Installation of Wien2k, parallelization, large scale applications with WIEN2k

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WIEN2k- hardware/software

- WIEN2k runs on any Linux platform from PCs, Macs, workstations, clusters to supercomputers
- Intel **I7** quad (six)-core processors with fast memory bus (2-4 Gb/core, Gbit-network, SATA disks). 1000-1500 € /PC,
  - *with a few such PCs you have a quite powerful cluster (k-parallel)*
  - *60 - 100 atom / cell, requires 2-4 Gb RAM/core*
  - *installation support for many platforms + compiler*
- Cluster of Intel Xeon based nodes with infiniband (probably 2x8 cores per node best because of memory access)
  - *mpi, Scalapack*
  - *up to 1000 atoms/cell*
- Fortran90 (dynamical allocation, modules)
  - *real/complex version (inversion)*
  - *many individual modules, linked together with C-shell or perl-scripts*
- *web-based GUI – w2web (perl)*

Required / optional software

- f90 compiler: **ifort** (gfortran)
- BLAS-library: **mkl**, (openblas) - most important for speed-up
  - ***mpi*** *+ Scalapack(mkl) + ELPA +* ***FFTW*** *(only for mpi-parallel version)*
- Linux utilities (not always installed by default)
  - *tcsh, perl5, ghostscript, gnuplot, pdf-reader*
  - *octave (structeditor)*
  - *python 2.7.x, numpy (BerryPI)*
  - *opendx (3D-plotting of NMR currents,….)*
- Xcrysden
- VESTA (structure visualization)
- DFTD3 (van der Waals bonding)
- LIBXC: (http://www.tddft.org/programs/octopus/wiki/index.php/Libxc)
- Wannier90, PHONOPY
- “unsupported software” (see www.wien2k.at; phonon, boltztrap,…)

Installation of WIEN2k

- Register via http://www.wien2k.at
- Create your $WIENROOT directory (e.g. ./WIEN2k)
- Download wien2k_XX.tar and examples (executables)
- Uncompress and expand all files using:
  - *tar –xvf wien2k_XX.tar*
  - *gunzip *.gz*
  - *./expand_lapw*
- This leads to the following directories:

./SRC	*(scripts, ug.ps)*
./SRC_aim	*(programs)*
…	
SRC_templates	*(example inputs)*
…	
SRC_usersguide_html	*(HTML-version of UG)*
example_struct_files	*(examples)*
TiC	

- siteconfig_lapw to compile programs (or: tar -xvf SRC_executables.tar)

siteconfig_lapw

```
   **************************************************
   *                      W I E N                   *
   *                 site configuration             *
   **************************************************
      S   specify a system
      C   specify compiler
      O   specify compiler options, BLAS and LAPACK
      P   configure Parallel execution
      D   Dimension Parameters
      R   Compile/Recompile
      U   Update a package
      L   Perl path (if not in /usr/bin/perl)
      Q   Quit
```

D: define NMATMAX (adjust to your hardware/paging!):
NMATMAX=10000 ➔ 1Gb (real) or 2Gb (complex) ➔ 50-100 atoms/unitcell
NUME=1000 ➔ number of eigenvalues (adjust to NMATMAX)

Compilation

- recommendation: **Intels Fortran compiler** (includes **mkl**)
  not anymore free for non-commercial usage, www.intel.com
  - *`which ifort`* → *tells you if you can use ifort and which version you have*
    - usually installed in **/opt/intel/..../bin/intel64 (ls ....)**
    - **include compilervars.csh** (and mklvars.csh) in your .bashrc/.cshrc file:
      - source /opt/intel/compilers_and_libraries_2017/linux/bin/compilervars.sh intel64
  - ***ifort 14 or later*** *(vers. 8.0, early 12.x are buggy and a bit different)*
    - dynamic linking recommended (depends on ifort version, requires system and compiler libraries at runtime, needs $LD_LIBRARY_PATH)
    - **Intel64 (em64t),** IA32 bit, IA64 bit (Itanium) - version
    - mkl-library: library-names change with every version, see:
      http://software.intel.com/en-us/articles/intel-mkl-link-line-advisor
    - siteconfig has default options and libraries which should work for any modern ifort version
      - -O (-O1 in buggy versions); -traceback (to get line numbers for runtime errors)
      - -FR (free format); -assume buffered_io (nobuffered in buggy 2017 versions)

compilation

- **gfortran + openblas** (gotolib, acml-lib, ATLAS-BLAS)
    - free
    - in sequential mode almost as fast as ifort+mkl (vector-cos missing)
    - quite complicated for mpi parallel version
- siteconfig has support for:
    - *ifort (LI)*
    - *ifort + SLURM batch system (LS)*
    - *gfortran (LG)*
    - *the standard siteconfig-options should work without modification for sequential (+ k-point parallel) compilation.*
    - *mpi installation requires that you* ***know*** *your mpi+scalapack+fftw*
- if you have no compiler, you can use the precompiled executables

userconfig_lapw

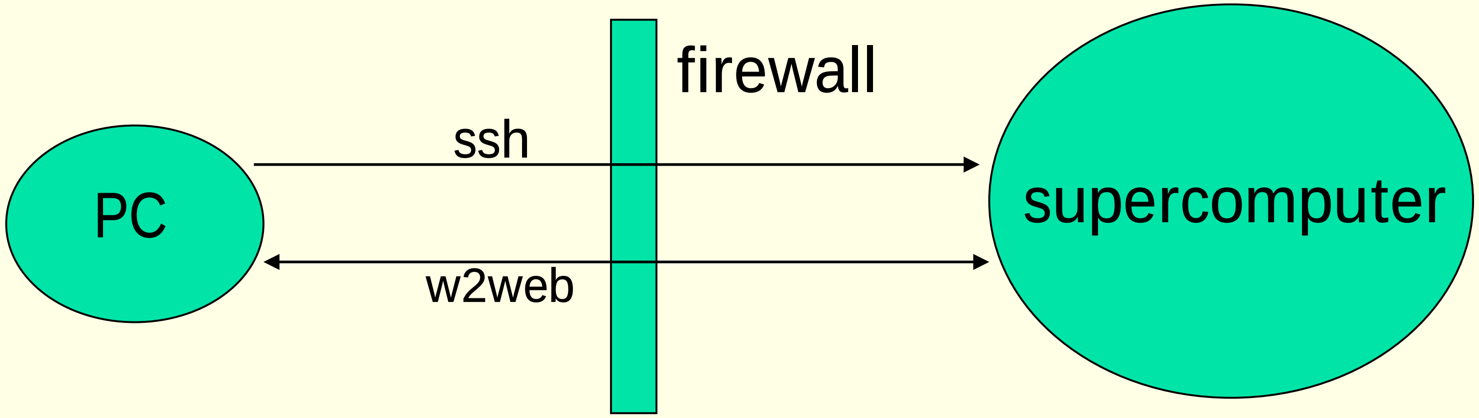
- Every user must run userconfig_lapw (setup of environment)
  - *support for tcsh and bash (requires .cshrc or .bashrc)*
  - *sets PATH to $WIENROOT, sets several variables and aliases*
    - $WIENROOT, $SCRATCH, $EDITOR, $PDFREADER, $STRUCTEDIT_PATH
    - SCRATCH directory (stores large files on local disks): /scratch

    - *pslapw: ps –ef | grep lapw*
    - *lsi: ls –als *.in*   lso: ls -als *.output**
    - *lss: ls –als *.scf*   lsc: ls -als *.clm**

- edit directly your .bashrc (.cshrc) file:
    - $OMP_NUM_THREADS = 1, 2 or 4 (for mkl+multi-core)
    - set a suitable prompt: hostname:dir (export PS1='\h:$PWD>‘)
    - $LD_LIBRARY_PATH (on some systems)
    - source ifort configuration (if not done by system admin)
    - include configurations (VARIABLES and PATH) for optional products (XCRYSDEN, PYTHON, PHONON, ...)

w2web

- w2web: acts as webserver on a userdefined (high) port.
  - *define user/password and port. (http://host.domain.xx:5000)*
  - *on remote system: ssh -X user@host; w2web*
  - *behind firewall create a „ssh-tunnel“:*
    - **ssh -fNL 5000:host:5000 user@host**



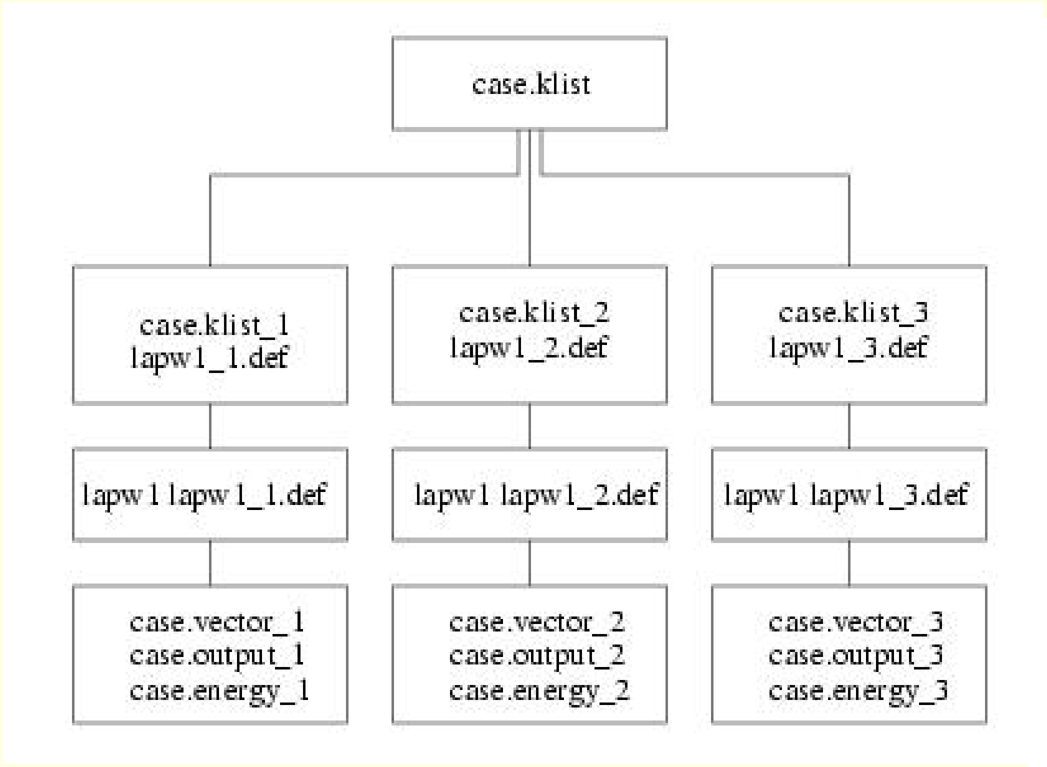
  - *~/.w2web/hostname/conf/w2web.conf: (configuration file)*
    - deny=*.*.*.*
    - allow=128.130.134.* 128.130.142.10
    - define execution types: NAME=commands (eg.: batch=batch < %f)

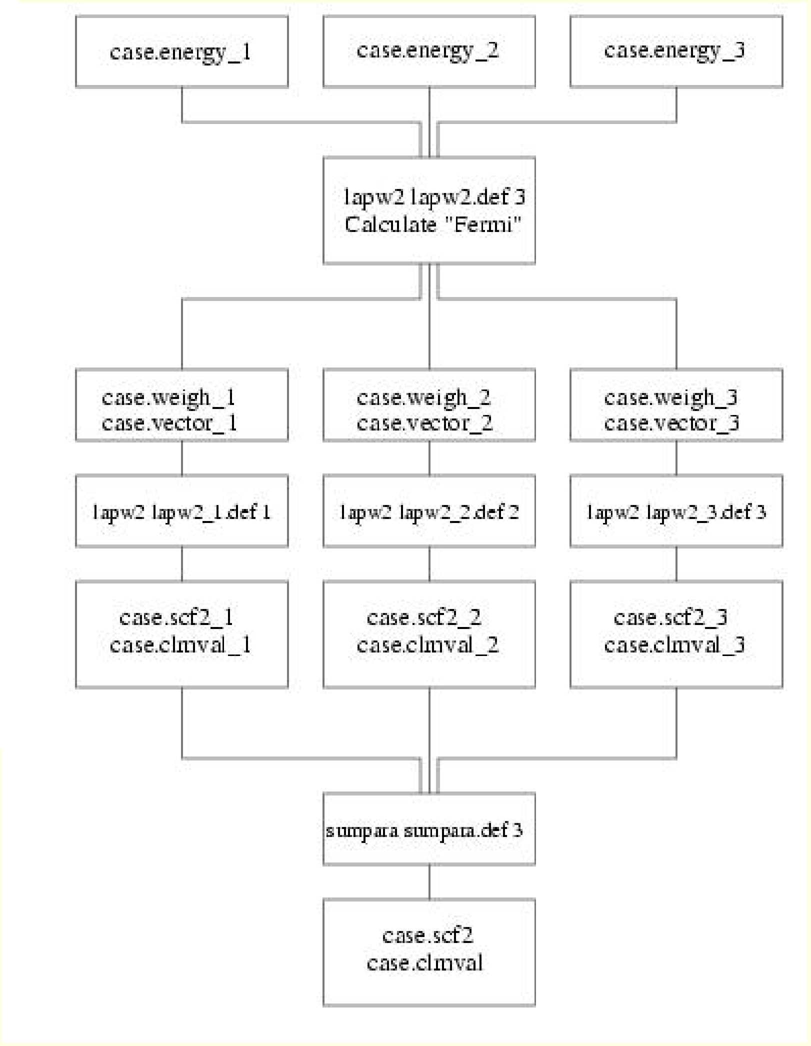
k-point Parallelization (lapw1+lapw2)

- very efficient parallelization even on loosely coupled PCs (slow network):
  - ***common NFS filesystem*** *(files must be accessible with the same path on all machines;   use /host1 as data-directory on host1)*
  - ***ssh without password*** *(private/public keys)*
    - ssh-keygen –t rsa
    - append .ssh/authorized_keys on remote host with id_rsa.pub of local host
    - .machines file:
      - 1:host1 (speed:hostname)
      - 2:host2
      - granularity:1 (1:10k+20k; 3: 3+6+3+6+3+6+rest ➔load balancing, not with $SCRATCH, -it
      - extrafine:1 (rest in junks of 1 k)
    - testpara (tests distribution); **run_lapw –p**
  - *case must fit into memory of one PC !*
  - *high NFS load: use local $SCRATCH directory (beware of accidental overwriting); run_lapw -p -scratch /scratch/pblaha]*
  - ***$OMP_NUM_THREADS=2*** *(parallel diag. (mkl) on multi-core CPU)*

Flow of parallel execution

lapw1para **lapw2para**



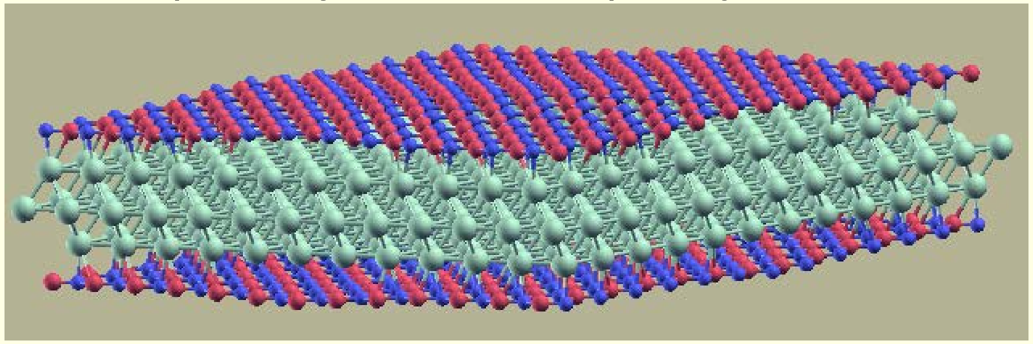

case.energy_1
case.energy_2
case.energy_3
lapw2 lapw2.def 3 Calculate "Fermi"
case.weigh_1 case.vector_1
case.weigh_2 case.vector_2
case.weigh_3 case.vector_3
lapw2 lapw2_1.def 1
lapw2 lapw2_2.def 2
lapw2 lapw2_3.def 3
case.scf2_1 case.clmval_1
case.scf2_2 case.clmval_2
case.scf2_3 case.clmval_3
sumpara sumpara.def 3
case.scf2 case.clmval

fine-grain mpi-parallelization

- for **bigger** cases (> 50 atoms) and **more** than **4 cores**
- fast network (~~Gbit~~, Myrinet, **Infiniband**, shared memory machines)
- **mpi** (you need to know which mpi is installed (mpich, open-mpi, **intel-mpi**, ..)
  - ***mpif90*** *or* ***mpiifort***
- **scalapack** (included in ifort): blacs-library depends on your mpi!!
  - *llibmkl_blacs_lp64.a or libmkl_blacs_openmpi_lp64.a or libmkl_blacs_intelmpi_lp64.a*
- **FFTW** (v. 2 or 3 ; mpi and sequ. version needed, -DFFTW2/3 in Makefiles)
- **ELPA** (at present use version 2015.11.001; optional, but faster than scalapack)
- .machines file:

1:host1:4 host2:4	8 mpi-parallel jobs on host1 and host2
lapw0:host1:4 host2:4	8 parallel jobs; atom-loops only + fft !!!

- simultaneous k-point and mpi-parallelization possible
  - *BN/Rh(111) nanomesh: cell with 1100 atoms*



  - NMAT=45000-80000; 64 cores, 1h / iteration; scales to at least 1024 cores

case.dayfile

- check how your computer is performing:

```
>   lapw1  -p          (07:09:28) starting parallel lapw1 at Sat Jun 21 07:09:2
4 number_of_parallel_jobs
     ne(1) 197.017u 1.750s 1:46.71 186.2%      0+0k 0+119520io 0pf+0w
     ne(1) 198.383u 1.943s 1:47.88 185.6%      0+0k 0+105192io 0pf+0w
     eos(1) 188.838u 1.553s 1:49.79 173.4%      0+0k 17288+106456io 0pf+0w
     eos(1) 187.964u 1.849s 1:42.29 185.5%      0+0k 24+106872io 0pf+0w
>   lapw2 -p           (07:11:38) running LAPW2 in parallel mode
      ne 60.015u 0.621s 1:10.52 85.9% 0+0k 0+21088io 0pf+0w
      ne 60.686u 0.634s 1:08.63 89.3% 0+0k 0+17688io 0pf+0w
      eos 60.428u 0.689s 1:18.04 78.2% 0+0k 14152+17688io 0pf+0w
      eos 59.942u 0.598s 1:18.60 77.0% 0+0k 24+17696io 0pf+0w
```

OMP_NUM_TREADS=2

```
>   lapw1  -p          (09:11:14) starting parallel lapw1 at Mon Jun 23 09:11:14
4 number_of_parallel_jobs
     susi(1) 254.613u 2.783s 2:16.95 187.9%     0+0k 0+119736io 0pf+0w
     susi(1) 257.553u 3.650s 2:18.71 188.3%     0+0k 0+107144io 0pf+0w
     planck(1) 299.348u 2.369s 3:03.88 164.0%   0+0k 13760+109696io 0pf+0w
     planck(1) 303.426u 2.783s 3:05.92 164.6%   0+0k 1664+107616io 0pf+0w
>   lapw2 -p -vresp    (09:25:17) running LAPW2 in parallel mode
      susi 23.078u 0.562s 0:13.24 178.4% 0+0k 0+34984io 0pf+0w
      susi 25.343u 0.552s 0:14.23 181.9% 0+0k 0+31584io 0pf+0w
      planck 22.181u 0.491s 1:54.13 19.8% 0+0k 56+31608io 0pf+0w
      planck 22.334u 0.476s 1:53.93 20.0% 0+0k 88+31608io 0pf+0w
```

somebody else is using planck
or the network is overloaded
(local SCRATCH)

iterative diagonalization for big cases:

- run_lapw -p -it -noHinv

```
 cycle 1     (Thu Oct 31 07:20:53 CET 2013)  (40/99 to go)

>   lapw0 -p    (07:20:53) starting parallel lapw0 at Thu Oct 31 07:20:53  2013
-------- .machine0 : 64 processors
264.604u 21.742s 0:40.76 702.5% 0+0k 591784+49768io 369pf+0w

>   lapw1  -up -p  -orb  (07:21:34) starting parallel lapw1 at Thu Oct 31
->  starting parallel LAPW1 jobs at Thu Oct 31 07:21:34 CET 2013
running LAPW1 in parallel mode (using .machines)
 r09n30 r09n30 r09n30 ....
6.558u 1.796s 29:08.54 0.4%     0+0k 16+520io 0pf+0w
....
cycle 3     (Thu Oct 31 07:50:53 CET 2013)  (40/99 to go)
...
>   lapw1 -it -up -p  -orb -noHinv   (09:31:52) starting parallel lapw1 at ...
 3.411u 0.908s 14:18.31 0.5%     0+0k 72+536io 0pf+0w
...
```

batch systems (see also our faq-page)

- submit a script to a queuing system (PBS, SGE, SLURM, ...)
- you can only specify total number of cores:
  - ***#$ -pe mpich 32*** *(specify 32 cores, but you don’t know the hosts)*
- get the machine names and write **.machines** on the fly:

```
set mpisize_per_k=16
set proclist=`cat $hostfile_tacc`          #  this will be different on your computer
set nproc=`cat hostfile_tacc | wc -l`
set i=1
while ($i <= $nproc )
echo -n '1:' >>.machines
@ i1 = $i + $mpisize_per_k
@ i2 = $i1 - 1
echo $proclist[$i-$i2] ':1' >>.machines
set i=$i1
end
echo 'granularity:1' >>.machines
echo 'extrafine:1' >>.machines
```

- you can combine k- and mpi-parallelization ($mpisize_per_k)
  - *32 cores: 2 k-points, 16 mpi-jobs/k-point*

Getting help

- *_lapw –h „help switch" of all WIEN2k-scripts
- help_lapw:
  - *opens usersguide.pdf; Use ^f keyword to search for an item („index")*
- html-version of the UG: ($WIENROOT/SRC_usersguide/usersguide.html)
- http://www.wien2k.at/reg_user
  - *FAQ page with answers to common questions*
  - *Update information: When you think the program has an error, please check newest version*
  - *Textbook section: DFT and the family of LAPW methods by S.Cottenier*
  - *Mailing-list:*
    - subscribe to the list (always use the same email)
    - full text search of the „digest" (your questions may have been answered before)
    - posting questions: Provide sufficient information, locate your problem (case.dayfile, *.error, case.scf, case.outputX).
    - „My calculation crashed. Please help." This will most likely not be answered.

WIEN2k_17.1

- always use latest version (**bug fixes**, improved performance, new features, **better** and **new utilities**)
  - *much better **siteconfig_lapw***
  - ***non-local van der Waals option** (probably most promising)*
  - *configure_int (for easier partial DOS configuration)*

- eventually: use prebuilt executables from our website !!

- a new Wien2k version is usually coming at least once a year