O.29 Memory parallelization of DFPT in Abinit

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The solution of the Sternheimer equation allows the variational calculation of the second order derivative of the total energy.

$$P_{I^\perp}(H^{(0)} - \epsilon_i^{(0)})P_{I^\perp} \mid \psi_i^{(1)}\rangle = -P_{I^\perp}H^{(1)} \mid \psi_i^{(0)}\rangle \tag{O.1}$$

where $P_{I^\perp}$ is the projector on the subspace orthogonal to the ground state valence electrons. In Abinit this is exploited, starting from a DFT $H^{(0)}$, to calculate many response properties such as phonon frequencies and dielectric constants. The Sternheimer equation is simple to parallelize over bands i, as the orthogonality condition for $\psi_i^{(1)}$ is defined by projection on the (fixed) $\psi_j^{(0)}$ (instead of the habitual O(N^3) algorithms to orthonormalize a set of vectors). Up to version 9.1, however, this level of parallelization was only over the work load: the wave functions for all bands were present on all of the processors for a given k-point. For large systems this quickly explodes the available memory, and does not scale to HPC.

I will present the modifications made to the DFPT part of Abinit to enable memory parallelization as well, with some of the intricate re-distribution of work arrays, to ensure the orthogonalization and matrix element calculations (ie all operations involving two band indices) are carried out in a distributed manner. In this way the allocated memory for wavefunctions is rapidly decimated. The next steps to further distribute DFPT grids on very large systems and HPC architectures will be discussed as a perspective.