Extension of the computation of density to non-diagonal band occupations with the KGB parallelization

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As it solves a model corresponding to a perturbed Hamiltonian, DMFT produces non-diagonal occupations (in the band space) when converting the results to the DFT Kohn Sham band space. Non-diagonal occupations were an obstacle to use DMFT with the KGB parallelization because of the required mixing of Kohn Sham bands that are not available to the current MPI process. As a consequence DMFT computation were before this work only possible with the simpler and less efficient K parallelization.
My first master internship was dedicated to the extension of the existing code to solve this problem. I implemented alongside the density computation the possibility to use non-diagonal occupations even in the case where only a subset of the bands are available to a given process.
After a few reminders on the parallelization modes of Abinit and the way wave functions are distributed among processors, I will present the way I solved this problem, using natural orbitals in one case, and point-to-point communications in another case. I will then exhibit the effect of my work on computations on large systems. This work opens the door to studies of multi-atoms problems like phonons or defects with DFT+DMFT. It could also be used to implement further methods implying the use of non-diagonal occupations in Abinit.