Fast Parallel I/O on Cluster Computers

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Abstract

Today’s cluster computers suffer from slow I/O, which slows down I/O-intensive applications. We show that fast disk I/O can be achieved by operating a parallel file system over fast networks such as Myrinet or Gigabit Ethernet.

In this paper, we demonstrate how the ParaStation3 communication system helps speed-up the performance of parallel I/O on clusters using the open source parallel file system (PVFS) as testbed and production system. We will describe the set-up of PVFS on the Alpha-Linux-Cluster-Engine (ALiCE) located at Wuppertal University, Germany. Benchmarks on ALiCE achieve write-performances of up to 1 GB/s from a 32-processor compute-partition to a 32-processor PVFS I/O-partition, outperforming known benchmark results for PVFS on the same network by more than a factor of 2. Read-performance from buffer-cache reaches up to 2.2 GB/s. Our benchmarks are giant, I/O-intensive eigenmode problems from lattice quantum chromodynamics, demonstrating stability and performance of PVFS over Parallel in large-scale production runs.

Keywords: Cluster Computing, Parallel File System, ParaStation, Lattice QCD

1 Introduction

Within the past years commodity-off-the-shelf (COTS) clusters have evolved towards cost-effective general-purpose HPC devices. Such systems, self-made and commonly denoted as Beowulf computers [1], show up increasingly on
the TOP500 list [2]. While gigabit network technology (Gigabit-Ethernet, Myrinet) along with error-correcting zero-copy-communication software [3,4,5] have boosted communication-intensive number-crunching tasks, I/O-intensive computations have not benefited from cluster computers to the same extent. The reason was the relatively slow I/O capability of clusters.

Today, a promising approach to achieve fast I/O on cluster computers is to utilize distributed disks and their aggregate bandwidth by means of a parallel file system (PFS). A PFS is designed to make the entire disk capacity of the I/O-nodes available to all the compute-nodes and to allow the parallel file access of the compute nodes to be translated into real parallel disk access. Physically, files are stored on a given partition of cluster nodes by distributing the data of the given file, for instance in a round robin fashion. In contrast to standard network file systems, a PFS provides concurrent parallel access to store or read the file from all nodes of a parallel application. In a typical implementation, a set of compute-nodes reads and writes data to another set of I/O-nodes that host the physical resources of the PFS. The two sets of nodes may be identical, may partly overlap or may even be distinct. In principle this concept allows for scalability of the I/O-rate with the number of I/O-nodes, provided that (i) the number of compute-nodes is large enough to saturate the capacity of the I/O-nodes—this is usually the case as soon as the number of compute-nodes equals the number of I/O-nodes—and (ii) the network delivers full bi-sectional bandwidth—this is, for instance, the case for crossbar or multi-stage crossbar topologies.

Distributed file systems like NFS or AFS are not suited for concurrent high-bandwidth file-access as required in I/O-intensive cluster computing applications. In these systems, parallel data accesses of compute nodes are serialized by file servers. Therefore, they can not be called “parallel” file systems. There exist commercially available parallel file systems (sometimes platform dependent), for example the General Parallel File System GPFS (IBM [6]). Currently, the only known open source parallel file system, working in a stable manner, and freely available for Linux under the GNU General Public License, is the Parallel Virtual File System (PVFS) developed at Clemson University and Argonne National Laboratory [7]. PVFS is devised as a truly parallel file system for use on cluster computers. The communication back-end of the standard distribution of PVFS is based on the TCP/IP protocol. Therefore, PVFS can readily be operated on top of any network supporting TCP/IP.

In this paper we consider PVFS boosted by the Myrinet communication network [8] of the Alpha Linux Cluster Engine (ALiCE) located at Wuppertal University, Germany [9]. There are several error-correcting and package-loss-safe communication sub-systems available, designed to drive Myrinet: e.g. the vendor-provided GM software [8], SCore [4], and the ParaStation system [5], developed at Karlsruhe University. On ALiCE, we are using ParaStation.
ParaStation implements the concept of virtual nodes, operating in close interaction with queuing systems like PBS [10]. The communication system provides safe multi-user operation and outstanding stability, not to mention the comfortable single-point-of-administration management by means of the ParaStation-daemons. System crashes are tidily cleaned-up without any user interference. Most important in our context is however the communication bandwidth under ParaStation. A special kernel module routes TCP/IP via the ParaStation communication system and renders Myrinet an additional IP-network with full bi-sectional bandwidth. In this manner, the superior bandwidth from ParaStation as Myrinet driver can be exploited.

Combining parallel file systems like PVFS with ParaStation perfectly meets the demands of an application from the post-simulation phase of a large scale Monte Carlo project in lattice-quantum chromodynamics (LQCD). We are evaluating giant eigenproblems [11], which are very data-intensive, on cluster computers. The eigenvectors are required for the construction of correlations between two quark loops. Such creation and annihilation of quarks originate from the quantum fluctuations of the QCD vacuum, according to Heisenberg’s uncertainty principle. They are considered affectual to the unusually large mass of the $\eta'$-meson [12]. In our simulations, we have to compute $O(1000)$ low eigenvectors of the fermionic matrix, which describes the dynamics of the quarks. The size of each vector is $O(10^6)$.

Typically, about 10 GB of I/O is carried out in data-intensive production steps of about 10 minutes compute time on 16 to 64 processors; actually several thousands of such runs are performed. Without parallel I/O, reading or writing lasts between 10 and 30 minutes. PVFS helps cut down the read and write times to about 20 seconds.

The paper is organized as follows: in Section 2 we present the new TCP/IP kernel module included in ParaStation and describe the connectivity of ALiCE and its specific PVFS implementation. Section 3 gives benchmarks for the components of the I/O-machinery, including disk-speed and TCP/IP node-to-node rates. The results of the PVFS benchmarks are shown in Section 4 along with a comparison with Ref. [13]. We are in the position to test PVFS/ParaStation within a large-scale application from lattice quantum chromodynamics, described in Section 5. Finally we summarize and give a short outlook on the novel parallel file system ClusterFile that is currently under development at the IPD, University of Karlsruhe [14].
2 Technical Background

For cluster applications based on IP-communication to benefit from ParaStation’s performance, a TCP/IP kernel module has been introduced on top of the ParaStation communication system. In this manner, stable communication with gigabyte bandwidth is provided for the parallel virtual file system (PVFS) as implemented on the 128-node Alpha-Linux-Cluster-Engine ALiCE.

2.1 TCP/IP kernel module with ParaStation

Many cluster applications neither use MPI nor the low-level communication API as for instance provided by ParaStation. To benefit from ParaStation’s performance for such applications, an additional TCP/IP module was developed at the Institute for Programs and Data Structures, University of Karlsruhe.

This module provides a network driver interface to the Linux kernel, just as any other Ethernet card driver does. This way, virtually any Ethernet protocol that is supported by the kernel can be transported over Myrinet. In practice, most applications will use the TCP (or UDP) over IP protocol.

Internally, the module uses the kernel variant of the ParaStation low-level communication interface to send raw Ethernet datagrams to any other host in the cluster. This interface supports a set of basic communication operations, since at this level we don’t need more functionality. Packet (dis)assembling for instance is done by the kernel. Upon startup, a so-called kernel-context is obtained from the ParaStation module. This reserves a certain number of communication buffers in the memory of the Myrinet network adapter card and instructs the driver to listen for messages addressed to the TCP/IP module. Secondly, a call-back mechanism is established: whenever such a message arrives, an interrupt is risen and the ParaStation interrupt handler calls a method of the TCP/IP module which in turn hands the message to the Linux network stack. If a message is to be sent, the network stack functions call a method of the module that was registered upon initialization, handing the message over to the ParaStation module.

In order to address other nodes in the cluster, the TCP/IP driver module (in fact an Ethernet driver) maps the ParaStation node identification number (ParaStation ID) onto Ethernet hardware addresses. The administrator can set up static ARP tables that map IP addresses to these hardware addresses. This

\footnote{The intended use is the reason for the somewhat misleading name of the module. It should better be called Ethernet driver for ParaStation.}
is necessary, as the driver does not support broadcast messages that would be 
required to enable automatic ARP functionality. However, if IP addresses are 
chosen such that the ParaStation ID (the node number counted from 0) equals 
the IP address minus one, the static ARP tables can be omitted. In this case, 
any driver module in the cluster can guess ParaStation IDs from IP addresses 
and thus generate fake ARP reply messages.

2.2 *ALiCE setup*

The Alpha-Linux-Cluster-Engine ALiCE is an assembly of 128 Compaq DS10 
workstations [9]. ALiCE, located at the University of Wuppertal (Germany), 
is fully operational since the end of 2000. The machine is equipped with Alpha 
21264 EV67 processors, with 2 MB cache, operating at a frequency of 616 MHz. 
With 256 MB ECC memory for each processor, the total amount of memory is 
32 GB. The disk space of 10 GB per node adds up to about 1.3 TB in total. The 
nodes are interconnected by a $2 \times 1.28$ Gbit/s Myrinet network configured as 
a multi-stage crossbar with full bi-sectional bandwidth. The M2M-PCI64A-2 
Myrinet cards utilize a 64 bit/33 MHz PCI bus.

Figure 1 shows the hardware plan of the inter-node connection of ALiCE. A 
full crossbar is realized by three switch-stages (where each octal switch ac-
tually consists of two stages) employing the $2 \times 4$ Myrinet M2M-oct-SW8 
switches and 8 Myrinet M2M-dual-SW8 switches. The hardware latency is 
about 100 ns per switch stage, far below the total latency (software and hard-
ware) of 17.1 $\mu$s.

We have extended the network in order to incorporate an external file and 
archive server as well as to provide gigabit links to external machines for the 
purpose of fast on-line visualization. To this end, we have exchanged two of 
the 8 M2M-dual-SW8 switches by two M2M-SW16 switches, as sketched in 
Figure 2. This way, we could avoid an inhomogeneous number of hardware 
stages of the multi-stage crossbar network.

2.3 *PVFS partitioning*

On ALiCE, we run 4 different PVFS partitions with 32-nodes each. This par-
titioning fits well with the compute-partitions, chosen such as to optimize the 
compute performances of our applications. Each PVFS partition (/pvfs1 to 
/pvfs4) is represented by a mount point on each node and on the file server. 
Mounting PVFS on the file server enables us to copy UNIX files with Para-
Station TCP/IP speed from the external RAID to PVFS. For each partition,
Fig. 1. Myrinet multi-stage crossbar network.
the last node plays the rôle of the management node. The entire set-up is displayed in Figure 3.
3 Performance of Basic I/O-Devices

The proper interpretation of the benchmark results presented in Section 4 requires some background knowledge about the features of ALiCE’s basic I/O-components, i.e., file system performance, TCP/IP and MPI data rates.

3.1 Local file system performances

The ALiCE DS10 nodes are equipped with 10 GB Maxtor IDE disks. We have carried out tests on local file systems, formatted with ReiserFS, by means of bonnie++ [15]. Write and read-performances are determined for a series of file sizes, from 10 MB up to 2 GB. In order to reveal buffer-cache effects, we have adjusted the “dirty buffer” parameter to two different values, 40 % and 70 %. Our results are given in Figure 4.

![Figure 4. Local file system performances on ALiCE.](image)

The bonnie++ benchmark works as follows: the given file is written and read back immediately. We observe the write performance to buffer cache of 60 MB/s to fall to about 23 MB/s at a file size of 100 and 200 MB, for 40 and 70 % dirty buffers, respectively. Asymptotically, the performance is decreasing to about 19 MB/s. Being able to read from the buffer cache, the subsequent

\[\text{read 40\%} \quad \text{write 40\%} \quad \text{read 70\%} \quad \text{write 70\%}\]

2 5400 rpm versions.

3 The standard behavior of the Linux kernel is to start flushing buffer pages as soon as the given percentage of memory available for buffer cache is “dirty”. A buffer page is called dirty if it changed in memory but has not yet been written to disk.
read operation shows a bandwidth of more than 280 MB/s for small files. At a file size of about 200 MB, the speed drops down to 24 MB/s.

3.2 TCP/IP performance via ParaStation

On ALiCE, we can choose TCP packages to be routed via Fast Ethernet or alternatively—using the new TCP/IP kernel module described in Section 2.1—via ParaStation/Myrinet. The ttcp benchmark issues TCP/IP packets over a point-to-point connection to determine the uni-directional TCP/IP speed, cf. Figure 5. The performance is seen to saturate at 93 MB/s.

![Fig. 5. Performance test by ttcp via ParaStation.](image)

It is instructive to compare these results with the outcome of the Pallas send-receive MPI benchmark [16], see Figure 6.

For the send-receive case (i.e. the bi-directional situation), the performance levels off at a total bandwidth of about 175 MB/s (adding up the data rates of both directions). As the PALLAS benchmark does not provide uni-directional measurements, we have prepared corresponding send and receive programs and found a saturation of the uni-directional MPI-performance at about 140 MB/s, cf. Figure 7. The data rate via TCP/IP is only about 34% smaller than via MPI, in spite of the overheads of the full-fledged TCP/IP implementation. Still this leaves room for improvement, since on a cluster there exists a priori knowledge of the paths to all IP destinations, therefore one could try to set up a slim TCP/IP protocol. Moreover, a double error checking is carried out, one on the ParaStation level, and a second one on the TCP/IP level.
Fig. 6. Performances of the send-receive Pallas MPI-benchmark on ALiCE.

Fig. 7. MPI-performance for uni-directional communication.

4 File System Benchmarks

Our benchmarks follow Ref. [13], where performance results on 60 nodes of the Chiba-City cluster at Argonne National Laboratory have been reported. This cluster is equipped with the same Myrinet version as ALiCE. This will enable us to compare our results using TCP/IP over ParaStation on an Alpha system with TCP/IP over the Myrinet/GM software on a Pentium cluster. Since loading and discharging large amounts of data to the cluster constitute a crucial bottleneck for data-intensive production runs on clusters, we include performances with respect to reading from and writing to UNIX files located on an external RAID.
4.1 Concurrent read/write performance

Our test code works as follows: a new PVFS file, common to \(P\) compute processes, is opened on \(N\) I/O-nodes. Concurrently the same amount of data \(S\) is written from each of the \(P\) processes (virtual partitioning) to disjoint parts of the file. PVFS stripes the data onto the \(N\) I/O-nodes (physical partitioning) with a stripe size of 64 kB.

After the data is written, we close the file and reopen it again in order to reshuffle the same data back to the compute-nodes. The bandwidth for write and read operations is computed from the maximum of the wall clock execution times achieved on all the \(P\) compute-nodes.

We vary \(P\) in the range \(P = 1 \ldots 64\), and repeat each measurement for \(N = 4\), \(N = 16\) and \(N = 32\) I/O-nodes. The amount of data \(S\) written and read per compute-node is chosen proportional to the number \(N\) of I/O-nodes, \(S/N = \text{const}\) (here we follow closely the benchmark of Ref. [13]). The reasoning is that although we vary the number of I/O-nodes, the buffer-cache will be saturated for one and the same number of compute-nodes. Indeed this behavior is borne out in Figure 8, which shows the cumulative throughput for the write operation.

![Figure 8. Concurrent write performance.](image)

We followed Ref. [13] and have carried out 5 measurements in each case. The smallest and the largest results were discarded and the remaining ones have been averaged. Actually, the five values did not differ by more than 2 % in any of the measurements.
As we see from Figure 8, the performance quickly reaches a plateau for each I/O-partition. There is no visible impact from the number of compute-nodes as long as the buffer-cache of the I/O-nodes is not saturated. This occurs when the number of compute-nodes is greater than 50. The amount of data written and read on every I/O-node is \( P \cdot S/N \), so it is greater than 100 MB for \( P > 50 \) and \( S/N = 2 \text{ MB} \).

The write performance reaches between 29 and 35 MB/s for each I/O-node, not exhausting the bonnie++ figures of Section 3.1 or the TCP/IP speed, see Figure 5. However, we achieve about 30% faster write performances than reported in Ref. [13]. Visually comparing the Figure 6 in Ref. [13] with Figure 8 we recognize the substantially improved stability of our curves, a well known feature of the communication sub-system ParaStation.

After buffer-cache saturation, the performance drops down to a value which is about 18% smaller than expected from the hard disk performance benchmarks displayed in Figure 4.

As the read operation is carried out directly after the write, with only a synchronizing barrier in between, the read process can draw the data directly from buffer-cache. As explained above, dirty buffers are written to disk if their size exhausts the limit of 100 MB. However, they remain in memory and can be read back at a rate limited only by the memory bandwidth. Thus, Figure 9 shows no loss of performance throughout the test range.

It is gratifying to find that each I/O-node can send with a speed varying between 56 MB/s and 75 MB/s, since several sockets are served simultaneously. This performance is just 20% slower than the measured point-to-point performance via TCP/IP, but still about 45% slower than the actual capabilities of ParaStation as seen in MPI applications, see Figure 6. The maximal performance reaches more than 1800 MB/s for 32 I/O-nodes.

We should remark, that the read test seems to be rather artificial. Actually, it would be more meaningful given a hard disk with a read performance faster than 75 MB/s. In general, a real application reads data from disk and not from buffer-cache. In that case, one expects a saturation below hard disk read performance, as demonstrated in Section 5.

In order to test the raw throughput of the disk, i.e. without utilizing the buffer cache, a modified benchmark was used. Now, a huge amount of data (multiple times the size of the buffer cache) is created and written to several files. After

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4 In fact the buffer-cache itself is not saturated, but at this point the amount of “dirty buffers” has reached 40% of the whole buffer-cache, see Section 3.1. With no other program running at the same time, almost all of the main memory is used for the buffer-cache, and 40% of 256 MB yield 100 MB, as observed.
writing and closing the last file, it is very unlikely that any data from the first files is still present in the buffer cache. A subsequent read operation will therefore be forced to read directly from hard-disk. Figure 10 shows the result of this benchmark.

Obviously the throughput for read operations from PVFS drops dramatically within such realistic setup. In the case of 4 I/O-nodes the read performance drops to about 13 MB/s per I/O-node. Nevertheless a total read performance of 300 MB/s can be achieved if all 32 I/O-nodes are utilized.
The results presented so far have used a stripe size of 64 kB, the default value of PVFS. Taking a stripe size as large as the amount of data a given compute-node has to write, we achieve about 920 MB/s writing from 32 compute-nodes to 32 I/O-nodes. The corresponding read-operation achieves up to 2200 MB/s using the cache. Without a full cache, performance is lower.

A second important feature—as far as data-intensive computations on clusters are concerned—is the speed for charging and discharging the system. A high throughput is is crucial for the success of computer experiments that work on data sets much larger than the PVFS disk space available. In this case one has to retrieve (store) data from (to) an external TB-size repository.

Distributing UNIX files onto PVFS from the archive in principle could proceed with the TCP/IP performance of about 92 MB/s. Actually, the limiting factor is the disk performance of the file server. Our RAID delivers or stores at about 25 MB/s. In practice this limitation poses no real problem, since data staging can be carried out asynchronously to the parallel applications on the cluster.

5 Fast I/O for Giant Eigenproblems in Lattice Field Theory

In the following, we demonstrate how PVFS/ParaStation enables us to compute huge eigensystems on cluster computers. Such computational problems arise in the post simulation phase of Monte Carlo simulations of lattice quantum chromodynamics (LQCD). We aim at computing $O(1000)$ low eigenvectors of the so-called fermionic matrix, which describes the dynamics of quarks in the gluon background field. The size of each vector is $O(10^6)$. Typically about 10 GB I/O is carried out in production runs of length $\approx 30$ minutes on 32 processors of ALiCE. In practice, we have to perform thousands of such runs.

5.1 Physical problem

Non-perturbative lattice quantum chromodynamics (LQCD) deals with the determination of hadronic properties and interactions [17]. Particularly important observables are given by the mass spectrum of bound quark states, as for instance the masses of hadrons like the $\pi$-Meson and the rho $\rho$-Meson. Among these particles, hadronic states that can be classified as singlet representation of the flavor-SU(3) group play a special rôle. They are characterized by contributions of so-called non-valence objects. More precisely, their correlation functions, $C_{\eta}(t_1 - t_2)$, the quantities which allow to extract the physical properties of the hadrons by exploring their decay in time, $\Delta t = t_1 - t_2$, contain
contributions from correlators between closed virtual quark-gluon loops. These “non-valence” objects are nothing but a manifestation of quantum mechanical vacuum fluctuations, which follow from Heisenberg’s uncertainty principle as applied to relativistic field theory. From a physical point of view, flavor singlet objects are particularly intriguing, as they are sensitive to (and thus allow to explore) the topological structure of the QCD vacuum.

The reliable determination of disconnected diagrams has been a long-standing issue ever since the early days of LQCD. It can be traced back to the numerical problem of getting information about functionals of the complete inverse fermionic matrix $M^{-1}$.\footnote{In contrast to flavor singlet observables, non-singlet masses are far simpler to compute: they imply the solution of a few systems of linear equations of type $Mx = b$, the discrete analogue of Dirac’s equation with source term.}

First attempts in this direction started only a few years ago, using the so-called stochastic estimator method (SE)\cite{18} for the computation of the trace of $M^{-1}$. This approach requires to solve a linear system $Mx = \xi$ on hundreds of source vectors $\xi$, with $\xi$ being noise vectors that are $Z_2$ of Gaussian distributed.

In Ref.\cite{11}, we have shown how to estimate the mass of the $\eta'$ meson just using a set of low-lying eigenmodes of $M$. Strictly speaking, our approach deals with the matrix $Q$, the hermitian form of $M$, the eigenvectors of which form an orthogonal base\cite{19}:

$$Q = \gamma_5 M. \quad (1)$$

The Wilson-Dirac matrix is given by

$$M_{x,y} = 1_{cs} \delta_{x,y} - \kappa \sum_{\mu=1}^{4} (1_s - \gamma_\mu) \otimes U_\mu(x) \delta_{x,y-\mu}$$
\[+ (1_s + \gamma_\mu) \otimes U_\mu(x-\mu) \delta_{x,y+\mu}. \quad (2)\]

The symbols $\gamma_\mu$ stand for the $4 \times 4$ Dirac spin matrices. The $3 \times 3$ matrices $U_\mu \in \text{color-SU}(3)$ represent the gluonic vector field, thus $1_{cs}$ is a $12 \times 12$ unit-matrix in color and spin space. $M$ is a sparse matrix in 4-dimensional Euclidean space-time with matrix valued stochastically distributed coefficient functions of type $(1_s \pm \gamma_\mu) \otimes U_\mu(x)$ at site $x$.

Once the low-lying modes are computed, it is possible to approximate the full inverse matrix $Q^{-1}$ and those matrix functionals or functions of $Q$ which are sensitive to small eigenvalues, i.e. long-range physics.
5.2 Numerical procedure

In LQCD, hadronic masses are extracted from the large-time behavior of correlation functions. The correlator of the flavor non-singlet π-meson is defined as

\[ C_\pi(t = t_1 - t_2) = \left\langle \sum_{\vec{x},\vec{y}} \text{Tr} \left[ Q^{-1}(\vec{x}, t_1; \vec{y}, t_2) Q^{-1}(\vec{y}, t_2; \vec{x}, t_1) \right] \right\rangle_U, \tag{3} \]

while the flavor singlet η’ meson correlator is composed of two terms, the first corresponding to the propagation of a quark-antiquark pair from \( \vec{x} \) to \( \vec{y} \) without annihilation in between and the second one being characterized by intermediate pair annihilation:

\[ C_{\eta'}(t_1 - t_2) = C_\pi(t_1 - t_2) - 2 \left\langle \sum_{\vec{x},\vec{y}} \text{Tr} \left[ Q^{-1}(\vec{x}, t_1; \vec{x}, t_1) \right] \text{Tr} \left[ Q^{-1}(\vec{y}, t_2; \vec{y}, t_2) \right] \right\rangle_U. \tag{4} \]

The brackets \( \langle \ldots \rangle_U \) indicate the average over a canonical ensemble of gauge field configurations. For large time separations \( t \), the respective correlation functions are dominated by the ground state, because the higher excitations die out and therefore become proportional to \( \exp(-m_0 t) \). \( m_0 \) is the mass of the particle associated to the correlation function.

As already mentioned, the π-correlator (3), equivalent to the first term of the η’-correlator, is obtained by solving the linear system

\[ M(\vec{x}, t_1; \vec{y}, t_2) c(\vec{y}, t_2) = \delta(\vec{1}, 1; \vec{x}, t_1); \tag{5} \]

on 12 source vectors (here located at site \((\vec{1}, 1))\). Of course, the statistics could be improved by averaging over many sources; however this becomes prohibitively expensive as the effort increases with the number of sources.

The second term in eq. (4),

\[ \sum_{\vec{x},\vec{y}} \text{Tr} \left[ Q^{-1}(\vec{x}, t_1; \vec{x}, t_1) \right] \text{Tr} \left[ Q^{-1}(\vec{y}, t_2; \vec{y}, t_2) \right], \tag{6} \]

depends on the diagonal elements of \( Q^{-1} \). The inverse can be expanded in terms of the eigenmodes weighted by the inverse eigenvalues:

\[ Q^{-1}(\vec{x}, t_1; \vec{y}, t_2) = \sum_i \frac{1}{\lambda_i} \frac{|\psi_i(\vec{x}, t_1)\rangle \langle \psi_i(\vec{y}, t_2)|}{\langle \psi_i|\psi_i \rangle}, \tag{7} \]

where \( \lambda_i \) and \( \psi_i \) are the eigenvalues and the eigenvectors of \( Q \) respectively. We found that we can approximate the sum on the right hand side by restriction.
to $O(300)$ lowest-lying eigenvalues and their corresponding eigenvectors. Due to the factor $1/\lambda_i$, one expects that the low-lying eigenmodes will tend to dominate the sum. Our procedure is called truncated eigenmode approximation (TEA).

We compute the eigensystem by means of the implicitly restarted Arnoldi method, a generalization of the standard Lanczos procedure. A crucial ingredient of our approach is a Chebyshev acceleration technique. The spectrum is transformed such that the Arnoldi eigenvalue determination becomes uniformly accurate for the entire part of the spectrum we aim for. A comfortable parallel implementation of IRAM is provided by the PARPACK package [20].

We work on a space-time lattice of size $16^3 \times 32$. Taking into account the Dirac and color indices, the Dirac matrix acts on a $12 \times 16^3 \times 32 = 1.572.864$ dimensional vector space. This explains why the inversion of the entire Dirac matrix is not feasible since this would need about 40 TB memory space, whereas the determination of 300 low-lying eigenvectors leads to about 7.5 GB memory space only. Our computations are based on canonical ensembles of 200 field configurations with $n_f = 2$ flavors of dynamical sea quarks. Such kind of ensembles have been generated at 5 different dynamical quark masses in the framework of the SESAM full QCD project [21]. It takes us about 3.5 Tflop-hours to solve for 300 low-lying modes per ensemble for each quark mass. Altogether we aim at $O(30)$ valence mass/coupling combinations. First physical results of our computations can be found in Refs. [11,22,23,24].

5.3 Benchmarks

The typical compute partitions used for the TEA on ALiCE range from 16 to 64 nodes, depending on the number of eigenmodes required for the approximation as well as on the memory available. Each node reads its specific portion of a given eigenmode corresponding to the sub-lattice assigned to this node. In our case, a simple regular space decomposition of the $16^3 \times 32$ lattice in $z$ and $t$ directions is applied.

Physically, the 300 eigenmodes for each field configuration are stored as a single large file in round-robin manner. In case of a stripe-size that corresponds to the size of an entire time-slice of the lattice, each time-slice will be assigned to exactly one processor by PVFS.

In our application we use MPI-IO calls (MPI_File_read_at()) instead of standard I/O to read from the PVFS. In Table 1 performance averages over four measurements are presented. The results fluctuate only marginally.

As to be expected from Figure 10 the throughput for read-operations is as
Table 1
Read and write performances for three compute partitions.

| # of compute nodes | 16 | 32 | 64 |
|-------------------|----|----|----|
| # of eigenmodes   | 100| 200| 300|
| read performance per I/O-node [MBytes/s] | 11.9 | 13.3 | 11.1 |
| write performance per I/O-node [MBytes/s] | 11.9 | 13.4 | 13.2 |

high as 13 MB/s, which is the actual hard-disk performance. The effective throughput for write-operations is about 10 % less than achieved in Figure 8, most likely a remaining MPI-IO overhead.

5.4 Gain

A production step includes reading eigenmodes and computing observables. Typically the computation takes about 10 minutes. Another 10 minutes are needed for loading all 300 modes from the local disk. Loading the data from an external archive (which is the usual procedure since local disks do not provide enough capacity for an entire ensemble of field configurations and eigenmodes) lasts about 30 minutes. This large mismatch between compute time and I/O time (where the processors are idling) renders standard clusters very inefficient for such type of computational problems, denoted as \textit{data-intensive}.

PVFS via ParaStation/Myrinet cuts down the I/O-times to less than 20 seconds for both reading and writing. This is a substantial acceleration compared to local or remote disk I/O. With these improvements we were able to enter large-scale productions with thousands of read-compute-write sequences to be carried out. After several months of continuous heavy duty we find the I/O system to behave remarkably reliable and stable, with no failure encountered so far.

6 Future Perspectives: ClusterFile

Most parallel file systems, including PVFS, distribute the files stripe-wise over the I/O-nodes. However, parallel applications provide their specific data structures that are often accessed in form of regular patterns called the “virtual” or “logical” partitioning of the data. The access pattern studies [25,26,27] have shown that the performance and scalability of parallel scientific applications with intensive parallel I/O-activity suffer significantly from the mismatch between virtual partitioning and physical placement of file data. This may result in an under-utilization of disk and network bandwidths and in a decreased
For the above mentioned reasons, it is important that a parallel file system offers support for flexible physical partitioning. On one hand one would wish a fully developed PFS to be able to “translate” efficiently from any physical partitioning of the files on the I/O-nodes of the PFS to any virtual partitioning and vice versa, on the other hand one would like to control the physical data layout on the PFS. So far, this goal is only partly realized by PVFS. Therefore, we decided to develop a novel parallel file system, called ClusterFile [14], that addresses these issues.

In its present state, ClusterFile presents architectural similarities with PVFS, in so far that several I/O-daemons are responsible for storing the data on I/O-nodes with one central meta-data manager. The clients must link to a library that provides transparent file system access.

Unlike PVFS, ClusterFile employs a file partitioning model, that allows the arbitrary distribution of data over a cluster, in regular or irregular patterns. The model is optimized for regular patterns, since most frequently used data structures of parallel scientific applications are multidimensional arrays [25], partitioned into chunks among parallel processes.

The file model of ClusterFile is used for both physical and logical partitioning. A file is physically partitioned into sub-files. As an example, it is possible to spread a file over several disks using a block-cyclic distribution or any other regular and irregular distribution as for instance supported by High Performance Fortran [28].

A file may be logically partitioned between several processors by means of views. A view is a sequential window to an eventually non-contiguous subset of a file and can be used exactly in the same way as a file. An important advantage of using views is that it relieves the programmer from complex index computation. Additionally, it also provides hints on potential future access patterns and can be used for matching the physical to the logical distribution. For instance, if a file is striped in round-robin manner over the disks while the parallel processes of an application set block-cyclic views, it could be better for performance to convert the physical layout into a conforming block-cyclic distribution.

The processes of a parallel application access a shared file in many cases at nearly equal times. This observation suggests the design of collective I/O operations. Their main goal is to coalesce many small I/O requests of several cooperating processes into a few large requests. The two main categories of collective I/O are two-phase [29] and disk-directed [30] operations. The two-phase I/O consists of a file access step that is independent of the virtual partitioning, and a shuffle-phase in which the access data is distributed according
to the access pattern. The MPI-IO library, which is implemented on top of PVFS and ClusterFile utilizes the two-phase method since it is not aware of the physical file partitioning. ClusterFile implements a version of the disk-directed method, in which the requests are gathered at I/O nodes, coalesced, before access is performed, and the result is returned to the compute nodes. This approach has the advantage that it can exploit the relationship between physical and logical partitionings, whereas the two-phase method separates the operation into two distinct steps.

In the future we plan to test ClusterFile on ALiCE and to perform a detailed comparison with PVFS. We expect the collective I/O implementation of ClusterFile to perform better than that of MPI-IO, due to the above mentioned reasons.

Another important step will be the incorporation of cooperative caching policies [31] that allow the buffer-caches of I/O- and compute-nodes to interact. The goal is to provide a global caching policy that provides a better utilization of buffer-caches and avoids unnecessary disk requests.

7 Summary

We have demonstrated that the ParaStation3 communication system speeds up the performance of parallel I/O on cluster computers such as ALiCE. I/O-benchmarks with PVFS using Parastation over Myrinet achieve a throughput for write-operations of up to 1 GB/s from a 32-processor compute-partition, given a 32-processor PVFS I/O-partition. These results out-perform known benchmark results for PVFS on 1.28 Gbit Myrinet by more than a factor of 2, a fact that is mainly due to the superior communication features of ParaStation. Read-performance from buffer-cache reaches up to 2.2 GB/s, while reading from hard-disk saturates at the cumulative hard-disk performance. The I/O-performance achieved with PVFS using ParaStation enables us to carry out extremely data-intensive eigenmode computations on ALiCE in the framework of lattice quantum chromodynamics. In the future the I/O-system will be utilized for storing and processing mass data in high energy physics data analysis on clusters.

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