Hands-on IRVSP/IR2TB/IR2PW/IR2PH

Source code:
https://github.com/zjwang11/IR2PW
https://github.com/zjwang11/UnconvMat

Ref:

Gao, J. et al. "IRVSP: to obtain irreducible representations in the VASP", Comput. Phys. Comm. 261, 107760 (2021).
Zhang, R. et al. "Large shift current, π Zak phase and unconventional nature of Se and Te", Phys. Rev. Research 5, 023142 (2023).

Ruihan Zhang 2025/6/3

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1 Installation

1) **lib_irrep_bcs.a**

```
$ tar -zxvf lib_irrep_bcs.tar.gz
$ cd lib_irrep_bcs
$ ./configure.sh
$ make
$ cd ../
```

2) **pos2aBR**

```
$ tar -zxvf src_pos2aBR.tar.gz
$ cd src_pos2aBR
$ ./configure.sh
$ source ~/.bashrc
$ make
$ cd ../
```

3) **irvsp**

```
$ tar -zxvf src_ir2pw_vasp.tar.gz
$ cd src_ir2pw_vasp
$ make
$ cd ../
```

4) **ir2tb**

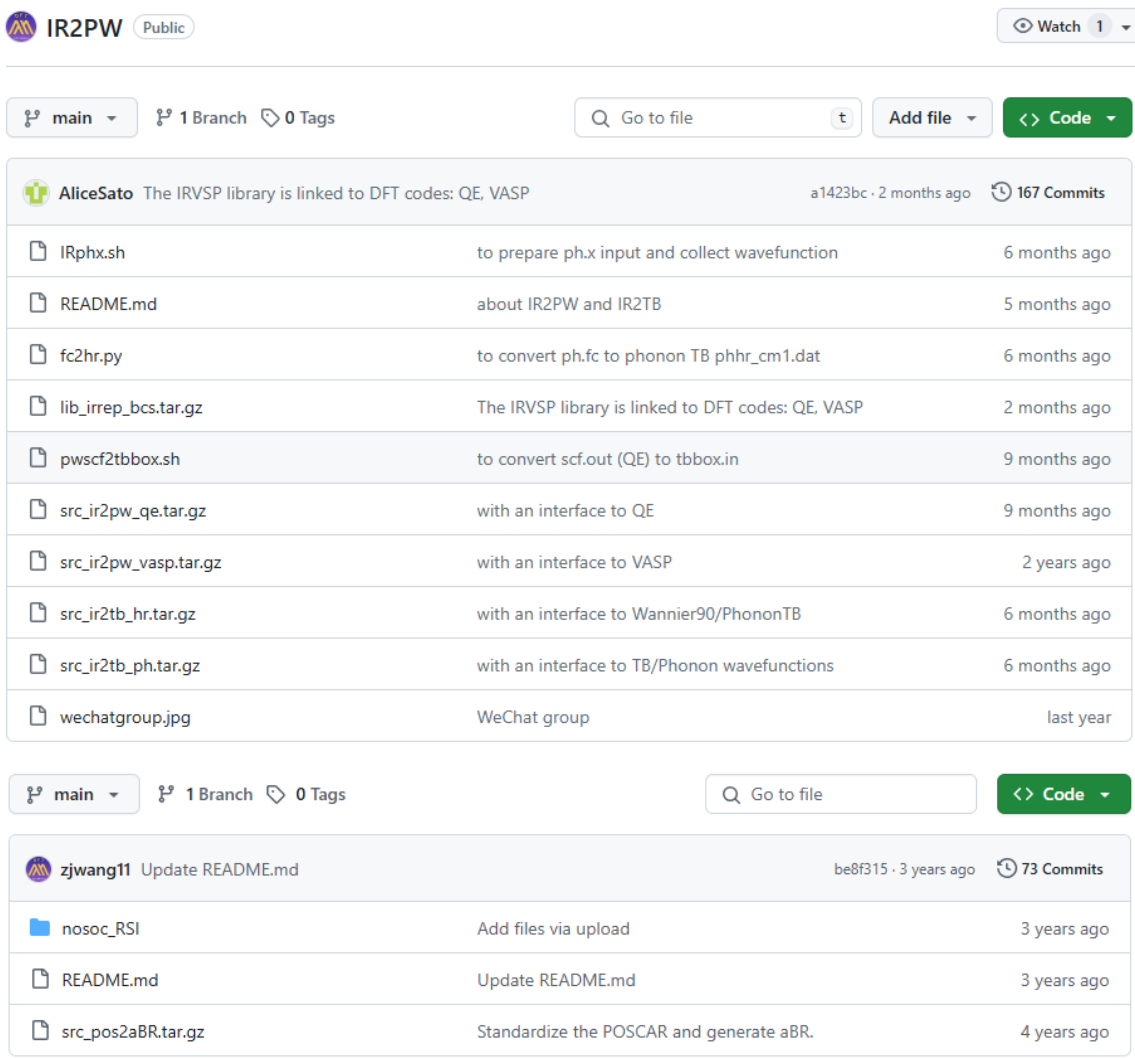
```
$ tar -zxvf src_ir2tb_hr.tar.gz
$ cd src_ir2tb_hr
$ make
$ cd ../
```

5) **ir2pw**

```
$ tar –zxvf src_ir2pw_qe.tar.gz
$ cd src_ir2pw_qe
$ make
$ cd ../
```

6) **ir2ph**

```
$ tar -zxvf src_ir2tb_ph.tar.gz
$ cd src_ir2tb_ph
$ make
$ cd ../
```



https://github.com/zjwang11/IR2PW

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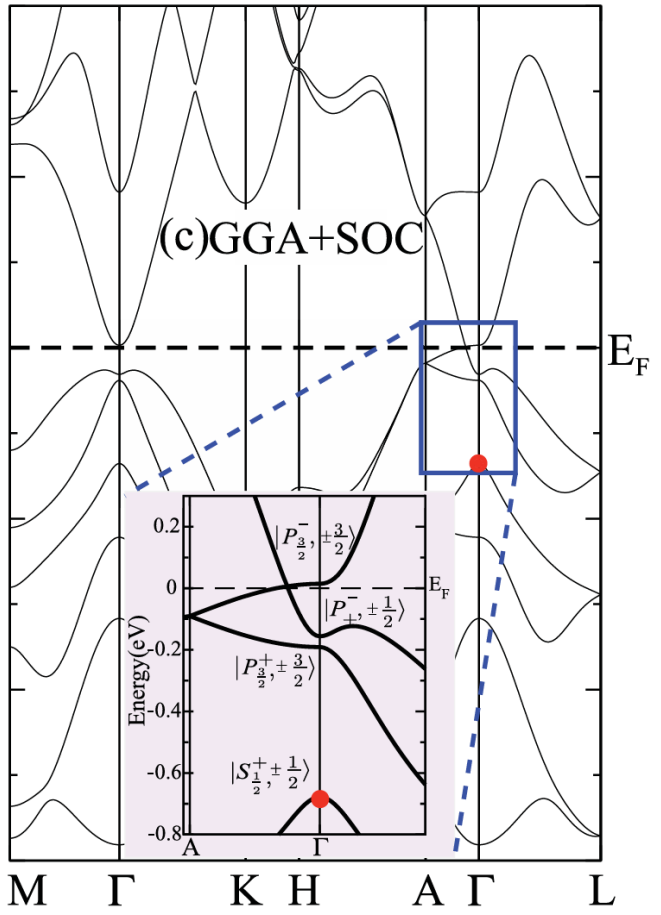
2 Example 1: find Dirac points from Na_3Bi

- In first-principles calculations, we often need to find band-crossing (or gap). If the k-points are not dense enough, it may be difficult.
- Here we take the Na_3Bi as an example to introduce how to calculate the Irreducible representations (Irreps) of different k-points to find Dirac points by using IRVSP/IR2TB/IR2PW.

band structures with spin-orbit coupling



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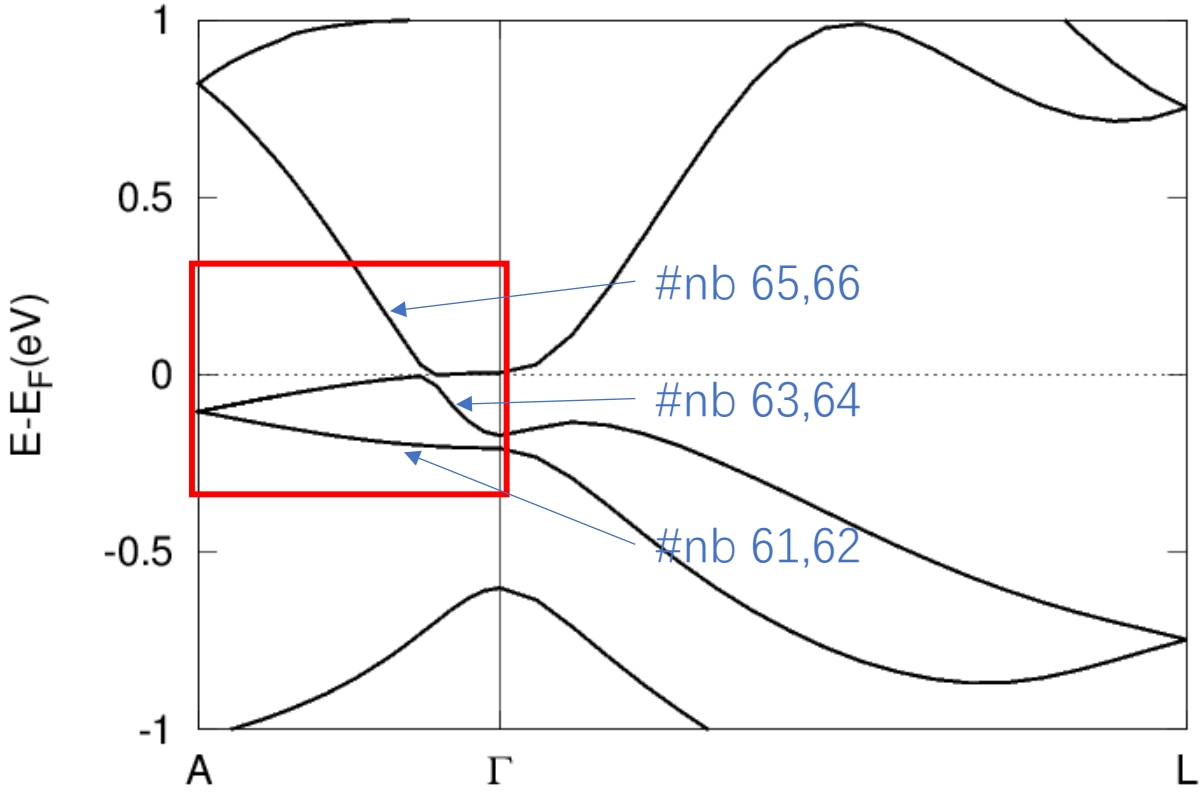
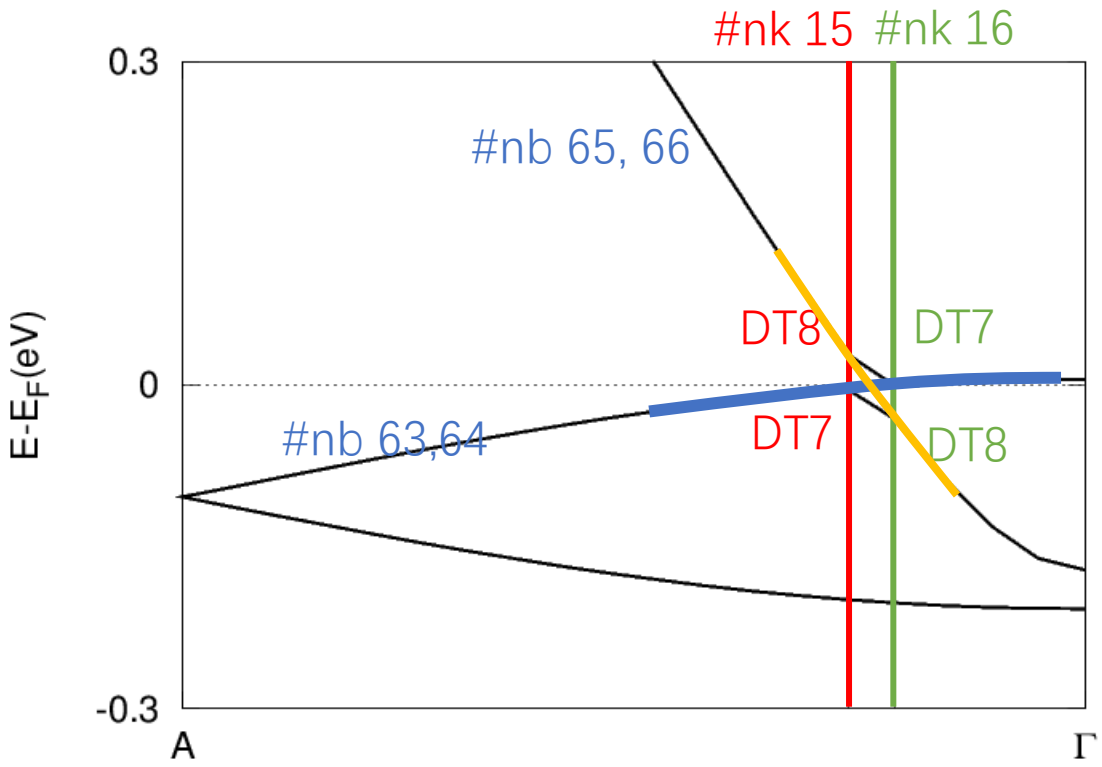
Through the analysis of the band structure, we find that there may be a band-crossing on the $A - \Gamma$ path near the Fermi energy.



We can see that the orders of BRs at No. 15 k-point and No. 16 k-point are different, so there is a symmetry-protected band-crossing on the $A - \Gamma$ path near the Fermi energy.

There is actually a Dirac point between #nk 15 and #nk 16.



IRVSP: Get Irreps in the band structures from VASP.

Step 1: Prepare the POSCAR file (taking Na_3Bi as an example).

Step 2: Symmetrize your POSCAR and get the atomic band representations (ABRs).

Step 3: do VASP scf and band calculations.

Step 4: Run IRVSP: read wavefunctions from WAVECAR and symmetry operations from OUTCAR to compute Irreps.

Make sure the following programs are compiled: phonopy, pos2aBR, vasp, irvsp
Enter EX_Na3Bi/vasp and run the following commands.

Shell commands

```
$ phonopy --symmetry --tolerance 0.01 -c POSCAR
$ pos2aBR > ABR.out
  ### do VASP scf calculation ###
$ cp INCAR.scf  INCAR (set “ISYM = 2; ICHARG =  2; LCHARG = .T. ”)
$ mpirun -np $ncpu $vasp_ncl  > out
  ### do VASP band calculation ###
$ cp INCAR.b  INCAR (set “ISYM = 2 ; ICHARG =  11; LWAVE = .T.”)
$ mpirun -np $ncpu $vasp_ncl  > out
  ### run IRVSP ###
$ irvsp –sg 194 –nb 61 66 > outdir1
$ vi outdir1
```

IR2TB: Get Irreps from tight-binding Hamiltonians.

Step 1: Prepare the POSCAR file (taking Na_3Bi as an example).

Step 2: Symmetrize your POSCAR and get the ABRs.

Step 3: Run IR2TB: read tbbox.in and soc_hr.dat to compute Irreps.

Make sure the following programs are compiled: phonopy, pos2aBR, ir2tb
Enter EX_Na3Bi/tb and run the following commands.

Shell commands

$ phonopy --symmetry --tolerance 0.01 -c POSCAR

$ pos2aBR > ABR.out

run IR2TB

$ vim tbbox.in (contains atomic orbitals, positions, k-points, lattice vectors and symmetry operations.)

$ vim soc_hr.dat (tight-binding Hamiltonian in Wannier90 format.)

$ ir2tb –sg 194 –nb 9 14 > outdir2

$ vi outdir2

IR2PW: Get Irreps in the band structures from QE.

Step 1: Prepare the POSCAR file (taking Na_3Bi as an example).

Step 2: Symmetrize your POSCAR and get the ABRs.

Step 3: do QE scf and band calculations.

Step 4: Run IR2PW: read wavefunctions from ./${outdir}/${prefix}.save and symmetry operations from ./nscf_b.out to compute Irreps.

Make sure the following programs are compiled: phonopy, pos2aBR, QE, ir2pw
Enter EX_Na3Bi/qe and run the following commands.

Shell commands

$ phonopy --symmetry --tolerance 0.01 -c POSCAR

$ pos2aBR > ABR.out

do QE scf calculation

$ vim scf.in (set “calculation = ‘scf’; verbosity = ‘high’”, put POSCAR_std in scf.in)

$ mpirun -np $ncpu $pw.x < scf.in > scf.out

do QE band calculation

$ vim nscf_b.in (set “calculation = ‘bands’; verbosity = ‘high’”)

$ mpirun -np $ncpu $pw.x < nscf_b.in > nscf_b.out

run IR2PW

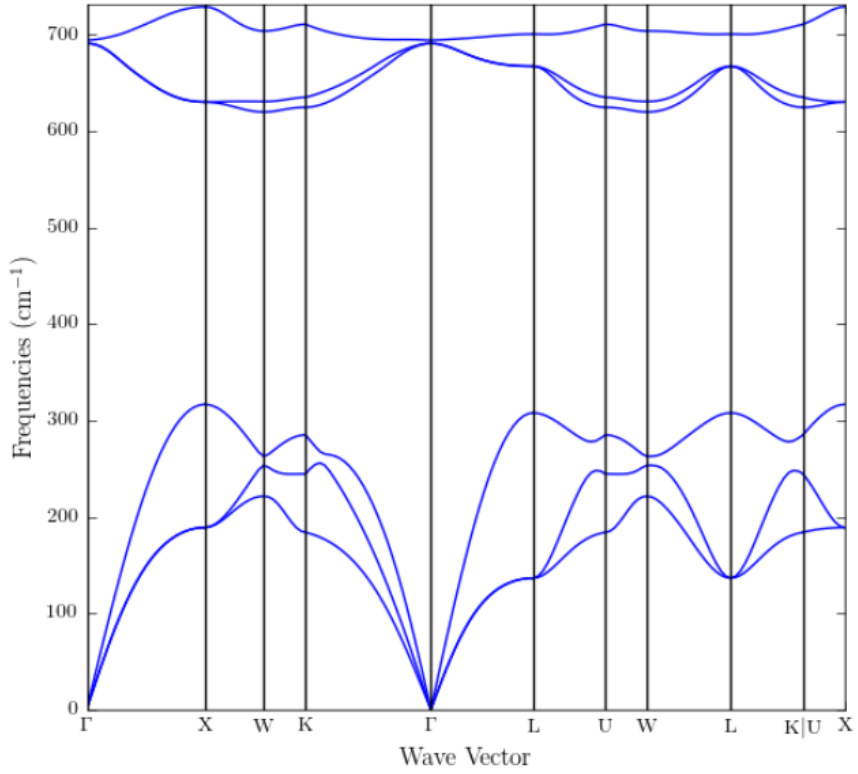
$ ir2pw –sg 194 –nb 81 86 > outdir3 (read nscf_b.out and /tmp/pwscf.save)

$ vi outdir3

3 Example 2: Get the phonon Irreps from BAs.

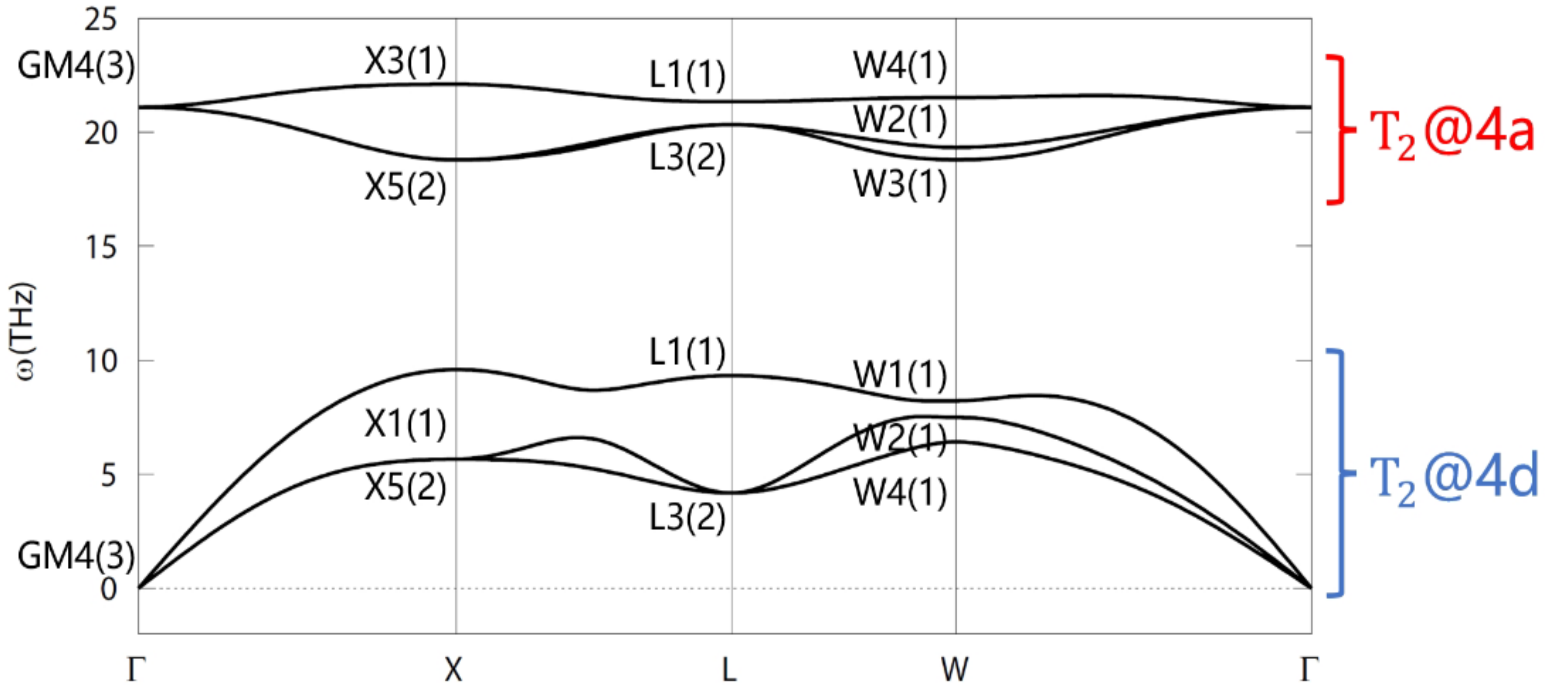
MATERIAL	ID:	DOI:
BAs	**mp-10044**	**10.17188/1185076**

- Here we take the BAs as an example to introduce how to calculate phonon Irreps by using IR2PH.



https://legacy.materialsproject.org/materials/mp-10044/

Atom	WKP(q)	Symm.	Vibrations(ρ)	ABRs(ρ@q)
B	4a (0,0,0)	$-43m$	$p_x, p_y, p_z : T_2$	T_2@4a
As	4d (3/4,3/4,3/4)	$-43m$	$p_x, p_y, p_z : T_2$	T_2@4d



Note that the gap of phonons can be understood as well-separated phonon modes. We can diagnose topological / unconventional at any well-separated phonon modes.

IR2PH: Get the phonon Irreps from QE.

Step 1: Prepare the POSCAR file (taking BAs as an example).

Step 2: Symmetrize your POSCAR and get the ABRs.

Step 3: do QE scf and phonon calculations and generate tbbox.in and ph_wf.dat.

Step 4: Run IR2PH: read tbbox.in and ph_wf.dat to compute Irreps.to compute Irreps.

Make sure the following programs are compiled: phonopy, pos2aBR, QE, ir2pw
Enter EX_BAs and run the following commands.

Shell commands

```
$ phonopy --symmetry --tolerance 0.01 -c POSCAR
$ pos2aBR > ABR.out
  ### do QE scf calculation ###
$ vim scf.in  (set “calculation = ‘scf’; verbosity   = ‘high’”)
$ mpirun -np $ncpu $pw.x < scf.in > scf.out
  ### do QE phonon calculation ###
$ mpirun -np $ncpu $ph.x < q${i}.inp > q${i}.out (${i}=0, 1, 2, 3)
  ### generate tbbox.in and ph_wf.dat ###
$ python dyn2wf.py 4
$ ./pwscf2tbbox.sh  216
  ### run IR2PH ###
$ ir2ph –sg 216 –nb 1 3 > outdir13
$ ir2ph –sg 216 –nb 4 6 > outdir46
```

Thank you !!!