



AiiDA and YAMBO, current status and developments.

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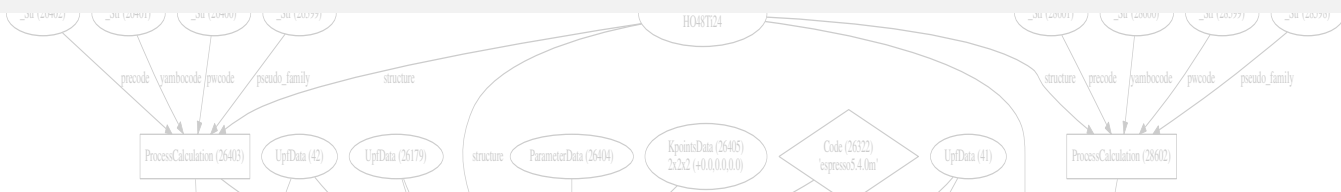
2017



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Contributors

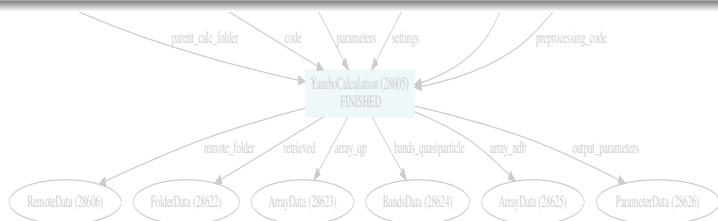


People

- 1 Michael Atambo (CNR-NANO)
- 2 Andrea Ferretti (CNR-NANO)
- 3 Antimo Marrazzo (EPFL)
- 4 Prandini Gianluca (EPFL)
- 5 Contributions from Henrique Miranda (from related yambopy project) [Univ of Luxembourg].

Can be obtained at

- 1 https://bitbucket.org/prandini/yambo_input
- 2 https://bitbucket.org/prandini/yambo_parser
- 3 Also take a look at MAX deliverable D3.2 (Month 12)



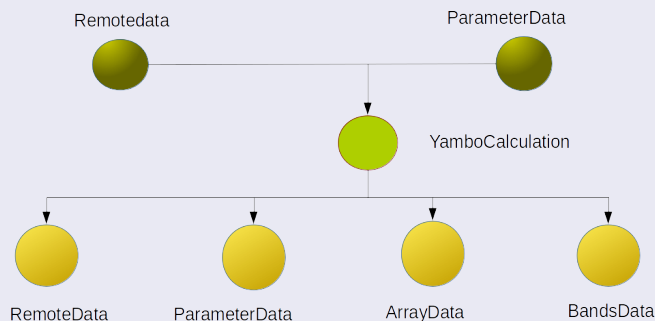
Internal Design

Input

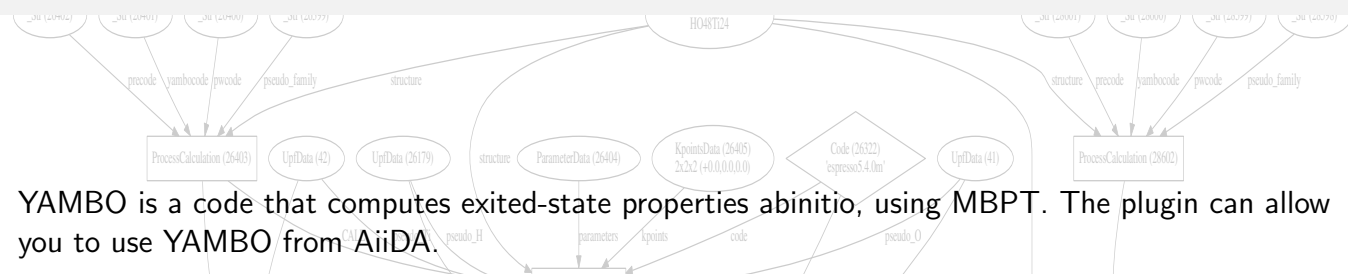
- 1 Inputs passed in as Key-value pairs,
- 2 No duplication of yambo input directives in AiiDA plugin code.
- 3 Yambo can add/remove directives without changes to input generation code (ease of maintenance)

Output

- 1 Parses Report files, and databases after a calculation, stores the result.



Current Status

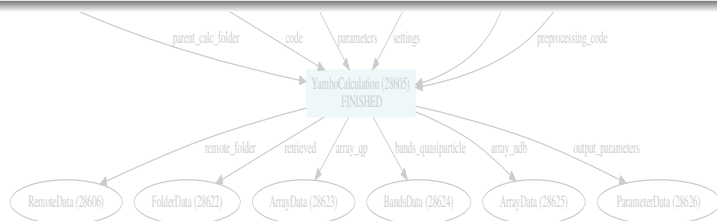


Present Functionality in the (Input) Plugin

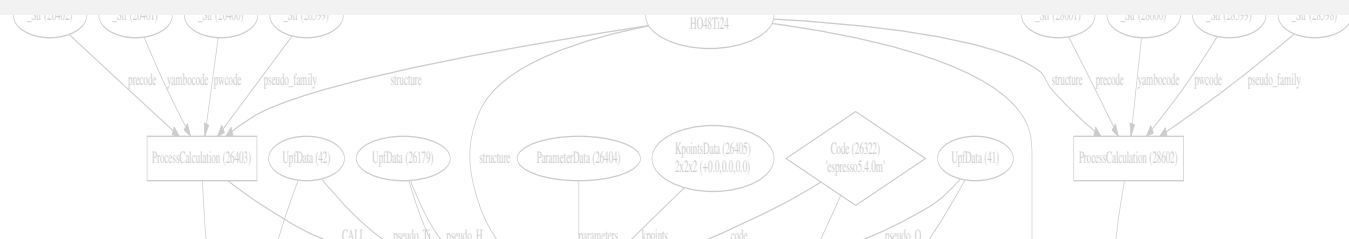
- 1 Support for RPA (response function) computations.
- 2 Support for COHSEX QP corrections.
- 3 Support for GW (Plasmon Pole Approx.) QP corrections.
- 4 Fine grained control of the files retrieved after calculations.

Present Functionality in the (Output) Plugin

- 1 Parsing YAMBO report file (BandsData, Calculation state).
- 2 Parsing YAMBO NetCDF database files (these files have full precision numerical results).



Future Enhancements and Maintenance

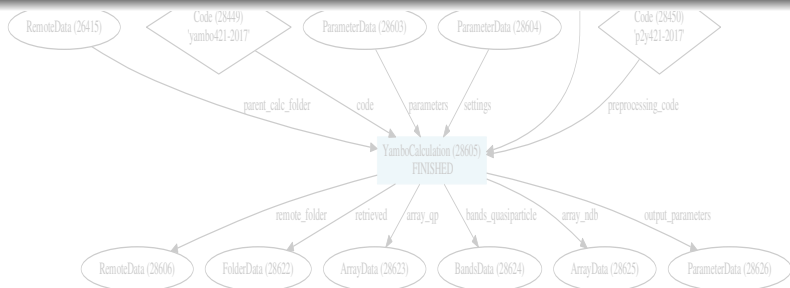


Planned features

- 1 Adding support for BSE (optics) computations with Yambo.
- 2 Adding support for RA (full frequency) computations with Yambo.
- 3 New tool to extrapolate GW QP corrections over convergence parameters (to be used within workflows).

Maintenance

- 1 Output parser will be maintained and updated to reflect changes to YAMBO Database format (foreseen).



YAMBO Workflows

Basic Workflows

- 1 YamboWorkflow: supports PW inputs runs SCF+NSCF+GW with restarts for interrupted calculations,
- 2 This work is still ongoing.
- 3 Also automatic restarts (for interrupted jobs) will be supported by the workflows.

Advanced Workflows:

- 1 YamboConvergenceWorkflow: Automates convergence tests for GW calculations, using YamboWorkflow as a sub workflow.
- 2 This will involve deeper considerations about convergence parameters and thresholds for GW Quasiparticle corrections.

End User Solutions

- 1 Development of ROBUST interface for users that just works.
- 2 Example: Given a structure, the workflow should provide as output the converged GW band gap.

Technical Challenges

- 1 A methodology to give end users and estimate of the required CPU and memory resources given a structure.
- 2 New AiiDA workflow API (may mean changes to the plugin).
- 3 Yambo converter (p2y), needed careful handling until it supports parallization, (recently solved).