Cache oblivious storage and access heuristics for blocked matrix–matrix multiplication

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We investigate effects of ordering in blocked matrix–matrix multiplication. We find that submatrices do not have to be stored contiguously in memory to achieve near optimal performance. Instead it is the choice of execution order of the submatrix multiplications that leads to a speedup of up to four times for small block sizes. This is in contrast to results for single matrix elements showing that contiguous memory allocation quickly becomes irrelevant as the blocksize increases.

I. INTRODUCTION

In current state–of–the–art algorithms for large scale electronic structure calculations probably the most important operation is sparse matrix–matrix multiplication. To name but a few important applications, sparse matrix–matrix multiplication is a computational kernel of: (1) density matrix purification1–8, (2) density matrix minimization8–14 (3) density matrix perturbation theory15–17, (4) computation of interior eigenpairs of potential matrices18–20, and (5) time–dependent response calculations21–24. Since matrices occurring in electronic structure calculations often have a natural blocked structure arising from local atom centered basis functions, performance can be dramatically improved by using a blocked data structure25–28. In addition, the sparse blocked matrix–matrix multiply is important in many other fields as for example the evaluation of matrix functions including the matrix exponential, the matrix inverse29, inverse factorizations30–33, and multigrid methods34 where local blocking may occur.

CPUs and memory of modern computer architectures work at different speeds. Main memory operates at lower speeds to reduce the price and power consumption of computers. Direct access to main memory causes the CPU to stall for several, sometimes hundreds of cycles. To achieve decent computer performance cache memory that store frequently accessed data was introduced into modern CPU designs. Cache memory works at speeds comparable with the CPU but typically has only a size of about 0.1% to 1% of computer main memory. The cache stores data in chunks, so–called cache lines, which are usually on the order of tens of bytes long. A memory manager controls storing and evicting data from these cache lines using heuristics (a typical algorithm called Least Recently Used (LRU), eviction the least recently used cache line when trying to store a new one) and it prefetches subsequent lines when sequential memory access is detected or explicit machine language instructions are given to the CPU. When implementing a data intensive algorithm, both of these cache features – LRU eviction and hardware prefetching – can be used to optimize performance.

Previous research into ordering effects for the matrix–matrix multiply has been focused on either the dense or the very sparse case. In the dense case, block recursive algorithms have drawn much attention35–38. In the case of sparse matrices, Toledo39 found better than 2× speedups with the use of locality enhancing orderings based on space filling curves. Here, we are interested in the intermediate case of matrix–matrix multiplication involving sparse matrices with local blocking, as occurs with local basis functions, finite element methods40 or reordering schemes41–43.

The performance of blocked matrix–matrix multiplication depends on (1) the performance of block operations and (2) how blocks are stored and accessed. Block operations can be delegated to some standard linear algebra library optimized for the particular platform44–48. Here, we focus on (2), exploring the effects of orderings for small blocks, consistent with our interest in the intermediate case of locally blocked sparse matrices.

This article is organized as follows: In section II we describe in more detail the locality issues we are addressing. In section III we discuss our results and finally, in section V we conclude.

II. DATA LOCALITY

Data locality is known to be important for achieving good performance of matrix multiplication on modern computer architectures39. In addition, Translation Lookaside Buffer (TLB) misses can significantly impact performance45. In this study we will focus on the locality problem.

A. Effects of ordering on performance

We divide an $N \times N$ matrix into submatrices of size $b \times b$, where $b$ is the blocksize. We choose $b$ so that the resulting blocked matrix will consist of $n \times n$ submatrices. We assume for simplicity that $n b = N$. The matrix product can be written as a combination of submatrix products,

$$C_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj} \quad \{i, j \in [1..n]\} \ .$$

(1)
FIG. 1: A qualitative illustration of the performance of a blocked matrix multiplication with perfect locality and no locality.

The \( n^3 \) products may be evaluated in any order and we are free to choose the precise ordering of execution and the allocation of the matrix blocks. Algorithm 1 illustrates this point.

Algorithm 1 General matrix multiplication algorithm

Allocate \( n^2 \) submatrix blocks for \( A \), \( B \), and \( C \).

for all \((i, j, k)\) in blocked matrix product of eq. (1) do

Multiply blocks \( A_{ik} \) and \( B_{kj} \).

Add result to block \( C_{ij} \).

end for

Considering that we use a highly optimized matrix multiplication function on the block level, what performance gain, if any, can we hope to achieve by arranging the blocks in a particular order? Clearly, we can construct the two limiting cases easily, “perfect locality” and perfect non-locality or “no locality”. We construct two tests: In the first test we multiply the same 2 blocks (e.g. \( A_{11} \) and \( B_{11} \) to get \( C_{11} \)) \( n^3 \) times; in this way perfect locality is obtained since the computer’s memory manager can keep the three submatrices in cache throughout the whole operation. In the second test we randomize the multiplication and the allocation order of the blocks. This will break most of the locality since memory prefetches are only possible in the rare event that two blocks are close together in memory and the time between two multiplication steps in which a particular block is reused is very long and will almost certainly lead to a cache miss. If ordering effects are significant for performance, we expect to find results qualitatively similar to those shown in Fig. 1.

B. Space filling curves for optimized locality

It is well known that ordering matrix elements in memory along locality preserving space filling curves improves the performance of matrix operations due to memory subsystem design issues. Bader and Zenger applied this idea to dense matrix–matrix multiplication. They devised a block recursive scheme which allocates the matrix elements along a Peano curve and reorders the multiplications of matrix elements to optimize locality. They point out that such a scheme is cache oblivious and platform independent. Compared to the standard library MKL, Bader and Zenger find that the reordered matrix–matrix multiplication yields competitive performance when processor specific optimization techniques, e.g. Intel’s Streaming Single Instruction, Multiple Data Extensions (SSE), are turned off. In the following we will apply the idea of improving locality by ordering to blocked matrices with blocks larger than single matrix elements.

Figure 2 illustrates the recursive construction of the Peano curve ordering of the matrix elements. This defines the matrix element index ordering and also the ordering of the matrix elements in memory. The Peano ordering does not uniquely define a multiplication order and we chose the multiplication order that maximizes locality according to Bader and Zenger.

C. Temporal vs. spatial locality

Locality can be divided into two types: spatial and temporal locality. Spatial locality is the kind of locality one achieves by allocating data contiguously in memory. Such locality takes advantage of the hardware prefetch – after operations on a block are finished, the next one can be found ready in the cache. Temporal locality on the other hand means that data needed is already present in cache because it was used in a previous computational step and does not have to be loaded from memory. The impact of this locality is related to the cache line management algorithm (e.g. LRU). From a programmer’s point of view, spatial locality concerns may influence the choice of the submatrix allocation method, whereas temporal locality concerns may influence the choice of execution order of the matrix multiplication.

It is reasonable to assume that by ordering the blocked matrix product along a Peano curve, we optimize both
spatial and temporal locality, just as is the case for single matrix elements\textsuperscript{35,36}. In the following we refer to the case in which both spatial and temporal locality are optimized along a Peano curve as “temporal and spatial locality”. We want to separate the two types of locality and understand how each of them affects performance.

We can destroy spatial locality by avoiding any kind of contiguous memory allocation during the matrix block allocation. Elements within the matrix blocks are of course still allocated in contiguous memory since we want to be able to multiply matrix blocks by calling a standard generalized matrix–matrix multiply (\texttt{gemm}). However, we randomize the allocating order of the submatrix blocks, which makes it unlikely that two consecutive blocks are close to each other in memory, and break in this way contiguous allocation on the inter–block level. Since allocation order does not affect the multiplication order, and therefore temporal locality, we can measure the effect of temporal locality by itself and compare with our result for full Peano curve ordering. In the following we will refer to this non–contiguous case as “temporal locality”. We expect the performance to lie somewhere between the 2 idealized curves indicated in Fig. 1.

III. RESULTS

In the previous section we discussed four different strategies of computing a blocked matrix–matrix product with different data locality features: “perfect locality”, “temporal and spatial locality”, “temporal locality”, and “no locality”. Here we present the performance for the blocked matrix–matrix multiplication with these locality features for block sizes ranging from 3 to 200, on two different computer architectures. All calculation were performed on a single CPU.

The results shown in Fig. 3 were obtained on an AMD Opteron 248 system clocked at 2.2 GHz with 8 GiB\textsuperscript{51}.

FIG. 3: Opteron 248: Comparison of the blocked matrix multiplication performance for different ordering. The dense case is shown as reference and represents the performance of a dense matrix multiplication.

FIG. 4: Xeon Woodcrest: Comparison of the performance of Peano curve ordering and Peano curve multiplication ordering with no spatial locality.

FIG. 5: Opteron 248: Speedup of blocked matrix multiplication compared to the case of no locality. Speedup is given in percentage and a speedup of 100\% means a doubling of performance.

FIG. 6: Xeon Woodcrest: Speedup of blocked matrix multiplication.
of main memory, using the GotoBLAS\textsuperscript{45} library. The results shown in Fig. 4 were obtained on an Intel Xeon Woodcrest 5150 system clocked at 2.66 GHz with 8 GiB of main memory, using GotoBLAS\textsuperscript{45}.

We generate 2 random square matrices of size $N \times N$, where $2000 \leq N \leq 6000$. These matrices are blocked into submatrices of size $b \times b$, the block size. The type of test determines the allocation method of the submatrix blocks and the execution order of the multiplication. We time the multiplication with the CPU time as reported by the operating system. The performance is defined as $P = \left(2N^3 + 4N^2\right) / t$, where $t$ is the CPU time measured, taking into account one multiplication and one addition per term in eq. (1), one memory read operation per matrix element, and one write operation per matrix element of the $C$ matrix. We repeat each test 30 times to average out any fluctuations in the timing.

On both platforms, we find that ordering has a profound effect on performance. The difference between a blocked multiplication with perfect locality and without locality is significant (see section II A for a definition of the terms “perfect locality” and “no locality”). This point is emphasized in Figs. 5 and 6, which show the relative speedup achieved over the case of “no locality”.

The performance of the dense matrix test is independent of the matrix size for $N > 2000$. As a reference we also show in Figs. 3 and 4 the performance of the \texttt{gemm()} library call in the large matrix limit. The “dense” result has to be seen as an upper limit of what can be achieved for large matrices. Due to the fact that libraries such as GotoBLAS tune their performance with regards to large matrices, we should expect a drop in performance for small matrices. This is the reason why our results indicate that a blocked approach becomes less efficient as the block size decreases.

We clearly find that full Peano curve ordering achieves a performance which is close to perfect locality. This agrees with earlier findings by Bader and Zenger\textsuperscript{36}. In the case of temporal locality, we find that the matrix multiplication achieves near perfect locality performance as well (“temporal locality” refers to the case where we separately allocate submatrix blocks so that they are not contiguous in memory, see section II C). The relative speedup achieved by temporal ordering is almost identical to the speedups achieved by Peano curve ordering or the case of perfect locality. This is in contrast to the results for single matrix elements. This shows that spatial locality becomes quickly irrelevant as the blocksize increases. We believe that this result has not been appreciated until now.

IV. DISCUSSION

A closer look at how modern computer memory managers operate reveals that one might expect our finding that performance of matrix–matrix multiplication is controlled by temporal locality, and not spatial locality. As pointed out in the introduction, the cache is organized in cache lines of fairly limited size. In the case of the Opteron 248, a cache line contains 64 bytes. The Opteron’s memory manager will prefetch cache line $n + 3$ when it notices access to cache line $n$, followed by access to cache line $n + 1$, which is true also for the case of a descending access pattern. The total size of a typical cache is much larger than the size of a single cache line and is typically on the order of 0.1% to about 1% of main memory. In the case of the Opteron 248, the size of cache is 1 MiB. The size of cache of the Xeon Woodcrest architecture on the other hand is 4 MiB, which is, at least partly, responsible for the delayed rise of the multiplication performance when compared to the Opteron. To remind the reader, we refer to spatial locality as having to do with prefetching and temporal locality as referring to data being reused and therefore already present in cache. We conclude that cache line size and memory prefetch are the relevant features regarding spatial locality and total cache size is what matters for temporal locality. Given that a cache line is very small we do not expect hardware prefetch effects and therefore spatial locality to matter for the submatrix sizes we studied. Temporal locality, on the other hand, is important up to relatively large submatrix blocks given the different length scale of the total cache size.

V. CONCLUSIONS

We find that ordering effects for blocked matrix multiplications is important for performance confirming earlier findings by other researchers\textsuperscript{26,35,36}. The performance gain is due to increased locality. By breaking down the block locality into two types, spatial and temporal locality, we find that temporal locality gives near perfect locality by itself and that spatial locality can be neglected. This has important implications for the implementation of any blocked matrix multiplication method. The programmer should worry about the execution order of the multiplication, but can safely ignore any concerns regarding contiguous memory allocation. This allows for greater flexibility for blocked matrix data structures.

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