Acceleration of the transcorrelated method for solids KEITARO SODEYAMA, MASAYUKI OCHI, University of Tokyo, REI SAKUMA, Chiba University, SHINJI TSUNEYUKI, University of Tokyo — To calculate the electronic structures of solids including electron correlation effects, we have developed the transcorrelated (TC) method. In the TC method, a many-body wave function is represented by a correlated wave function $F\Phi$, where $\Phi$ is a single Slater determinant and $F$ is a Jastrow function, $F = \exp[-\sum_{i<j} u_{ij}]$. $u_{ij}$ is a two-body function called Jastrow factor. The many-body Hamiltonian $H$ is similarity transformed to an effective Hamiltonian $H_{TC} = F^{-1}HF$ with up-to-three-body interaction. One-electron orbitals in the Slater determinant $\Phi$ and their orbital energies are optimized by solving a set of Hartree-Fock-like single particle equations derived by minimizing the variance of the $H_{TC}$. We have confirmed that the total energy calculations for solids using the TC method were feasible enough to determine the lattice constants and bulk moduli. However, it required a lot of computational time for solid that scales as $O(N_k^3 N_{\text{band}}^4)$. In this presentation, we will demonstrate that the CPU cost can be reduced by orders of magnitude after revising the algorithm.