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Linear Scaling NanoScience Simulations for Petascale Computing[1] ZHENGJI ZHAO, LIN-WANG WANG, JUAN MEZA, LBNL — There are many large-scale nanoscience problems that require *ab initio* accuracy total energy calculations and atomic relaxations. Unfortunately, the traditional direct *ab initio* method scales as $O(N^3)$, where N is the number of atoms in the system, and most of the $O(N)$ methods studied in the last decade have various numerical convergence problems and computer parallelization issues. In this talk, we present an alternative $O(N)$ method which divides the whole system into small fragments. By combining the fragments in an ingenious pattern, the artificial boundary effects of the spatial division can be canceled out. As a reasult, the difference between this method and the direct *ab initio* calculation is smaller than errors introduced by other numerical approximations, and the method scales almost linearly to the number of processors. We have used this method to calculate nanostructures with more than ten thousand atoms using thousands of processors under the conventional planewave pseudopotential approach. We will demonstrate that this approach provides a practical way for future petascale computation in materials/nanomaterials science.

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