Hyper-Systolic Processing on APE100/Quadrics: 
$N^2$-Loop Computations

Th. Lippert$^a$, G. Ritzenhöfer$^a$, U. Glässner$^b$, H. Hoeber$^a$, A. Seyfried$^b$, and K. Schilling$^a,b$

$^a$HLRZ, c/o KFA-Jülich, D-52425 Jülich, Germany and DESY, Hamburg, Germany
$^b$Department of Physics, University of Wuppertal, D-42097 Wuppertal, Germany

Abstract

We investigate the performance gains from hyper-systolic implementations of $n^2$-loop problems on the massively parallel computer Quadrics, exploiting its 3-dimensional interprocessor connectivity. For illustration we study the communication aspects of an exact molecular dynamics simulation of $n$ particles with Coulomb (or gravitational) interactions. We compare the interprocessor communication costs of the standard-systolic and the hyper-systolic approaches for various granularities. We predict gain factors as large as 3 on the Q4 and 8 on the QH4 and measure actual performances on these machine configurations. We conclude that it appears feasible to investigate the thermodynamics of a full gravitating n-body problem with $O(10000)$ particles using the new method on a QH4 system.

1 Introduction

Many grand challenge tasks in computational science involve the solution of $n^2$-loop problems, demanding for algorithms and techniques viable on parallel machines. One would wish to increase the number of processors proportional
to $n^\alpha$ such as to achieve a computational complexity of $O(n^{2-\alpha})$ per processor. This strategy sets the goal towards the limit of low granularity!

In this paper we treat, as a prototype of an $n^2$-loop problem, the molecular dynamics of $n$ equal particles with long range Coulomb forces. Computationally, this implies repeated calculation of all interparticle distances $r_{ij}$ within the full system. The state-of-the-art system size in molecular dynamics with an exact treatment of such long-range forces is at present of $O(10,000)$, requiring machines in the 10 GFlops range.

On a massively parallel computer with $p$ processors and distributed memory, the coordinates of the particles are assigned to different processors and therefore interprocessor movement of data becomes a considerable cost factor in the computation of two particle forces. In the limit of low granularity, i.e. $p \approx n$, interprocessor communication is in fact the major performance bottleneck. This holds particularly true for machines with next-neighbour interprocessor communication networks as e.g. the APE100/Quadrics system, manufactured by Alenia Spazio S.P.A. or the 16k node machine under construction at Columbia University. It is therefore crucial to gear algorithms to render low communicational overhead on such machines for computing $n^2$-loop problems.

An earlier proposal to implement $n^2$-loop systems on the massively parallel computer Quadrics has been presented by Paolucci. His parallel approach rests upon the replicated data method in conjunction with global summations over the whole machine and arrives at a total communicational complexity of $O(n^4p^3)$.

In this paper we will fathom the power of systolic array computation. The latter is a rather general technique to organize data flow on parallel systems that implies the potentiality to improve the interprocessor communication complexity for $n^2$-loop problems. In systolic loop processing, on a $p$ processor machine working on $n$ particle dynamics with long range forces, the latter is of order $O(np)$, as each of the $n$ data elements has to be communicated to $p$ processors.

Recently, we have introduced the concept of hyper-systolic array processing. This novel parallel algorithm is an extension of the standard-systolic method.

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1In Ref. [1], Parisi discusses the limiting case of $O(const.)$ complexity per processor on computers with arbitrarily large parallelism.

2Closely related problems are protein folding, polymer dynamics with long range forces, signal processing, or fully coupled neural nets.
In this approach, the data flow is reorganized such that the interprocessor communication is reduced to order $2n(2\sqrt{\frac{p}{2}} - 1)$ for an array of $n$ particles, at no additional computational cost. This is accomplished at the expense of only a modest amount of additional storage.

Hyper-systolic data piping is structurally related to the so-called postage stamp problem in Additive Number Theory which can serve to classify all possible hyper-systolic flow patterns. Needless to say the hyper-systolic concept is very general and can be applied to all sorts of $n^2$-computations, as e.g. matrix computations \cite{8, 9}.

In this work we shall benchmark the hyper-systolic concept for solving $n^2$-loop problems on the Quadrics system. For assessing performance gains, we choose the 1-dimensional standard-systolic method as our reference point. We will present an efficient mapping of 1-dimensional systolic arrays onto the 3-dimensional network of the Quadrics. In our setup, one hyper-systolic movement is performed in $\leq 3$ interprocessor communication steps.

## 2 Systolic Array Implementation

We consider for definiteness the computation of the local Coulombic forces within an n-body problem

$$\vec{y}_i = \vec{F}(\vec{x}_i) = \sum_{\substack{j=1 \atop j \neq i}}^{n} \frac{\vec{x}_i - \vec{x}_j}{|\vec{x}_i - \vec{x}_j|^3}, \quad i = 1, \ldots, n, \quad (1)$$

the evaluation of which represents the computational bottleneck.

Let us assume for a start the limit of granularity $g$ to be $g = n/p = 1$. Our standard-systolic loop approach to compute Eq. (1) proceeds by mapping the processors onto a 1-dimensional periodic chain (GRA\cite{3}), see Fig. 1. The information on the location of the physical system in configuration space, $\vec{x} = (\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_n)$, is distributed over the compute system such that each processor $p_i$ holds in its local memory the coordinate $\vec{x}_i$ as its ‘resident vector’. Besides the local resident vector $\vec{x}_i$ there is a local migrating vector $\vec{x}'_i$, that originally coincides with $\vec{x}_i$. During a systolic step, $\vec{x}'_i$ is shifted cyclically onto the right hand next-neighbour processor on the 1-dimensional systolic

\footnote{This name was chosen as a mnemonic to the 20th century Roman traffic solution Grande Raccordo Anulare.}
chain GRA. After completion of this systolic move, the computation of the local pairings is performed in parallel and the results are accumulated into a resident result array $y'$. After $n - 1$ such systolic steps, Eq. 1 is fully computed\textsuperscript{4}.

In Fig. 2a, we illustrate the mapping of the 1-dimensional systolic array onto the Quadrics processor topology: on a Quadrics Q4, with $n = p = 32$. The processors of the Q4 are arranged in a $8 \times 2 \times 2$-grid that is toroidally closed\textsuperscript{5}.

One must differentiate between a movement on the logical, systolic chain GRA and its actual hardware realization, in terms of interprocessor communications: one systolic movement to the next neighbour processor on GRA amounts to three steps on the interprocessor links, as depicted in Fig. 2:

**Step 1:** cyclical shift to next neighbour in $y$-direction,

**Step 2:** cyclical shift to next neighbour in $z$-direction, at $y = 1$ only,

**Step 3:** cyclical shift to next neighbour in $x$-direction, $y = 1$, $z = 1$ only.

For the entire systolic process, $3(p - 1)$ such interprocessor communication operations are needed. Therefore the communicational complexity of standard-systolic computations on the Quadrics is $3p(p - 1)$.

Proceeding to the case of $n > p$, we partition the systolic array into $\frac{n}{p}$ subarrays and distribute each subarray across the machine. From the point of view of interprocessor communication the pairings of coordinates from different subarrays present no additional complication. The total number of interprocessor communication operations is now found as $3n(p - 1)$, while the total number of computation operations remains unaltered, $n(n - 1)$.

\textsuperscript{4}One invokes Newton’s *actio = reactio* to reduce the amount of computation by a factor two.

\textsuperscript{5}The mapping of systolic arrays with $n = p$ onto other Quadrics configurations, like Q16, QH2, and QH4 is straightforward.
Figure 2: Systolic movement. a) Initial state: Mapping of a 1-dimensional systolic array with $n = 32$ onto the 3-dimensional Quadrics Q4 with $p = 32$ processors. The systolic chain is periodically closed. b) Final state: reached after 3 steps. The coordinate system is given to specify the Quadrics’ $8 \times 2 \times 2$ processor grid.
3 Hyper-Systolic Algorithm

The hyper-systolic reorganization of the computation of Eq. 1 will enable us to reduce the complexity of interprocessor communication to $O(np^2)$; thus, interprocessor communication ultimately becomes negligible compared to the pure computational complexity, on machines with a very large number of processors.

Quadrics machines allow for an efficient realization of hyper-systolic array computing, due to their 3-dimensional cubic connectivity

3.1 Definition: Regular Base Algorithm

The hyper-systolic data movement generalizes the standard-systolic one by increasing the number of resident arrays from one to $k$, with $k \ll p$ and introducing cyclical shifts with strides $a_t \geq 1$.

Let us give an operational description of the hyper-systolic algorithm for extreme granularity $g = 1$:

1. For a given array $x$ of length $n$, $k$ arrays $\hat{x}_t$ are generated by shifting the original array $x$ $k$ times by strides $a_t$, and copying $x$ to $\hat{x}_t$ in step $t$, $1 \leq t \leq k$. The variable stride $a_t$ of the shifts must be chosen such that
   (a) all pairings of data elements occur at least once, and
   (b) the number of equal pairings as well as
   (c) the number of shifts $k$ as well as
   (d) the number of different strides $a_t$
   are minimized.

2. The required $n(n-1)/2$ results $\tilde{y}_t$ in Eq. 1 are successively computed and are added to $k$ resulting arrays $\tilde{y}_t$.

3. Finally, applying the inverse shift sequence, the arrays $\tilde{y}_t$ are shifted back to their proper locations and corresponding entries are summed up to build the elements of the final result array $y$.

\footnote{From the point of view of 1-dimensional systolic data arrangement and movement the 3-dimensional network of the Quadrics supports accelerated communication along transversal directions (wormhole communication).}
The interested reader can find the optimal solutions to this problem for $8 \leq p \leq 64$ in Ref. [7]. In general, one can resort to so-called regular base solutions which are very simple yet still in the optimal complexity class.

In the following we implement the hyper-systolic algorithm using the regular base:

$$A_{k=2K-1} = \left(0, 1, 1, \ldots, 1, K, K, \ldots, K\right),$$

with $K - 1$ shifts by stride $a_t = 1$ and $K$ shifts by stride $a_t = K$. The length of the base is $k = 2K + 1$. The shift constant $K$ is given by $K = \sqrt{\frac{p}{2}}$.

### 3.2 Implementation on the Q4.

For illustration we consider the case $n = 32$. The regular hyper-systolic base is given by

$$A_7 = \left(0, 1, 1, 4, 4, 4, 4\right),$$

leading to the storage of eight arrays as depicted in Fig. 3. By inspection one finds all pairings of the numbers 1 to 32 within the columns, i.e. within the 32 local memories.

![Hyper-systolic data movement on the Q4 for $n = 32$ using the regular base $A_7 = (0, 1, 1, 4, 4, 4, 4)$.](image)

The systolic chain $x$ is mapped in the very same way as in section 2 for stride $a_t = 1$. The shifts by the stride $K = 4$ present a novel feature of the hyper-systolic method: from Fig. 4 it can be seen that such a hyper-shift, on the Q4, is performed by just one communication operation to the next-neighbour in $x$-direction.
Thus the communicational complexity of the regular base hyper-systolic method on the Q4 is improved compared to the scaling law in Ref. [7], that has been derived for constant communicational cost for all strides, and is given by 

\[ R = \frac{3n(p-1)}{2n(4\sqrt{\frac{p}{2}} - 1)} \simeq 3 \sqrt{\frac{p}{32}} = 3. \]  \hspace{1cm} (4)

This result holds also for the case \( n > p \) where we partition the array into \( \frac{n}{p} \) subarrays and compute all relevant interactions\(^7\).

\(^7\)Recently, the so called Half-Orrery algorithm has been presented in Ref. [10]. This method also belongs to the class of hyper-systolic algorithms. In principle, it can, as is the case with the approach presented here, make usage of the symmetry inherent in Eq. [4]. The communication, however, is not reduced compared to the standard-systolic way, and moreover on the Quadrics, additional back-shifts have to be performed. Thus Half-Orrery is not competitive on Quadrics.
3.3 Implementation on the QH2 and QH4

The 256-node Quadrics QH2 is arranged as an $8 \times 4 \times 8$ lattice. The procedure underlying Eq. 3 needs to be generalized as $\sqrt{128}$ is not integer. We can utilize the decomposition $\frac{p}{2} = KK'$ and select the base

$$A_{k=K-1+K'} = \left(0,1,1,\ldots,1,K,K,\ldots,K\right),$$

$$K - 1 \quad K'$

(5)

For the QH2, the favourite base reads

$$A_{23} = \left(0,1,1,1,1,1,1,8,8,8,8,8,8,8,8,8,8,8,8,8,8\right).$$

(6)

Note that a stride by 8 can be performed with 2 communication operations only, analogous to the shifts on the Q4. It turns out that the ratio $R$ between standard-systolic and hyper-systolic data communication expense theoretically is about 7.2.

The QH4 with 512 processors and $8 \times 8 \times 8$ topology readily lends itself to the regular hyper-systolic base, Eq. 3, again with a stride of $K = 16$. Constrained by the topology, a shift with a stride of 16 has to be accomplished within 3 communication operations by 2 strides of length 8, and theoretically a gain in communicational expense of a factor of 8 can be achieved. It is interesting to note that asymmetric processor grids can increase the hyper-systolic performance: e.g., if the $16 \times 8 \times 4$-topology is realized, the gain factor is about 10. With a $4 \times 4 \times 32$-topology, the gain is optimized further to 12.

4 Performance Results

4.1 Performance Tests on the Q4

The hyper-systolic computation of the interaction given by Eq. 1 on Quadrics machines has been developed and first tested on the 32-node Q4 at Wuppertal University, Germany. In order to speed up the purely computational part of the program we have employed block matrices in form of register declarations for the compute intensive part. As the number of registers is limited to 128 per processor, this approach amounts to an additional second blocking in form of loop-unrolling in the number of particles per processor $\frac{p}{2}$. Thus, the array of
\( \frac{n}{p} \) elements is subpartitioned into \( q \) parts. In our three-dimensional molecular dynamics example with Coulombic forces we are able to perform computations on 2 arrays of up to 6 particles, \( i.e., \ 6 \times 6 \) coordinate pairings can be treated while no recourse to the local memory is needed. We emphasize that both the standard-systolic and the hyper-systolic methods use the identical optimized code concerning this local computational part.

We have measured the total run times, \( t_{total} = t_{cpu} + t_{ipc} \), and the pure interprocessor communication times \( t_{ipc} \) as a function of the total number of particles \( n \).

As a result we show the performance plot of the Q4 in Fig. 5. The total time expense (total) and the pure communication time (ipc) for one computation of all forces are plotted for both the standard-systolic (sys) and the hyper-systolic (hys) algorithms. As expected, for both methods, we find a linear increase in communicational and a quadratic behaviour of the total time expense, as we are working on a fixed machine size, with constant number of processors \( p \).

Figure 5: Overall time (total) and communication time (ipc) vs. the number of particles for one interaction time-step on the 32-nodes Quadrics Q4 for the systolic and the hyper-systolic method.
The insertion zooms the curves in a regime of $n$ that is common in practical computations on a machine with the number and performance of processors as provided by the Q4 ($\#$ of particles $< 500$ for the Q4). We find here that both advantages of the hyper-systolic method lead to their full pay-off: the communication time is drastically reduced and together with the smaller amount of computation operations, the total time expense is diminished by more than a factor of two. For example, one interaction step on 192 particles requires 4.2 milliseconds in the systolic case compared to 1.8 milliseconds in the hyper-systolic mode.

Fig. 6 plots the ‘inefficiency factor’, $t_{total}/t_{cpu}$, for both algorithms. The

Figure 6: $t_{total}/t_{cpu}$ as function of the number of particles on the Q4.

threshold behaviour of the inefficiency factor in the region $n \leq 150$ reflects the characteristics of the Quadrics register structure: for the registers to be filled without bubbles, one needs at least a set of $2 \times 6$ particles, while the communication time increases proportional to $n$. Notice that communication plays a much smaller rôle for the hyper-systolic method and even for a granularity of $g = 32$, i.e. $n = 1024$, the performance in the standard-systolic approach is still considerably affected by communication.

In Fig. 6, we display the gain factors $\frac{t_{sys}}{t_{hys}}$ separately, in terms of the total, the
net computational and the interprocessor communication overhead times. On

![Figure 7: Gain factor $\frac{t_{sys}}{t_{hys}}$ for overall time (total), net computation (cpu) and interprocessor communication (ipc) times as measured on the Q4.](image)

the Q4, we actually achieve a gain factor of about 3.2 in communication time across the entire granularity range, to be compared to the predicted value of 3. The startup behaviour of the three curves at small $n$ again reflects the filling of the registers. The overall gain reaches its maximum in the range of 128 to 192 particles, whereupon the competing complexities are leading to more modest improvements. Yet, the hyper-systolic mode still results in an attractive gain of 60% for 1024 particles, at granularity 32!

Let us turn next to efficiency measurements. Counting the computation of an inverse square root with 18 floating point operations, we assign 35 floating point operations to the computation of each $r_{ij}$ in Eq. 1 on the 3-dimensional problem. Fig. 8 presents the flop rates as measured with the hyper-systolic method on the Q4 (in units of its peak performance) for the computation of the Coulomb interaction. Before the registers are fully exploited ($< 150$ particles on the Q4), the performance is small as expected. For larger values of $n$, however, a remarkably high performance can be achieved for the full $n$-body computation of the Coulomb force in three dimensions. In terms of the peak performance of the Quadrics Q4, i.e. 1.6 Gflop, nearly 50% can be
reached in the limit of large $n$. In real life, one would consider the Q4 to be the adequate Quadrics configuration for treating 200 to 500 particles; in this range we observe efficiencies between 20 and 30% of the peak performance.

4.2 Performance Tests on the QH4

Next we extend our performance measurements to the QH4 configuration which is equipped with 512 processing nodes and usually configured as $8 \times 8 \times 8$ grid.

As explained above, we expect an improvement in interprocessor communication by about a factor of 8 on the QH4 (as compared to 3 on the 32-node Q4)$^8$. The results of our QH4 benchmark are displayed in Fig. 8, which is the analogue to the Q4 plot in Fig. 5. The insertion zooms the granularity range $g \leq 8$. Characteristic for the hyper-systolic algorithm is the fact that, even for $g = 1$, $t_{ipc}$ is one order of magnitude smaller than $t_{cpu}$. In the whole

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$^8$On top of that, there should be additional, computational gains with respect to the Q4.
Figure 9: Total time (total) and communication time (ipc) vs. the number of particles for one interaction time-step on the 512-nodes Quadrics QH4 for the systolic and the hyper-systolic method.

range of granularities investigated, for the hyper-systolic method, the size of $t_{ipc}$ is marginal, whilst the standard-systolic computation is dominated by communication overhead, up to the point $g = 16$.

The QH4 inefficiency factor, as shown in Fig. 10 is very reminiscent to Fig. 6, featuring again the effects of register filling in form of the characteristic threshold behaviour at small $n$. The important message to be drawn from this plot is the finding that in the relevant intermediate region of say $g < 16$, hyper-systolic are by far superior to standard-systolic implementations in performance. Note that in the asymptotic regime of very large granularity the machine can be viewed more and more as an assembly of independently working processors; in this ‘scalar’ limit, communication ceases to dominate for both systolic varieties, but our $n^2$-loop computation approaches the creeping mode!

In Fig. 11 we display the gain factor for the hyper-systolic implementation on the QH4 for particle numbers up to 35,000. It is not surprising after our theoretical discussion in section 3.3 to find an improvement of $> 8$ in the interprocessor communication time throughout the observed $g$ range. Here we
reach a slightly improved level for the gain in CPU-time as the computations contribute more heavily (larger $n$ as compared to the Q4 case). The improved communication time boosts the peak in the overall gain factor from 2.8 on the Q4 to 3.5 on the QH4.

Finally it is rather gratifying to find a high efficiency level for the QH4 in terms of its peak performance, see Fig. [12]. The efficiency of the QH4 in the hyper-systolic implementation of molecular dynamics saturates at a value close to 60%, crossing the 50% mark at granularity 20. Even at low granularity like $g \approx 6$ we observe efficiencies in the ball-park 30 to 40 %!

5 Summary

We have investigated standard-systolic and hyper-systolic computations for a prototype $n^2$-loop problem on the massively parallel computer Quadrics.

A next-neighbour data movement on the logical systolic chain “GRA” is real-
Figure 11: Ratio $\frac{t_{sys}}{t_{hys}}$ for total time (total), pure computation (cpu) and interprocessor communication (ipc) on the QH4.

ized in form of three interprocessor communication steps, the hyper-systolic data movement can be performed in one interprocessor communication step on the Q4, two steps on the $8 \times 4 \times 8$ QH2 and three steps on $8 \times 8 \times 8$ QH4, respectively.

As expected, our measurement reveals a gain factor of $\approx 3$ in communication time compared to the standard-systolic computation, on the Quadrics Q4. In this way, we verified a performance of up to 750 Mflops in molecular dynamics with exact long range gravitational forces for acceptable granularity. Saturation would be reached at about 50% of the theoretical peak performance of the machine.

Even more encouraging results were subsequently found in measurements on the largest actually built member of the Quadrics line, the QH4, where the cpu-power can be exploited even for small granularity. The performance saturates for $n > 32k$ near 60% of the peak performance, i.e. nearly 15.5 Gflops, for long-range Coulomb interactions.

According to the results, on the QH4, it appears realistic to perform molecular
dynamics simulations with $O(16k)$ particles in 6 days compute time with a length of $10^6$ molecular dynamics time steps.

We thus conclude that the APE100/Quadrics architecture should no longer be considered as special purpose machines for lattice QCD. Instead they should be viewed as powerful devices that can solve just as well many other bottleneck problems of Computational Science belonging to the wide class of $n^2$-loop problems.

In two consecutive papers we will evaluate the impact of the hyper-systolic approach on other bottleneck problems in HPCN such as matrix products and fast Fourier transforms.

**Acknowledgements**

Part of this investigation has been carried out at ENEA/Casaccia. Th. L., G. R. and K. S. thank Profs. N. Cabibbo and A. Mathis for their kind hospitality. We are indebted to Dott. R. Guadagni and Dott. R. Canata for their support.
The work of Th. L. is supported by the Deutsche Forschungsgemeinschaft DFG under grant No. Schi 257/5-1.

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