

A new test system for ABINIT, bottom-up approach on structured data

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As a big open source project ABINIT need facilities to ensure the stability of its features. These facilities take the form of around a thousand tests checking numerical precision of a specific feature. The historic program running tests use a naive line by line algorithm comparing each floating point value on each line. This method has its advantages but also have some limitations.

During my internship at MODL/UCLouvain I have been working on a brand new system for writing and running tests in a bottom-up fashion that addresses the limitations of the old style testing method. Those tests are based on two key concepts. First, they work on structured machine-readable data written in YAML in the ABINIT output file. Second they are defined by a flexible configuration file also based on YAML.

I will present the principles of this new system and the implications on the ABINIT developer work flow. The goal is also to collect feedback from the ABINIT community. This work aims at helping improving the overall quality of ABINIT and at providing the tools for a new approach of the validation of ABINIT features.