

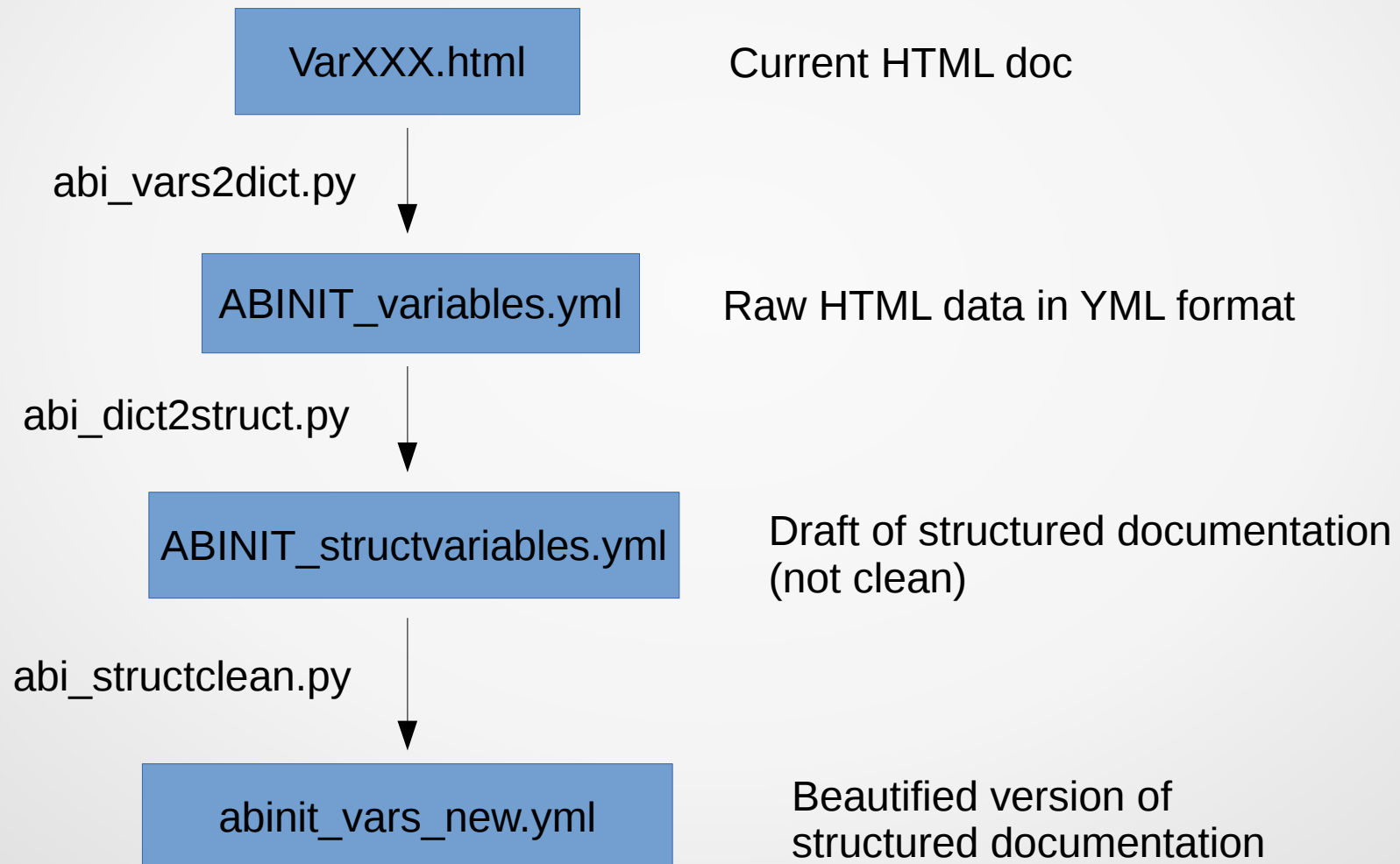
Beautification 2015: Towards a structured documentation

From HTML → YAML

01/10/2014 : Correction !

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What is already done ...



What is already done (2) ...

...



abinit_vars_new.yml

Beautified version of
structured documentation

AUTOMATIC

Then, I started cleaning stuff ...

abinit_vars.yml

MANUAL

What should you do ?

- 1) Correcting current `abinit_vars.yml` (today !)
- 2) Cleaning `abinit_vars` (afterwards)

GUI

You can modify
abinit_vars.yml
by hand !

And/or

Use the GUI...

- `java -jar Abivars.jar (`
`java -jar Abivars.jar n`

Live DEMO !

The screenshot shows a window titled "Input variables" with a menu bar containing "File" and "Edit". On the left is a list of variables, with "iatsph" selected. The main area displays the configuration for "iatsph":

Name	iatsph	Edit
Section	vargs	Edit
Default	[1.. natsph]	Edit
	Comment: null	See error Del error
Dimensions	null	Edit
	Comment: null	See error Del error
Type	integer	Edit
Mnemo	Index for the ATomic SPHeres of the atom-projected density-of-states	Edit
Category		Edit
Description	This input variable is active only in the prtDOS=3 case or if pawfatbnd=1 or 2. It gives the number of the natsph atoms around which the sphere for atom-projected density-of-states will be built, in the prtDOS=3 case. The radius of these spheres is given by ratsph . If pawfatbnd=1 or 2, it gives the number of the natsph atoms around which atom-projected band structure will be built.	Edit

YML specifications

- !variable
 - defaultval
 - text: description of the variable (in HTML)
 - dimensions
 - ...
 - varname: 'myvariable'

YML specifications : general things

- All the links to a variable should become '[[varname]]'
- !TODO for cleaning part : check and transform all
varname to '[[varname]]'

Values : dimensions

- If value is a scalar => dimensions: 'scalar'
- Else, should be a list of value.

Example: for `rprimd(3,3)`, should become

- 3
- 3

Example: for `xred(natom,3)`, should become

- '[[natom]]'
- 3

- dimensions: null is reserved for errors in principle (ask me if you need something else !)

Values : dimensions

- Only use simple formulas for expressions
- max, abs, ... + - * /
- Because we want to be able to parse it !
- If you needed something 'non-standard', please tell me !
- Example: dmatpawu
 - $2 * \max([\text{lpawu}]) + 1$
 - $2 * \max([\text{lpawu}]) + 1$
 - $\max([\text{nsppol}], [\text{nspinor}])$
 - $'[\text{natpawu}]'$

Values: defaultval

- Defaultval: null means there is No default !
- There might be default value depending on other variables
 - => Use !valuewithconditions (see after)
- There might be range of values
 - => Use !range (see afterwards)
- There might be list of values => use YAML list syntax:
 - val1
 - val2
- Otherwise should be expressions

Values: defaultval

- You can use !valuewithconditions
- Is a dictionary:

!valuewithconditions

defaultval: 'value by default'

cond1: 'val1'

cond2: 'val2'

Values: defaultval

- Example, diemixmag:
- HTML code was : Default is diemixmag= diemix when iprcel=0 or $70 < \text{iprcel} < 80$ or $\text{iscf} < 10$ (SCF mixing on potential), else diemixmag= - diemix
- Should be replaced by:

!valuewithconditions

defaultval: -[[diemix]]

' $70 < \text{[[iprcel]]}$ and $\text{[[iprcel]]} < 80$ ': '[[diemix]]'

' $\text{[[iscf]]} < 10$ ': '[[diemix]]'

' $\text{[[iprcel]]} == 0$ ': '[[diemix]]'

„SELECT CASE“ spirit:

Takes the first condition that is true
Else take defaultval

Default

```
if 70 < iprcel and iprcel < 80 : diemixmag = diemix  
else if iscf < 10 : diemixmag = diemix  
else if iprcel == 0 : diemixmag = diemix
```

Comment: null

Ed

See e

Del e

Values: defaultval

- You can also use !range:

!range

start: 1

stop: N

- Example iatsph
- Html code was 1, 2, ... `natsph`
- Should be replaced by:

!range

start: 1

stop: '[[natsph]]'

How to tackle problems

- In general, use comments to describe the default value or the dimensions of the variable.
- Try not to use comments unless it is really needed for the human being to understand
- Conflicts or Requirements are not tackled yet by this YML file
 - Explicit them in comment :
 - requires: [[varname]]
 - requires: CONDITION
 - excludes: [[varname]]
 - excludes: CONDITION
- If the value is related to the way Abinit is compiled
 - MPI_IO, ETSF_IO, ... might be CONDITION in „requires, excludes, everywhere“
 - MPI_IO, ETSF_IO, ... are compilation flags

Check the HTML !

- Afterwards, you can try 'abi_struct2html'
- `python abi_struct2html [-f file_name.yml]`
- It generates html files in 'html_output/'
 - ABINIT_allvariables.html : link to all variables
 - ABINIT_varXXX.html : variables by category
- The links have been replaced by html links, everything should work
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- NB: you need pyyaml