Helpdoc &
QE emacs modes

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What is “helpdoc” ?

- a small utility in `dev-tools/` that transforms `INPUT_*.def` into `INPUT_*.html|txt` and `PWgui` help files, **etc.**

Why helpdoc ?

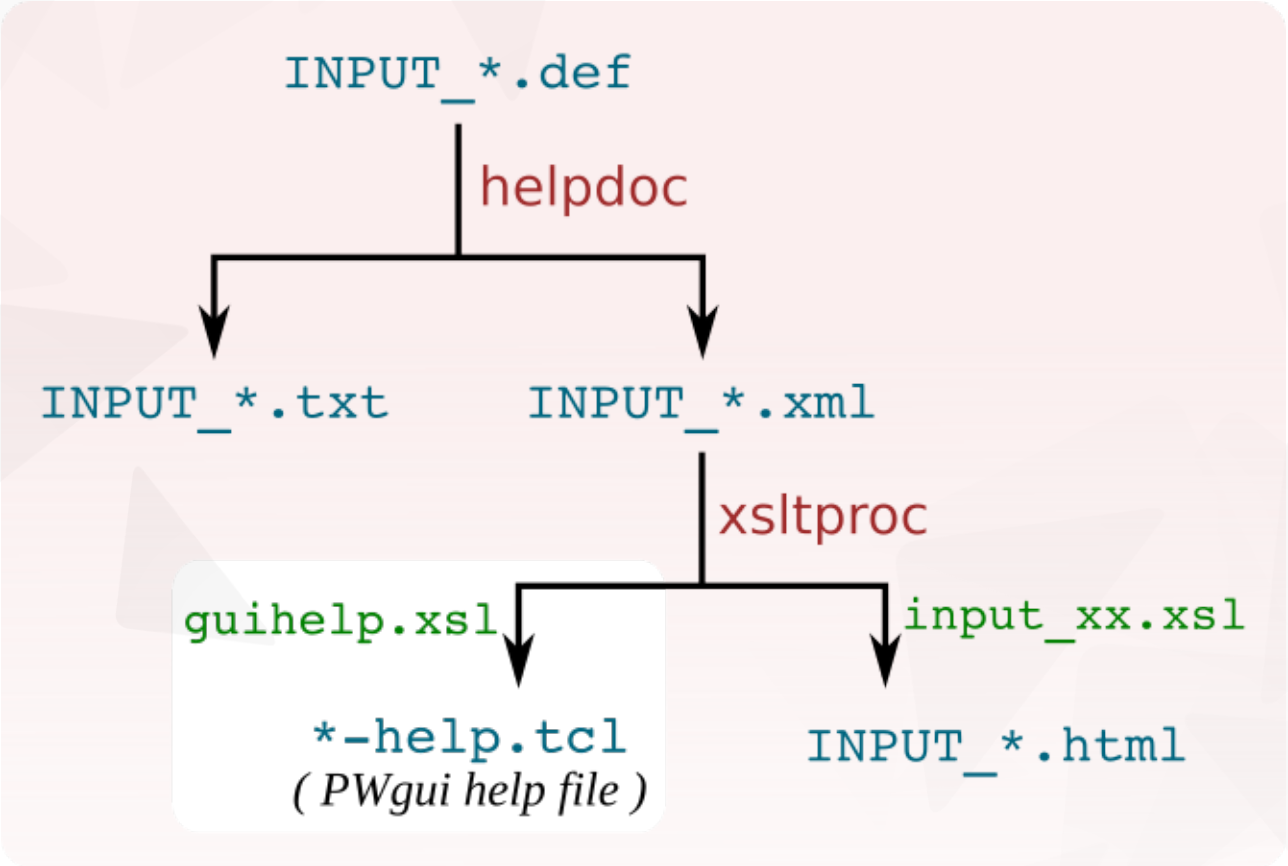
- in the “old” days the usage of a `*.x` program was explained with a plain text `INPUT_*` file

- Basic idea of **helpdoc:**
  - to make `INPUT_*` computer semantic → *this can be exploited in a number of ways*
  - to yield a more user friendly documentation

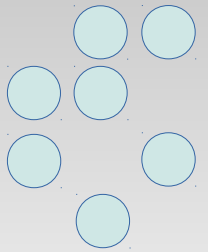
  - transformation of `INPUT_*` files should not involve much human effort

Helpdoc: how it works

- a small utility in `dev-tools/` that transforms `INPUT_*.def` into `INPUT_*.html|txt` and `PWgui` help files, **etc.**



Helpdoc's *.def markup



- *.def markup is more compact than XML markup

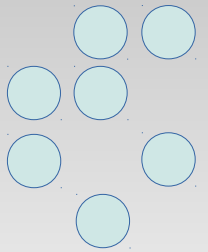
- **def:**

```
var etot_conv_thr -type REAL {
      default { 1.0D-4 }
      info {
         convergence threshold on total energy (a.u) for ...
      }
}
```

- **XML:**

```
<var name="etot_conv_thr" type="REAL">
      <default> 1.0D-4 </default>
      <info>
         convergence threshold on total energy (a.u) for ...
      </info>
</var>
```

Helpdoc's `*.def` markup



- **How to:**

  take an existing `*.def` file and use it as a template

- syntax is shortly explained in `dev-tools/README.helpdoc`

- syntax/structure is formally described by the schema: `dev-tools/helpdoc.schema`

Text is treated as pre-formatted

```
var wf_collect -type LOGICAL {
  default { .FALSE. }
  info {
        This flag controls the way wavefunctions are stored to disk :

        .TRUE.  collect wavefunctions from all processors, store them
                into the output data directory "outdir"/"prefix".save,
                ...

                .FALSE. do not collect wavefunctions, leave them in temporary
                        local files (one per processor). The resulting format
                        ...

        Note that this flag has no effect on reading, only on writing.
  }
}
```

ident is skipped

recommended width ~ 70 – 80 characters

wf_collect	LOGICAL
Default:	.FALSE.

```
This flag controls the way wavefunctions are stored to disk :

.TRUE.  collect wavefunctions from all processors, store them
        into the output data directory "outdir"/"prefix".save,
        ...

        .FALSE. do not collect wavefunctions, leave them in temporary
                local files (one per processor). The resulting format
                ...

Note that this flag has no effect on reading, only on writing.
```

Helpdoc: new features

- *option* variables: options can be semantically defined via `options`

```
var smearing -type CHARACTER {
    default { 'gaussian' }
    options {
      info { Available options are: }
      opt -val {'gaussian', 'gauss'} {
         ordinary Gaussian spreading (Default)
      }
      opt -val {'methfessel-paxton', 'm-p', 'mp'} {
         Methfessel-Paxton first-order spreading
         (see PRB 40, 3616 (1989)).
      }
      ...
    }
}
```

smearing	CHARACTER
Default:	'gaussian'

Available options are:

'gaussian', 'gauss' :
ordinary Gaussian spreading (Default)

'methfessel-paxton', 'm-p', 'mp' :
Methfessel-Paxton first-order spreading
(see PRB 40, 3616 (1989)).

'marzari-vanderbilt', 'cold', 'm-v', 'mv' :
Marzari-Vanderbilt cold smearing
(see PRL 82, 3296 (1999))

Helpdoc: new features

- the following are automatically turned into hyperlinks:

```
PRB 40, 3616 (1989)
PRL 82, 3296 (1999)
arXiv:cond-mat/0504077
doi: 10.1038/srep24603
http://www.quantum-espresso.org/
```

- `@`-prefixed tags within the text, i.e.: `@tag { text }`
  - hyperlinks:

    `@ref identifier` *(identified = variable, namelist, card name)*
    `@link document` *(document = external file, web-page)*

  - primitive HTML tags for fancier formatting: `@b`, `@i`, `@u`, `@br`, `@hr`, `@p`

Helpdoc: @*tag* example

```
var ion_dynamics -type CHARACTER {
  options {
    info {
       See also: @link README.ion_dynamics

       @b CASE ( @ref calculation == 'relax' )
    }
    opt -val 'bfgs' {
       @b (default) use BFGS quasi-newton algorithm,
       based on the trust radius procedure, ...
    }
    ...
  }
}
```

ion_dynamics CHARACTER

See also: README.ion_dynamics

CASE (calculation == 'relax')

'bfgs' :
(default) use BFGS quasi-newton algorithm,
based on the trust radius procedure,
for structural relaxation

'damp' :
use damped (quick-min Verlet)
dynamics for structural relaxation

Various usage of helpdoc

- `INPUT_*.def` files can be exploited in a number of ways

(1) **html** description of input files ✓

(2) semi-automated updating of **PWgui** ✓

(3) templated automatic generation of **QE emacs modes** ✓

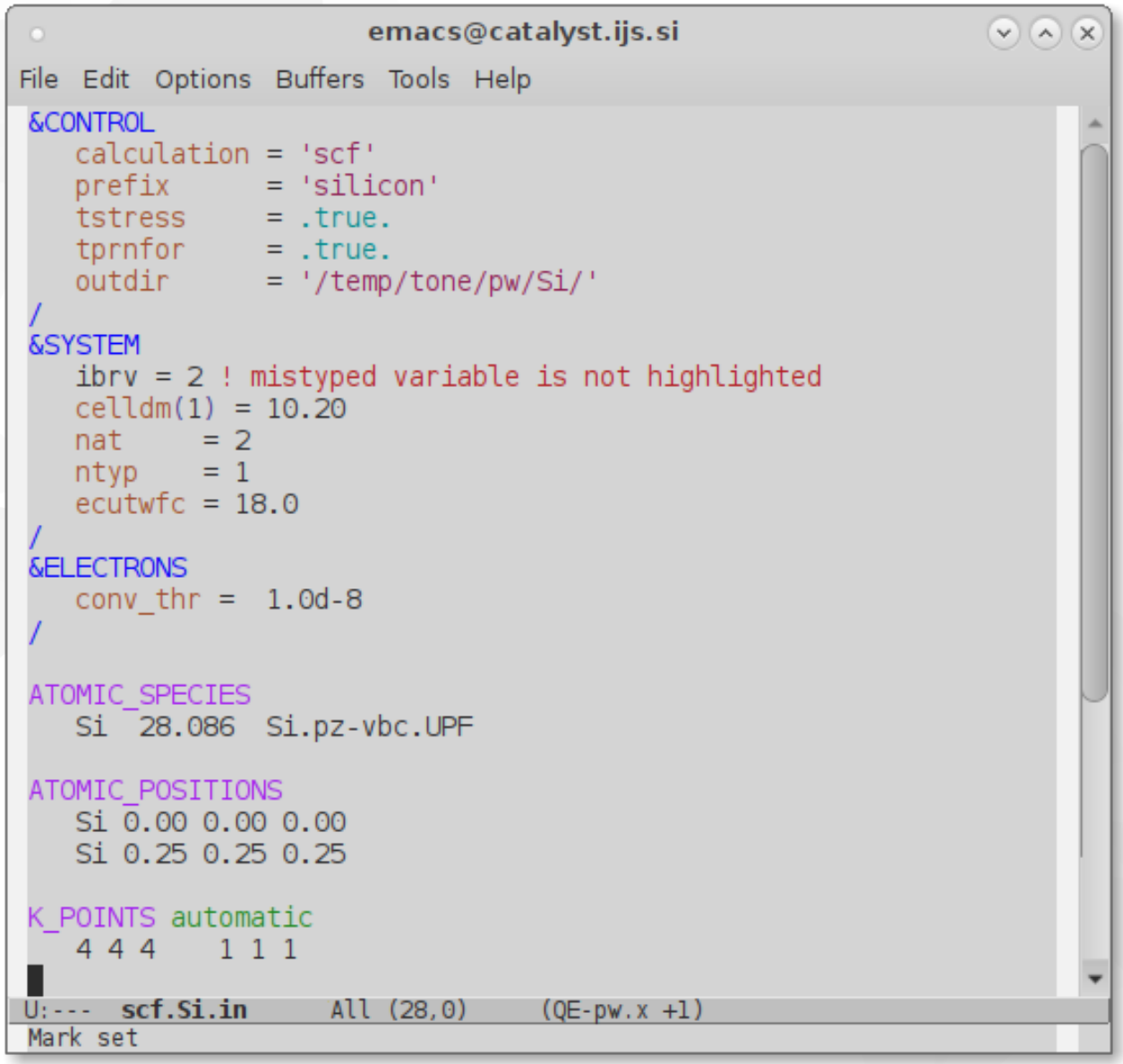
(4) semi-automated updating of **pwtk** (scripting interface for PWscf)

QE emacs modes

- *a collection of **Emacs** major-modes for making the editing of **Quantum ESPRESSO** input files easier and more comfortable with Emacs*

- `syntax-highlighting`
- `auto-indentation, auto-completion`
- `several utility commands`

QE emacs modes



QE emacs modes

- available modes:

  specific: `pw, neb, cp, ph, ld1, pp`

  generic: `qe`

- some useful commands:
  - `M-X prog-insert-template`
    (currently available for: `pw, neb, pp, projwfc, dos, bands`)
    Notice: *exemplar inputs required for other programs !!!*

  - `M-X prog-NAMELIST`
  - `M-X prog-CARD`
  - `M-X prog-variable`

Thank you for your attention !