Generalized Hyper-Systolic Algorithm

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Abstract

We generalize the hyper-systolic algorithm proposed in [1] for abstract data structures on massive parallel computers with $n_p$ processors. For a problem of size $V$ the communication complexity of the hyper-systolic algorithm is proportional to $\sqrt{n_p}V$, to be compared with $n_pV$ for the systolic case. The implementation technique is explained in detail and the example of the parallel matrix-matrix multiplication is tested on the Cray-T3D.

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1 Introduction

In a near future Teraflops supercomputers will be available from many vendors. A possible architecture to achieve such a high performance is based on massive parallelism. Many powerful processors (PE) are linked together. Each of them can access his own local memory which is usually relatively large. The communications between the PE’s is performed by a fast network. Using this architecture the hope is to obtain a linear speedup in the number of PE’s. This is, of course, not possible because the overhead of the communications increases with the number of PE’s.

The overhead due to the communications can be encountered in many algebraic problems. For example, let us assume we have two matrices $A$ and $B$ of size $V$ which are distributed among the PE’s, then the simple operation $A \cdot B$ needs inter processor communications. The volume of the data which have to be communicated is then proportional to $n_p$ keeping the size of the matrices fixed. In fact the volume of private data owned by one PE is proportional to $V/n_p$. Using an usual systolic algorithm the matrix-matrix multiplication needs that each PE communicates his local portions of the matrices to each PE so that the volume of the communicated data will be $n^2/n_p V$ which is proportional to $n_p$.

The granularity of a problem is considered to be the average size of tasks to be performed in parallel. A problem of size $V$ implemented in parallel on $n_p$ processors has a granularity $g$ proportional to $V/n_p$. If the granularity of the problem is very large the inter processor communication becomes irrelevant compared with the time spent for the local computations. But if the granularity of the problem is small the overhead due to the communication is a serious obstacle to the wanted speedup. In fact, using an usual systolic algorithm, the data to be communicated is proportional to $V n_p$ and because we can assume that each PE can communicate data in parallel, the overhead time is constant in the number of PE’s $V n_p/n_p = V$. The computer time needed to solve a problem of granularity $g$ is then proportional to $\tau = a \cdot \frac{V}{n_p} + b \cdot V$ where $a$ and $b$ are constants. Asymptotically in $n_p$ this time reach a plateau given by the overhead time $b \cdot V$.

Of course, performance can be obtained by increasing the size of the problem so that the granularity remains constant. This is nice, but usually it is not what one needs in real applications. In fact, one may also needs speedup by more or less maintaining constant the size of the problem. It is then an important task to find new algorithms that need less inter processors communications even at low granularity. This is possible exploiting the fact that usually at low granularity there is abundance of memory.

Recently, it was proposed an hyper-systolic algorithm for organizing the data
communications related to the problem

\[ y_i = \sum_j f(x_i, x_j) \] (1)

where \( x_i \) and \( y_i \) are some data stored on the \( i \) PE and \( f \) is some function. It was shown that the volume of the communicated data was proportional to \( \sqrt{n_p} \) for fixed size of the problem\(^2\). This algorithm can be useful in various fields of applications, like \( n \)-body dynamics, polymer chains, protein folding or signal processing.

Equation (1) describes a small class of problems. Of course, the hyper-systolic algorithm can be generalized for a more large class of problems with global communication and with a more complicate data structure. We consider the following generalized problem

\[ C_{i\text{mype}} = \bigoplus_{i_p \text{ over all PE}} f(A_{i\text{mype}}, B_{i_p}) \]

where now \( A, B \) and \( C \) are abstract data structures, \( f \) is some operations on \( A \) and \( B \) which has an output with the same data structure type of \( C \) and \( \bigoplus \) is an associative and commutative operation on the data structure of type \( C \). The portions of the data owned by the different PE’s are denoted by the subscript \( i_p \). The index \( i_{\text{mype}} \) characterizes the local PE.

For example, if one considers the matrix-matrix product the same formalism can be applied. In this case \( A_{i\text{mype}} \) and \( C_{i\text{mype}} \) are the portions of the matrices \( A \) and \( C \) stored locally on the PE \( i_{\text{mype}} \) and \( B_{i_p} \) is the portion of the matrix \( B \) stored on the remote PE \( i_p \). The product \( f(A_{i\text{mype}}, B_{i_p}) = A_{i\text{mype}} \ast B_{i_p} \) is a generalized matrix product which takes care how the matrices are distributed among the PE’s (column-like, row-like or block-like) and the operator \( \bigoplus \) is a direct sum on the respective \( n_p \) linear subspaces of \( C_{i\text{mype}} \).

The hyper-systolic algorithm replicas a volume of data proportional to \( \sqrt{n_p} V / n_p \) coming from the portions of \( A \) and \( B \) stored on \( O(\sqrt{n_p}) \) different PE’s, and uses all possible combinations of them to built \( O(\sqrt{n_p}) \) different portions of \( C \) which are then sent back to the original PE’s. The communication directions are chosen so that all PE’s receive all needed data. In this case the amount of data to be communicated is only proportional to \( V \sqrt{n_p} \) for a fixed size \( V \) of the problem. Then the time needed to solve a problem of granularity \( g \) is \( \tau = a \cdot \frac{V}{n_p} + b \cdot \frac{V}{\sqrt{n_p}} \) where \( a \) and \( b \) are some constants. Now the overhead time \( b \cdot \frac{V}{\sqrt{n_p}} \) vanishes asymptotically in the number of PE’s.

\(^2\)In the original work of [1] it is showed that the communicated data is proportional to \( n_p^{3/2} \) if one increase the size of the problem linearly in \( n_p \).
In this paper we discuss in details the hyper-systolic algorithm for an abstract data structure and then we consider the useful example of the matrix-matrix product which is one of the most hard problem in linear algebra operations on massive parallel computers and also mimics all aspects of more general applications. We also report the gain in performance against the usual systolic algorithm tested on the Cray-T3D.

2 Generalized Algorithm

We consider a massive parallel computer built up by a set of \( n_p \) PE’s labeled by \( S_{PE} = \{i_p \in \{0, ..., n_p - 1\}\} \) and a network connecting the PE’s \( N = \{b_{ij}|i, j \in S_{PE}\} \). The index \( i_{mype} \) denotes the local PE. We define a set of three data structures \( \hat{D} = \{\hat{A}, \hat{B}, \hat{C}\} \). Each PE owns a portion of \( \hat{D} \). We denote this portion by \( \hat{D}_{i_p} \). For three variables \( A \in \hat{A}, B \in \hat{B} \) and \( C \in \hat{C} \) we want to compute

\[
C_{i_{mype}} = \bigoplus_{i_p} f(A_{i_{mype}}, B_{i_p})
\]

where \( f: \{\hat{A}_{i_{mype}}, \hat{B}_{i_{mype}}\} \to \hat{C}_{i_{mype}} \) is some operations on the local \( \hat{A} \) and \( \hat{B} \) which has an output of type \( \hat{C} \) and \( \bigoplus: \{\hat{C}_{i_{mype}}, \hat{C}_{i_{mype}}\} \to \hat{C}_{i_{mype}} \) is an operation with associative and commutative properties on the data structure of type \( \hat{C} \) with output of type \( \hat{C} \).

The usual systolic algorithm works as follow

**Algorithm 1 Systolic Algorithm**

\[
do \forall i_p \in S_{PE} \n
get B_{i_p} \text{ from PE } i_p \n
C_{i_{mype}} = C_{i_{mype}} \bigoplus f(A_{i_{mype}}, B_{i_p}) \n\od
\]

where the communication routine \( \text{get} \) represents a shift sequence optimized for the used architecture. We do not go into the details of how this routine organizes the shifts because it is standard.

The idea of the hyper-systolic algorithm is to allocate on each PE a set of replicas \( \{D_{i_{mype}}^k \in D_{i_{mype}}|k \in I\} \). The set of integer \( I = \{0, ..., K\} \) contains the index of the replicas of \( D_{i_{mype}} \) that we want to memorize on each PE. Each replica \( A^k \) and \( B^k \) has to be filled with a copy of some remote portion of \( A \) and \( B \). Then many combinations of these portions can be used to find many contributions to \( f(A_{i_{mype}}, B_{i_p}) \). These have then to be sent back to the right PE’s. To control all the directions of communications one has to ensure that all needed contributions occur. This can be done by defining a mapping \( \phi \) from \( S_{PE} \times I \) to \( S_{PE} \) by the following algorithm
Algorithm 2

\[
\text{do } \forall i_p \in S_{PE} \\
i_{tmp} = i_p \\
\text{do } \forall k \in I \\
\quad \phi(i_p, k) = i_{tmp} - \Gamma_k \\
\quad \text{while } \phi(i_p, k) < 0 \text{ do} \\
\quad \quad \phi(i_p, k) = \phi(i_p, k) + n_p \\
\quad \text{od} \\
\quad i_{tmp} = \phi(i_p, k) \\
\text{od} \\
\text{od}
\]

where the \( \Gamma_k = \{0, \gamma_1, ..., \gamma_K\} \) with \( \gamma_i \) positive and integer. The dimension of the vector \( \Gamma \) has to be chosen with \( K \) minimal so that

\[
\forall m \in S_{PE} : m = \gamma_i + \gamma_{i+1} + ... + \gamma_{i+j} \text{ or } m = n_p - (\gamma_i + \gamma_{i+1} + ... + \gamma_{i+j}) \quad (3)
\]

with \( 0 \leq i + j \leq K \). How to determine the appropriate vector \( \Gamma \) is discussed in [1]. The best choice of the vector \( \Gamma \) is called the best basis. The best basis has dimension \( K \simeq \sqrt{n_p} \). There is no analytical recipes for finding the best basis for a given number of PE’s. One has to try all combinations of numbers and select the ones which satisfy (3). But this can be a very hard computational problem for a large number of PE’s. For the allowed configurations of the Cray-T3D we have enumerate the best basis in Table 1. Fortunately, there exists a regular basis which is very easy to be found and has dimension \( K \simeq \sqrt{2 \cdot n_p} \). This basis is given by

\[
\Gamma = (1, 1, ..., 1, K, K, ..., K) \quad (4)
\]

where \( K \) is the integer part of \( \sqrt{2n_p} \). In any case the choices of \( K \) are of order \( O(\sqrt{n_p}) \).

The mapping \( \phi \) is local to each PE and it is equal for each PE. It contains all informations about the location of the data \( D \) which has to be communicated to fill the \( K \) replicas. The definition (3) ensures that all combinations of PE’s occurs at least once. To ensure that only one PE will compute the combination \( f(A_{ tympe }^{k_1}, B_{ tympe }^{k_2}) \) and send it back to the right PE one has to check the multiplicity of the occurrence of this combination among the PE’s defining a multiplicity table \( M \) going from \( I^2 \) to \{0, 1\}. All informations about the multiplicity of the operations can be read from the mapping \( \phi \). \( M \) takes the value 0 when a duplicate of the combination \( f(A_{ tympe }^{k_1}, B_{ tympe }^{k_2}) \) is encountered. This table controls that in the operation \( \oplus \) the elements contributes only once by switching off the PE’s which duplicates this operation when \( M(k_1, k_2) = 0 \).
Algorithm 3

\[
M(\phi(i_{mype}, k_1), \phi(i_{mype}, k_2)) = 1 \quad \forall k_1, k_2 \in I
\]

\[
do \quad i_p = 0, i_{mype} - 1
\]

\[
do \quad \forall k_1, k_2, k_3, k_4 \in I
\]

\[
\quad \text{if } (\phi(i_{mype}, k_1) = \phi(i_p, k_3) \text{ and } \phi(i_{mype}, k_2) = \phi(i_p, k_3)) \text{ then}
\]

\[
\quad \quad M(\phi(i_{mype}, k_1), \phi(i_{mype}, k_2)) = 0
\]

\[
\quad \fi
\]

\[
\odo
\]

The hyper-systolic algorithm can then be organized as following: one gets from the remote PE’s selected by the \(\phi\) mapping the \(K\) portions of data \(\{A, B\}\) needed to built all \(K^2\) combinations \(f(A_{i_{mype}}^{k_1}, B_{i_{mype}}^{k_2})\) among the replicas. Then one sums up these combinations in the respective replica \(C_{i_{mype}}^{k_1}\) according to the operation \(\oplus\) and controlling the multiplicity. Now one has to synchronize\(^3\) all PE’s to be sure that all have done their job. Then one has to send back according to the exact reverse \(\phi(i_{mype}, k)\) sequence all \(C_{i_{mype}}^{k_1}\) and sum up them to the result local \(C\) according with \(\oplus\).

Algorithm 4 \textit{Hyper-Systolic Algorithm}

\[
do \quad \forall k \in I
\]

\[
\quad \text{get } A_{i_p} \text{ from PE } i_p = \phi(i_{mype}, k) \text{ and store in } A_{i_{mype}}^{k}
\]

\[
\quad \text{get } B_{i_p} \text{ from PE } i_p = \phi(i_{mype}, k) \text{ and store in } B_{i_{mype}}^{k}
\]

\[
\odo
\]

\[
do \quad \forall k_1, k_2 \in I
\]

\[
\quad \text{if } M(k_1, k_2) = 1 \text{ then } C_{i_{mype}}^{k_1} = C_{i_{mype}}^{k_1} \oplus f(A_{i_{mype}}^{k_1}, B_{i_{mype}}^{k_2})
\]

\[
\odo
\]

\[
\quad \text{synchronize}
\]

\[
do \quad \forall i_p \in S_{PE}, k \in I
\]

\[
\quad \text{if } \phi(i_p, k) = i_{mype} \text{ then}
\]

\[
\quad \quad \text{get } C_{i_p}^{k} \text{ from PE } i_p \text{ and store in } T \in \hat{C}_{i_{mype}}
\]

\[
\quad \quad C_{i_{mype}} = C_{i_{mype}} \oplus T
\]

\[
\quad \fi
\]

\[
\odo
\]

This pseudo-code can be used to implement any parallel problem satisfying eq. (4). As a test example we have implemented the product of two matrices on the Cray-T3D. We have distributed the matrices so that each PE owns some fixed portion of

\(^3\)Of course, the synchronization is needed only on MIMD architectures.
rows or columns of the matrices. We have tested the algorithm for matrices with
dimensions going from $16 \times 16$ to $2048 \times 2048$ real entries on 2 to 256 PE’s. We
have measured the ratio between the time spent to communicate data for the systolic
against the hyper-systolic algorithm. This ratio expresses the gain in computer time
for the communications. The hyper-systolic algorithm communicates three times a
volume of data equal to $K \cdot V$ (where $K$ is the integer part of $\sqrt{m_p}$ for the best
basis or the integer part of $\sqrt{2m_p}$ for the regular basis) and the systolic algorithm
communicates a volume of data equal to $n_p \cdot V$. In the ideal case we can assume
that the networks is able to transfer data in parallel with the same speed for both
algorithms then the ideal ratio is

$$R_{\text{ideal}} \simeq \frac{n_p}{3 \cdot \sqrt{n_p}} = \frac{\sqrt{n_p}}{3} \text{ best basis}$$

$$R_{\text{ideal}} \simeq \frac{n_p}{3 \cdot \sqrt{2 \cdot n_p}} = \frac{\sqrt{n_p}}{3\sqrt{2}} \text{ regular basis}$$  \hfill (5)

Of course, the hyper-systolic algorithm can not have an ideal ratio against the sys-
tolic algorithm because it involves communications to more remote PE’s than in the
systolic case. This eventually can overload the network and slow down the commu-
nications. However, if the topology of the network is a $d$–torus with $d \geq 2$ this
effect should be negligible because there exist many paths which connect each pair
of PE’s. Only if $d = 1$ then a 1–torus is a circle some problem can arise because for
connecting a pair of PE’s there exist only two paths. In fig. 1 we plot the measured
ratio averaged on the different dimensions of the matrices. We see that the measured
values lies near the ideal case as expected from the topology of the Cray-T3D.

3 Conclusion

We have generalized the hyper-systolic algorithm proposed by [1]. This algorithm
is able to handle a vast class of massive parallel problems which need global com-
munications. It reduces significantly the overhead due to the communications when
compared with the usual systolic algorithm. As an example we have implemented
the algebraic problem of multiplying two large matrices in parallel. In our example
we have observed a speedup of the communications of about $\sqrt{n_p}$ using the best basis
and $\sqrt{n_p \cdot \frac{3}{2}}$ using the regular basis.

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| $n_p$ | $K$ | $\Gamma$ |
|------|------|---------|
| 2    | 1    | 1       |
| 4    | 1 1 2| 1 1 2   |
| 8    | 1 2 4| 1 2 4   |
| 16   | 6    | 1 1 1 4 4 8 |
| 32   | 8    | 1 1 12 3 10 8 20 4 |
| 64   | ?    | ?       |
| 128  | ?    | ?       |
| 256  | ?    | ?       |

Table 1: The best basis for the configurations of the Cray-T3D at the EPFL, Switzerland. The basis for 128 and 256 PE’s could not be found.

References

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W. Smith, Comput. Phys. Commun. 62 (1991) 229
Figure 1: Average ratio between the time spent to communicate data for the systolic algorithm against the hyper-systolic one for the example of the matrix-matrix product. The squares are obtained using the best basis, the crosses using the regular basis. The lines represent the ideal cases for the best basis (solid) and regular basis (dashed), respectively. The errorbars of the average over the different matrix dimensions are smaller than the plotted symbols.