A new test system for Abinit

Bottom-up approach on structured data

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Why do we test ?

We have to test to

- Find bugs
- Grant quality of the physical results
- Prevent breaking old features working on new ones

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The need of a new comparison method

Caracteristics of the current comparison method

- Linear comparison of lines
- Extracting of every floating point and individual comparison
- One tolerance, used as absolute and relative, for the whole test
- Auxiliaries tolerances used if the main one is not respected

Strength :

- Systematic/comprehensive top-down approach
- Strict by design
- Does not require specific format of the output, except for the first character of the line
- Just work ™

Flaws :

- Linear analysis fail if the number of significant line differ
- Unaware of physics
- Hardly any extension possibilities
- Very rigid configuration leads to weakening the whole test when a few lines are hard to get right

Some quantitative insight

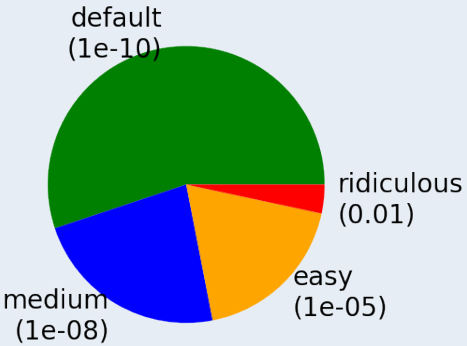
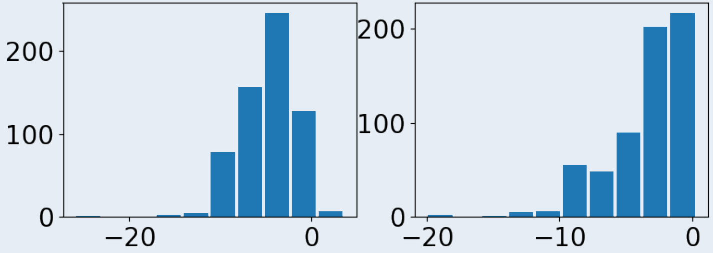


Figure: Repartition of the main fldiff tolerances in the pool of tests



Repartition of the auxiliary tolerances in the pool of tests:
(left) $\log_{10}$ of absolute tolerance, peak between -5 and -2
(right) $\log_{10}$ of relative tolerance, peak between -1.5 and 0

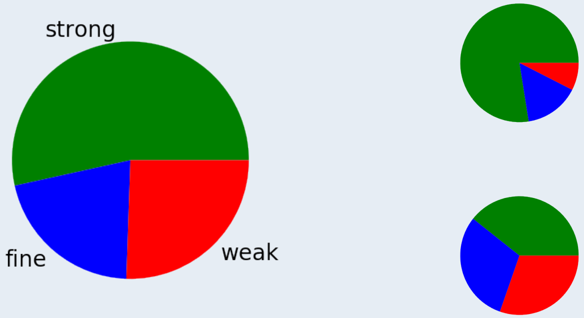


Figure: "Quality" of tests according to their tolerances (left: all, top right: v3 only, bottom right: v8 only)

The solution proposed

Caracteristics of the new comparison method

- Based on structured data in the form of YAML documents embeded in the main output file
- YAML documents produced by Fortran
- Bottom-up approach
- Configured with a separate file also written in YAML
- Aware of the "iteration state"
- Testing side written in Python and integrated with the existing testsuite
- Integration of Numpy and Pandas

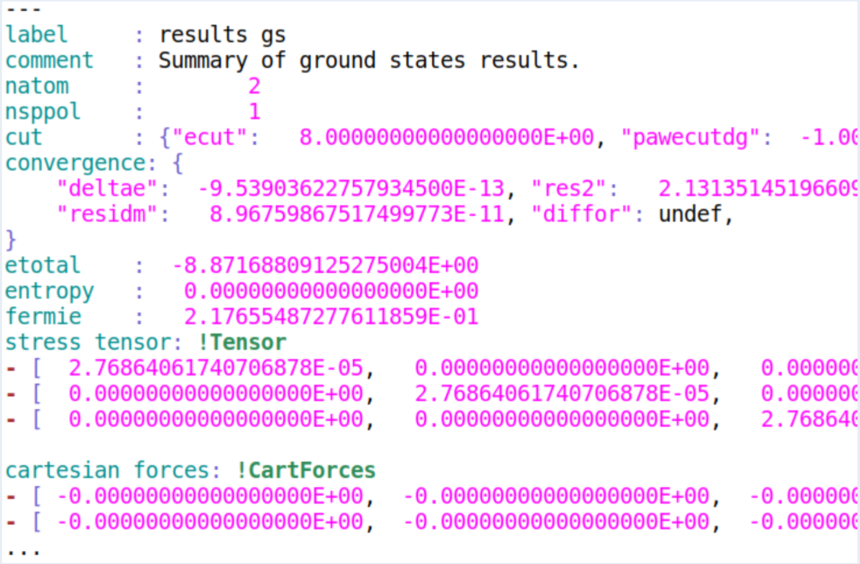
Strength:

- Great flexibility
- Open lots of new possibilities
- Backward compatible: YAML documents can be ignored and the test bot will behave as it did before
- Allow physics aware analysis
- Matching of tester and reference documents is done through label and iteration state

Flaws:

- Ask for more configuration when enabled
- Have to be configured for each test and each physical quantity
- Brand new, need real world testing

The two methods are complementary and will be used together.



```
---
label       : results gs
comment     : Summary of ground states results.
natom       :         2
nsppol      :         1
cut         : {"ecut":   8.00000000000000000E+00, "pawecutdg":  -1.00
convergence: {
    "deltae":  -9.53903622757934500E-13, "res2":   2.13135145196609
    "residm":   8.96759867517499773E-11, "diffor": undef,
}
etotal      :  -8.87168809125275004E+00
entropy     :   0.00000000000000000E+00
fermie      :   2.17655487277611859E-01
stress tensor: !Tensor
- [  2.76864061740706878E-05,   0.00000000000000000E+00,   0.000000
- [  0.00000000000000000E+00,   2.76864061740706878E-05,   0.000000
- [  0.00000000000000000E+00,   0.00000000000000000E+00,   2.768640

cartesian forces: !CartForces
- [ -0.00000000000000000E+00,  -0.00000000000000000E+00,  -0.000000
- [ -0.00000000000000000E+00,  -0.00000000000000000E+00,  -0.000000
...
```

Figure: Example of a YAML document in ABINIT output

Producing a YAML document on the Fortran side

Two level of API:

- `m_neat`: high-level API, should be called in computations routines
- `m_yaml_out`:low-level API, actually produce YAML documents, supposed to be called only from `m_neat`.

Additional toolboxes:

- `m_stream_string`: variable-size string type, can be used as a buffer to build a YAML document
- `m_pair_list`: structure to store key-value pairs, keys are strings and values integers, real numbers or strings.

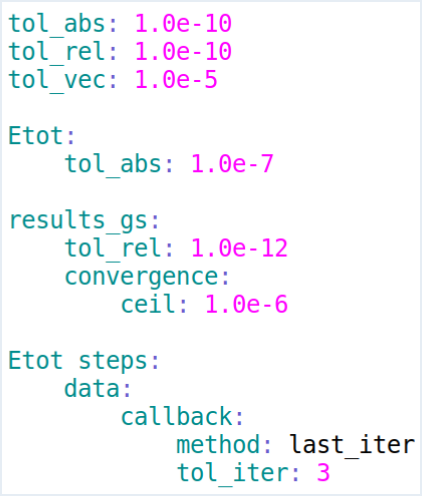
1. Use `m_pair_list` to store values as the computation go on:
   ```
   call pl%set("Etot", r=etot_val)
   ```
2. Pass data to a `m_neat` routine you wrote before
3. It will call `m_yaml_out` routines to build a document and use `stream_wrtout` to output it
   ```
   call yaml_single_dict("Etot", "", pl, 30, 100, stream=mydoc)
   call stream_wrtout(mydoc, iout)
   ```

Python-side entry points

- Input file TEST_INFO section and YAML test configuration
- `structures.py`
- `conf_parser.py`

YAML FILE

Actual test configuration belongs here. Define the rules for each piece of data and the logic of the test.

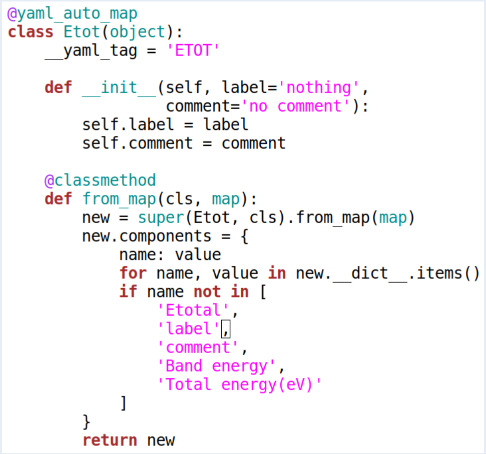


```yaml
tol_abs: 1.0e-10
tol_rel: 1.0e-10
tol_vec: 1.0e-5

Etot:
    tol_abs: 1.0e-7

results_gs:
    tol_rel: 1.0e-12
    convergence:
        ceil: 1.0e-6

Etot_steps:
    data:
        callback:
            method: last_iter
            tol_iter: 3
```

Figure: An example of YAML configuration file

Tags and structures

YAML provides facilities to have specialized logic for some data structures.

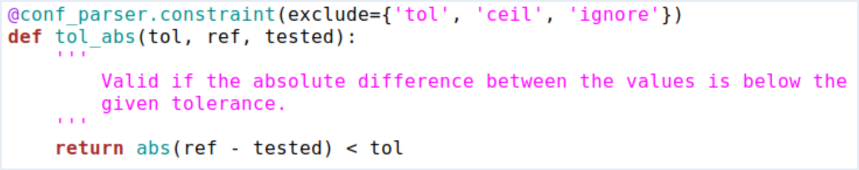


```python
@yaml_auto_map
class Etot(object):
    __yaml_tag = 'ETOT'

    def __init__(self, label='nothing',
                 comment='no comment'):
        self.label = label
        self.comment = comment

    @classmethod
    def from_map(cls, map):
        new = super(Etot, cls).from_map(map)
        new.components = {
            name: value
            for name, value in new.__dict__.items()
            if name not in [
                'Etotal',
                'label',
                'comment',
                'Band energy',
                'Total energy(eV)'
            ]
        }
        return new
```

Figure: Example of a structure definition

Constraints and parameters

Here are defined the rules used in YAML configuration file.
The actual comparison functions (constraints) belong here as well as their parameters declarations.



```python
@conf_parser.constraint(exclude={'tol', 'ceil', 'ignore'})
def tol_abs(tol, ref, tested):
    '''
        Valid if the absolute difference between the values is below the
        given tolerance.
    '''
    return abs(ref - tested) < tol
```

Figure: Example of constraint definition

What is coming next

We need you !

How you can help:

- Read the documentation (located at `~abinit/doc/developers/new_testsuite.md`), give us feedback on it
- Add YAML testing to your old tests
- Use YAML testing in your new tests

New opportunities

- Parameterized tests
- Test starting from precomputed binaries
- Strongly noisy tests giving stable processed quantities
- New processing in test (linear regression, statistics, simpler consistency tests...)

I want to express my gratitude to Jean-Michel Beuken for his help with the test farm and the building process of ABINIT. I also want to thank Matteo Giantomassi and Xavier Gonze for giving me the possibility of doing this work and for their supervision.

Thank you for your attention !

Questions ?