# SPECIAL ISSUE PAPER

# **Understanding parallelism in graph traversal on multi-core** clusters

Huiwei Lv  $\cdot$  Guangming Tan  $\cdot$  Mingyu Chen  $\cdot$  Ninghui Sun

Published online: 23 May 2012 © Springer-Verlag 2012

**Abstract** There is an ever-increasing need for exploring large-scale graph data sets in computational sciences, social networks, and business analytics. However, due to irregular and memory-intensive nature, graph applications are notoriously known for their poor performance on parallel computer systems. In this paper we propose a new hybrid MPI/Pthreads breadth-first search (BFS) algorithm featuring with (i) overlapping computation and communication by separating them into multiple threads, (ii) maximizing multi-threading parallelism on multi-cores with massive threads to improve throughputs, and (iii) exploiting pipeline parallelism using lock-free queues for asynchronous communication. By comparing it with traditional MPI-only BFS algorithm, we learned several valuable lessons that would help to understand and exploit parallelism in graph traversal applications. Experiments show our algorithm is 1.9× faster than the MPI-only version, capable of processing 1.45 billion edges per second on a 32-node SMP cluster. At a large scale, our algorithm is 1.49× than the MPI-only BFS algorithm in Combinatorial BLAS Library with 6,144 cores.

**Keywords** Breadth-first search · Graph algorithms · Hybrid MPI/Pthreads programming · Lock-free queues

H. Lv ( $\boxtimes$ ) · G. Tan · M. Chen · N. Sun State Key Laboratory of Computer Architecture, Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China

e-mail: lvhuiwei@ncic.ac.cn

H. Lv

Graduate School of Chinese Academy of Sciences, Beijing, China

# 1 Introduction

Graphs have been extensively used to abstract complex systems and interactions in emerging "big data" applications, such as social network analysis, WWW, biological systems and data mining. With the increasing growth in these areas, petabyte-sized graph datasets are produced for knowledge discovery.

Graph applications are typical examples of irregular applications, whose performance improvements are notoriously difficult on parallel computer systems [14]. They are different from the traditional computing intensive applications in various ways. Graph computations are often completely data-driven, there is a higher ratio of data access to computation than for scientific computing applications. Moreover, the data in graph problems are typically unstructured and highly irregular, which leads to poor locality of graph algorithms.

On the other side, there is an emerging trend to use hybrid programming model on multi-core clusters. With increasing numbers of cores per node, multi-core clusters provide a natural programming paradigm for hybrid programs, where OpenMP is used for intra-node data sharing between multi-cores and MPI for communication between nodes, minimizing communication and synchronization overhead. However, whether the hybrid programming model outperforms the MPI-only depends on specific problems being considered [8, 13, 19]. It is still not clear how BFS performs with hybrid programming models, or what kinds of parallelism it can exploit.

Breadth-first search (BFS) is a basic building block for many important graph applications. The newly announced Graph500 benchmark [1], which ranks supercomputers based on their performance on data-intensive applications, chose BFS as their first representative program. In this paper we present a new hybrid MPI/Pthreads BFS algorithm



on multi-core clusters. By comparing it with the traditional MPI-only version, we also made several findings. Specifically, we make the following contributions:

- We propose a new hybrid parallel BFS algorithm on a distributed memory system with multi-core processors. The algorithm exploits both intra-node and internode parallelism: core-level and memory-level parallelism to improve throughput on multi-core architectures, and pipeline-level parallelism of asynchronous communication to improve scalability on distributed memory architectures.
- We implement our parallel BFS algorithm with hybrid MPI/Pthreads programming. Experimental results show our algorithm is 1.9× faster than the MPI-only version in Graph 500 benchmark with 32 nodes, and 1.49× than the MPI-only version in Combinatorial BLAS Library with 6,144 cores.
- We learn several valuable lessons that would help to understand and exploit parallelism in graph traversal applications on multi-core clusters.

The rest of the paper is organized as follows, Sect. 2 briefly introduces Graph500 benchmark and our experiment platform. Section 3 reports analysis of the MPI-only implementations of Graph500. Section 4 presents our new hybrid algorithm, whereas Sect. 5 shows experimental results. Section 6 describes the related works. Finally, Sect. 7 concludes this paper.

# 2 Background

In this section we give a brief introduction to the Graph 500 benchmark and its BFS algorithm. We also describe the architectural parameters of our multi-core cluster.

# - Graph 500.

Graph 500 [1] is a set of large-scale benchmarks for data-intensive applications to complement the Top 500 [2]. It has gained attention from both academia and industry since the benchmark was first released for ranking supercomputers in 2010. Graph 500 use synthetic Kronecker graphs [12] which follow power law distributions. In order to save space, an adjacency array (or list) representing sparse graph is transformed into compressed sparse row (CSR). Table 1 summarizes the graph datasets used in this paper. The graph size is determined by two parameters: "Scale" and "Edge factor", where the total number of vertices N equals  $2^{Scale}$ , and the number of edges, M = edgefactor \* N.

In order to compare the performance of Graph 500 implementations across a variety of architectures, a new performance metric is adopted in Graph 500. Let time be the measured execution time for running BFS. Let m be the

**Table 1** Graph datasets used in this paper. Graphs are generated using synthetic Kronecker graph generator in Graph 500

Scale	Vertices number	Edge factor	Memory usage
30	1.07 billion	16	272 GB
29	537 million	16	136 GB
28	268 million	16	68 GB
27	134 million	16	34 GB
26	67 million	16	17 GB
25	34 million	16	8.5 GB

number of input edge tuples within the component traversed by the search, counting any multiple edges and self-loops. The normalized performance rate *traversed edges per second (TEPS)* is defined as: TEPS = m/time.

# - Serial BFS algorithm.

A graph G(V, E) is composed of a set of vertices V and a set of edges E. Given a graph G(V, E) and a root vertex  $r \in V$ , the Breadth-First Search (BFS) algorithm explores the edges of G to traverse all the vertices reachable from r, and it produces a breadth-first tree rooted at r. In the level-based algorithm a current queue (CQ) is used to record all vertices at current level l. Each vertex is fetched from CO and explored, that is, its neighboring vertices are visited, then are stored into a next queue (NQ) if they are visited for the first time. In some cases, the traversal path traces are recorded so that we can backtrace the BFS tree. Therefore, we set the parent of v to be u or array  $P[v] \leftarrow u$  if v is identified as a neighboring vertex of u during the processing of exploring u at current level. Correspondingly, vertex v is inserted into queue NO for the exploration of the next level. At the end of each level, we reset the current queue CQ to be the next queue NQ. The traversal finishes when there are no more vertices in NO.

# Multi-core cluster architecture.

Our experiment platform is a multi-core cluster, connected by Infiniband network. In our experiments, we use two different scales: 32 and 512 nodes. Each node is an SMP architecture with two Xeon X5650 CPUs (Westmere), which are connected through Intel QuickPath Interconnect (QPI). The Xeon X5650 has six cores, each supports simultaneous multithreading (SMT) up to two threads. Table 2 summarizes its architectural parameters.

# 3 MPI-only BFS algorithm and analysis

In this section we first introduce an MPI-only BFS algorithm in the Graph 500 benchmark, then perform some experimental analyses to identify bottlenecks.



Node	SMP
Number of CPUs	2
Processor	Intel X5650
Number of cores	6
Number of threads	12
Core frequency	2.66 GHz
L1 cache size	384 KB
L2 cache size	1536 KB
L3 cache size	12 MB
Memory type	DDR3-1333
QPI Speed	6.4 GT/s
Interconnect	Infiniband

40 Gb/s (4X QDR)

Rate

```
Algorithm 1: MPI-only parallel BFS algorithm
   Input : G(V, E), source vertex r
   Output: Array P[1..n] with P[v] holding the parent
   Data: outbuf[o]:Array of outgoing buffers
  while true do
       foreach u \in CQ do
2
           check incoming vertices and insert them to NQ;
3
           u \leftarrow Dequeue\ CO;
4
5
           foreach v adjacent to u do
               o = getowner(v);
6
               if o = rank then
                   if P[v] = \infty then
                        P[v] \leftarrow u, NQ \leftarrow Enqueue\ v;
                       NQ\_Count \leftarrow NQ\_Count + 1;
10
               else
11
                   outbuf[o] \leftarrow v, outbuf[o] \leftarrow u;
12
                   if outbuf[o] is full then
13
                       MPI\_Isend(outbuf[o]);
14
       flush outbuf and send finish message;
15
       MPI_Allreduce(&NQ_Count, &Sum);
16
       if Sum = 0 then break;
17
       Swap(CQ, NQ), NQ \leftarrow \emptyset;
18
```

Algorithm 1 describes the MPI-only parallel BFS algorithm. First we partition the graph among the processes. Let each process own N/p vertices and all the outgoing edges from those vertices, where N is the number of all vertices, and p is the number of all processes. Every pro-

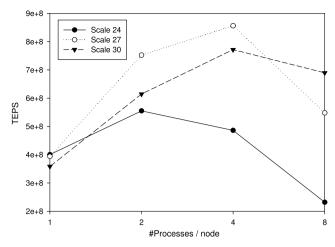


Fig. 1 Scalability of MPI-only BFS on a 32-node cluster for Kronecker graphs at different scales

cess only maintains the status of vertices it owns, and only the owner process of a vertex can identify whether it is newly visited or not. All the adjacencies of the vertices in the current frontier need to be sent to their corresponding owner process (getowner(v)). In practice, each process creates p-1 message buffers (outbuf[o]), each buffer is assigned to another process except itself. To overlap computation and communication as much as possible, message passing between processes use non-blocking  $MPI\_Isend$  and  $MPI\_Irecv$  (line 14, line 3).

**Observation 1** MPI-only BFS scales poorly across multiple nodes due to extremely intensive MPI communication with long latency.

Figure 1 plots the scalability of MPI-only BFS (Algorithm 1). We fix the number of nodes and problem scale, and change the number of processes per node to see the scalability of the program. As we can see in the figure, when the number of processes per node changes from four to eight, the performance degrades. The communication cost overwhelms the benefit of increase in process numbers. Thus it is necessary to eliminate domain decomposition at node level using hybrid approach.

**Observation 2** On a single multi-core node, multi-threading BFS performs better than MPI.

Next we compare the MPI-only algorithm with an OpenMP implementation of BFS program in Graph  $500^1$  on a single node. The OpenMP parallelism is exploited for all vertices at current level (vertices in CQ). As we can see in Fig. 2, the OpenMP-only BFS outperforms MPI-only BFS

<sup>&</sup>lt;sup>1</sup>For fairness, we optimize the original program with bitmap technique as the MPI program does.

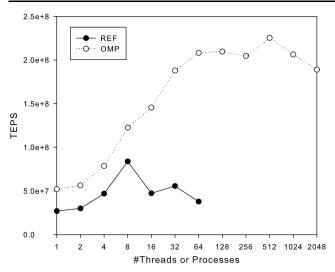


Fig. 2 MPI-only BFS (REF) vs. OpenMP-only BFS (OMP) performance on a single node

enormously, and its performance continues to increase even if its number of threads exceeds the number of cores per node. The improvement is from memory level parallelism. A deep profile finds out that the bandwidth of BFS increases as the number of threads grows (discussed in Fig. 6, Sect. 5). In fact, a similar result is observed in previous work [3] that shows Nehalem can hide the memory latency by keeping a number of read requests in flight.

Based on these observations, we will design a hybrid algorithm in the next section.

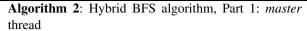
# 4 Hybrid BFS algorithm

In this section we describe the design of a new hybrid MPI/Pthreads BFS algorithm. *The key idea is to keep events as asynchronous as possible*. Our strategies include: (i) separating computation and communication into multiple threads to achieve overlapping; (ii) leveraging multithreading mechanism on multi-core architecture to tolerate latency; (iii) using lock-free algorithms to efficiently execute asynchronous operations.

- Separating communication from computation.

The first step is to separate computation from communication. We group all operations into computation and communication, then assign them to two different threads: a *master* thread (Algorithm 2) and many *traversal* threads (Algorithm 3). The former is in charge of communication among different MPI processes, and the latter are in charge of traversing vertices at the current BFS level. We choose to use one *master* thread and many *traversal* threads based on the observation that one core is capable of saturating the lanes of the PCIe network link.

Algorithm 2 describes the work of the *master* thread: repeatedly check the incoming and outgoing buffers, insert in-



```
Data: Sum: overall number of vertices in all NO
   trav finish: indicates whether all traversal threads are
   finished in this level
   barr start: barrier for all threads
   barr trav: barrier for all traversal threads
   barr_all: barrier for all threads
 1 while true do
2
       barrier wait(&barr start);
3
       while not trav finish do
          check incoming vertices and insert them to NQ;
4
          for o ∈ [0..size − 1] do
5
              MPI Test(&outreg[o], &flag);
6
7
              if flag then DEQUEUE(OUTBUF);
          for o \in [0..size - 1] do
8
              if real \ count[o] = BUFLEN then
9
                  MPI_Isend(outbuf[o], BUFLEN,
10
                  \&outreq[o]);
       flush outbuf and send finish message;
11
       MPI Allreduce(&NQ Count, &Sum);
12
       barrier_wait(&barr_all);
13
```

coming vertices to *NQ* and send *outbuf* out. Line 7 checks the status of *outbuf*, if it is full, then sends its content to another corresponding process. At the same time, vertices received in line 6 will be inserted to *NQ*. The data structures are described in Fig. 3.

- Fine-grained parallel traversal.

**if** Sum = 0 **then** break;

 $Swap(CQ, NQ), NQ \leftarrow \emptyset;$ 

14

15

Traversal threads first synchronize with the master thread at start (line 2), then partition vertices in CQ between themselves (line 3). After that, each traversal thread starts to traverse its vertices (lines 4–11). There are two different kinds of vertices here: the first kind is local vertices, they are visited and inserted to local NQ; the other kind is remote vertices, they will be inserted to outbuf and sent to other processes. After traversing all its neighbors, traversal threads synchronize with the master thread and wait for it to finish its job, then start another level (lines 12–15).

The *outbuf* is shared among all *traversal* threads and *master* thread. It is a multiple-producer single-consumer problem which involves mutual exclusion. Generally speaking, locks are sufficient when there are not too many threads. However, to leverage multi-threading mechanism of multicore processors, high number of threads are used to maximize multi-threading parallelism (as the Observation 2 in Sect. 3 indicates). In this situation, the cost of locks would be



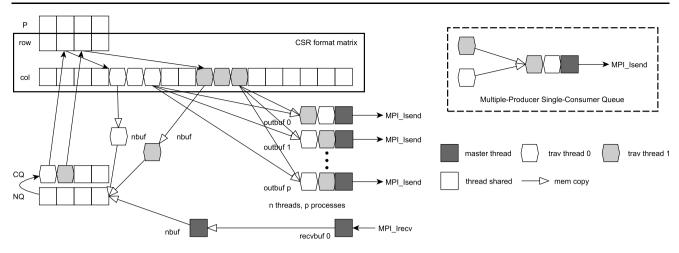


Fig. 3 Data structures used in hybrid BFS

# **Algorithm 3**: Hybrid BFS algorithm, Part 2: *traversal* threads

```
1 while true do
       barrier_wait(&barr_start);
2
3
       partition CO between threads, get my astart and
       foreach u \in CQ[qstart..qend] in parallel do
4
           foreach v adjacent to u do
5
               o = getowner(v);
              if o = rank then
7
                   if P[v] = \infty then
8
                       P[v] \leftarrow u, NO \leftarrow Enqueue v;
                       NQ\_Count \leftarrow NQ\_Count + 1;
10
              else ENQUEUE(OUTBUF[O],U,V)
11
       barrier_wait(&barr_trav);
12
       trav finish = true;
13
       barrier_wait(&barr_all);
14
       if Sum = 0 then break;
15
```

too high. Therefore, we need to find another way to implement a highly effective multiple-producer single-consumer queue. In the next subsection we will propose a lock-free multiple-producer single-consumer queue to solve this problem.

 Lock-free based pipeline parallelism for asynchronous communication.

The key data structure used in our hybrid BFS algorithm is a multiple-producer single-consumer lock-free queue, which brings asynchrony into parallel BFS and exploits additional pipeline parallelism for communication. As we can see in Fig. 3, multiple *traversal* threads insert outgoing vertices into the queue, while *master* thread is waiting to consume the queue by sending vertices out. The algorithm

**Algorithm 4**: Enqueue and dequeue functions for a multi-producer single-consumer lock-free queue. ENQUEUE(OUTBUF,U,V): Insert vertices u and v into queue outbuf. DEQUEUE(OUTBUF): Empty the queue

```
Input: u: vetex to be inserted
         v: another vertex to be inserted
         outbuf: the buffer queue, it uses two variable
  count and real count to record buffer head position
  and actual vertex number in the queue respectively.
  Function: ENQUEUE(OUTBUF,U,V)
1 while count > BUFLEN do yield();
c = fetch\_add(\&count, 2);
3 while c \ge BUFLEN do
     while count \ge BUFLEN do yield();
     c = fetch\_add(\&count, 2);
6 outbuf[c] = v;
7 outbuf[c+1]=u;
8 c = fetch\_add(\&real\_count, 2);
  Function: DEQUEUE(OUTBUF)
9 real_count \leftarrow 0;
```

of the lock-free queue is described in Algorithm 4. The ENQUEUE(OUTBUF,U,V) function first checks whether the buffer is full by repeatedly checking (lines 2–5) the *count* variable. Atomic *fetch\_add()* is used here to get a position *c* in the buffer. After insert the vertices (lines 6–7), *real\_count* records the actual vertex count in the buffer. The DEQUEUE() function simply resets *count* and *real\_count* to zero, note that *real\_count* should be cleared first, then *count*.

# 5 Experimental results

10 count  $\leftarrow 0$ ;

In this section we report the experimental results of our proposed hybrid BFS algorithm, as well as the lessons we learned.



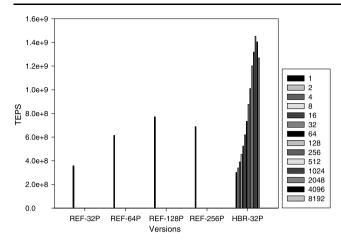


Fig. 4 HBR vs. REF on a 32-node cluster

Our new hybrid algorithm is implemented with MPI (OpenMPI-1.4.2) and POSIX Pthreads on a standard Linux environment. BFS's performance is evaluated by TEPS, and the graph datasets are described in Sect. 2. Our experiment platform is described in Sect. 2. In all experiments each measurement runs BFS 64 times from different starting vertices and reports the harmonic mean of TEPS. For brevity, we use following abbreviations when plotting the figures: *REF* for the MPI-only BFS algorithm in Graph 500 [1], *HBR* for our hybrid algorithm, and *CBL* for the MPI-only BFS algorithm in Combinatorial BLAS Library [6].

Lesson 1 A careful orchestration of core level parallelism, memory level parallelism and pipeline parallelism, gives a big boost to performance.

Figure 4 plots the performance of MPI-only (REF) and hybrid (HBR) algorithms. The graph data size is scale 30 (1.07 billion vertices). On the left side of the figure are the performance results of REF of four different configurations. "REF-32P" denotes running REF with 32 processes on our 32-node cluster. The highest TEPS scores of REF is 7.72e+08, achieved by "REF-128P". On the right side is the performance results of HBR with different number of threads per process. The highest TEPS scores of HBR is 1.45e+09, achieved with 2048 threads per process, which is  $1.9\times$  faster than REF's best performance. We use 32 MPI processes for HBR because our exhaustive experiments (Fig. 5) show that the best configuration is one MPI process per node.

Figure 5 presents performance trend of *HBR* with different configurations. Let process number remain the same "256P" (i.e. 8 processes per node), we see a drop of performance when the number of thread per process increases. However, with "32P" (i.e. 1 process per node), the performance continually increases until the thread number reaches 2048.

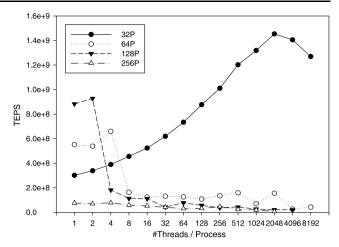
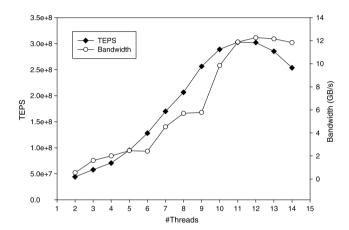


Fig. 5 HBR with different process and thread numbers



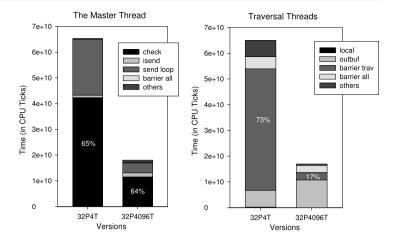
**Fig. 6** Bandwidth and TEPS of *HBR* vs. Thread Numbers. Running *HBR* at scale 24 with one process on a single node

Lesson 2 Massive fine-grained thread parallelism not only takes advantage of memory level parallelism in state-of-the-art multi-core architecture, but also improves load balancing.

An important optimization is the use of *massive* number of threads (much more than the number of hardware cores). This finding echoes the results in the previous work [16]: state-of-the-art multi-core processors support memory level of parallelism, e.g., Intel Nehalem's fill buffers allow a maximum of 10 concurrent memory requests. It is one of the most notable features that make a difference between data-intensive graph applications and traditional scientific computing applications. By contrast, if programs are CPU-bound, using more number of threads than the number of physical cores will lead to poor performance. Figure 6 plots the relationship between program bandwidth and number of threads per process. Running *HBR* with one process on a single node, as the number of threads increases, the bandwidth of *HBR* increases. As a result, its TEPS increases cor-



**Fig. 7** Time profiling information for the *master* thread and *traversal* threads of *HBR* 



respondingly benefiting from the bandwidth increase. There are knees where the performance begins to degrade when the number of threads continues to increase. When the number of threads is larger than some threshold, the overhead of thread context switch can not be mitigated by the improved memory access performance with more concurrent memory requests.

Another reason for massive threads is better load balancing. Massive threading can shorten workload gaps among different threads, i.e., with more threads, each thread is doing less and finishes more quickly. Figure 7 profiles execution time distribution of several main components in our HBR program. It compares the case of 4 threads and 2048 threads. On the right side of the figure, the barrier time ("barrier tray") of traversal threads reduces significantly from 73 % to 17 % despite the number of threads waited at the barrier increases. Another benefit is reduced waiting time for buffers. The left side of Fig. 7 gives the time profiling information for the *master* thread. The most time consuming part "check" (lines 4–5 of Algorithm 2) reduces more than a half in absolute value when changed from 4 threads to 2048. As the total communication volume remains the same, it means that the *master* thread spends less time in waiting for the outbuf and incoming buffers to become ready.

Lesson 3 Hybrid programming improves scalability of the BFS algorithm.

At a small scale of 384 cores, both *REF* and *HBR* achieve good scalability. Figure 8 plots the weak scalability of *HBR* and *REF* with no more than 384 cores. Fix the graph size on each node to scale 25, experiment on 2 nodes runs scale 26, 4 node runs scale 27, and so on. *REF* use 8 processes per node and *HBR* use 1 process per node, with 1024 threads per process.

At a larger scale of 6,144 cores, *REF* did not finish weak scalability test because its exponential space cost growth in communication buffers leads to memory overflow. Instead, we compare the strong scalability of *HBR* and *REF* at a

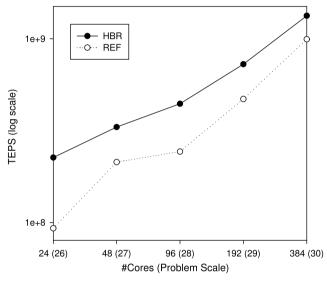


Fig. 8 HBR vs. REF: weak scalability with no more than 384 cores

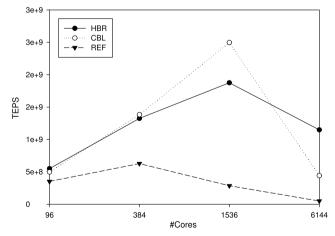


Fig. 9 HBR, CBL and REF: scale 26, strong scaling with 6,144 cores

smaller problem scale in Fig. 9, along with *CBL*, an MPIonly BFS algorithm in Combinatorial BLAS Library [6]. At scale 26, both *HBR* and *CBL* scales better than *REF*.



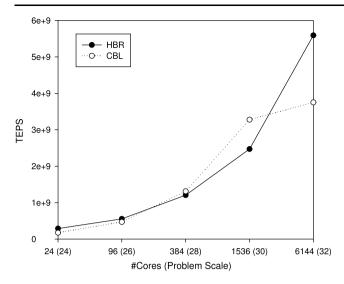


Fig. 10 HBR vs. CBL: weak scaling with 6,144 cores

Figure 10 compare the weak scalability of HBR and CBL with 6,144 cores. As we can see in the figure, HBR achieves 5.60e+09 TEPS with 6,144 cores at scale 32, 1.49× better than CBL.

#### 6 Related works

Earlier works on Cray XMT/MTA [5, 15] and IBM Cyclops-64 [18] prove that both massive threads and fine-grained data synchronization improve BFS performance. With the recent progress of multi-core and SMT, this technique can be popularized to more commodity users. Agarwal et al. [3] achieved performances on Intel Nehalem EP and EX processors comparable to special purpose hardwares like Cray XMT and Cray MTA-2, and first identified the capability of commodity multi-core systems for parallel BFS algorithms. Our algorithm also proves the feasibility of using massive threads for BFS on commodity processors. As for asynchrony, the similar idea of asynchronous algorithm is also used in optimizing communication between SPE and SPU for running BFS on STI CELL processors [17].

Buluç and Madduri [7] managed to run hybrid BFS modified from Graph 500 on a 40,000-core machine. They use a improved 2D partition to reduce communication overhead, which based on Yoo et al.'s work [20] on BlueGene/L. It is a significant work to run BFS at such large scale. However, the performance of the 2D hybrid version is roughly the same as the 2D MPI-only version. The major disadvantage of MPI/OpenMP is its BSP like synchronization. In this paper we provide a new approach to overlap communication and computation by introducing a multiple-producer single-consumer lock-free queue between computation and communication threads.

Lock-free algorithms design requires deep understanding of an algorithm and the underlying system. Bader and

Cong [4] developed a lock-free algorithm for computing the minimum spanning forest (MSF) of sparse graphs on symmetric multiprocessors. Kang and Bader [10] further developed a transactional memory (TM) algorithm for it. Leiserson and Schardl [11] also use a lock-free data structure as a key component in their work-efficient parallel BFS. Agarwal et al.'s algorithm [3] use a lock-protected single-producer single-consumer lock-free queue based on the FastForward [9] algorithm. We modify that into multiple-producer single-consumer lock-free queue using atomic instructions instead of locks.

# 7 Conclusion

In this paper we propose a new hybrid breadth-first search algorithm, and present a comprehensive comparison with the MPI-only version. Our experimental analysis leads to several findings, which would be valuable for other researchers who want to understand and exploit parallelism in parallel BFS on multi-core clusters. The hybrid BFS algorithm exploits three kind of parallelism: core level, memory level, and pipeline level. Experiments show our algorithm outperforms the MPI-only algorithm significantly. One important lesson we learned in the experiments is to use massive number of threads to take advantage of memory level parallelism in state-of-the-art multi-core processors. We chose Pthreads as our thread library and managed to run our program with thousands of threads per node. However, for fine-grained programs like BFS, the overhead of thread context switch is still too large. For future works, we believe that a user level lightweight threading mechanism will increase the performance further.

**Acknowledgements** The authors gratefully acknowledge Erlin Yao and the anonymous reviewers for their helpful comments on previous drafts of this work.

This work is supported by National 863 Program (2009AA01A129), the National Natural Science Foundation of China (61003062, 60925009, 60921002, 60803030, 61033009, 60921002, and 60925009) and 973 Program (2011CB302502 and 2011CB302500).

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**Huiwei Lv** is a Ph.D. student at State Key Laboratory of Computer Architecture, Institute of Computing Technology, Chinese Academy of Sciences. His research interests include High Performance Computing and Parallel Simulation of Many-core Processors.



Guangming Tan became Associate Professor at National Research Center for Intelligent Computing Systems, ICT, CAS in 2010. His research interests include Parallel algorithms and programming on Multi/Many-core architectures.



Mingyu Chen is a Professor at State Key Laboratory of Computer Architecture, Institute of Computing Technology, Chinese Academy of Sciences. His research interests include HPC Architecture, Operating System and Parallel Computing.



Ninghui Sun is the Director of the Institute of Computing Technology, Chinese Academy of Sciences. His research interests include Parallel Architecture and Distributed Operating System.

