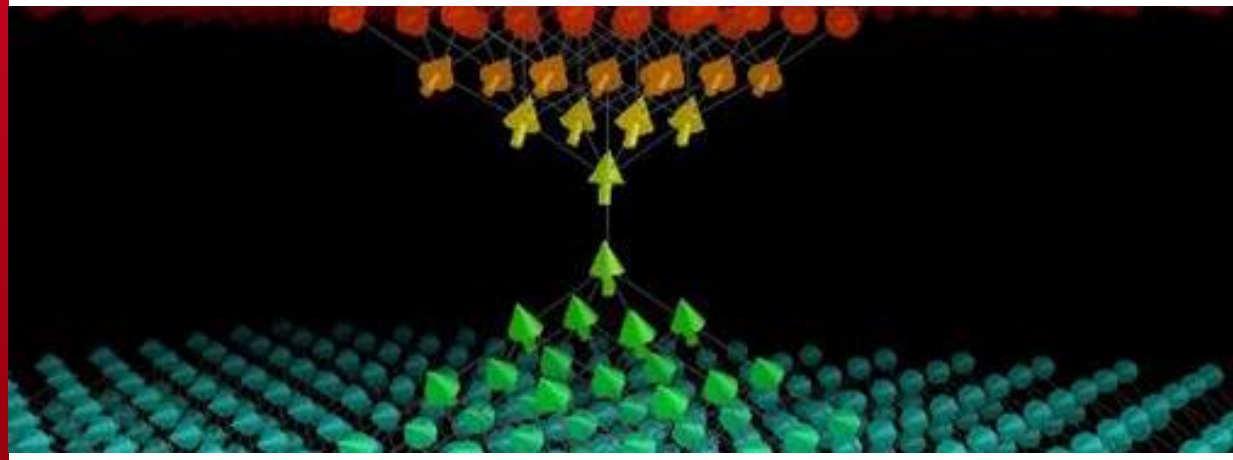
DE LA RECHERCHE À L'INDUSTRIE

(Paris, France)

(Copenhagen, Denmark)

MAGNETISM IN DFT
HANDS ON



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PREREQUISITE

- Create the directory july3 in your home directory

```
mkdir july3
```

- download the hands on of July 3 (named hands-on.tar) and save it to the july3 directory

Depending on the way you proceed you may have to untar your file

```
cd july3
tar -xvf hands-on.tar
```

This will generate a series of directories and files

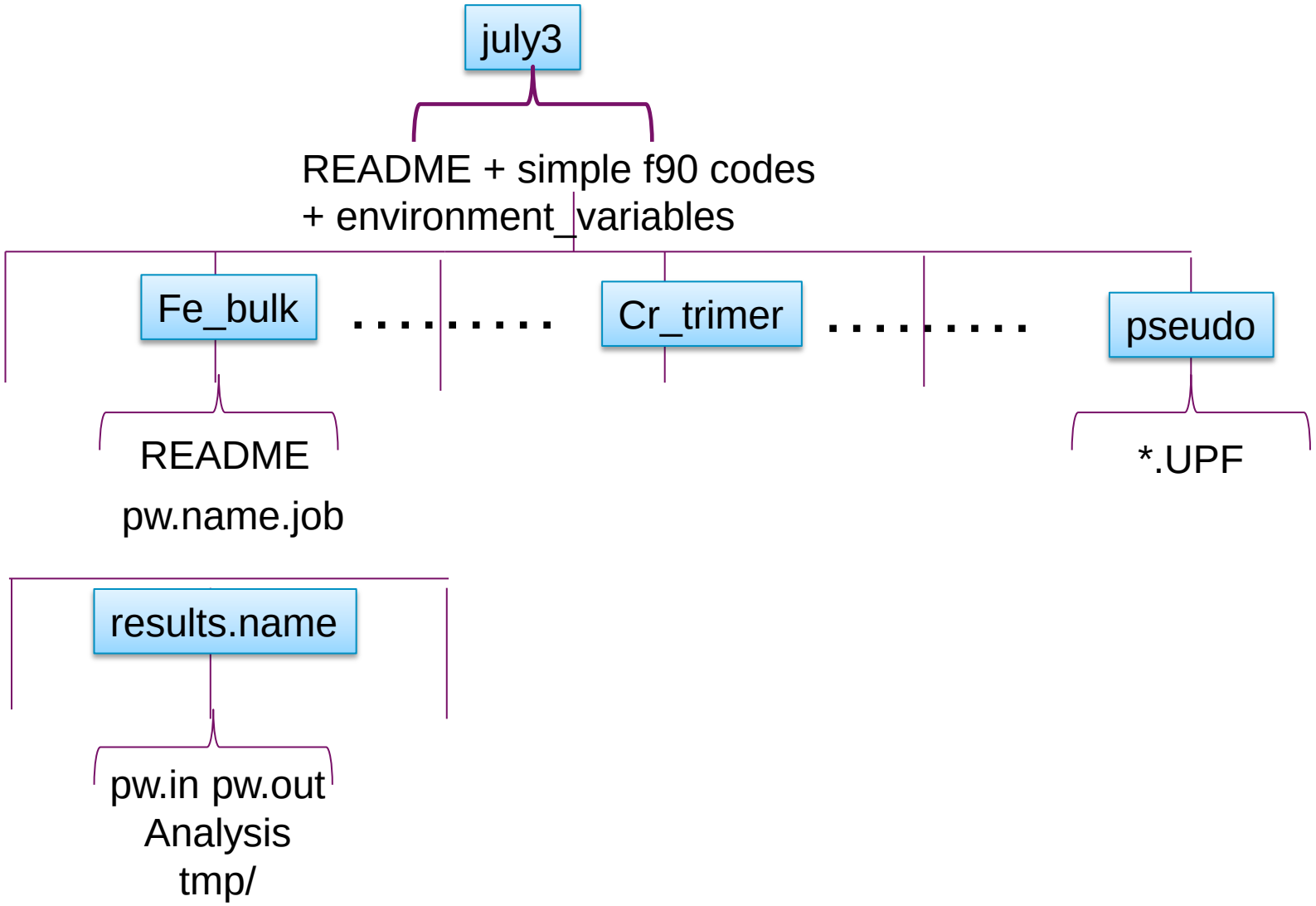
```
README      environment_variables      make_bands.f90

Fe_bulk/    Fe_surf/    Cr_bulk/    Cr_trimer/    Fe_wire/    pseudo/
```

- Compile the f90 code `make_bands.f90`

```
gfortran -o make_bands.x make_bands.f90
```

TREE OF DIRECTORIES



HOW TO RUN THE HANDS ON EXAMPLES

- Go into the first example directory `Fe_bulk`

```
cd Fe_bulk
```

- List the content of this directory by the command `ls`

open the README file where you will find all necessary instructions

```
gedit README
```

You will also find several files that are bash scripts with a generic name `pw.name.job`

```
pw.alat.job    pw.band.job    pw.dos.job    pw.fsm.job
```

The task of these scripts is it to generate a series of input for QE and subsequently runs QE with these inputs files.

- You can run the `pw.name.job` script by simply typing the command

```
./pw.name.job
```

QE will run in a directory named `results.name` which will contain the input and output files of QE as well as the `outdir` directory of QE `tmp/`

EXAMPLE 1

- Run `pw.alat.job`

```
./pw.alat.job
```

It should take a few minutes to run… be patient….

In the meanwhile….

- Go into `results.alat`

And look at what is going on for example check scf convergency or visualize the structure with xcrysden..

At the end of the run the script extract from pw.scf.out two quantities: total energy and magnetization for a series of lattice parameters that are saved in two separate files.

```
@# alat Etot
alat1 Etot1
alat2 Etot2
……..
alatN EtotN
```

You can then plot E(alat) and M(alat) with `xmgrace`

THANK YOU FOR YOUR ATTENTION

QUESTIONS?

COMMENTS?