FFT for the APE Parallel Computer

THOMAS LIPPERT, KLAUS SCHILLING, FEDERICO TOSCHI,
SVEN TRENTMANN, RAFFAELE TRIPICCIONE

HLRZ c/o KFA-Jülich and DESY
D-52425 Jülich, Germany

Dipartimento di Fisica, Università di Pisa
Piazza Torricelli 2, I-56126, Pisa, Italy,
and
INFN, Sezione di Tor Vergata,
Via della Ricerca Scientifica 1, I-00133, Roma, Italy.

INFN, Sezione di Pisa, c/o
I-56010 S. Piero, Pisa, Italy

Received

We present a parallel FFT algorithm for SIMD systems following the ‘Transpose Algorithm’ approach. The method is based on the assignment of the data field onto a 1-dimensional ring of systolic cells. The systolic array can be universally mapped onto any parallel system. In particular for systems with next-neighbour connectivity our method has the potential to improve the efficiency of matrix transposition by use of hyper-systolic communication. We have realized a scalable parallel FFT on the APE100/Quadrics massively parallel computer, where our implementation is part of a 2-dimensional hydrodynamics code for turbulence studies.

Keywords: FFT; Transpose Algorithm; Hyper-Systolic

1. Introduction

The efficient implementation of Fast Fourier Transforms (FFT) on parallel high performance computers is of tantamount importance in order to warrant broad scientific and industrial application of these systems.

The ongoing development of new high speed low cost parallel computers with Teraflops performance, designed primarily to solve problems in lattice quantum field theory\textsuperscript{1–4}, generates interest in other scientific and commercial fields with Tera-computing needs. There are quite a few such applications for which one would like to spend 10 to 1000 sustained Teraflopshours. However, low cost parallel systems go along with certain architectural restrictions as \textit{e.g.} next-neighbour connectivity\textsuperscript{5,6}. Numerical procedures like FFT that involve non-local inhomogeneous interproces-
Th. Lippert et al.

sor communication patterns are therefore hard to implement efficiently on these machines. The communication bottleneck of FFT is even more serious on single addressing machines like APE100, referred to as SISAMD in the following\(^a\), where the individual processing units do not provide indexed local addressing\(^1\).

The substantial cost-factor of FFT on parallel computers arises from ‘bit-inversion’ of the location of each input data element and from the pair-wise decimation of the bit-inverse ordered array elements\(^7\). As a result, FFT is harassed by frequent non-contiguous memory accesses. On a standard computer, this fact implies repeated cache misses, while on a parallel machine it translates into non-local interprocessor communication.

A well known strategy to carry out FFT on parallel systems for a dimensionality \(\geq 2\) is based on the splitting of the \(d\)-dimensional FFT into \(d\) 1-dimensional FFT’s\(^7\). This approach\(^b\) is known as the ‘Transpose Algorithm’\(^8\). Let us start from a \(d\)-dimensional data field with coordinates \(i_1, i_2, \ldots, i_d, i_k = 0, \ldots, n_k - 1\). The field may be distributed such that one axis (coordinate \(i_1\)) is spread across the processors, while the other axes are locally assigned to the processors. In this case, the 1-dimensional FFT can be computed on the local axes (coordinates \(i_2, \ldots, i_d\), i.e. for each coordinate \(i_k\) in parallel without access to remote memory. However, as at least one axis has to be distributed across the processors, a reordering of the data field between distributed and local axes is required. Such a reordering of the data elements is equivalent to a matrix transposition. So the generic task is to devise an efficient Transpose Algorithm for distributed array layout\(^8\).

In Ref. 9, a promising implementation of the Transpose Algorithm, adapted to mesh-based SIMD computers with next-neighbour connectivity, has been discussed. A \(k\) dimensional field of volume \(V\) is assigned to the processors within a \(d\)-dimensional toroidal mesh network. The transposition of the field is performed in a three-step procedure: first the data field is skewed (like rendering a matrix skew). This step is followed by interprocessor communication. The final step is an inverse skewing.

The authors of Ref. 9 specify a pattern for the interprocessor communication adapted to \(d\)-dimensional mesh architectures like APE. For the 3-dimensional connectivity of APE100/Quadrics they reached the gratifying result that the interprocessor communication can be performed with complexity of \(V/p^2\) data communication operations per processor, where \(V\) is the data volume.

The two local skewing steps at the beginning and the end of the transposition have to be carried out according to the machine’s addressing capabilities: on SIMD or MIMD machines, skewing is nothing but a local data assignment. An extra difficulty arises on SISAMD computers since they lack local addressing. The lack of local addressing at first sight renders the skewing phase non-scalable, i.e., each processor has to carry out its copy operations separately. This leads to an unac-

\(^a\) SISAMD: Single Instruction Single Addressing Multiple Data

\(^b\) A second standard procedure, the ‘Bit-Exchange’ algorithm, is better suited for hyper-cubic architectures than mesh computers.
ceptable performance degradation on SISAMD machines\textsuperscript{c}. We will largely overcome this problem, by introducing a novel skewing algorithm that proceeds in \( \log p \) steps.

Starting out from Ref. 9, we construct a general transpose algorithm for FFT, that can be implemented in a scalable manner on any parallel architecture. For this purpose, we first associate the data field to a 1-dimensional ring of systolic cells\textsuperscript{10}, that can perform both computations and communication (to neighbouring cells). Our systolic ring can be readily mapped onto any parallel machine’s processor connectivity. One way to do this for APE100/Quadrics has been presented in Ref. 11. We can reduce the time expense of systolic interprocessor communication along the systolic ring by application of hyper-systolic data movement\textsuperscript{12,13}. Implemented on a \( d \)-dimensional mesh, each processor has to perform \( O(V/p^{d-1}) \) communication operations on average.

One particular target implementation system of our FFT will be the European Teraflops system of 1998, APEmille\textsuperscript{2}. APEmille is designed as SIMD machine with next-neighbor connectivity.

There are of course many Tera-computing applications where efficient parallel FFT algorithms will be of use, \( e.g. \) spectral methods in global climate modeling, turbulent fluid dynamics or quantum chromodynamics. The latter two will serve us as examples for illustration and benchmarking of the Transpose Algorithm.

The implementation of a 1-dimensional FFT on APE which is important for signal processing applications will be presented in an upcoming publication\textsuperscript{14}.

### 2. Transpose Algorithm on a Systolic Ring

We construct a Transpose Algorithm as implemented on a 1-dimensional systolic array with toroidal topology.

#### 2.1. Data assignment

Let us consider a 2-dimensional data field (matrix) \( M \) of size \( p \times p \), where \( p \) is the number of processors of the parallel system. Each element \( m_{ji}, i = 0, \ldots, p-1, j = 0, \ldots, p-1 \), can be considered as sub-matrix. This structure will allow for easily generalization to data arrays of size \( V = m \times n = \frac{m}{p} \times \frac{n}{p} \times p \times p \) with rectangular shape.

In the following, we assume that the implementation network supports the embedding of a 1-dimensional ring topology. Along the ring, circular shifts in an homogeneous pattern can be performed.

To achieve a universal Transpose Algorithm we are going to discuss the method as implemented on an array of systolic cells that can perform compute, store and communication operations. For illustration, in Fig. 1, a 1-dimensional ring with \( p = 8 \) cells is sketched. The cells are connected to their next neighbours by direct communication lines. The cells can perform communication operations to the next

\textsuperscript{c}Ref. 9 discusses the implementation of the Transpose Algorithm for Multi-controller APE systems that can partly overcome the SISAMD restrictions.
neighbours in a homogeneous pattern as well as synchronous compute operations with equal load, on cell resident data. This systolic array concept is simple enough to be mapped efficiently onto practically any parallel architecture and thus is the adequate framework for the construction of a “universal” Transpose Algorithm.

The initial data assignment on the systolic ring is given in Fig. 2. The data elements are indexed following standard matrix notation. Note that matrix elements with equal second coordinate $i$ are all assigned to cell $i$, while their first coordinate refers to their local address.

Figure 1: Systolic array of 8 systolic cells forming a systolic ring.

Figure 2: Assignment of the $p \times p$ data array $M$ to the $p$-cell ring.
2.2. Transposition

The transposition of $M$ proceeds within 3 steps, a pre-skewing step, that does not involve interprocessor communication, a row-shifting step, requiring interprocessor communication and finally a re-skewing step, again without interprocessor communication:

1. Pre-Skewing. The matrix $M$ is locally skewed along the columns. The $i$-th column is shifted upward by a circular shift of stride $i$. After finishing this process for all columns $i$, the diagonal elements of the original matrix are located in the first row, see Fig. 3.

The skewing procedure is given in the pseudo-code representation of Algorithm 1.

```
Algorithm 1 Pre-Skewing.
    foreach cell $i = 0 : p - 1 \in$ systolic array
        for $j = 0 : p - 1$
            $m_{j,i} = m_{[(j+i)\text{mod}_p],i}$
        end for
    end foreach
```

Note, that in each step different cells act on different internal addresses. As all cells of a systolic array perform equal operations per definition, skewing is not a systolic process! However, we will demonstrate in appendix A how skewing can be performed in form of a systolic process, within $p \log p$ steps. Therefore, by mapping of the systolic array onto a SISAMD systems we are able to perform skewing in a scalable manner. Of course on SIMD and MIMD systems skewing is trivial as it can be carried out by usage of local addressing facilities.
2. **Row-shifting.** In the second phase, the rows of \( M \) are shifted along the ring. After the shift, the rows are assigned to a local memory location determined as follows: the \( j \)-th row is circularly shifted by a distance of \( j \) cells to the right and subsequently is copied from storage location \( j \) to storage location \( (p - j) \mod p \). The procedure is given in Algorithm 2.

**Algorithm 2** Row-Shifting.

```plaintext
foreach cell \( i = 0 : p - 1 \in \text{systolic array} 
for j = 0 : p - 1 
m_{j,i} = m_{[(p-j) \mod p, (i+j) \mod p]} 
end for 
end foreach
```

The corresponding data locations after completion of phase 2 are illustrated in Fig. 4.

![Figure 4: \( p \times p \) data array \( M \) after row-shifting.](image)

We emphasize that in any step, each cell acts on the same local addresses. Therefore, the row-shifting is a systolic process and, mapping the systolic array onto the processors of a parallel computer, local address computations are not required.

3. **Re-Skewing.** In a last step, the matrix \( M \) is skewed downwards, in analogy to the pre-skewing step. The \( i \)-th column is shifted by a circular shift of stride \(-i\). The final data arrangement is depicted in Fig. 5.
The pseudo-code representation of the re-skew step is given in Algorithm 3.

**Algorithm 3** Re-Skewing.

```plaintext
foreach cell \( i = 0 : p - 1 \in \text{systolic array} \\
for j = 0 : p - 1 \\
m_{j,i} = m[(j-i+p)\mod p,i] \\
end for
end foreach
```

For FFT in more than 1 dimensions, two such transposition have to be carried out. In Algorithm 4, we give a pseudo-code template for parallel FFT in two dimensions:

**Algorithm 4** 2-dimensional parallel FFT.

```plaintext
call 1-d-FFT ! on local axis 
call transpose 
call pre-skew 
call row-shift 
call re-skew 
call 1-d-FFT ! on local axis 
call transpose 
call pre-skew 
call row-shift 
call re-skew
```

For the description of FFT we refer to Ref. 7.

### 3. Mapping on APE100/Quadrics

The ring of systolic cells together with their functionality can readily be mapped onto the processors of a parallel machine that supports a 1-dimensional ring topology. We are going to describe the mapping for APE100/Quadrics.
3.1. The APE100/Quadrics parallel system

The parallel system APE100 has been designed primarily for quantum chromodynamics computations on a lattice. Its commercial version goes under the name Quadrics. The diagram Fig. 6 depicts the Quadrics system: compilation and program submission as well as I/O tasks are carried out on a front-end workstation. The so-called Z-CPU manages the instruction stream (synchronous for all computing nodes) and performs global integer arithmetics.

The programming language TAO looks FORTRAN like. It supports so-called syntagmas, structs which are very useful for efficient programming. TAO supports a local address space whereas communication from and to remote memories uses additional global address bits.

The compute nodes perform the local floating point operations. They are composed of memory, a floating point unit called MAD, and the communication chips. The MAD is able to perform 2 floating point operations within one clock cycle, that is \((25\text{MHz})^{-1}\). Thus, one processor has a peak speed of 50 Mflops.

The smallest configuration of the Quadrics computers is a Q1, a unit of 8 compute nodes, called a board. The nodes are connected by 6 communication links to their neighbor nodes in a 3-dimensional grid, see Fig. 6. Larger machines like the 32-node Q4 or the 512-node QH4 are composed of several boards. The network topology of the large system is hard-wired. A 512-node Quadrics QH4 is typically configured as an \(8 \times 8 \times 8\)-grid, toroidally closed in each direction.

In order to transfer one 32-bit word from the memory of the neighboring processor to the memory of the local processor, apart from start-up times, 8 clock cycles are needed in the ideal case. In practical applications, this limit can not be reached completely, however.

APE100/Quadrics is the European pathway towards Tera-computing. The APE groups in Pisa and Roma are currently developing their next generation of SIMD machines, the parallel APEmille systems. This machine will exhibit a com-
The APEmille architecture is extremely similar to APE100 (same topology and interconnectivity). Improvements, beyond much higher performances, include integer and double precision arithmetic.

As the most important extension to the present APE100 architecture all processing nodes may access their own local memories using different local addresses. Thus, APEmille will overcome the local addressing restrictions of APE100, allowing to implement algorithms that could not scale on APE100 machines.

A second advantage is the more general long-distance routing capability. Indeed, rigid communications can be set-up at arbitrary distances and automatically handled by the network (cut-through-routing). Again, this simplifies coding of the systolic moves and reduces communication latency. Furthermore, the APE100 software will be upward compatible for APEmille, and FFT-packs developed for APE100 can readily be ported onto APEmille.

3.2. Embedding a 1-dimensional ring on Quadrics

As has been shown in detail in Refs. 11 and 16, the 3-dimensional network of the Quadrics can be exploited to emulate the 1-dimensional ring functionality and to carry out shifts of any stride.

On a 3-dimensional grid based machine, the shifts can be described by a sequence of hardware communication operations in each of the three directions. We encode the stride $a_l$ in terms of the distance between processor 0 and processor $l$ on the systolic ring, by

$$l = l_2 + l_1p_2 + l_0p_2p_1 = a_l,$$  \hspace{1cm} (1)

with $p_i$ being the number of processors in direction $i$, and $l_i$ the coordinates of processor $l$ in direction $i$ on the 3-dimensional processor grid, the total number of processors being $p = p_0p_1p_2$. The cost function $C(a_l)$ in units of hardware communication operations is given as

$$C(a_l) = l_0 + l_1 + l_2.$$  \hspace{1cm} (2)

The total cost function $C_t$ is the sum of the individual $C(a_l)$ over all circular shifts with stride $a_l$, $a_l = 0, \ldots, p - 1$:

$$C_t = \sum_{l_2=0}^{p_2-1} \sum_{l_1=0}^{p_1-1} \sum_{l_0=0}^{p_0-1} (l_2 + 1 + l_1 + 1 + l_0 + 1) = \frac{p}{2} (p_0 + p_1 + p_2 + 3).$$  \hspace{1cm} (3)

In practise, one can exploit hardware communication for each axis in both directions. Hence, the average cost per shift can be reduced by a factor of 2, and on a 3-dimensional machine with next-neighbour connectivity the wall clock time for interprocessor communication decreases like

$$t_{ipc} \propto \frac{1}{p} (p_0 + p_1 + p_2 + 6),$$  \hspace{1cm} (4)
for a fixed size $V$ of the data array.

4. Benchmarking the Transpose Algorithm on APE100/Quadrics

We have mapped the FFT based on the systolic Transpose Algorithm onto several Quadrics parallel SISAMD computers. Here we present timing results and scaling. In the next section we discuss two physics case studies where FFT can play an important rôle.

For a 32-node APE100/Quadrics Q4 system and a 512-node QH4 system we give detailed timing results. We plot the total execution times against the matrix size $V$, cf. Fig. 7. On both machines the asymptotic behaviour is reached when the length of the stream set involved in row-shifting is larger than 32 data elements. For stream smaller than 32 elements we are faced with a start-up time effect. The

![Graph showing the relationship between matrix size and execution time for 32 and 512 nodes.](image)

**Figure 7:** Double log plot of transposition vs. matrix size $V$ on a 32-node Quadrics Q4 and a 512-node Quadrics QH4.

The two curves intersect each other for about $n = 1024$.

In order to test the scaling law, Eq. 4, we plot the times for interprocessor communication for a fixed matrix size of $2048 \times 2048$ complex elements on various Quadrics platforms, against the number of processors (see Fig. 8). A fit to the data according to $t \propto p^\alpha$ reveals an exponent $\alpha$ of $-0.76$. The naive expectation
from Eq. 4 for cubic machine topologies would be \(-0.66\). However, the actual
topologies were \(V_{(p=512)} = 8 \times 8 \times 8\), \(V_{(p=256)} = 8 \times 8 \times 4\), \(V_{(p=128)} = 8 \times 4 \times 4\), and
\(V_{(p=32)} = 8 \times 2 \times 2\).

5. Applications of FFT on APE100/Quadrics

The work described in the previous section has been motivated by the need to have
a fast FFT in some physics applications of ours. The solution of these problems
can benefit considerably from the power of APE computers.

5.1. 2-dimensional FFT: Kraichnan model

In order to simulate the Kraichnan model\(^{15}\), an efficient 2-dimensional FFT trans-
form was required. The Kraichnan model is a toy model which has attracted much
interest recently, because of its analytical simplicity with respect to the full Navier-
Stokes equations. An often studied problem of turbulence is the anomaly of the
scaling exponents in the inertial range. In order to get reliable numerical values for
these exponents, huge computer simulations are required.

This toy model describes a passive scalar \(T(x, t)\) which moves in a velocity field
which is synthetically generated with a given scaling exponent \(\xi\). One studies the
scaling exponent $\xi_T$ of the passive scalar as a function of $\xi$. The relevant equations are:

$$\partial_t T + (\mathbf{u} \cdot \nabla) T = \chi \nabla^2 T + f$$

$$\langle f(x, t)f(y, t') \rangle = \delta(t - t') C(|x - y|)$$

$$\langle v_i(x, t)v_j(y, t') \rangle = D^{\alpha \beta}(x - y) \delta(t - t'). \quad (5)$$

$$D^{\alpha \beta}(x) = D(0) \delta^{\alpha \beta} - d^{\alpha \beta}(x)$$

$$d^{\alpha \beta}(x) = D \left( (d + \xi - 1) \delta^{\alpha \beta} - \xi \frac{x^\alpha x^\beta}{|x|^2} \right) |x|^\xi$$

The random force $f(x, t)$ is delta correlated in time and Gaussian with correlator $C$ (a function with support of the order of size of the system) in space. The velocity field is $\mathbf{u}$, its statistical properties are given by Eq. 5 and, as it is clear from the expression for $D^{\alpha \beta}$, the incompressibility condition is fulfilled. The exponent $\xi$ is just the scaling exponent imposed on the velocity field (relevant values are in the range $[0, 2]$).

The main practical problem for the simulation of a system of this kind are the huge size of the system (i.e. $8192 \times 8192$) and the fact that a new velocity field is required at each time step.

The velocity field with the required statistical properties given by Eq. 5 is easily generated in Fourier space just by extracting random gaussian amplitudes (for the $k$ modes) with given variance $\sim k^{-1-\xi/2}$. The direction of the $k$-th component $\mathbf{u}_k$ is choosen such that $\mathbf{k} \cdot \mathbf{u}_k = 0$. In addition, with FFT, periodic boundary conditions are automatically fulfilled.

Alternative algorithms could be used for the generation of the velocity field, but, since the required statistical property is non-local, they would face the non-locality problem anyway and communication between different processors would become very heavy. In the case of our problem, a further major performance gain can be achieved in a very simple way. Since we need a specific geometric mapping of the variables only in real space, we can skip a transposition step by generating transposed amplitudes in $k$ space. This is of course true in several interesting cases, when we need to go to $k$ space in order to make some computation and then we want to come back to real space.

The FFT which has been described in this article has been implemented on a 512-node QH4 machine and has been optimized for working with very large lattice sizes (i.e. $8192 \times 8192$ elements). We are able to compute an FFT on the corresponding date set of about 512 Mbyte in 4 seconds. This means that we are working at about 9% of the peak performance for the above problem. If we perform the complete FFT including the back-transposition, we achieve about 6% of the peak performance.
5.2. 4-dimensional FFT: Quantum chromodynamics

In principle, the above Transpose approach to parallel FFT could be applied for systems of any dimensionality $\geq 2$. However, from a practical point of view, in the implementation of FFT on parallel systems we meet rather different situations: on a low dimensional lattice, the length of the axes obviously can be much larger than that of a high dimensional lattice. However, the length of at least two axes must be as large as the length of the systolic ring, otherwise we would have to pad with zeroes and would loose efficiency.

This situation occurs e.g. in simulations of lattice quantum chromodynamics\textsuperscript{17} (QCD). QCD is formulated on a 4-dimensional euclidean space-time lattice. Some aspects of QCD simulations, like e.g. gauge fixing\textsuperscript{18}, Fourier acceleration of Krylov solvers\textsuperscript{19} or accelerated updates might involve FFT\textsuperscript{20}.

We can not go into detail of lattice QCD here, but rather discuss the FFT implications of a 4-dimensional field $f(x_0, x_1, x_2, x_3)$. This field is assigned onto a finite 4-dimensional lattice of size $x_0 = 0, \ldots, p_0 - 1$, $x_1 = 0, \ldots, p_1 - 1$, $x_2 = 0, \ldots, p_2 - 1$, and $x_3 = 0, \ldots, p_3 - 1$. Typical sizes of QCD lattices range between $16^4$ and $64^4$ sites, hence on massively parallel systems with $p > 100$, the direct application of the approach described above would not be adequate for these applications.

However, the systolic FFT idea can be readily generalized: In the case of the 2-dimensional FFT on a 3-dimensional grid computer, one axis was distributed while the other was local on the systolic ring. Handling the 4-dimensional FFT on a 3-dimensional grid computer one has more than one option.

A very natural choice is to stick to the lexicographic data layout of the 4-dimensional QCD lattice. This leads to introduce many systolic rings along the grid axes of a given dimension. On a 3-dimensional grid the set of axes along a given direction is specified by fixing two grid coordinates orthogonal to the direction, say coordinates $x_0$ and $x_1$. Then, we can consider the axes specified by $x_0$ and $x_1$ of our 4-dimensional system as a number of $p_0 p_1$ systolic rings. On each ring, coordinate $x_2$ of the 4-d system is laid out while $x_3$ is local. Therefore, each of the rings corresponds to the situation we have encountered in the above case of 2-dimensional FFT. The Transpose Algorithm introduced above applies readily to this situation.

The order of local axes 4-dimensional FFT is schematically illustrated in Fig. 9. Initially, we perform the FFT along the third dimension, regarded as local at this time. Next, we transpose axis 2 with axis 3 and perform the FFT along the second axis being local now. This transposition is carried in parallel for all coordinates $x_0$ and $x_1$. It is obvious how the process can be continued. In the second step, we fix dimension 0 and 3 and transpose axis 1 with 2. Hence we can FFT axis 1, being local now. In the third step, we fix dimension 2 and 3, transpose axis 0 and 1 and can perform FFT on axis 0 being local now. Finally, we transpose axis 3 with 0 and re-arrive in the original data layout. Algorithm 5 gives the pseudo-code.
Figure 9: Schematical view of 4-dimensional FFT on a 3-dimensional processor grid.

Algorithm 5 4-dimensional parallel FFT on 3-dimensional processor grid.

```
call 1-d-FFT(axis 3)
call transpose(axis 2 and 3)
call 1-d-FFT(axis 2)
call transpose(axis 1 and 2)
call 1-d-FFT(axis 1)
call transpose(axis 0 and 1)
call 1-d-FFT(axis 0)
call transpose(axis 3 and 0)
```

6. Summary

We have presented a novel scalable parallel algorithm for matrix transposition and its application within FFT. Universality of the method is achieved by assignment of the data onto an abstract systolic ring that can be readily mapped onto any parallel system. For mesh systems the use of the hyper-systolic communication structure improves the communicational complexity considerably. In our scheme we can avoid computation of local addresses. Thus, in particular for SISAMD systems like APE100/Quadrics, the implementation of efficient FFT became feasible.

We have implemented the FFT scheme within a 2-dimensional simulation of the Kraichnan model for passive advection. Further, we suggested an implementation of 4-dimensional FFT applied within lattice quantum chromodynamics. In the first application the FFT performs with an efficiency of about 9% of the peak performance of the system, in a general application we reach about 6%.

On the European Teraflops system APEmille to come there is no restriction as to local addressing. Pre-skewing and Re-skewing will benefit mostly. Coding will be straightforward and the computation significantly faster (about an order of magnitude for a 512 node machine compared to on APE100/Quadrics). On APEmille, we expect to achieve a performance for FFT of about 15% of the theoretical peak performance.

To set the numbers achieved on APE100 and expected on APEmille into per-
spective we can compare with results from general purpose parallel machines. On
the Cray T3E for an 8 node partition, the 3-dimensional FFT on complex data per-
forms with 10 % of the peak performance using the optimized scientific library\textsuperscript{21}. On the Hitachi SR2201, a $8k \times 8k$ complex data array is Fourier transformed with a speed of 30 % of the machine’s peak performance\textsuperscript{22}.
Currently we are working on an efficient realization of 1-dimensional FFT.

**Acknowledgements.** The numerical tests in this work have been carried out on
a 512-node QH4 system at INFN, Pisa, Italy and the 256-node QH2 and 128-node
QH1 at the University of Bielefeld, Germany. We thank the staff of these centers
for their support. We thank Dr. R. Vogelsang, Cray/ZAM Jülich, Germany and
Dr. P. Haas, RUS, Stuttgart, Germany for benchmarking the Cray T3E and the
Hitachi SR2201. Th. L. is indebted to Paolo Palazzari for many useful discussions
and the construction of the APE100/Quadrics cost function tables. The work of
Th. L. is supported by the Deutsche Forschungsgemeinschaft DFG under grant
No. Schi 257/5-1. F. T. thanks K. S. and Th. L. for their friendly hospitality at
HLRZ/Jülich, where part of this work was performed.

**Appendix**

**A: Skewing on SISAMD Computers**

The first and last phases in the matrix transposition presented above involve the
representation of $M$ in skew order. On systems with indexed addressing facilities
skewing is just a local address computation. However, for SISAMD systems like
APE100/Quadrics, skewing is more difficult as its naive implementation spoils scal-
ability.

```
Algorithm 6 Skewing for SISAMD systems.
    foreach cell $i = 0 : p - 1 \in$ systolic array
        for $q = 0 : l - 1$
            $g = h \mod 2^q$
            where $g_q > 2^q$
            for $j = 0 : p - 1$
                $m_{j,i} = m_{(j+2^q),i}$
            end for
        end for
    end foreach
```

In order to solve this problem we have developed a systolic skewing algorithm
that avoids indexed addressing and shows logarithmic complexity. Thus the method
is well suited for SISAMD systems.

We start from the initial data configuration as illustrated in Fig. 2. Let $p$
be a number $2^l$, $l \in \mathbf{N}$, and let $h$ number the cells from 0 to $p - 1$ along the
systolic ring. Taking $g_q = h \mod 2^q$, $q = 0, \ldots, l - 1$, we can partition the cell array
successively in $\frac{p}{2}, \frac{p}{4}, \ldots, 2$ parts of equally numbered sequences. In each step we can
impose a conditional statement that is true where $g_q > 2^q$. There a local memory shift operation by a stride of $2^q$ is executed. After l such steps, the data array is represented in skew order. The process is illustrated as pseudo-code in Algorithm 6.

B. Skewing by Translation Invariance

An alternative to pre and re-skewing as presented above can be constructed by usage of the translation invariance of the system. The task is to calculate a Fourier transformed function $\tilde{f}_j$ (we consider one dimension) that is computed from the real space function $f_i$, $i = 0, \ldots, N-1$ which is a vector $f_i = g_{(i+k)\mod N}$, translated by $k$ elements. The Fourier transform

$$\tilde{f}_j = \sum_{i=0}^{N-1} f_i \exp \frac{2\pi ji}{N}$$

(6)

can be written in terms of $g$:

$$\tilde{f}_j = \sum_{i=0}^{N-1} g_{(i+k)\mod N} \exp \frac{2\pi ji}{N}$$

$$= \exp \left( -\frac{2\pi jk}{N} \sum_{i=0}^{N-1} g_{(i+k)\mod N} \exp \frac{2\pi j(i+k)}{N} \right)$$

$$= \exp \left( -\frac{2\pi jk}{N} \sum_{i=0}^{N-1} g_i \exp \frac{2\pi jl}{N} \right).$$

(7)

The translation in real space amounts to the application of a mode dependent phase factor in Fourier space. Similarly, a translated left hand side is computed using corresponding phase factors.

A 2-dimensional FFT as given in Algorithm 4 can be performed on SISAMD systems omitting 3 skewing steps. However, one re-skewing step remains:

**Algorithm 7** 2-dimensional parallel FFT using translation invariance.

- call 1-d-FFT-pre-skew
- call row-shift
- call 1-d-re-skew-FFT-pre-skew
- call row-shift
- call re-skew

We note that in the actual implementation of this method one has to carefully address precision issues.

References

1. C. Battista et al.: ‘The APE-100 Computer: (I) the Architecture’, Int. J. of High Speed Computing 5 (1993) 637.
2. R. Tripiccione, in: F. Karsch, B. Monien, and H. Satz (eds.), Proceedings of the International Conference "Multi-scale Phenomena and their Simulation", ZiF, Bielefeld, Sep. 30 - Oct. 4, 1996, (World Scientific, Singapore, 1997), pp. 91.
3. I. Arsenin et al. in: T. D Kieu et al. (edts.), Lattice 95, Proceedings of the International Symposium on Lattice Field Theory, Melbourne, Australia, 1995, Nucl. Phys. B (Proc. Suppl.) 47 (1996) 804.
4. N. Christ, in: F. Karsch et al. (edts.), Proceedings of the International Conference “Multi-scale Phenomena and their Simulation”, ZiF, Bielefeld, Sep. 30 - Oct. 4, 1996, to appear.
5. B. Parhami, ‘SIMD Machines: Do They Have a Significant Future?’, The Fifth symposium on the frontiers of massively parallel computation, McLean, VA, 1995, http://www.ece.ucsb.edu/Faculty/Parhami/FMPC95-SIMD-Panel.html
6. G. S. Almasi and A. Gottlieb Highly Parallel Computing, (Redwood City, California, Benjamin/Cummings Publishing Company, 1994).
7. H. Press et al.: Numerical Recipes (Cambridge University Press, 1989)
8. V. Kumar, A. Grama, A. Gupta, and G. Karypis: Introduction to Parallel Computing, (Redwood City, California, Benjamin/Cummings Publishing Company, 1994).
9. N. Cabibbo and P.S. Paolucci, ‘SIMD algorithm for matrix transposition’, preprint ROME-963-1993.
10. N. Petkov: Systolic Parallel Processing, (Amsterdam: North-Holland, 1992).
11. Th. Lippert, U. Glässner, H. Hoeber, G. Ritzenhöfer, K. Schilling and A. Seyfried, ‘Hyper-Systolic Parallel Processing on APE100/Quadrics: I. N^2 Loop Computations’, Int. J. of Mod. Phys. C 7 (1996) 485-501.
12. Th. Lippert, A. Seyfried, A. Bode, K. Schilling: ‘Hyper-Systolic Parallel Computing’, Preprint Server HEP-LAT 9507021, Preprint WUB 95-13, HLRZ 32/95, accepted for publication in IEEE Trans. of Parallel and Distributed Systems.
13. Th. Lippert and K. Schilling: ‘Hyper-Systolic Matrix Multiplication’, in: Proceedings of the International Conference on Parallel and Distributed Processing Techniques and Applications, PDPTA’96, August 9-11, 1996, Sunnyvale, California, Hamid R. Arabnia (edt.) (C.S.R.E.A. Press, 1996, p. 919).
14. Th. Lippert, K. Schilling, F. Toschi, S. Trentmann, and R. Tripiccione, ‘1-Dimensional FFT for the APE Parallel Computer’, in preparation.
15. R. H. Kraichnan, Phys. Fluids 11, 945 (1968)
16. P. Palazzari, Th. Lippert and K. Schilling: ‘Simulated Annealing Techniques for the Communication-Efficient Hyper-Systolic Parallel Computing on APE100/Quadrics’, in: L. Grandinetti et al. (edts.), Proceedings of NATO Advanced Research Workshop on High Performance Computing, Technology and Applications Cetraro, Italy - June 1996 (NATO ASI Series, Kluwer, 1996).
17. Rothe, H. J.: Lattice Gauge Theories, World Scientific, Singapore (1992).
18. K. Schilling and H.Suman, ‘A Comparative Study of Gauge Fixing Algorithms for QCD’, hep-lat/9306018.
19. N. Cabibbo and P.S. Paolucci, ‘SIMD algorithm for matrix transposition’, preprint ROME-963-1993.
20. R. Vogelsang, Cray/ZAM Jülich, Germany, private communication.
21. P. Haas, RUS Stuttgart, Germany, private communication.
22. The FFT software and related publications are available under (http://www.hlrz.kfa-juelich.de/HLRZ/HighEnergy/AQUA)