Simulating the Performance of Scalapack with Clue

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Abstract. This paper describes CLUE, a tool for the accurate performance assessment and prediction of clusters of symmetric multiprocessors (SMPs). By using CLUE, the performance of different cluster configurations consisting of processing elements, memory, network etc. may be evaluated. The generated performance analysis may then guide potential cluster customers in their decision for one particular configuration.
Using CLUE, hardware therefore can be adapted to individual software features, reversing the currently used techniques of adapting high-performance software to hardware features (as used, for instance, in FFTW, PHIPAC, or the ATLAS tool).

1. Introduction

In the last few years high-performance hardware has changed dramatically. Until quite recently, shared memory parallel vector processor (PVP) computers and distributed massively parallel processing (MPP) machines dominated the field of supercomputing. Nowadays high-performance computing has turned towards clusters of shared memory symmetric multiprocessors (SMPs). Most of these clusters are built using custom processors, as well as custom interconnection devices and memory. Accordingly, clusters of SMPs appear in a multitude of different configurations, ranging from teraflops machines to small clusters, comprising several PCs or workstations. The large number of possible configurations makes it difficult to decide which particular structure is suitable to solve a particular class of problems under certain performance requirements, and of course under given financial constraints. To aid this process of evaluating computer clusters the simulation and assessment tool CLUE (*clu*ster *e*valuator) has been developed. This paper describes CLUE and gives some results gathered in numerical experiments.

1.1 PC Clusters

As the performance of commodity computer and network hardware increases and prices decrease, building parallel computer systems from off-the-shelf components has attracted more and more attention. The current price / performance ratio of a PC cluster is often ten times better than that of traditional supercomputers. PC clusters scale reasonably well, are easy to construct and only the hardware has to be paid for as most of the software is free. Meanwhile several entries of the top 500 supercomputer list[1] are clusters of off-the-shelf SMPs.
Often PC clusters do not contain any proprietary hardware components and thus are trivially reproducible. Commodity software like the Linux operating system, PVM (Geist et al. [6]) and MPI (Gropp et al. [7]) are used for developing parallel programs.
Usually a server node controls the whole cluster and serves files to the client nodes. These nodes can be thought of as a (multi) CPU plus a memory package which can be plugged into the cluster, just like a CPU or memory module can be plugged into a motherboard. PC clusters used for high-performance computing are often referred to as *Beowulf clusters*.[2] Typical configurations are, for example, a compound of several computers connected via Fast Ethernet or faster networks like Gigabit Ethernet, Myrinet or SCI (Scalable Coherent Interface).
Yielding a form of parallel computers, PC clusters fall somewhere in between MPPs (Massively Parallel Processors) and NOWs (Networks of Workstations). They profit from developments in both architectures. MPPs are usually larger than PC clusters and use faster networks. Typical problems when programming MPPs are load and data distribution, granularity, and minimizing the communication

[1] http://www.netlib.org/benchmark/top500.html
[2] http://www.beowulf.org

overhead. Programs, which are not too fine grained, can be ported from MPPs to PC clusters easily and achieve there a satisfactory performance. When programming NOWs, in most cases algorithms are designed to utilize unused cycles of powerful workstations. These algorithms have to be tolerant of load variations and have to use dynamic load balancing. All programs running on NOWs run at least as good on dedicated PC clusters.
Often PC clusters are used as a (relatively cheap) platform for large production codes which were running for many years on Unix workstations. It would be difficult to adapt these codes to the requirements of the hardware, thus it is important to configure the cluster according to the requirements of the code. This was one of the reasons for the development of CLUE.

1.2 Hardware

In this paper two specific PC clusters are investigated.

The Vienna Cluster was built and operated by the authors. It consists of five dual 350 MHz Pentium II systems ($p = 10$) with 256 MB main memory, 512 KB Level 2 cache and local 4.5 GB hard discs. The nodes are connected via a switched Fast Ethernet network (measured bandwidth: 12.5 MB/s).

The Aachen Cluster, a Siemens hpcLine PC cluster, consists of 16 dual processor boards equipped with 400 MHz Pentium II processors ($p = 32$), 512 KB Level 2 cache, 512 MB main memory and local 4 GB hard discs. The nodes communicate either via switched Fast Ethernet or SCI (Scalable Coherent Interface; measured bandwidth: 80 MB/s). The SCI network is configured as a two-dimensional torus.

For more details see Hlavacs et al. [8].

1.3 Algorithms

The following ScaLapack routines were chosen to demonstrate the usefulness and the reliability of CLUE.

Cholesky Factorization. `SCALAPACK/pdpotrf` is a routine which computes the Cholesky factorization $U^T U$ of a symmetric, positive definite matrix A. As the computation proceeds, elements of A are overwritten with elements of U. A and U are stored in a block-cyclic two-dimensional way using identical block sizes in both dimensions.

LU Factorization. `SCALAPACK/pdgetrf` computes the LU factorization PLU of a general matrix A. The output matrices U and L are stored in place of the input matrix A which is distributed in a two-dimensional block-cyclic manner using identical block sizes in both dimensions.

Matrix Multiplication. The routine `PBLAS/pdgemm` multiplies two matrices: $C = AB$. All three $n \times n$ matrices are distributed in a two-dimensional block-cyclic way. Identical block sizes are used in both dimensions and for all matrices.

2. The Simulation Tool CLUE

CLUE is based on MISS-PVM, the *Machine Independent Simulation System for PVM 3* (Kvasnicka, Ueberhuber [9]). CLUE is meant to support the development of software for parallel computers which are not yet available and to carry out reproducible performance assessments in environments with constantly changing load characteristics (like NOWs). CLUE also makes the debugging of parallel programs easier. Using CLUE, reliable information can be obtained to reach the optimum decision on hardware configurations (processing elements and communication networks) before actually purchasing this hardware. Thus, hardware can be adapted to individual software features, reversing the currently used techniques of adapting high-performance software to hardware features (as used, for instance, in FFTW [4,5], Phipac [1], or the Atlas tool [10]). To exploit these features of CLUE, it is not necessary to rewrite existing code or create additional one (neither in C nor in Fortran). PVM based code can be used without modification. CLUE's favorable properties are achieved by establishing a virtual layer which does not have to be tampered with when developing software. The *Virtual Layer for PVM 3* is situated between the user

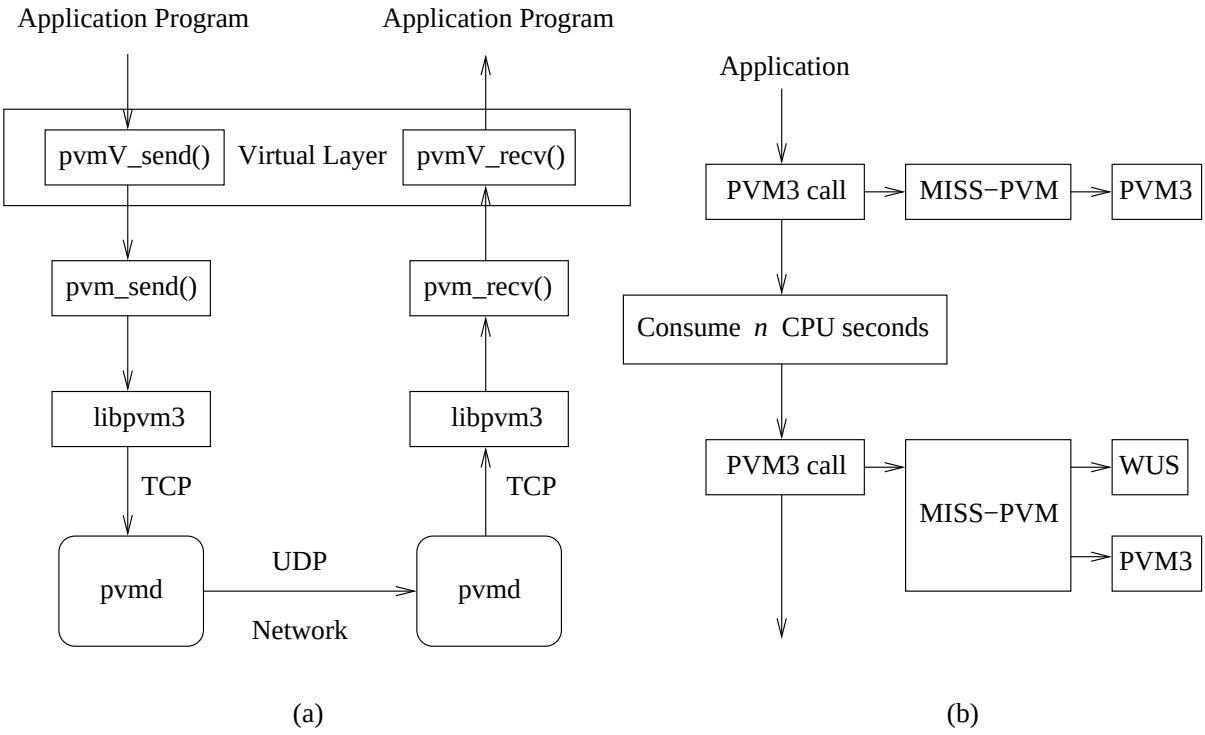

Figure 1: (a) Position of the Virtual Layer for PVM. (b) Interaction of application and virtual layer.

program and PVM 3 (see Fig. 1 (a)). All calls to PVM 3 are redirected to CLUE subroutines performing virtual timing and virtual machine adaptation. They eventually pass on the calls (in a modified form) to PVM 3.

Use of the virtual layer is possible without the necessity to modify the user program. It is sufficient to use different include files and to link the user program to additional libraries. The virtual layer generates output files which trace calls to communication subroutines. These trace files are the input of post-mortem visualization.

This tracing technique has two major advantages over conventional trace file writing. The *Virtual Layer for PVM 3* (i) uses its own simulated *system time*, and (ii) makes a *virtual machine* available to the user. The virtual time is advanced by measuring the CPU time consumed between two successive calls to the virtual layer (see Fig. 1 (b)) and the simulated time for communication. The virtual machine may represent a wide variety of real machines which may even be non-existent or not available at the moment. Machine parameters are read from a file when CLUE is started. These parameters may be changed dynamically during simulation.

The virtual layer allows to compare program runs on computers having different communication latency and computation speed (independent of actual load characteristics). For instance, reproducible experiments for the assessment of load balancing strategies on irregularly loaded NOWs can be made easily and quickly.

High level communication libraries like the BLACS (Dongarra et al. [2,3]) can be simulated very comfortably. Once the high level library routines (based on PVM) have been recompiled, no further modifications are needed. The user program is linked with the new library. The result is a program that performs the same task as before, except that it writes an output file (if required) and can be simulated on virtual machines.

For small programs usually the whole simulation runs on one processor. For large programs (especially those performing compute intensive tasks) the overall execution time is often a prohibitive factor in simulation. Therefore, in cases which require much time or main memory, the simulation can be distributed to several processors.

3. Numerical Experiments

3.1 Measurement, Modeling, and Simulation

Up to now, two Beowulf clusters have been examined. On both clusters, measurements have been carried out to obtain the following communication related parameters. (i) *Send time*: The time the sender spends in the send call. (ii) *Transmission time*: The difference between the send time and the time the message needs to be received by the receiver. Fig. 2 shows the send and transmission times observed on the Vienna cluster. Both sender and receiver run on the same node, thus the message is not sent over the network. The piecewise linear model used for the simulation in shown as well.

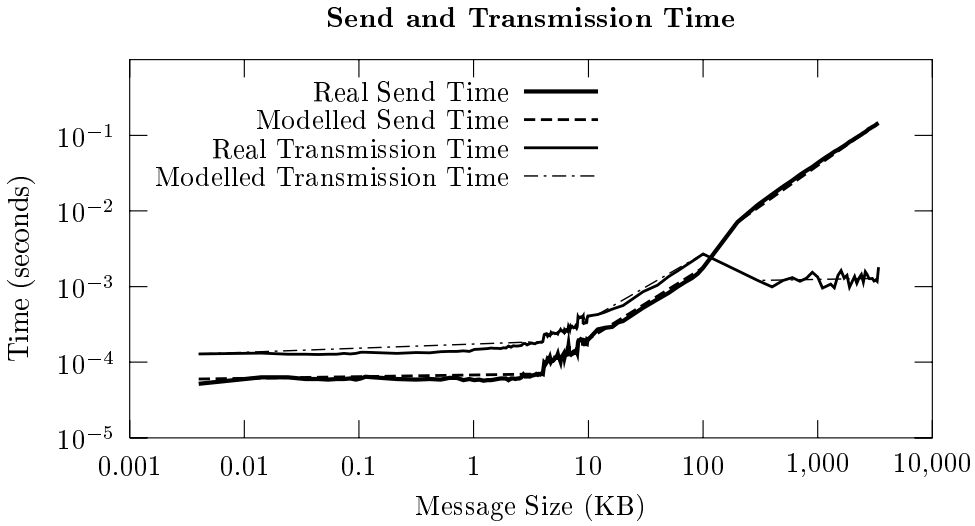

Figure 2: Send and transmission time for the Vienna cluster. Sender and receiver are on the same node.

Additionally, for the case of sending messages from one sender to several receivers at the same time, contention has been observed that increases both the send and transmission time. This is important for those cases, where all tasks synchronize, and one of the tasks then sends out messages to one or several others to redistribute work or results.
Each cluster was simulated by using two communication modes (intra- and inter-node) and by using a contention model. This method achieves sufficiently accurate results even on the torus-shaped network of the Aachen cluster.
Measured computation time is modified by a computational factor. For example, each processor of the Aachen cluster was measured to be 10 % faster than one of the processors of the Vienna cluster.
The SCI network of the Aachen cluster was only available for the MPI version of the BLACS. Thus, communication parameters and performance data of the real runs were measured on the Aachen cluster using the MPI version of the BLACS, whereas the simulation runs were carried out on the Vienna cluster using the PVM version of the BLACS.

3.2 Results

In order to obtain widely applicable results, the three algorithms described above have been chosen to be simulated on the two clusters. 2000 × 2000 matrices were chosen to set up problems of a sizeable computational complexity.
Moreover, these problems are imposing substantial main memory requirements on the simulating node.
The simulation runs were carried out to answer the following questions. (i) Do the real observations and the simulated runs have the same qualitative properties? (ii) Do the real observations and the simulated runs have the same quantitative properties? (iii) Can the simulation results be used to evaluate the performance of workstations clusters a priori?
In Fig. 3, the observed and simulated wall times are plotted against the processor grid used. Such a grid or 2-dimensional mesh is always assumed to define the topology of the parallel computer, even if in reality this is a cluster of SMPs connected over a bus, star or ring topology. Each processor is assigned a

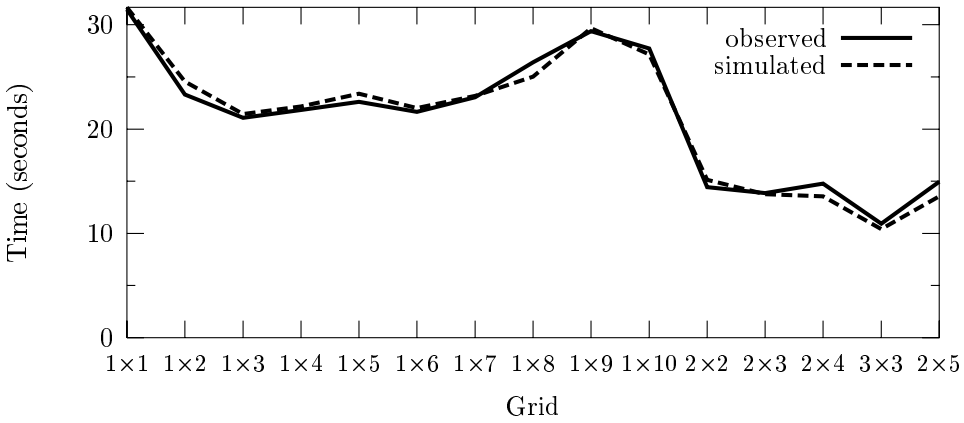

Figure 3: Cholesky factorization of a 2000×2000 matrix on the Vienna cluster. Blocksize 100.

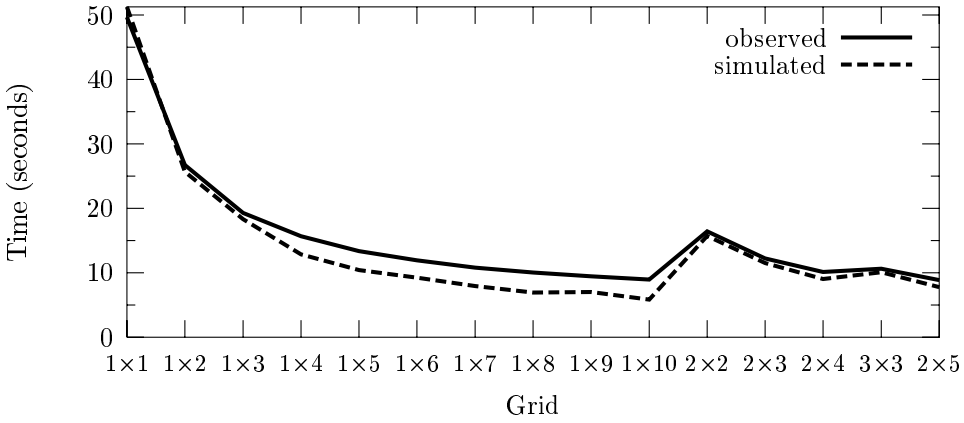

Figure 4: LU factorization of a 2000×2000 matrix on the Aachen cluster. Blocksize 50.

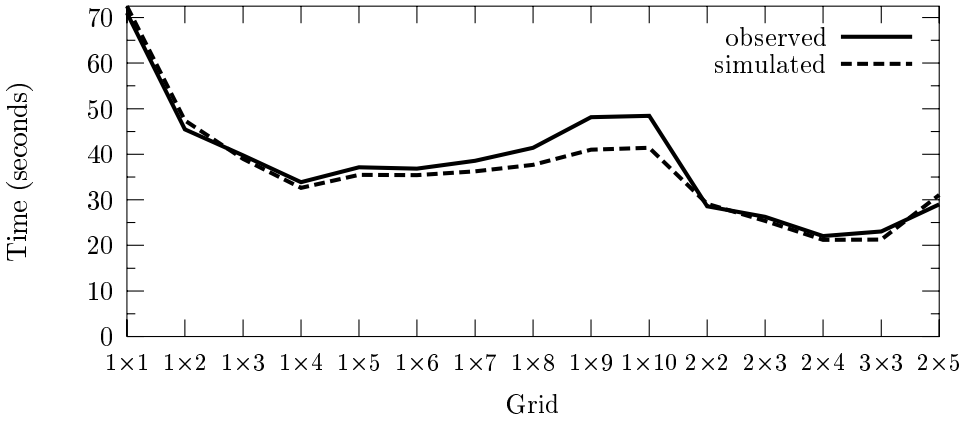

Figure 5: Multiplication of a 2000×2000 matrix on the Vienna cluster. Blocksize 500.

place in the virtual mesh topology. Basically, an $N \times M$ grid means that $N \times M$ processors were used to compute the task. The relation of N to M defines the communication pattern used, which has a strong influence on efficiency as the diagrams show.
The diagrams reveal the answers to the above questions. (i) The real observations and the simulated runs have the same qualitative properties. (ii) The real observations and the simulated runs have the same quantitative properties. (iii) The simulation results can be used to evaluate the performance of workstations clusters a priori, since the important variatons in execution time are at the correct places.

4. Summary and Conclusions

In this paper the new simulation tool CLUE is described. This tool is meant to investigate the performance behavior of clusters of SMPs.
Simulation results obtained for a PC cluster with slow communication (using Fast Ethernet) turned out to be very accurate. Both qualitative and quantitative performance behavior can be simulated highly satisfactory.
Simulating the performance of PVM versions of ScaLAPACK and the PBLAS does not require any modification of the PVM code. Simulating MPI versions by using PVM versions on a different type of node is more demanding. Still, performance diagrams indicate that the qualitative behavior of the parallel programs is described accurately whereas quantitative results are sometimes a little misleading.
It may be concluded, that performance comparisons between different clusters of SMPs are possible, though experiments must be carefully designed and results have to be interpreted cautiously. The qualitative behavior of parallel programs running on clusters of SMPs can be simulated accurately.
Using CLUE it is possible to analyze the behavior of parallel programs and predict their performance, depending on cluster parameters. Simulation results can be used to investigate the influence of different parameters of the simulated workstation or PC cluster, in order to plan new hardware configurations or make an educated choice between several alternatives.
Future work will include the development of improved network models to simulate various topologies.
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5. References

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