Towards PetaFlops Computing with IBM Blue Gene

Norbert Attig and Friedel Hoßfeld

Jülich Supercomputing Centre (JSC)
Forschungszentrum Jülich GmbH
52425 Jülich
n.attig@fz-juelich.de
f.hossfeld@fz-juelich.de

Abstract: Driven by technology, Scientific Computing is rapidly entering the PetaFlops era. The Jülich Supercomputing Centre is focusing on the IBM Blue Gene architecture to provide computer resources of this class to its users. Details of the system will be discussed and applications will be introduced which significantly benefit from this new architecture.

1 Introduction

In many areas, numerical simulations are the essential method for achieving innovative, high-quality results. Driven by the rapid development in computer technology, this insight has dramatically increased the requirements of computational scientists with respect to application performance, memory, data storage and data transfer capabilities [BHL05, Ko06]. Currently, only high-performance supercomputers with a large number of processors are capable to fulfil these needs.

The Jülich Supercomputing Centre, one of three national supercomputing centres, has implemented a dual supercomputer concept to provide computational scientists with adequate computing resources. On one side, a moderately parallel cluster serves about 150 user groups from academia and research institutions. This system allows the development of parallel codes as well as the execution of small to mid-size projects. For applications which scale up to thousands of processors, on the other side, IBM Blue Gene systems are available, serving as Leadership-class systems addressing the PetaFlops scale. Here, a much smaller number of projects are granted to give selected researchers the opportunity to get new insights into complex problems which were out of reach before.

2 IBM Blue Gene systems at JSC

When in 2004/2005 the IBM Blue Gene technology became available, the Jülich Supercomputing Centre recognised the potential of this architecture as a Leadership-class system for capability computing applications. In early summer 2005, Jülich started testing a single Blue Gene/L rack with 2,048 processors [AW05]. It soon became obvious that many more applications than initially expected were ported to efficiently run on the Blue Gene architecture. Therefore, in January 2006 the system was expanded to 8 racks with 16,384 processors, funded by the Helmholtz Association. The 8-rack system has successfully been in operation for almost two years now. Today, about 30 research groups, which were carefully selected with respect to their scientific quality, run their applications on the system using job sizes between 1,024 and 16,384 processors.

In early 2007, Research Centre Jülich decided to order a powerful next-generation Blue Gene system. In October 2007, a 16-rack Blue Gene/P system with 65,536 processors was installed [SW07], mainly financed by the Helmholtz Association and the State of North Rhine Westphalia. With its peak performance of 222.8 TFlop/s, Jülich's Blue Gene/P – alias JUGENE – is currently the biggest supercomputer in Europe and ranked No 2 worldwide.

The important differences between Blue-Gene/P and Blue Gene/L largely concern the processor and the networks while the principal build-up of Blue Gene/L was kept unchanged. Key features of Blue Gene/P are:

- 4 PowerPC® 450 processors are combined in a fully 4-way SMP (node) chip which allows a hybrid programming model with MPI and OpenMP (up to 4 threads per node).
- The network interface is fully DMA (Direct Memory Access) capable which increases the performance while reducing the processor load during message handling.
- The available memory per processor has been doubled.
- The external I/O network has been upgraded from 1 to 10 Gigabit Ethernet.

A key feature of this architecture is its scalability towards PetaFlops computing based on low power consumption, small footprint and an outstanding price performance ratio.

3 Running Applications on Blue Gene

Due to the fact that the Blue Gene systems are well balanced in terms of processor speed, memory latency, and network performance, many applications scale reasonably up to large numbers of processors. More surprising was that so many applications could be ported to and run efficiently on this new architecture which in a forerunner version was mainly designed to perform lattice quantum chromo dynamics (LQCD) codes. Blue Gene applications at JSC cover a broad spectrum ranging from LQCD to MD codes like CPMD and VASP, materials science, protein folding codes, fluid flow research, quantum computing and many, many others.

The performance and the scaling behaviour of the applications are continuously being improved in close collaboration between the user support team at JSC and the corresponding computational scientists. For example, a code from theoretical elementary particle physics runs now on Blue Gene/P at nearly 40 % of the peak performance compared to about 25 % on Blue Gene/L. In this context Blue Gene Scaling Workshops, where experts from Argonne National Laboratory, IBM and Jülich help to further optimise some important applications are highly welcome. Computational scientists from many research areas take the chance to improve their codes during these events and then later apply for significant shares of Blue Gene computer time to tackle unresolved questions which were out of reach before.

References

[AW05] Attig, N., Wolkersdorfer, K.: IBM Blue Gene/L in Jülich: A First Step to Petascale Computing. In inSiDE, 3, 2005, 2, S. 18-19

[BHL05] Bode, A., Hillebrandt, W., Lippert, T: Petaflop-Computing mit Standort Deutschland im europäischen Forschungsraum, Bedarf und Perspektiven aus Sicht der computergestützten Natur- und Ingenieurwissenschaft. "Scientific Case" im Auftrag des BMBF, Bonn, 2005

[Ko06] Koski, K. et al.: "European Scientific Case for high-end computing". HPC in Europe Task Force, http://www.hpcineuropetaskforce.eu/draftdeliverables

[SW07] Stephan, M., Wolkersdorfer, K.: IBM BlueGene/P in Jülich: The Next Step towards Petascale Computing. In inSiDE, 5, 2007, 2, S. 46-47