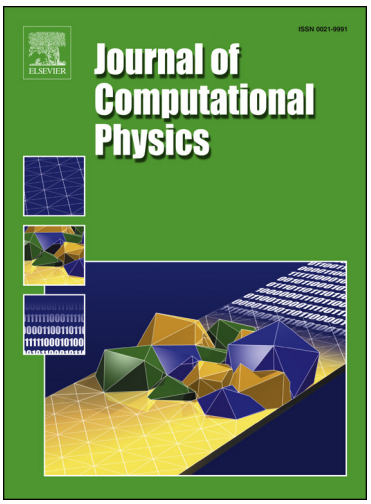
Accepted Manuscript



A parallel orbital-updating based plane-wave basis method for electronic structure calculations

Yan Pan, Xiaoying Dai, Stefano de Gironcoli, Xin-Gao Gong, Gian-Marco Rignanese, Aihui Zhou

PII: S0021-9991(17)30541-7
DOI: http://dx.doi.org/10.1016/j.jcp.2017.07.033
Reference: YJCPH 7480

To appear in: *Journal of Computational Physics*

Received date: 10 February 2017
Revised date: 10 June 2017
Accepted date: 17 July 2017

Please cite this article in press as: Y. Pan et al., A parallel orbital-updating based plane-wave basis method for electronic structure calculations, *J. Comput. Phys.* (2017), http://dx.doi.org/10.1016/j.jcp.2017.07.033

Highlights

- Propose three parallel orbital-updating based plane-wave basis methods for electronic structure calculations.
- These new methods can avoid the generating of large scale eigenvalue problems and then reduce the computational cost.
- These new methods allow for two-level parallelization which is particularly interesting for large scale parallelization.
- Numerical experiments show that these new methods are reliable and efficient for large scale calculations on modern supercomputers.