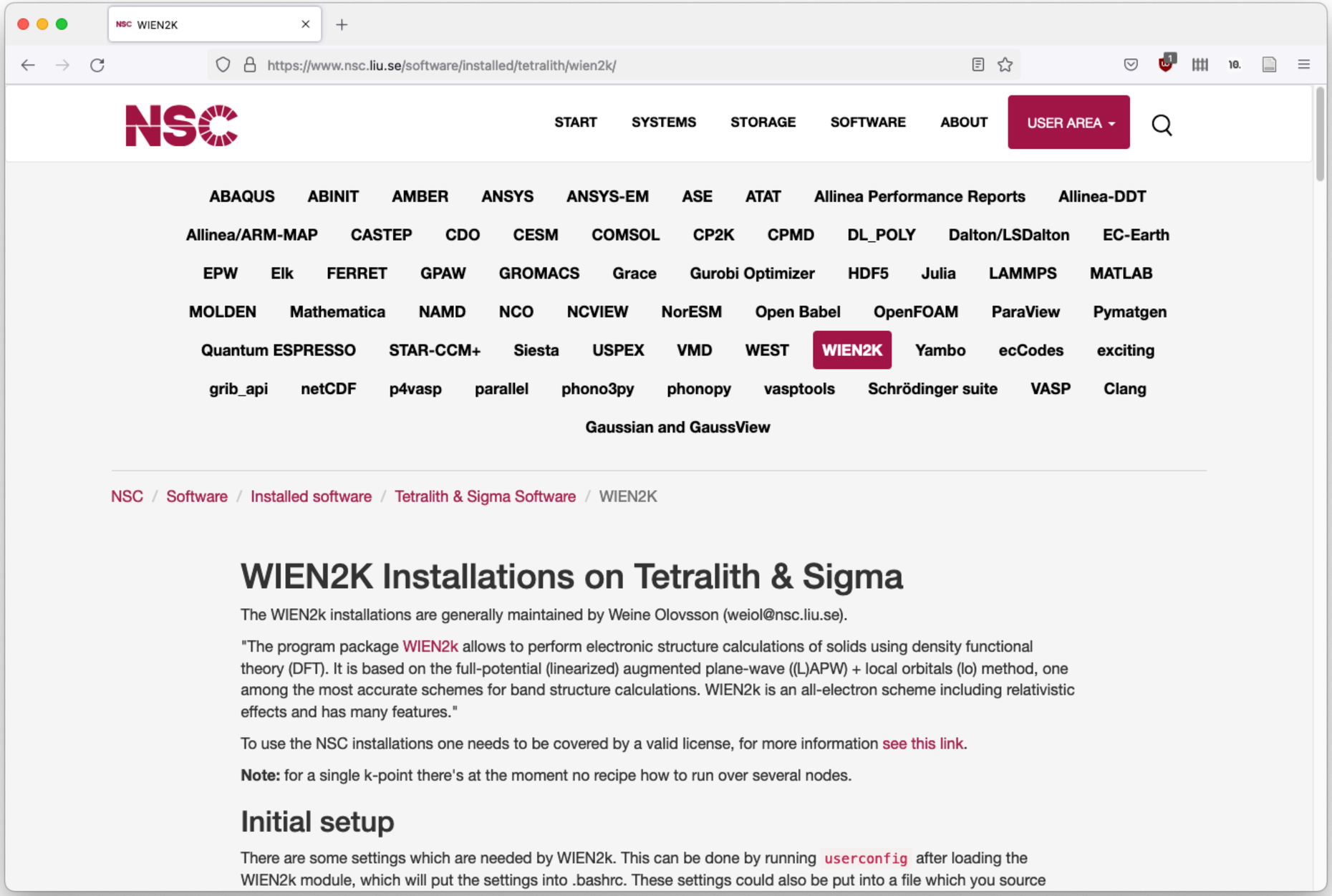
http://wien2k.at/events/ws2019/



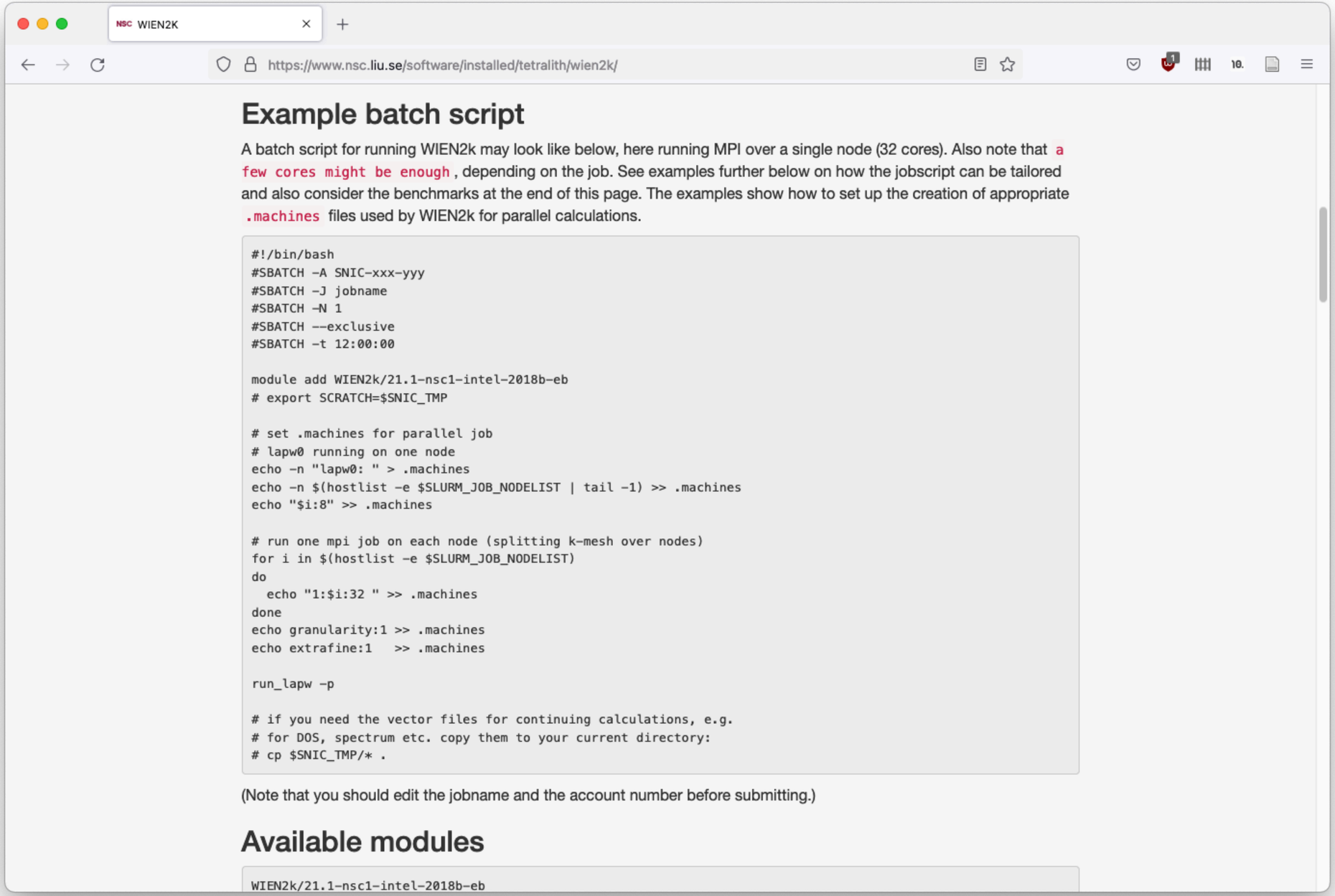
http://wien2k.at/onlineworkshop/



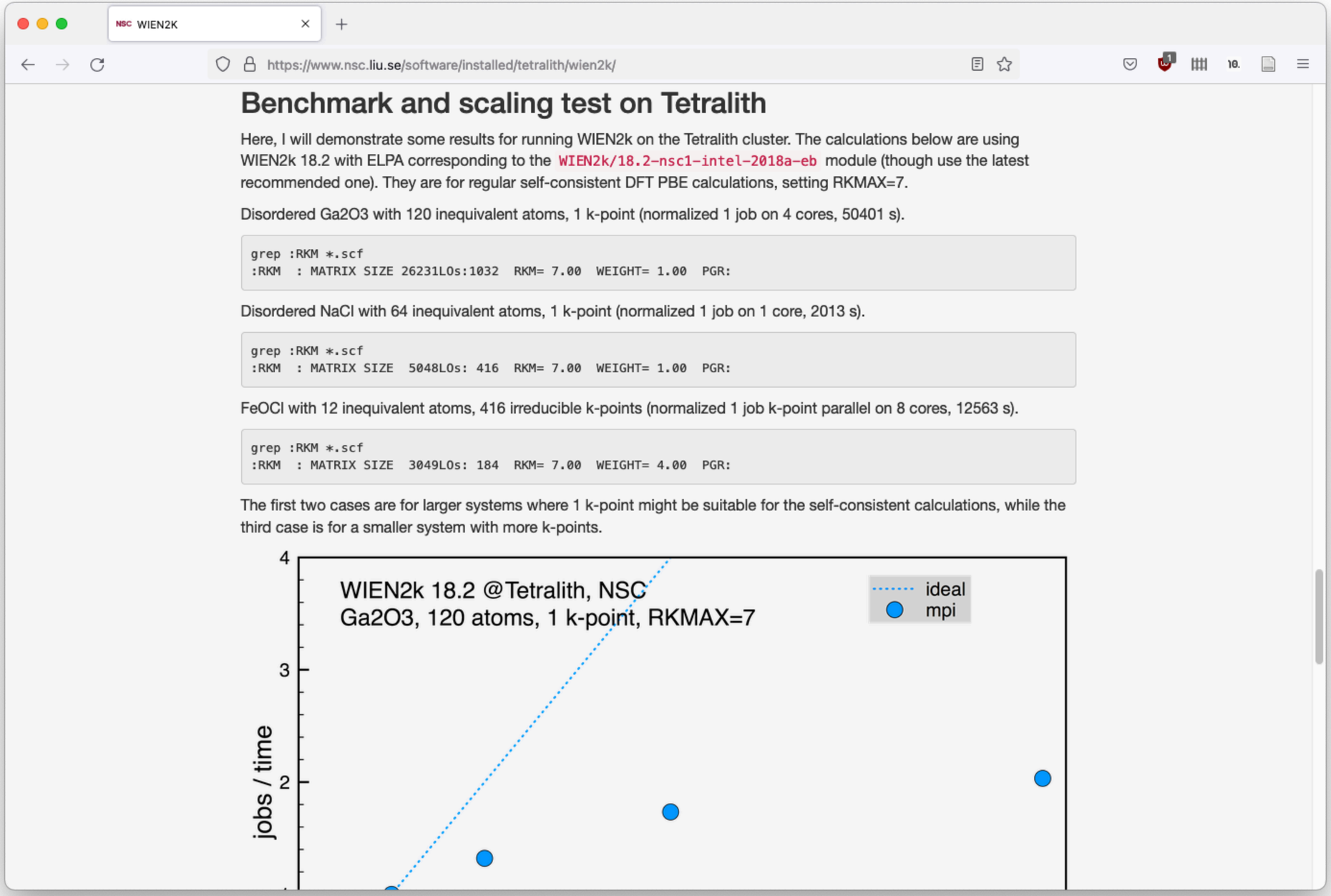
https://www.nsc.liu.se



https://www.nsc.liu.se/software/installed/tetralith/wien2k/



https://www.nsc.liu.se/software/installed/tetralith/wien2k/



https://www.nsc.liu.se/software/installed/tetralith/wien2k/

2. Setting up job

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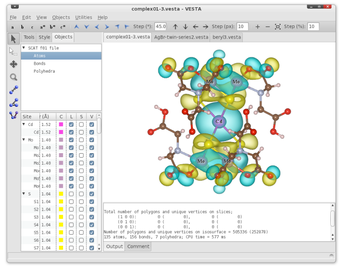
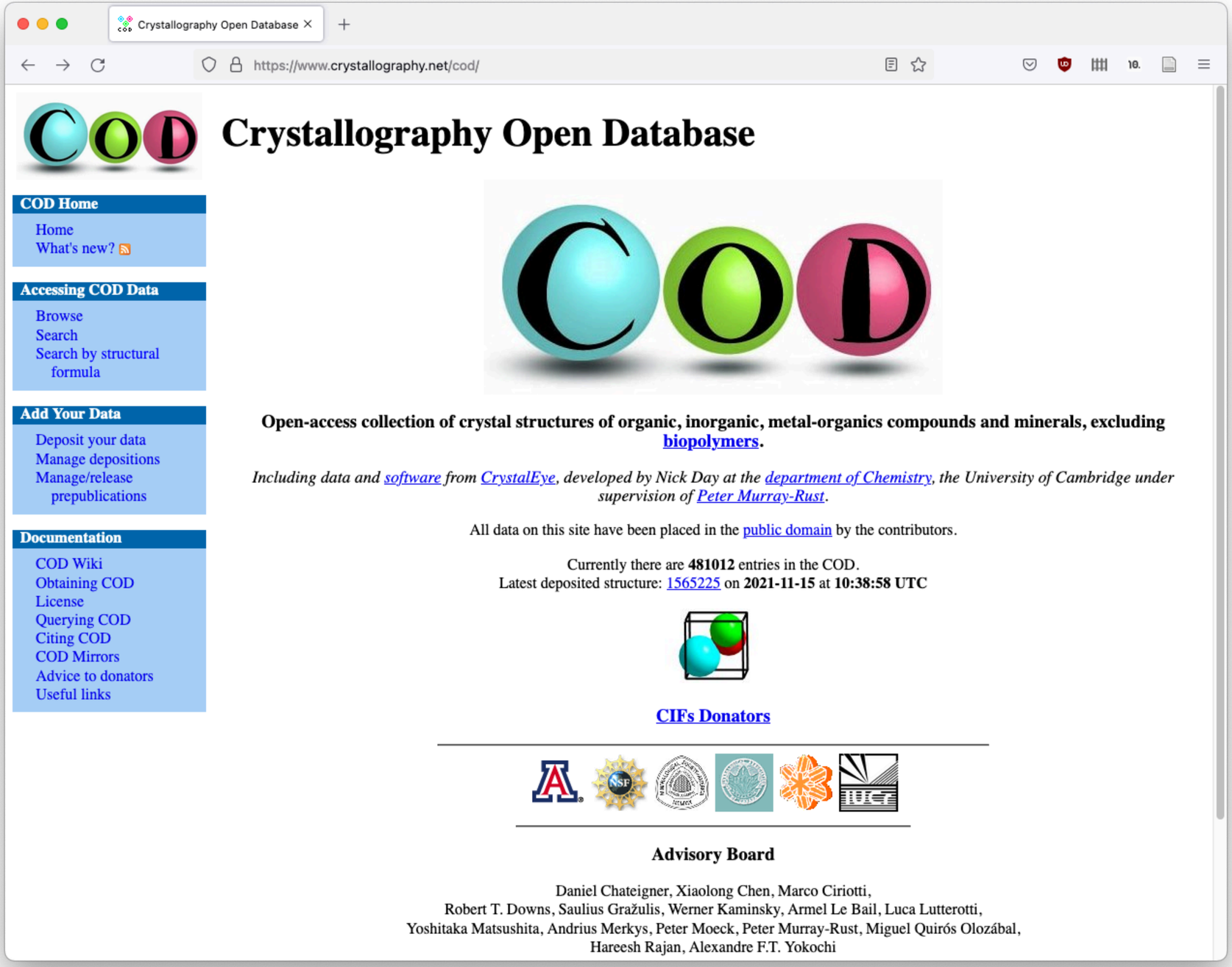
Typical workflow

- Prepare structure file: `cif2struct`, `supercell`
- Initialize calculation: `init_lapw` & w2web
- Prepare job script & submit
- Convergence, any problems?
- Post-processing, other steps
  - DOS, band structure, …

Prepare structure file

- WIEN2k structure file: `case.struct` → case = name of folder!
- Set up from scratch using w2web
- Convert from `.cif` file → `$ cif2struct`
  https://www.crystallography.net/cod/
- Create supercell from case.struct → `$ supercell`
  Might need to start from MULT=1
- Use ASE (convert, edit, …) e.g. convert POSCAR to .struct file
- Visualize e.g. with VESTA





https://www.crystallography.net/cod/

experimental structures in .cif format!

Initialize calculation

- Some basic settings needed:

```
export EDITOR="vi"
export SCRATCH=./
```

```
$ module load WIEN2k/21.1-nsc1-intel-2018b-eb
$ mkdir test; cp test.struct test; cd test
$ init_lapw
```

- Sets up structure symmetry and input files

  `sgroup` important for correct symmetry!

- Quite many files generated!

Example: h-BN supercell setup

- From .cif to .struct
- Reduce .struct symmetry (MULT=1)
- Create a 4x4x2 supercell
- If interested in 1st B atom position, break supercell symmetry by tagging it in .struct

init_lapw

```
[weiol@tetralith1 t1]$ init_lapw
 next is setrmt
Automatic determination of RMTs. Please specify the desired RMT reduction
compared to almost touching spheres.
Typically, for a single calculation just hit enter, for force minimization
use 1-5; for volume effects you may need even larger reductions.

Enter reduction in %
enter
Use old or new scheme (o/N)
enter

 specify nn-bondlength factor: (usually=2) [and optionally dlimit, dstmax (about
  1.d-5, 20)]
 DSTMAX:   27.9450136800000
 iix,iiy,iiz           2           2           2   37.8548400000000
   37.8548400000000        50.3513760000000
 NAMED ATOM: B 1       Z changed to IATNR+1000 to determine equivalency

   ERROR !!!!!!!!!!!!!!
 RMT(  1)=2.00000 AND RMT(100)=2.00000
 SUMS TO 4.00000 GT NNN-DIST= 2.73194

...

 WARNING: Mult not equal. PLEASE CHECK outputnn-file
 WARNING: Mult not equal. PLEASE CHECK outputnn-file

...
```

nn

```
  NN created a new t1.struct_nn file
NN created a new CASE.STRUCT_NN FILE
0.347u 0.019s 0:00.44 79.5%0+0k 0+0io 0pf+0w
atom  Z   RMT-max   RMT
 1   5.0  1.29   1.29
 2   5.0  1.29   1.29

...

 126   7.0  1.43   1.43
 127   7.0  1.43   1.43
 128   7.0  1.43   1.43
file    t1.struct_setrmt   generated
Do you want to accept these radii; discard them; or rerun setRmt (a/d/r):
enter
 next is nn
>   nn (16:20:46)  specify nn-bondlength factor: (usually=2) [and optionally dlimit, dstmax
(about
  1.d-5, 20)]
enter
```

case.outputnn

```
opens a new file “t1.outputnn” in vi

blebleble
H                           128
              RELA
 18.927420 18.927420 25.175688 90.000000 90.000000120.000000
       1    0.08333333   0.16666667   0.12500000
                  1
 NAMED ATOM: B 1       Z changed to IATNR+1000 to determine equivalency
B 1        NPT=  781  R0=0.00010000 RMT=    1.2900   Z:  5.0
                     1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
       2    0.33333333   0.16666667   0.12500000
                  1
B          NPT=  781  R0=0.00010000 RMT=    1.2900   Z:  5.0
                     1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
       3    0.58333333   0.16666667   0.12500000
                  1
B          NPT=  781  R0=0.00010000 RMT=    1.2900   Z:  5.0
                     1.0000000 0.0000000 0.0000000
                     0.0000000 1.0000000 0.0000000
                     0.0000000 0.0000000 1.0000000
       4    0.83333333   0.16666667   0.12500000
                  1
...

quit file with :q
```

sgroup

```
...

 WARNING: Mult not equal. PLEASE CHECK outputnn-file
 WARNING: ityp not equal. PLEASE CHECK outputnn-file

  NN created a new t1.struct_nn file
NN created a new CASE.STRUCT_NN FILE
0.358u 0.010s 0:45.45 0.7%0+0k 0+0io 0pf+0w
-----> check in  t1.outputnn  for overlapping spheres,
       coordination and nearest neighbor distances
nn has created a new struct file with different multiplicities
-----> DO YOU WANT TO USE THE NEW t1.struct_nn file (y/n)
enter
-----> continue with sgroup or edit the t1.struct file (c/e)
enter
```

case.outputsgroup

```
opens a new file “t1.outputsgroup” in vi

warning: !!! Number of inequivalent atoms has changed.
         !!! Old value= 128     New value= 30

warning: !!! Struct file is not consistent with space group found.

-------------------------------------------------------------------

Bravais lattice: Hexagonal

     a             b             c
 18.92742000    18.92742000   25.17568800
     alpha         beta          gamma
 90.00000000    90.00000000   120.00000000


===== Decomposition of new basis vectors over input basis =====
 1.000000   0.000000  0.000000  <--- 1
 0.000000   1.000000  0.000000  <--- 2
 0.000000   0.000000  1.000000  <--- 3

==== Number of atoms in cell: 128
==== Atom positions:

 0.00000000   0.00000000  0.00000000
 B1
...

quit file with :q
```

sgroup: output

```
 next is sgroup
>   sgroup (16:24:17) 0.002u 0.006s 0:00.00 0.0%0+0k 0+0io 0pf+0w
  Names of point group: -6m2  -6m2    D3h
  Names of point group: m      m      Cs
  Names of point group: mm2    mm2    C2v
  Names of point group: mm2    mm2    C2v
  Names of point group: mm2    mm2    C2v

...

  Names of point group: m      m      Cs
  Names of point group: mm2    mm2    C2v
  Names of point group: mm2    mm2    C2v
  Names of point group: -6m2  -6m2    D3h
warning: !!! Struct file is not consistent with space group found.
Number and name of space group: 187 (P -6 m 2)
warning: !!! Number of inequivalent atoms has changed.
         !!! Old value= 128     New value= 30
warning: !!! Struct file is not consistent with space group found.
-----> check in  t1.outputsgroup  for proper symmetry, compare
       with your struct file and later with  t1.outputs
       sgroup has also produced a new struct file based on your old one.
       If you see warnings above, consider to use the newly generated
       struct file, which you can view (edit) now.
-----> continue with symmetry (old case.struct) or use/edit t1.struct_sgroup ? (c/e)
e
```

- edit to use `sgroup` suggestion, check file & quit with :q (if using vi)

sgroup: new struct

```
-----> Do you want to use the new struct file  ? (y/n)
y
```

- accept new struct file (otherwise old one used)

```
patchsymm has found inconsistencies in your struct file
it comes probably from rounding errors in the last digits of your positions
Site  39 Ops  2 New:    0.58333333   0.16666666   0.25000000 Diff: -0.10000D-07 0.00000D+00 0.00000D+00 <
Site  40 Ops  2 New:    0.83333334   0.41666667   0.25000000 Diff:  0.00000D+00-0.10000D-07 0.00000D+00 <
Site  41 Ops  2 New:    0.58333333   0.41666667   0.25000000 Diff:  0.10000D-07 0.10000D-07 0.00000D+00 <
Site  42 Ops  2 New:    0.58333333   0.16666666   0.75000000 Diff: -0.10000D-07 0.00000D+00 0.00000D+00 <
Site  43 Ops  2 New:    0.83333334   0.41666667   0.75000000 Diff:  0.00000D+00-0.10000D-07 0.00000D+00 <

...

Site  44 12 Ops 12 New:    0.58333333   0.41666667   0.75000000 Diff:  0.10000D-07 0.10000D-07 0.00000D+00 <
Site 106 23 Ops 12 New:    0.33333334   0.16666667   0.00000000 Diff:  0.11102D-15 0.10000D-07 0.00000D+00 <
Site 107 23 Ops 12 New:    0.83333333   0.16666667   0.00000000 Diff: -0.10000D-07-0.10000D-07 0.00000D+00 <
Site 108 23 Ops 12 New:    0.83333333   0.66666666   0.00000000 Diff:  0.10000D-07-0.22204D-15 0.00000D+00 <
Site 122 28 Ops 12 New:    0.33333334   0.16666667   0.50000000 Diff:  0.11102D-15 0.10000D-07 0.00000D+00 <
Site 123 28 Ops 12 New:    0.83333333   0.16666667   0.50000000 Diff: -0.10000D-07-0.10000D-07 0.00000D+00 <
Site 124 28 Ops 12 New:    0.83333333   0.66666666   0.50000000 Diff:  0.10000D-07-0.22204D-15 0.00000D+00 <
do you want to use t1.struct_patchsymm ? (Y/n)
enter
```

- symmetry problem!? Accept patch (usually)  restarts from beginning!

sgroup: again

```
next is sgroup
>   sgroup (16:32:11) 0.002u 0.004s 0:00.01 0.0%0+0k 0+0io 0pf+0w
  Names of point group: -6m2  -6m2    D3h
  Names of point group: m      m      Cs
  Names of point group: mm2    mm2    C2v

...

Number and name of space group: 187 (P -6 m 2)
-----> check in  t1.outputsgroup  for proper symmetry, compare
       with your struct file and later with  t1.outputs
       sgroup has also produced a new struct file based on your old one.
       If you see warnings above, consider to use the newly generated
       struct file, which you can view (edit) now.
-----> continue with symmetry (old case.struct) or use/edit t1.struct_sgroup ? (c/e)
enter
 next is symmetry
>   symmetry (16:32:16)  SPACE GROUP DOES NOT CONTAIN INVERSION
0.020u 0.012s 0:00.07 42.8%0+0k 0+0io 0pf+0w
-----> check in  t1.outputs  the symmetry operations,
       the point symmetries and compare with results from sgroup
       if you find errors (often from rounding errors of positions), apply x patchsymm
-----> continue with lstart or edit the t1.struct_st file (c/e/x)
enter
```

- this time struct file seems OK!  …if not, might restart cycle again

lstart

```
next is lstart
 CREATE A NEW t1.inst FILE with PROPER ATOMS
 If necessary specify switches for instgen_lapw (or press ENTER):
 -up (default)   -dn   -nm (non-magnetic)   -ask
enter
 30 Atoms found:  with labels B 1  B 2  B 3  B 4  B 5  B 6  B 7  B 8  B 9  B 10 B 11 B 12 B 13 B
14 B 15 N 1  N 2  N 3  N 4  N 5  N 6  N 7  N 8  N 9  N 10 N 11 N 12 N 13 N 14 N 15
generate atomic configuration for atom 1 : B 1
generate atomic configuration for atom 2 : B 2
generate atomic configuration for atom 3 : B 3

...

generate atomic configuration for atom 29 : N 14
generate atomic configuration for atom 30 : N 15
>   lstart (16:33:53)   SELECT XCPOT:
  recommended: PBE    [(13) GGA of Perdew-Burke-Ernzerhof 96]
               LDA    [( 5)]
               WC     [(11)  GGA of Wu-Cohen 2006]
               PBESOL [(19) GGA of Perdew etal. 2008]
13
  SELECT ENERGY to separate core and valence states:
  recommended: -6.0 Ry (check how much core charge leaks out of MT-sphere)
  ALTERNATIVELY: specify charge localization
  (between 0.97 and 1.0) to select core state
-6
```

- selected PBE for XC and recommended energy separation between core/valence

case.outputst

opens a new file “t1.outputst” in vi

```
...

          E-up(Ry)      E-dn(Ry)   Occupancy   q/sphere  core-state
  1S     -13.270546    -13.249235  1.00  1.00    0.9989  T
  2S      -0.728058     -0.639738  1.00  1.00    0.2252  F
  2P*     -0.295469     -0.216441  1.00  0.00    0.2162  F

 TOTAL CORE-CHARGE:                      2.000000
 TOTAL CORE-CHARGE INSIDE SPHERE:        1.997822
 TOTAL CORE-CHARGE OUTSIDE SPHERE:       0.002178

...

          E-up(Ry)      E-dn(Ry)   Occupancy   q/sphere  core-state
  1S     -28.235802    -28.124001  1.00  1.00    1.0000  T
  2S      -1.460885     -1.124776  1.00  1.00    0.6338  F
  2P*     -0.610907     -0.304312  1.00  0.00    0.5866  F
  2P      -0.609450     -0.303079  2.00  0.00    0.5858  F

 TOTAL CORE-CHARGE:                      2.000000
 TOTAL CORE-CHARGE INSIDE SPHERE:        1.999991
 TOTAL CORE-CHARGE OUTSIDE SPHERE:       0.000009

...
```

quit file with :q

Continue…

```
Atomic configuration for atom: B 1   Z=   5.00
          E-up(Ry)      E-dn(Ry)   Occupancy   q/sphere  core-state
  1S     -13.270546    -13.249235  1.00  1.00    0.9989  T
  2S      -0.728058     -0.639738  1.00  1.00    0.2252  F
  2P*     -0.295469     -0.216441  1.00  0.00    0.2162  F

Atomic configuration for atom: N 1   Z=   7.00
          E-up(Ry)      E-dn(Ry)   Occupancy   q/sphere  core-state
  1S     -28.235802    -28.124001  1.00  1.00    1.0000  T
  2S      -1.460885     -1.124776  1.00  1.00    0.6338  F
  2P*     -0.610907     -0.304312  1.00  0.00    0.5866  F
  2P      -0.609450     -0.303079  2.00  0.00    0.5858  F
LSTART ENDS
1.101u 0.035s 0:47.38 2.3%0+0k 0+0io 0pf+0w
-----> continue with kgen or edit the t1.inst file and rerun lstart (c/e)
enter
```

- After this step, the setup of `case.in1/in1c` and `case.in2/in2c` starts

case.in1_st

opens a new file "t1.in1_st" in vi

```
WFFIL  EF= 0.50000        (WFFIL, WFPRI, ENFIL, SUPWF)
  7.00     10   4    ELPA pxq BL 64 (R-MT*K-MAX,MAX L IN WF,V-NMT,LIB)
  0.30    2  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0    0.30      0.0000 CONT 1
 1    0.30      0.0000 CONT 1
  0.30    2  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0    0.30      0.0000 CONT 1
 1    0.30      0.0000 CONT 1
  0.30    2  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0    0.30      0.0000 CONT 1
 1    0.30      0.0000 CONT 1
  0.30    2  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0    0.30      0.0000 CONT 1
 1    0.30      0.0000 CONT 1

...

  0.30    3  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0    0.30      0.0000 CONT 1
 0   -1.16      0.0010 CONT 1
 1    0.30      0.0000 CONT 1
  0.30    3  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0    0.30      0.0000 CONT 1
 0   -1.16      0.0010 CONT 1
 1    0.30      0.0000 CONT 1
K-VECTORS FROM UNIT:4   -9.0       1.5  1029   emin / de (emax=Ef+de) / nband
```

quit file with :q

case.in1_st

RKMAX

ELPA / SCALA

Energy range

```
opens a new file "t1.in1_st" in vi

WFFIL  EF= 0.50000        (WFFIL, WFPRI, ENFIL, SUPWF)
  7.00      10    4    ELPA pxq BL 64 (R-MT*K-MAX,MAX L IN WF,V-NMT,LIB)
  0.30     2  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0     0.30      0.0000 CONT 1
 1     0.30      0.0000 CONT 1
  0.30     2  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0     0.30      0.0000 CONT 1
 1     0.30      0.0000 CONT 1
  0.30     2  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0     0.30      0.0000 CONT 1
 1     0.30      0.0000 CONT 1
  0.30     2  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0     0.30      0.0000 CONT 1
 1     0.30      0.0000 CONT 1

...

  0.30     3  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0     0.30      0.0000 CONT 1
 0    -1.16      0.0010 CONT 1
 1     0.30      0.0000 CONT 1
  0.30     3  0       (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0     0.30      0.0000 CONT 1
 0    -1.16      0.0010 CONT 1
 1     0.30      0.0000 CONT 1
K-VECTORS FROM UNIT:4   -9.0       1.5  1029    emin / de (emax=Ef+de) / nband

quit file with :q
```

case.in2_st

```
opens a new file “t1.in2_st” in vi

TOT              (TOT,FOR,QTL,EFG,FERMI)
   -12.0   512.0   0.50 0.05  1   EMIN, NE, ESEPERMIN, ESEPER0, iqtlsave
TETRA    0.000      (GAUSS,ROOT,TEMP,TETRA,ALL      eval)
  0 0  2 0  3 3  4 0  5 3  6 0  6 6
  0 0  1 1 -1 1  2 0  2 2 -2 2  3 1 -3 1  3 3 -3 3  4 0  4 2 -4 2  4 4 -4 4  5 1 -5 1  5 3 -5 3
5 5 -5 5  6 0  6 2 -6 2  6 4 -6 4  6 6 -6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  2 0  3 3  4 0  5 3  6 0  6 6

...

  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  2 0  3 3  4 0  5 3  6 0  6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  1 1 -1 1  2 0  2 2 -2 2  3 1 -3 1  3 3 -3 3  4 0  4 2 -4 2  4 4 -4 4  5 1 -5 1  5 3 -5 3
5 5 -5 5  6 0  6 2 -6 2  6 4 -6 4  6 6 -6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  2 0  3 3  4 0  5 3  6 0  6 6
 12.00          GMAX
NOFILE        FILE/NOFILE  write recprlist

quit file with :q
```

case.in2_st

No. of electrons

Fermi-method

GMAX

```
opens a new file “t1.in2_st” in vi

TOT                (TOT,FOR,QTL,EFG,FERMI)
   -12.0    512.0    0.50 0.05  1    EMIN, NE, ESEPERMIN, ESEPER0, iqtlsave
TETRA     0.000       (GAUSS,ROOT,TEMP,TETRA,ALL      eval)
  0 0  2 0  3 3  4 0  5 3  6 0  6 6
  0 0  1 1 -1 1  2 0  2 2 -2 2  3 1 -3 1  3 3 -3 3  4 0  4 2 -4 2  4 4 -4 4  5 1 -5 1  5 3 -5 3
5 5 -5 5  6 0  6 2 -6 2  6 4 -6 4  6 6 -6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  2 0  3 3  4 0  5 3  6 0  6 6

...

  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  2 0  3 3  4 0  5 3  6 0  6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  1 1 -1 1  2 0  2 2 -2 2  3 1 -3 1  3 3 -3 3  4 0  4 2 -4 2  4 4 -4 4  5 1 -5 1  5 3 -5 3
5 5 -5 5  6 0  6 2 -6 2  6 4 -6 4  6 6 -6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  1 0  2 0  2 2  3 0  3 2  4 0  4 2  4 4  5 0  5 2  5 4  6 0  6 2  6 4  6 6
  0 0  2 0  3 3  4 0  5 3  6 0  6 6
 12.00          GMAX
NOFILE        FILE/NOFILE  write recprlist

quit file with :q
```

Continue...

```
-----> in  t1.in1_st  select   RKmax ( usually 5.0 - 9.0 ), LVNS and LOs
-----> in  t1.in2_st  select   GMAX and Fermi-Energy method
>   inputfiles prepared(16:41:50)
 inputfiles prepared
 inversion is NOT present
>   inputfiles for lapw1c/2c prepared, no inversion present(16:41:50)
 next is kgen
>   kgen(16:41:50)           12  symmetry operations without inversion
 inversion added (non-spinpolarized non-so calculation)
  NUMBER OF K-POINTS IN WHOLE CELL: (0 allows to specify 3 divisions of G)
1
```

```
opens the file "t1.klist"
         1         0         0         0         1  1.0 -7.0  1.5         1 k, div: (  1  1  1)
END
quit file with :q
```

```
 length of reciprocal lattice vectors:   0.383   0.383   0.250   1.154   1.154   0.751
           1  k-points generated, ndiv=           1           1           1
  2D-BZ: better use TEMP in case.in2
KGEN ENDS
0.001u 0.008s 0:29.49 0.0%0+0k 0+0io 0pf+0w
-----> check in  t1.klist  number of generated K-points
 WARNING: 2D-BZ, better use TEMP and not TETRA in case.in2
-----> continue with dstart or execute kgen again or exit (c/e/x)
enter
 next is dstart
>   dstart -c -p > & .mist(16:44:06)
```

case.outputd

```
opens a new file “t1.outputd” in vi

                                 ------------------------------------------------
                                   S T R U C T U R A L   I N F O R M A T I O N
                                 ------------------------------------------------


   SUBSTANCE                       = blebleble

   LATTICE                         = H
   LATTICE CONSTANTS ARE           =   18.9274200  18.9274200  25.1756880
   NUMBER OF ATOMS IN UNITCELL     =  30
   MODE OF CALCULATION IS          =
  convention (i,j)     (j)
                      ax ay az
                   (i) bx by bz
                       cx cy cz

...

rmt(min)*kmax =    7.00000
gmin =   10.85271
gmax =   12.00000


cutoff distance for superposition:    14.707
unitcell range:    2    2    2

...

quit file with :q
```

GMAX > GMIN ?

…and finishing

```
 C  T F
DSTART ENDS
8.383u 0.087s 0:09.21 91.8%0+0k 0+0io 0pf+0w

-----> check in  t1.outputd  if gmax > gmin, normalization
-----> new t1.in0 generated
-----> do you want to perform a spinpolarized calculation ? (n/y)
n
   init_lapw finished ok
```

- sgroup finds correct symmetry? Real or complex (case.in1/in1c)?
  - complex runs: don't forget -c flag!
- Select XC function & c/v e^- separation energy, core charge leak?
- RKMAX = 5 - 9 (H atom: 3 - 5) - bad scaling!
- Fermi-method: usually TEMP 0.002
- increase GMAX if warning in case.outputd
- k-points: shift or no shift? - DOS, spectroscopy, no shift!

Files & :log

```
[weiol@tetralith1 t1]$ ls
dstart.def        t1.bva      t1.in2_ls          t1.inq_st       t1.outputs         t1.rspup             t1.struct_sgroup
dstart.error      t1.clmsum   t1.in2_st          t1.inst         t1.outputsgroup    t1.sigma             t1.struct_st
kgen.def          t1.dayfile  t1.in2_sy          t1.kgen         t1.outputsgroup1   t1.sptdn             t1.test
:log              t1.in0      t1.inc             t1.klist        t1.outputst        t1.sptup             t1.vspdn_st
lstart.def        t1.in0_st   t1.inc_st          t1.nnshells     t1.potdn           t1.struct            t1.vsp_st
new_super.clmsum  t1.in0_std  t1.inm             t1.outputd      t1.potup           t1.struct_nn
nn.def            t1.in1c     t1.inm_restart_st  t1.outputkgen   t1.rsigma          t1.struct_orig
patchsymm.def     t1.in1_st   t1.inm_st          t1.outputnn     t1.rsp             t1.struct_patchsymm
symmetry.def      t1.in2c     t1.inq             t1.outputpatch  t1.rspdn           t1.struct_setrmt

[weiol@tetralith1 t1]$ cat :log
>   (init_lapw) options:
Wed Nov 17 16:18:27 CET 2021> (x_lapw) nn -f t1
Wed Nov 17 16:20:46 CET 2021> (x) nn
Wed Nov 17 16:24:17 CET 2021> (x) sgroup
Wed Nov 17 16:29:37 CET 2021> (x) patchsymm
Wed Nov 17 16:30:29 CET 2021> (x) nn
Wed Nov 17 16:31:45 CET 2021> (x) sgroup
Wed Nov 17 16:31:55 CET 2021> (x) patchsymm
Wed Nov 17 16:32:00 CET 2021> (x) nn
Wed Nov 17 16:32:11 CET 2021> (x) sgroup
Wed Nov 17 16:32:16 CET 2021> (x) symmetry
Wed Nov 17 16:33:53 CET 2021> (x) lstart
Wed Nov 17 16:41:50 CET 2021> (x) kgen
Wed Nov 17 16:44:06 CET 2021> (x) dstart -c -p
```

Quick initialization

- Can use if `case.struct` already properly setup

```
$ init_lapw -h
```
- check options

- Example: Al unit cell, 4000 k-pts, more states in core

```
$ init_lapw -b -red 0 -numk 4000 -ecut -4.5
```

- Example: NaCl 64 atoms perturbed supercell, 1 k-pt

```
$ init_lapw -b -red 0 -numk 1 -fermit 0.002
```

w2web

- The Wien2k Graphical User Interface (GUI)
- GUI alternative to scripts, such as `init_lapw`
- Good start for first time users
- Tool for structure setup
- Generate input files, check post-processing
- With experience, use scripts

w2web @NSC

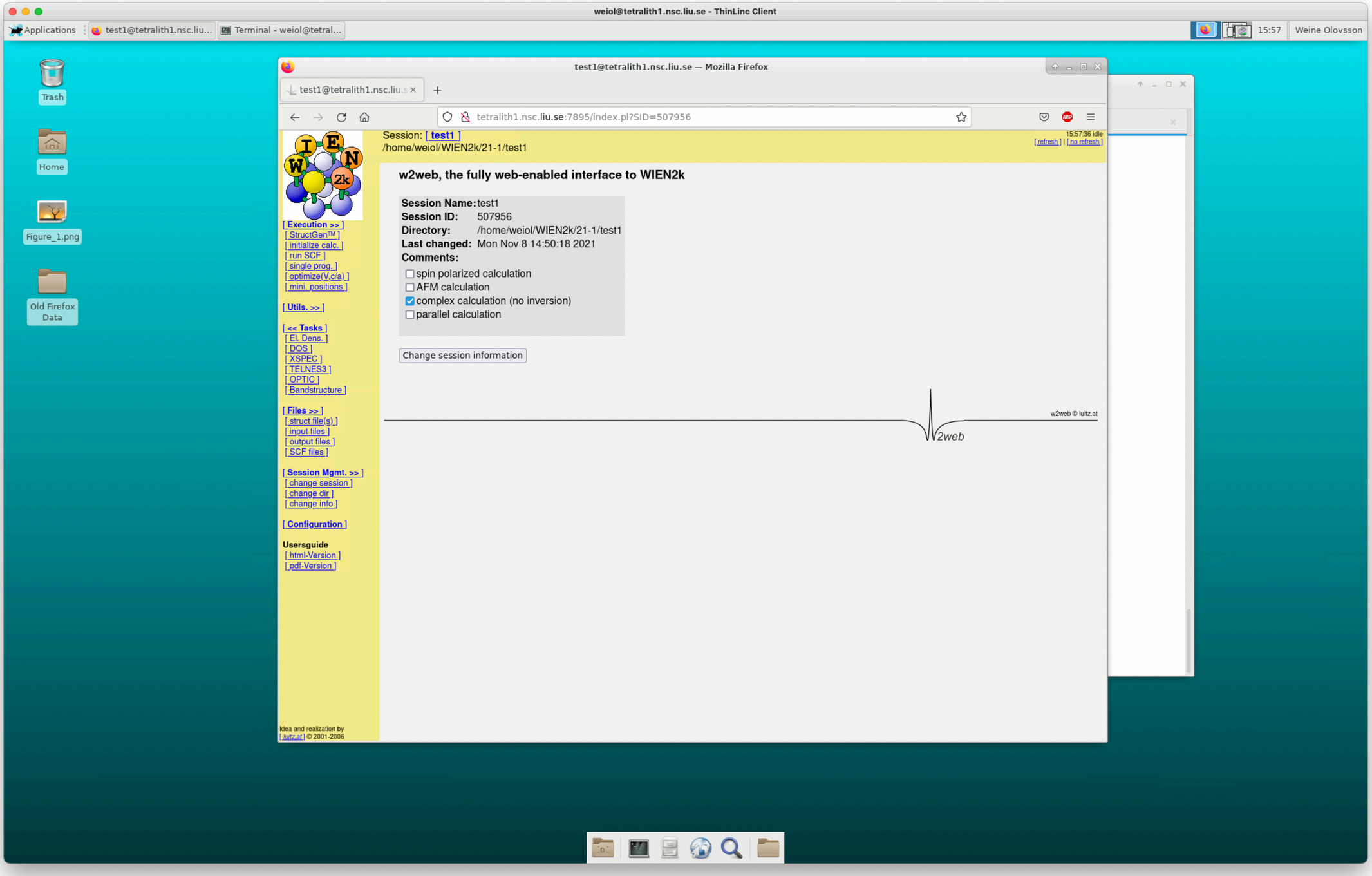
- Don’t use for heavy work! (login node)
- Login with ThinLinc virtual desktop & open terminal

```
$ module load WIEN2k/21.1-nsc1-intel-2018b-eb
$ w2web
```

- First time, set up with username & unique password
- Open link in Firefox Applications > Internet > Firefox
- When finished, close browser & w2web

```
$ ps -ef | grep w2web
$ kill -9 process-id
```

- find your w2web process & remove


weiol@tetralith1.nsc.liu.se - ThinLinc Client
Applications
test1@tetralith1.nsc.liu...
Terminal - weiol@tetral...
15:57
Weine Olovsson
Trash
Home
Figure_1.png
Old Firefox Data
test1@tetralith1.nsc.liu.se — Mozilla Firefox
test1@tetralith1.nsc.liu.s
tetralith1.nsc.liu.se:7895/index.pl?SID=507956
Session: [test1]
/home/weiol/WIEN2k/21-1/test1
15:57:36 idle
[refresh] | [no refresh]
w2web, the fully web-enabled interface to WIEN2k
Session Name: test1
Session ID: 507956
Directory: /home/weiol/WIEN2k/21-1/test1
Last changed: Mon Nov 8 14:50:18 2021
Comments:
spin polarized calculation
AFM calculation
complex calculation (no inversion)
parallel calculation
Change session information
w2web © luitz.at
[Execution >>]
[StructGen™]
[initialize calc.]
[run SCF]
[single prog.]
[optimize(V,c/a)]
[mini. positions]
[Utils. >>]
[<< Tasks]
[El. Dens.]
[DOS]
[XSPEC]
[TELNES3]
[OPTIC]
[Bandstructure]
[Files >>]
[struct file(s)]
[input files]
[output files]
[SCF files]
[Session Mgmt. >>]
[change session]
[change dir]
[change info]
[Configuration]
Usersguide
[html-Version]
[pdf-Version]
Idea and realization by
[luitz.at] © 2001-2006

3. Running job

Weine Olovsson
National Supercomputer Centre (NSC), Linköping University
SNIC training, online mini workshop @NSC 18th Nov 2021

LINKÖPINGS UNIVERSITET

Before running

- Initialization steps OK?
- Computational demand?
- Several steps with new/updated input files?

Small calculations

- Few atoms, DFT
- Run as serial job (or few cores) `$ run_lapw`
- Switch from ELPA to ScaLAPACK in `case.in1`

```
WFFIL  EF=.49676693479561029399   (WFFIL, WFPRI, ENFIL, SUPWF)
  7.00     10   4   ELPA pxq BL 64 (R-MT*K-MAX,MAX L IN WF,V-NMT,LIB)
  0.30    2  0      (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0    0.30     0.0000 CONT 1
 1    0.30     0.0000 CONT 1
K-VECTORS FROM UNIT:4   -7.5       1.5    5   emin / de (emax=Ef+de) / nband
```

```
WFFIL  EF=.49676693479561029399   (WFFIL, WFPRI, ENFIL, SUPWF)
  7.00     10   4   SCALA pxq BL 64 (R-MT*K-MAX,MAX L IN WF,V-NMT,LIB)
  0.30    2  0      (GLOBAL E-PARAMETER WITH n OTHER CHOICES, global APW/LAPW)
 0    0.30     0.0000 CONT 1
 1    0.30     0.0000 CONT 1
K-VECTORS FROM UNIT:4   -7.5       1.5    5   emin / de (emax=Ef+de) / nband
```

Heavy calculations

- Many inequivalent atoms, large basis set
- GW, hybrid calcs.
- Is it reasonable to run?
- Level of approximations
- Running efficiently (parallelization)

Job scripts: MPI

```
#!/bin/bash
#SBATCH -A SNIC-xxx-yyy
#SBATCH -N 1
#SBATCH --exclusive
#SBATCH -t 12:00:00

module add WIEN2k/12.1-nsc1-intel-2018b-eb
# export SCRATCH=$SNICTMP

# set .machines for parallel job
# lapw0 running on one node
    echo -n "lapw0: " > .machines
    echo -n $(hostlist -e $SLURM_JOB_NODELIST | tail -1) >> .machines
    echo "$i:8" >> .machines

# run one mpi job on each node (splitting k-mesh over nodes)
for i in $(hostlist -e $SLURM_JOB_NODELIST)
do
    echo "1:$i:32 " >> .machines
done
echo granularity:1 >> .machines
echo extrafine:1   >> .machines

run_lapw -p

# if you need the vector files for continuing calculations, e.g.
# for DOS, spectrum etc. copy them to your current directory:
# cp $SNIC_TMP/* .
```

- A job script “run.sh”
- Typical example
- 1 node = 32 cores
- 1 job with 32 MPI-ranks
- Submit with:
  `sbatch run.sh`

Monitoring calculations

- Size of calculation
```
$ grep :RKM *.scf
```
- Scf convergence
```
$ grep :ENE *.scf
$ grep :DIS *.scf
```
- Job run progress with timing

  `:log`
- Output messages, problems

  `case.dayfile`

  `slurm-1234567.out`

  `*error*`

- Did the calculation converge?

- Error files empty at finished run?

:log file example

```
>   (init_lapw) options:
Mon Nov  1 16:12:54 CET 2021> (x_lapw) nn -f t1
Mon Nov  1 16:12:55 CET 2021> (x) nn
Mon Nov  1 16:13:07 CET 2021> (x) sgroup
Mon Nov  1 16:13:19 CET 2021> (x) patchsymm
Mon Nov  1 16:13:24 CET 2021> (x) nn
Mon Nov  1 16:13:28 CET 2021> (x) sgroup
Mon Nov  1 16:13:41 CET 2021> (x) patchsymm
Mon Nov  1 16:13:42 CET 2021> (x) nn
Mon Nov  1 16:13:44 CET 2021> (x) sgroup
Mon Nov  1 16:13:46 CET 2021> (x) symmetry
Mon Nov  1 16:13:48 CET 2021> (x) lstart
Mon Nov  1 16:14:41 CET 2021> (x) kgen
Mon Nov  1 16:14:57 CET 2021> (x) dstart -c -p
>   (run_lapw) options: -p -i 100
Mon Nov  1 16:18:30 CET 2021> (x) lapw0 -p
Mon Nov  1 16:18:40 CET 2021> (x) lapw1 -p -c
Mon Nov  1 16:22:20 CET 2021> (x) lapw2 -p -c
Mon Nov  1 16:22:27 CET 2021> (x) sumpara -d
Mon Nov  1 16:22:28 CET 2021> (x) lcore
Mon Nov  1 16:22:28 CET 2021> (x) mixer
...
Mon Nov  1 17:03:30 CET 2021> (x) lapw0 -p
Mon Nov  1 17:03:44 CET 2021> (x) lapw1 -p -c
Mon Nov  1 17:07:13 CET 2021> (x) lapw2 -p -c
Mon Nov  1 17:07:19 CET 2021> (x) sumpara -d
Mon Nov  1 17:07:20 CET 2021> (x) lcore
Mon Nov  1 17:07:20 CET 2021> (x) mixer
Mon Nov  1 17:24:13 CET 2021> (x) kgen
Mon Nov  1 17:24:17 CET 2021> (x) kgen
Mon Nov  1 17:24:49 CET 2021> (x) lapw1 -c -p
Mon Nov  1 17:56:13 CET 2021> (x) lapw2 -c -p -qtl
```

$ init_lapw

run_lapw -p -i 100

scf end

$ x kgen

x lapw1 -c -p

x lapw2 -c -p -qtl

Output: case.dayfile

```
Calculating t1 in /proj/theophys/users/weiol/lapw/21-1/r-BN/hex/128at/t1
on n1145 with PID 56203
using WIEN2k_21.1 (Release 14/4/2021) in /software/sse/manual/WIEN2k/21.1/nsc1


    start       (Mon Nov  1 16:18:30 CET 2021) with lapw0 (100/99 to go)

    cycle 1     (Mon Nov  1 16:18:30 CET 2021)  (100/99 to go)

>   lapw0   -p  (16:18:30) starting parallel lapw0 at Mon Nov  1 16:18:30 CET 2021
-------- .machine0 : 8 processors
38.374u 2.925s 0:07.12 579.9%   0+0k 808+0io 24pf+0w
>   lapw1  -p   -c      (16:18:40) starting parallel lapw1 at Mon Nov  1 16:18:40 CET 2021
->  starting parallel LAPW1 jobs at Mon Nov  1 16:18:40 CET 2021
running LAPW1 in parallel mode (using .machines)
1 number_of_parallel_jobs
     n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145
n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145
n1145(1) 6153.646u 519.944s 3:38.54 3053.7%      0+0k 288+0io 4pf+0w
   Summary of lapw1para:
   n1145          k=1     user=6153.65    wallclock=218.54
6154.633u 520.753s 3:40.67 3025.0%      0+0k 1128+96io 9pf+0w
>   lapw2 -p     -c     (16:22:20) running LAPW2 in parallel mode
      n1145 126.920u 17.449s 0:05.09 2836.1% 0+0k 0+232io 0pf+0w
   Summary of lapw2para:
   n1145          user=126.92     wallclock=5.09
127.433u 17.769s 0:07.09 2047.8%        0+0k 0+336io 0pf+0w
>   lcore       (16:22:28) 0.177u 0.029s 0:00.31 61.2%  0+0k 0+0io 0pf+0w
>   mixer       (16:22:28) 1.039u 0.090s 0:01.26 88.8%  0+0k 0+0io 0pf+0w
:ENERGY convergence:  0 0.0001 0
:CHARGE convergence:  0 0.0000 0
ec cc and fc_conv 0 1 1

    cycle 2     (Mon Nov  1 16:22:30 CET 2021)  (99/98 to go)
```

Output: case.dayfile

```
    cycle 13    (Mon Nov  1 17:03:29 CET 2021)  (88/87 to go)

>   lapw0   -p  (17:03:30) starting parallel lapw0 at Mon Nov  1 17:03:30 CET 2021
-------- .machine0 : 8 processors
36.368u 2.203s 0:06.04 638.4%   0+0k 0+0io 0pf+0w
>   lapw1  -p   -c      (17:03:36) starting parallel lapw1 at Mon Nov  1 17:03:44 CET 2021
->  starting parallel LAPW1 jobs at Mon Nov  1 17:03:44 CET 2021
running LAPW1 in parallel mode (using .machines)
1 number_of_parallel_jobs
     n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145
n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145 n1145
n1145(1) 6085.728u 514.268s 3:26.94 3189.3%      0+0k 0+0io 0pf+0w
   Summary of lapw1para:
   n1145         k=1     user=6085.73    wallclock=206.94
6086.803u 514.944s 3:29.50 3151.1%      0+0k 0+96io 0pf+0w
>   lapw2 -p     -c     (17:07:13) running LAPW2 in parallel mode
      n1145 123.664u 17.198s 0:04.50 3130.0% 0+0k 0+232io 0pf+0w
   Summary of lapw2para:
   n1145         user=123.664    wallclock=4.5
124.181u 17.517s 0:06.39 2217.3%        0+0k 0+336io 0pf+0w
>   lcore       (17:07:20) 0.161u 0.025s 0:00.24 75.0%  0+0k 0+0io 0pf+0w
>   mixer       (17:07:20) 1.032u 0.092s 0:01.19 94.1%  0+0k 0+0io 0pf+0w
:ENERGY convergence:  1 0.0001 .0000208400000000
:CHARGE convergence:  0 0.0000 .0002632
ec cc and fc_conv 1 1 1

>   stop
```

Output: slurm-JOBID.out

```
 LAPW0 END
[1]    Done                          /software/sse/easybuild/prefix/software/impi/2018.3.222-
iccifort-2018.3.222-GCC-7.3.0-2.30/bin64/mpiexec.hydra -bootstrap ssh -np 8
-machinefile .machine0 /software/sse/manual/WIEN2k/21.1/nsc1/lapw0_mpi lapw0.def >> .time00
 LAPW1 END
[1]  + Done                          ( cd $PWD; $t $ttt; rm -f .lock_$lockfile[$p] )
>> .time1_$loop
LAPW2 - FERMI; weights written
 LAPW2 END
[1]    Done                          ( cd $PWD; $t $ttt $vector_split; rm -f .lock_$lockfile[$p]
) >> .time2_$loop
 SUMPARA END
 CORE  END
 MIXER END
ec cc and fc_conv 0 1 1
...
in cycle 13    ETEST: .0001015650000000   CTEST: .0014922
 LAPW0 END
[1]    Done                          /software/sse/easybuild/prefix/software/impi/2018.3.222-
iccifort-2018.3.222-GCC-7.3.0-2.30/bin64/mpiexec.hydra -bootstrap ssh -np 8
-machinefile .machine0 /software/sse/manual/WIEN2k/21.1/nsc1/lapw0_mpi lapw0.def >> .time00
 LAPW1 END
[1]  + Done                          ( cd $PWD; $t $ttt; rm -f .lock_$lockfile[$p] )
>> .time1_$loop
LAPW2 - FERMI; weights written
 LAPW2 END
[1]    Done                          ( cd $PWD; $t $ttt $vector_split; rm -f .lock_$lockfile[$p]
) >> .time2_$loop
 SUMPARA END
 CORE  END
 MIXER END
ec cc and fc_conv 1 1 1

>   stop
```

Job scripts: k-pt groups with MPI

```
...
#SBATCH -n 32
...
for i in $(hostlist -e $SLURM_JOB_NODELIST)
do
  echo "1:$i:16 " >> .machines
  echo “1:$i:16 " >> .machines
done
echo granularity:1 >> .machines
echo extrafine:1   >> .machines
...
```

- 1 node = 32 cores
- k-pts in 2 groups with 16 MPI-ranks
- e.g. calculation with 2 k-pts

```
...
#SBATCH -n 64
...
for i in $(hostlist -e $SLURM_JOB_NODELIST)
do
  echo "1:$i:4 " >> .machines
  echo “1:$i:4 " >> .machines
  echo “1:$i:4 " >> .machines
  echo “1:$i:4 " >> .machines
  echo "1:$i:4 " >> .machines
  echo “1:$i:4 " >> .machines
  echo “1:$i:4 " >> .machines
  echo “1:$i:4 " >> .machines
done
echo granularity:1 >> .machines
echo extrafine:1   >> .machines
...
```

- 2 nodes = 64 cores
- k-pts in 8 groups with 4 MPI-ranks per node

Job scripts: fully k-pt parallel

```
...
#SBATCH -n 32
...
for i in $(hostlist -e $SLURM_JOB_NODELIST)
do
  for j in {1..32}
  do
    echo "1:$i:1 " >> .machines
  done
done
echo granularity:1 >> .machines
echo extrafine:1   >> .machines
...
```

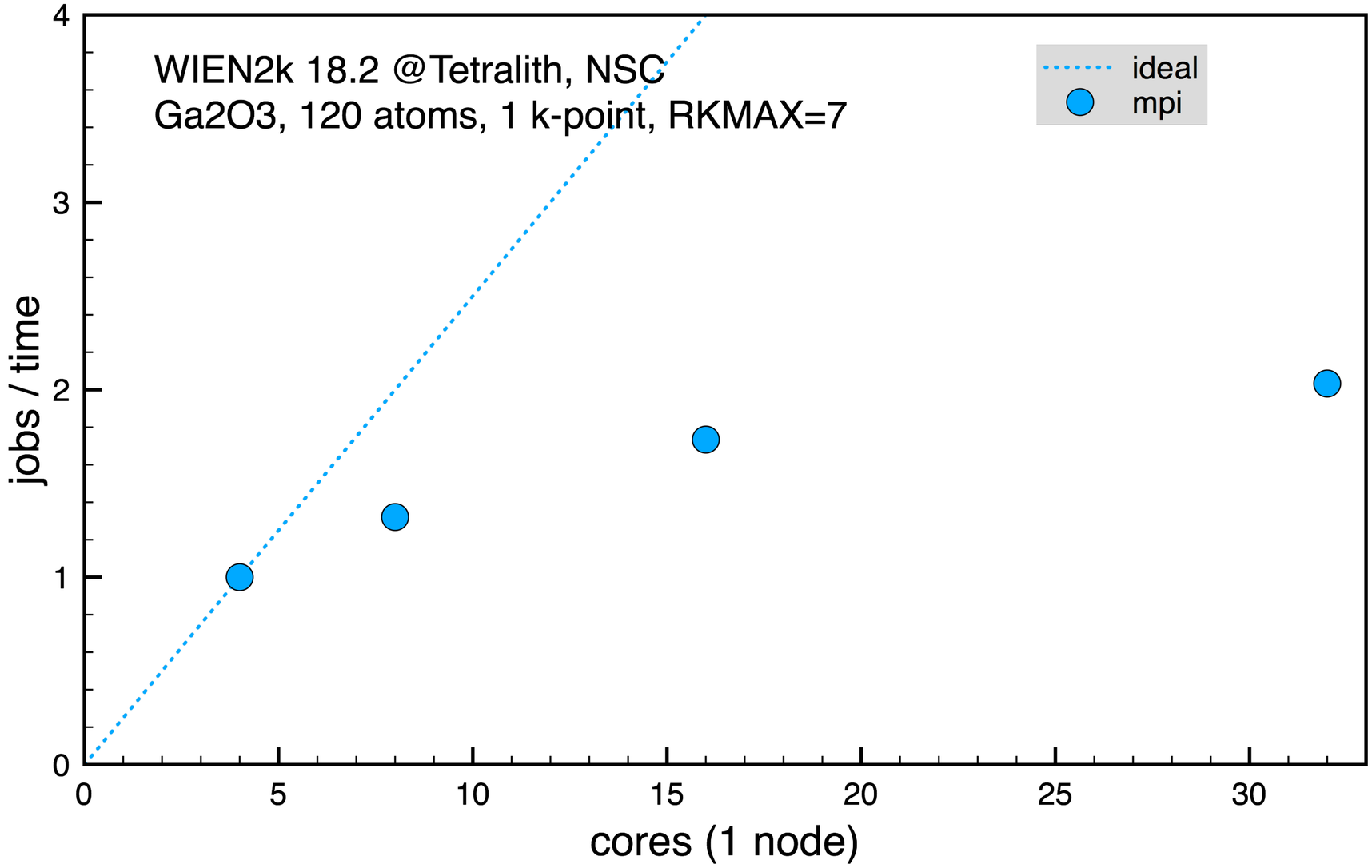
- 1 node = 32 cores
- 32 *independent* serial runs

```
...
#SBATCH -n 32
...
for i in $(hostlist -e $SLURM_JOB_NODELIST)
do
  for j in {1..16}
  do
    echo "1:$i:1 " >> .machines
  done
done
...
```

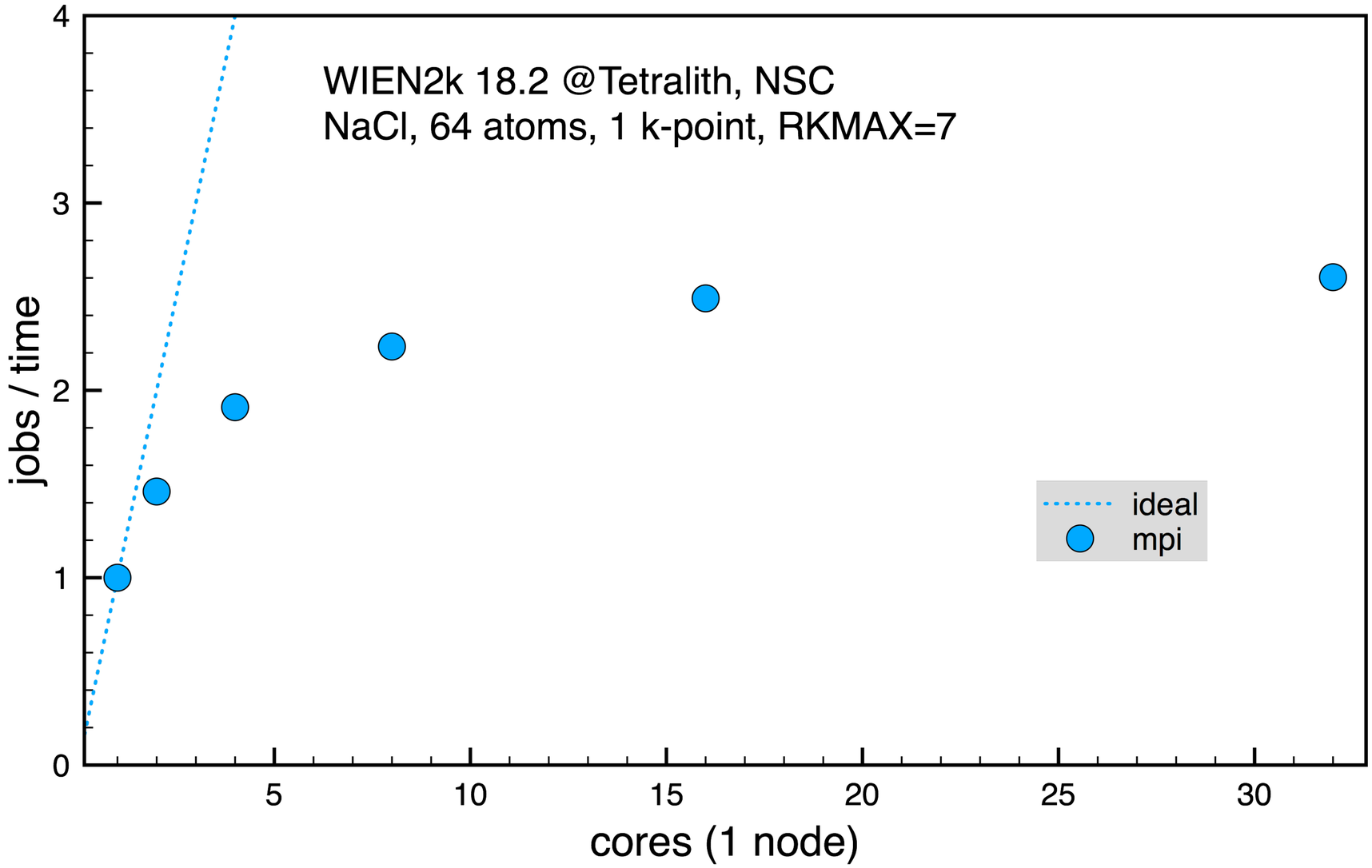
- 1 node = 32 cores
- 16 independent serial runs (half node)
- Idea: reducing memory usage

- A completely k-point parallel job, very efficient (“trivial” parallelism)

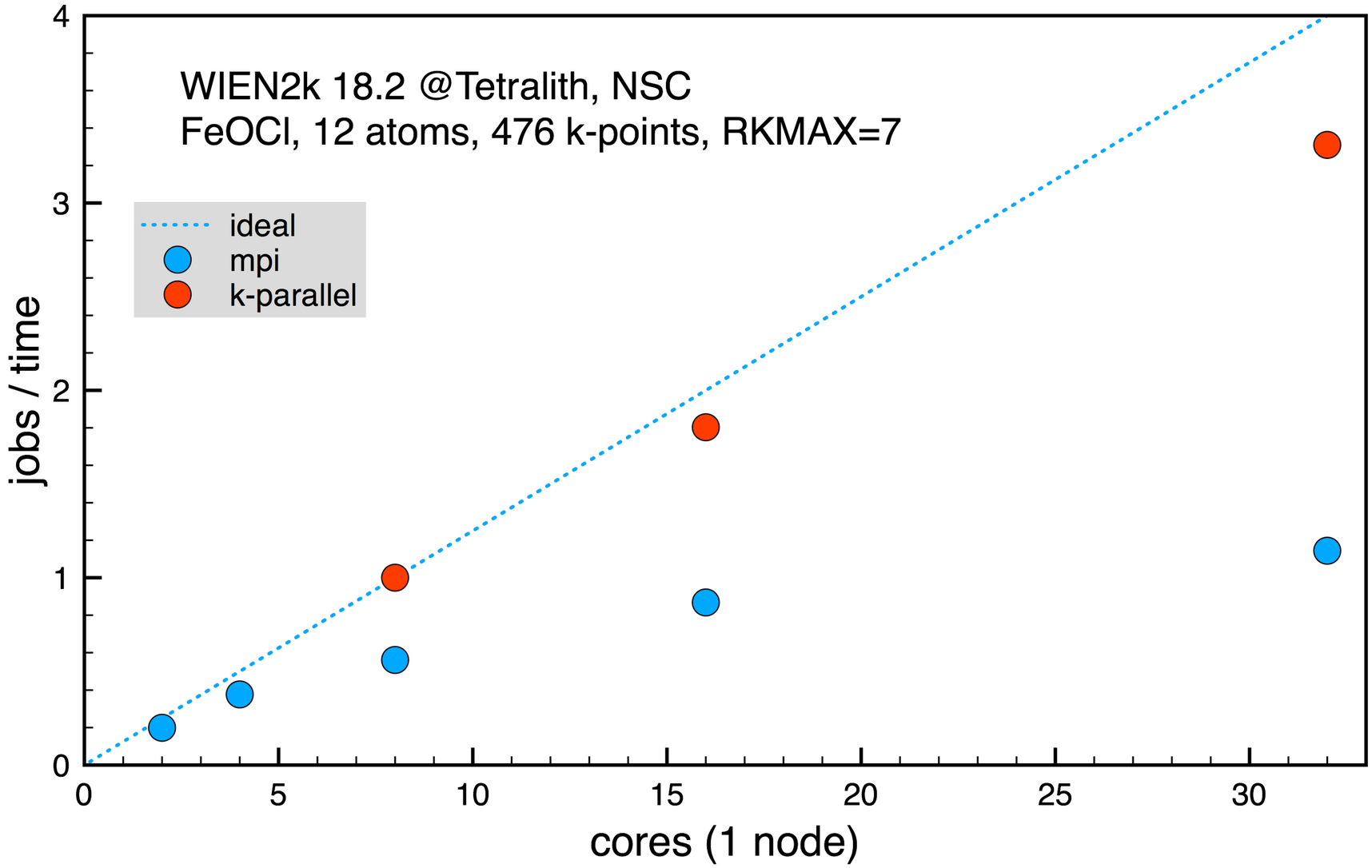
Ga2O3 120 atoms



NaCl 64 atoms



FeOCl 12 atoms



Further considerations

- Memory: allocate full node, reduce core usage
- OpenMP threading also available
- Iterative diagonalization, `run_lapw -p -it`
- Tool for “cleaning up” and saving a calculation

4. Hands-on & Questions

Weine Olovsson
National Supercomputer Centre (NSC), Linköping University
SNIC training, online mini workshop @NSC 18th Nov 2021

LINKÖPINGS UNIVERSITET

Hands-on & Questions

- Questions, on screen demonstration
- Your own WIEN2k case?
- Examples for hands-on:
  - Al metal unit cell
  - NaCl perturbed lattice, 64 atoms
  - h-BN, from .cif, build supercell