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

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

1. Introduction

The behavior of multilayer magnetic structures has become of great technological importance due to the applications in magnetic storage devices. The \textit{ab initio} calculations are widely used to calculate some characteristics of solids [1] and multilayer magnetic structures [2]. The main advantage of \textit{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, \textit{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 \textit{ab initio} calculations are VASP [3–5], Quantum Espresso [6], ABINIT [7].

High performance systems should be used for complex materials simulations 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 analyzed performance of the VASP package on OpenPOWER HPC 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 a maximum performance on OpenPOWER system with the GPUs.
2. Vienna Ab initio Simulation Package (VASP)

The central idea of DFT [3] is to consider the electron density \( \rho(r) \) instead of the full many-body wave functions \( \Psi(r_1, \ldots, r_N) \).

\[
\rho(r) = \langle \Psi| \sum_{i=1}^{N} \delta(r - r_i) |\Psi \rangle, \quad m(r) = \sum_{\nu=1}^{N} \Psi_{\nu}^*(r) \sigma \Psi_{\nu}(r)
\]

\[
\left\{ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{eff}} + \sigma \cdot B_{xc}(r) - \varepsilon_{\nu} \right\} \Psi_{\nu}(r) = 0, \quad B_{xc} = \frac{\partial E_{xc}[\rho(r), m(r)]}{\partial m(r)}
\]

In this work we used next methods and approximations:

(i) Projection augmented wave (PAW) method. The number of plane wave components is limited by the Cut-off Energy;

(ii) GGA (generalized gradient approximations);

\[
E_{xc}^{GGA}[n_\uparrow(\vec{r}), n_\downarrow(\vec{r})] = \int [\varepsilon[n_\uparrow(\vec{r}), n_\downarrow(\vec{r}), \nabla n_\uparrow(\vec{r}), \nabla n_\downarrow(\vec{r})] d\vec{r}
\]

(iii) Pseudopotential Perdew–Burke–Ernzerhof (PBE) [8];

(iv) Standard method Monkhorst–Pack grid. A regular grid in \( k \)-space [9].

3. VASP compilation

Official support of GPU appear in VASP from version 5.4.1, for our work we used version 5.4.4. VASP have one precompiled configuration file named \texttt{makefile.include} with a lot of parameters. Showing all parameters is redundancy and we present main part of it in table 1.

We use Intel Parallel Studio XE C/C++ with Intel MKL library to compile the VASP package on X86_64 architecture. The optimization flags were choosed \texttt{-O1} and \texttt{-O2} because compilation with harder optimization was not complete successfully. It was used Ubuntu 16.04 with 4.4.0-137 kernel. We used XIC 13.1.5 and Xlf 15.1.5 with including ESSL library on CentOS 7 with 3.10.0-514 kernel to compile VASP on IBM Power System S822LC.

| Compiler                  | Version | Flags                                                                 |
|---------------------------|---------|----------------------------------------------------------------------|
| IBM XL C/C++              | 13.1.5  | \texttt{-g -q64 -O3 -qarch=pwr8}                                      |
|                           |         | \texttt{-qtune=pwr8:st}                                               |
|                           |         | \texttt{-qfullpath -qsaveopt}                                         |
| IBM XL Fortran            | 15.1.5  | \texttt{-g -q64 -O3 -qarch=pwr8}                                      |
|                           |         | \texttt{-qtune=pwr8:st}                                               |
|                           |         | \texttt{-qfullpath -qsaveopt}                                         |
|                           |         | \texttt{-qflag=i:e -qsupress=cmpmsg}                                  |
| NVIDIA CUDA compilation tools | 8.0.61  | \texttt{-DCUDA_GPU -DRPROMU_CPROJ_OVERLAP}                            |
|                           |         | \texttt{-DCUFFT_MIN=28 -UscaLAPACK}                                  |
|                           |         | \texttt{-fPIC -DPADD_ -DMAGMA_WITH_MKL}                               |
|                           |         | \texttt{-DMAGMA_SETAFFINITY -DGPUTHMEM=300}                           |
|                           |         | \texttt{-DHAVE_CUBLAS}                                               |
| Intel Parallel Studio XE C/C++ | 2017    | \texttt{-O2 -f_com=no -free -w0}                                      |
| Intel Parallel Studio XE Fortran | 2017    | \texttt{-O1 -mkl=sequential -lstdc++}                                 |
4. Hardware information
IBM Power System S822LC is two socket HPC system with two POWER8 CPUs with 20 cores running at 4 GHz and interconnected with two NVidia Pascal P100 GPUs with high bandwidth (80GByte in and 80GByte out) NVLink 1.0 interface (figure 1). It is very important for exchange data between multiple GPUs and fast load data from CPU. The major goal of this system is efficiently using GPU units and accelerating calculations. A large part of HPC resources installed during the last decade are based on Intel CPUs. Novel generations of Intel CPUs present a wide spectrum of multicore processors [5]. Intel Core i7 4770 is desktop processor, but it is ”tock” model in Intel extensive strategy of microprocessor development – it is mostly complete 22 nm architecture. We compared IBM POWER8 with Intel Haswell because both architectures introduced in one year (2013) and had similar technical process (22 nm).

5. Model and simulation parameters
In this work we calculated energy and magnetic characteristics for multilayer Co/Cu[100] ferromagnetic structure to compare results obtained on CPU and GPU. The computed multilayer structure is shown at figure 2.

| Table 2. Simulation parameters |
|--------------------------------|
| Cutoff energy | 500 eV |
| K-points | 12 |
| Number of atoms | 36 |
| Thickness of vacuum layers | 5 Å |

6. Results of performance and accuracy comparison
We used three configurations to compare a VASP calculation times with similar INCAR parameters for IBM POWER8 CPU and Intel Haswell. We set LREAL=.FALSE. as described at VASP official documentation and use NCORE=1 with one MPI thread for GPU calculations. We do not use NVIDIA MPS system and do not set NSIM parameter clearly, but we know that it is important for large tasks especially. Core i7 have only 4 real cores and we run VASP with 4 processes only. On POWER8 we run VASP on 8 cores for using most part of one CPU.
Table 3. Comparison of the accuracy of the calculations performed on the CPU and GPU

| Architecture                  | Total magnetization | Free energy (eV)  |
|-------------------------------|---------------------|-------------------|
| Intel Core i7-4770 Haswell    | 40.646              | -202.20538224     |
| IBM POWER8                    | 40.646              | -202.20538199     |
| IBM POWER8+Nvidia P100        | 40.658              | -202.04101161     |

The results of magnetization and free energy calculations (table 3) are well correlated. The calculations with the GPU provide less accuracy but a value of the error is not so sufficient. The times of calculations are different for POWER8 system and Intel Core i7 (table 4). The one POWER8 thread was more efficient than one Intel thread for the VASP calculations. If we use GPU only with one MPI thread we have much better performance (table 4) than Intel or POWER CPUs even without optimizations of VASP parameters.

![Figure 3](image.png)

**Figure 3.** Dependence of execution time on used architecture.

Table 4. Execution times for different computing systems

| Architecture                  | Execution time   | Used memory | Number of threads |
|-------------------------------|------------------|-------------|------------------|
| Intel Core i7-4770 Haswell    | 38:23:54         | 6.91 Gb     | 4                |
| IBM POWER8                    | 14:27:20         | 6.67 Gb     | 8                |
| IBM POWER8+Nvidia P100        | 08:27:08         | 29.64 Gb    | 1                |

7. Conclusion

VASP is widely used by researchers to get characteristics of solids and multilayer magnetic structures. A one of the efficient ways to get results in less time is using of GPU especially in hybrid way with MPS daemon and multiple MPI threads. Therefore, to get maximum performance one need to optimize INCAR parameters for GPU, especially NCORE and NSIM. The values of acquired quantities and accuracy of GPU calculations are in a good agreement.
with CPU results. In order to use VASP efficiently with GPUs more memory is required in comparing with calculations on CPU.

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References
[1] Lejaeghere K, Bihlmayer G, Björkman T, et al 2016 Science 351 aad3000
[2] Kondrashov R A, Manonova M V, Povoroznuk E S, Prudnikov V V 2017 Lobachevskii J Math 38 940
[3] Kresse G and Furthmüller J 1996 Phys. Rev. B 54 11169
[4] Kresse G, Marsman M, Furthmüller J 2015 VASP THE GUIDE
[5] Stegailov V and Vecher V (2017) Efficiency Analysis of Intel and AMD x86_64 Architectures for Ab Initio Calculations: A Case Study of VASP. In: Voevodin V, Sobolev S (eds) Supercomputing. RuSCDays 2017. Communications in Computer and Information Science, vol 793. Springer, Cham
[6] Giannozzi P, Baroni S, Bonini N, et al 2009 Phys. Rev. B 21 395502
[7] Gonze X, Amadon B, Anglade P M, et al 2009 Comput. Phys. Commun. 180 2582
[8] Perdew J P, Burke K, Ernzerhof M 1996 Phys. Rev. Lett. 77 3865
[9] Monkhorst H J, Pack J D 1976 Phys. Rev. B 13 5188
[10] Sorokin A A, Makogonov S I, Korolev S P 2017 Scientific and Technical Information Processing 4 302