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Towards ab initio simulation of solid state materials at 10 nm scale[1] YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, G. MALCOLM STOCKS, DON M. NICHOLSON, ODBADRAKH KHORGOLKHUU, AURELIAN RUSANU, Oak Ridge National Laboratory — For the simulation of nanostructured materials and materials with structural defects, it is necessary to consider large size unit cells consisting of thousands or more atoms. It is especially true for our investigation of radiation damage effects on the structural materials. We found that for a reasonably high energy radiation, large unit cell samples at least at 10 nm scale are needed in order for allowing the thermal energy introduced into the sample by the radiation to have sufficient space to dissipate. In this presentation, we point out that, for ab initio electronic structure calculation of a system with a unit cell at such a large scale, it is essential to pay careful attention to numerical stability. We show some numerical pitfalls that will arise as a result of large number of atoms getting involved. The round-off errors accumulated in the calculation of long-range Coulomb interactions, in particular, can lead to divergence of self-consistent iterations. We discuss our approach for circumventing these numerical difficulties.

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Yang Wang
Pittsburgh Supercomputing Center, Carnegie Mellon University

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