A new massively parallel version of CRYSTAL for large systems on high performance computing architectures

The paper aims to address the scalability of the CRYSTAL code with respect to the number of cores and system size, providing end users with criteria for resource allocation and facilitating the tailoring of in-house computing facilities for different research groups. The hypothesis is that the new massively parallel version of CRYSTAL will exhibit good scalability with both system size and the number of cores.

The paper demonstrates that the new massively parallel version of CRYSTAL shows very good scalability with the number of cores at a fixed system size. It also provides insights into the performance of CRYSTAL for different HPC architectures and offers guidance on the number of cores to be used for MPPCRYSTAL runs.

The study involves internal tests to assess the scalability of the code with the system size and the number of cores. It also includes a comparison of the performance of different HPC architectures and the impact of different functionals on the computational efficiency.

The paper acknowledges the quadratic scaling with the system size for cells containing more than 200 irreducible atoms, which poses a limitation to the current version of the code.

The paper points out the need for major interventions on the code to address the quadratic scaling issue, particularly in revisiting the loop structure in the main routines, and the difficulty in disentangling the Fock diagonalization dependence on the system size.

The ideas presented in the paper have significant implications for potential applications in the field of computational chemistry and solid-state physics. The improved scalability of the new massively parallel version of CRYSTAL opens up opportunities for performing total energy calculations for systems with a relatively large size and for exploring future scopes in the development of the code to achieve linear scalability with respect to both the system size and the number of cores.

The paper concludes that the new massively parallel version of CRYSTAL is well-behaved in terms of scalability with the number of cores at a fixed system size. It also highlights the linear scaling for systems up to 200 atoms in the unit cell and the quadratic scaling for larger systems. The conclusion also outlines the ongoing and planned work to address the limitations of the code.