Ab initio calculation of multilayer magnetic structures by VASP on OpenPOWER high perfomance system

V. Borzilov[1,*], V. Lozhnikov[1], M. Mamonova[1], A. Mamonov[1], A. Sorokin[2], G. Baksheev[3], P. Prudnikov[1]

[1]Dostoevsky Omsk State University, Omsk, Russia
[2] Computing Center of Far Eastern Branch RAS, Khabarovsk, Russia
[3] Novosibirsk State University, Novosibirsk, Russia
*E-mail: BorzilovVO@omsu.ru

The behaviour of multilayer magnetic structures has become of great technological importance due to the applications in magnetic storage devices. The *ab initio* calculations are widely used to calculate some characteristics of solids [1] and multilayered magnetic structures [2]. The main advantage of *ab initio* approach is independence on experimental data. Unlike the case of semi-empirical methods, there is no need for calibration or fitting parameters. Thus, *ab initio* methods can also be used to calculate the characteristics of perspective systems, i.e., for prediction of properties of materials that have not yet been developed. Mainly used packages that can perform *ab initio* calculations are VASP [3], Quantum Espresso [4], ABINIT [5]. High perfomance systems should be used for complex materials modelling with large amount of atoms in supercell.

In this paper we calculated energy and magnetic characteristics for multilayer Co/Cu[100] ferromagnetic structure by VASP on POWER architecture. We analysed perfomance of VASP package on the OpenPOWER high perfomance system with several Pascal P100 GPU units in compare with calculation on POWER8 CPU only and on system with Intel architecture. We revealed that the VASP calculations achieve maximum perfomance on OpenPOWER System with the GPUs.

We would like to thank the IBM experts, who help us to optimize VASP package for IBM Power Systems S822LC. This research was supported by the grants 17-02-00279, 18-42-550003 of Russian Foundation of Basic Research and by the grant MD-6868.2018.2 of the President of the Russian Federation. The simulations were supported by the computational resources of Shared Facility Center "Data Center of FEB RAS" (Khabarovsk) [6]. Computations were performed with the methods and techniques, which were developed under the RFBR scientific project number 18-29-03196.

1. K. Lejaeghere, G. Bihlmayer, T. Björkman, et al., Reproducibility in density functional theory calculations of solids // Science – 2016 –V. 351 – aad3000 doi:10.1126/science.aad3000

2. R.A. Kondrashov, M.V. Mamonova, E.S. Povoroznuk, V.V. Prudnikov, First-principles investigations of the atomic structure and magnetic properties of Ni and Co films on Cu substrate // Lobachevskii Journal of Mathematics – 2017 – V. 38, P. 940–943. doi:10.1134/s1995080217050225

3. G. Kresse, J. Furthmüller, Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set // Phys. Rev. B – 1996 – V. 54, P 11169-11186. doi:10.1103/PhysRevB.54.11169

4. P. Giannozzi, S. Baroni, N. Bonini, et al., QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials // J. Phys.: Condens. Matter – 2009 – V. 21, P. 395502 doi:10.1088/0953-8984/21/39/395502

5. X. Gonze, B. Amadon, P.-M. Anglade, et al., ABINIT: First-principles approach to material and nanosystem properties // Comput. Phys. Commun. – 2009 –V. 180, P. 2582-2615 doi:10.1016/j.cpc.2009.07.007

6. A.A. Sorokin, S.I. Makogonov, S.P. Korolev, The Information Infrastructure for Collective Scientific Work in the Far East of Russia // Scientific and Technical Information Processing. – 2017. – V. 4, P. 302-304. doi:10.3103/S0147688217040153