Technical aspects related to high-throughput calculations with ABINIT.

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In this talk, I will present the approach employed in AbiPy to implement automatic ABINIT calculations. More specifically, I will discuss how we employ YAML and netcdf files to exchange information between Fortran and Python, the logic used in AbiPy to parallelize and optimize calculations at runtime and the protocol used to handle possible errors during the ab-initio computation. I will also discuss how to use the Fortran API of ABINIT to generate netcdf files that can interoperate seamlessly with our high-throughput infrastructure. In the last part, I will present some of the technical problems we are still facing and discuss possible approaches to address these issues.